Full wwPDB EM Validation Report (i)

Sep 20, 2026 – 07:58 am BST

PDB ID	:	7PIN / pdb_00007pin
EMDB ID	:	EMD-13444
Title	:	Stacked compact Dunaliella PSII
Authors	:	Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on	:	2021-08-22
Resolution	:	3.60 Å(reported)
Based on initial model	:	6KAC

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:

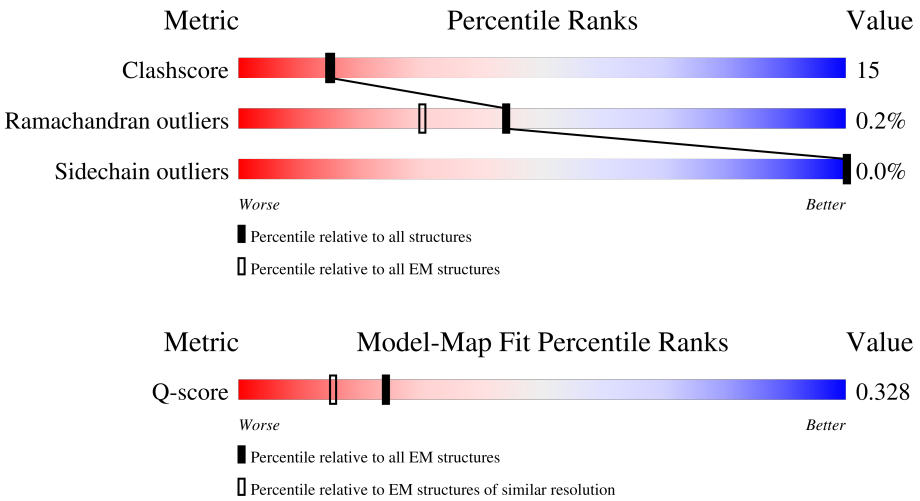
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.60 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	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	A	336	61% 70% 30%
1	A1	336	61% 63% 37%
1	a	336	54% 74% 26%
1	a1	336	70% 58% 42%

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Mol	Chain	Length	Quality of chain
2	B	484	74% 75% 25%
2	B1	484	66% 63% 37%
2	b	484	70% 69% 31%
2	b1	484	71% 68% 32%
3	V	32	94% 84% 16%
3	V1	32	69% 66% 34%
3	v	32	84% 84% 16%
3	v1	32	94% 59% 41%
4	C	449	55% 79% 21%
4	C1	449	42% 61% 38%
4	c	449	55% 81% 19%
4	c1	449	66% 63% 36%
5	D	348	63% 81% 19%
5	D1	348	63% 63% 37%
5	d	348	61% 73% 27%
5	d1	348	75% 61% 39%
6	E	76	92% 59% 41%
6	E1	76	50% 74% 26%
6	e	76	93% 75% 25%
6	e1	76	76% 67% 33%
7	F	31	74% 71% 29%
7	F1	31	58% 71% 29%
7	f	31	90% 52% 48%
7	f1	31	71% 58% 42%
8	H	67	84% 69% 31%

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Mol	Chain	Length	Quality of chain
8	H1	67	78% 63% 37%
8	h	67	88% 81% 19%
8	h1	67	84% 64% 36%
9	I	35	57% 80% 20%
9	I1	35	71% 54% 46%
9	i	35	60% 94% 6%
9	i1	35	74% 71% 29%
10	J	36	89% 83% 17%
10	J1	36	81% 75% 25%
10	j	36	86% 92% 8%
10	j1	36	81% 64% 36%
11	K	37	81% 78% 22%
11	K1	37	41% 68% 32%
11	k	37	76% 86% 14%
11	k1	37	73% 70% 30%
12	L	38	71% 84% 16%
12	L1	38	79% 74% 26%
12	l	38	74% 74% 26%
13	M	31	87% 84% 16%
13	M1	31	84% 74% 26%
13	m	31	84% 71% 29%
13	m1	31	77% 74% 26%
14	O	238	92% 77% 22%
14	O1	238	67% 65% 35%
14	o	238	94% 77% 23%

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Mol	Chain	Length	Quality of chain
14	o1	238	72% 72% 28%
15	P	187	100% 77% 23%
15	P1	187	98% 75% 25%
15	p	187	100% 72% 28%
15	p1	187	99% 73% 27%
16	T	30	83% 90% 10%
16	T1	30	83% 67% 33%
16	t	30	90% 70% 30%
16	t1	30	80% 77% 23%
17	W	44	95% 84% 16%
17	W1	44	75% 64% 36%
17	w	44	86% 73% 27%
17	w1	44	82% 57% 43%
18	X	30	97% 97% .
18	X1	30	57% 70% 30%
18	x	30	100% 67% 33%
18	x1	30	83% 77% 23%
19	Z	61	90% 90% 10%
19	Z1	61	52% 77% 23%
19	z	61	87% 87% 13%
19	z1	61	84% 80% 20%
20	N	222	94% 75% 25%
20	N1	222	37% 65% 34%
20	n	222	89% 77% 23%
20	n1	222	55% 65% 34%

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Mol	Chain	Length	Quality of chain
21	G	221	99% 75% 25%
21	G1	221	43% 71% 29%
21	g	221	97% 74% 26%
21	g1	221	62% 76% 24%
22	R	196	97% 82% 18%
22	R1	196	78% 82% 18%
22	r	196	98% 81% 19%
22	r1	196	78% 68% 32%
23	S	243	88% 82% 18%
23	S1	243	42% 72% 28%
23	s	243	90% 75% 25%
23	s1	243	75% 64% 36%
24	Y	222	83% 80% 20%
24	Y1	222	39% 68% 32%
24	y	222	83% 76% 23%
24	y1	222	66% 67% 33%
25	U	27	96% 63% 37%
25	U1	27	81% 59% 41%
25	u	27	100% 67% 33%
25	u1	27	96% 56% 44%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	C7Z	B	620	X	-	-	-
36	C7Z	B1	620	X	-	-	-
36	C7Z	b	620	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	C7Z	b1	620	X	-	-	-
41	LMK	C	527	X	-	-	-
41	LMK	C1	527	X	-	-	-
41	LMK	c	527	X	-	-	-
41	LMK	c1	527	X	-	-	-
45	RRX	H	101	X	-	-	-
45	RRX	H1	101	X	-	-	-
45	RRX	h	101	X	-	-	-
45	RRX	h1	101	X	-	-	-
48	CHL	G	601	X	-	-	-
48	CHL	G	605	X	-	-	-
48	CHL	G	607	X	-	-	-
48	CHL	G	609	X	-	-	-
48	CHL	G1	601	X	-	-	-
48	CHL	G1	605	X	-	-	-
48	CHL	G1	607	X	-	-	-
48	CHL	G1	609	X	-	-	-
48	CHL	N	601	X	-	-	-
48	CHL	N	605	X	-	-	-
48	CHL	N	606	X	-	-	-
48	CHL	N	607	X	-	-	-
48	CHL	N	609	X	-	-	-
48	CHL	N1	601	X	-	-	-
48	CHL	N1	605	X	-	-	-
48	CHL	N1	606	X	-	-	-
48	CHL	N1	607	X	-	-	-
48	CHL	N1	609	X	-	-	-
48	CHL	S	608	X	-	-	-
48	CHL	S1	608	X	-	-	-
48	CHL	Y	601	X	-	-	-
48	CHL	Y	606	X	-	-	-
48	CHL	Y	607	X	-	-	-
48	CHL	Y	609	X	-	-	-
48	CHL	Y1	601	X	-	-	-
48	CHL	Y1	606	X	-	-	-
48	CHL	Y1	607	X	-	-	-
48	CHL	Y1	609	X	-	-	-
48	CHL	g	601	X	-	-	-
48	CHL	g	605	X	-	-	-
48	CHL	g	607	X	-	-	-
48	CHL	g	609	X	-	-	-
48	CHL	g1	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	CHL	g1	605	X	-	-	-
48	CHL	g1	607	X	-	-	-
48	CHL	g1	609	X	-	-	-
48	CHL	n	601	X	-	-	-
48	CHL	n	605	X	-	-	-
48	CHL	n	606	X	-	-	-
48	CHL	n	607	X	-	-	-
48	CHL	n	609	X	-	-	-
48	CHL	n1	601	X	-	-	-
48	CHL	n1	605	X	-	-	-
48	CHL	n1	606	X	-	-	-
48	CHL	n1	607	X	-	-	-
48	CHL	n1	609	X	-	-	-
48	CHL	s	608	X	-	-	-
48	CHL	s1	608	X	-	-	-
48	CHL	y	601	X	-	-	-
48	CHL	y	606	X	-	-	-
48	CHL	y	607	X	-	-	-
48	CHL	y	609	X	-	-	-
48	CHL	y1	601	X	-	-	-
48	CHL	y1	606	X	-	-	-
48	CHL	y1	607	X	-	-	-
48	CHL	y1	609	X	-	-	-
49	LUT	G	621	X	-	-	-
49	LUT	R	620	X	-	-	-
49	LUT	n1	621	X	-	-	-
50	XAT	G	622	X	-	-	-
50	XAT	G1	622	X	-	-	-
50	XAT	N	622	X	-	-	-
50	XAT	N1	622	X	-	-	-
50	XAT	Y1	622	X	-	-	-
50	XAT	g	622	X	-	-	-
50	XAT	g1	622	X	-	-	-
50	XAT	n	622	X	-	-	-
50	XAT	r	621	X	-	-	-
50	XAT	r1	621	X	-	-	-
51	NEX	g	623	X	-	-	-
51	NEX	g1	623	X	-	-	-
53	ERG	R	626	X	-	-	-
53	ERG	R1	626	X	-	-	-
53	ERG	r	626	X	-	-	-
53	ERG	r1	626	X	-	-	-

2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 152240 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	336	2638	1721	432	468	17	1	0
1	a	336	2638	1721	432	468	17	1	0
1	A1	336	2638	1721	432	468	17	1	0
1	a1	336	2638	1721	432	468	17	1	0

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	484	3783	2480	630	663	10	0	0
2	b	484	3783	2480	630	663	10	0	0
2	B1	484	3783	2480	630	663	10	0	0
2	b1	484	3783	2480	630	663	10	0	0

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	V	32	227	152	37	38	0	0
3	v	32	227	152	37	38	0	0
3	V1	32	227	152	37	38	0	0
3	v1	32	227	152	37	38	0	0

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total 3483	C 2282	N 581	O 607	S 13	0	0
4	c	449	Total 3483	C 2282	N 581	O 607	S 13	0	0
4	C1	449	Total 3483	C 2282	N 581	O 607	S 13	0	0
4	c1	449	Total 3483	C 2282	N 581	O 607	S 13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total 2766	C 1824	N 454	O 477	S 11	0	0
5	d	348	Total 2766	C 1824	N 454	O 477	S 11	0	0
5	D1	348	Total 2766	C 1824	N 454	O 477	S 11	0	0
5	d1	348	Total 2766	C 1824	N 454	O 477	S 11	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	76	Total 621	C 404	N 102	O 115	0	0
6	e	76	Total 621	C 404	N 102	O 115	0	0
6	E1	76	Total 621	C 404	N 102	O 115	0	0
6	e1	76	Total 621	C 404	N 102	O 115	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total 252	C 172	N 42	O 37	S 1	0	0
7	f	31	Total 252	C 172	N 42	O 37	S 1	0	0
7	F1	31	Total 252	C 172	N 42	O 37	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	f1	31	252	172	42	37	1	0	0

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	67	503	334	76	92	1	0	0
8	h	67	503	334	76	92	1	0	0
8	H1	67	503	334	76	92	1	0	0
8	h1	67	503	334	76	92	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	35	279	190	42	46	1	0	0
9	i	35	279	190	42	46	1	0	0
9	I1	35	279	190	42	46	1	0	0
9	i1	35	279	190	42	46	1	0	0

- Molecule 10 is a protein called PsbJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	J	36	266	183	40	43	0	0
10	j	36	266	183	40	43	0	0
10	J1	36	266	183	40	43	0	0
10	j1	36	266	183	40	43	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	K	37	297	207	43	47	0	0
11	k	37	297	207	43	47	0	0
11	K1	37	297	207	43	47	0	0
11	k1	37	297	207	43	47	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	38	313	209	51	52	1	0	0
12	l	38	313	209	51	52	1	0	0
12	L1	38	313	209	51	52	1	0	0

- Molecule 13 is a protein called PsbM.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	31	234	159	33	42	0	0
13	m	31	234	159	33	42	0	0
13	M1	31	234	159	33	42	0	0
13	m1	31	234	159	33	42	0	0

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	238	1820	1149	295	370	6	0	0
14	o	238	1820	1149	295	370	6	0	0
14	O1	238	1820	1149	295	370	6	0	0
14	o1	238	1820	1149	295	370	6	0	0

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	187	1444	916	242	285	1	0	0
15	p	187	1444	916	242	285	1	0	0
15	P1	187	1444	916	242	285	1	0	0
15	p1	187	1444	916	242	285	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	T	30	247	171	36	39	1	0	0
16	t	30	247	171	36	39	1	0	0
16	T1	30	247	171	36	39	1	0	0
16	t1	30	247	171	36	39	1	0	0

- Molecule 17 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	W	44	332	215	53	63	1	0	0
17	w	44	332	215	53	63	1	0	0
17	W1	44	332	215	53	63	1	0	0
17	w1	44	332	215	53	63	1	0	0

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	X	30	201	132	32	37	0	0
18	x	30	201	132	32	37	0	0
18	X1	30	201	132	32	37	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	x1	30	201	132	32	37	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	61	457	312	68	76	1	0	0
			Total	C	N	O	S		
19	z	61	457	312	68	76	1	0	0
			Total	C	N	O	S		
19	Z1	61	457	312	68	76	1	0	0
			Total	C	N	O	S		
19	z1	61	457	312	68	76	1	0	0

- Molecule 20 is a protein called LHCII M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	N	222	1703	1100	277	321	5	0	0
			Total	C	N	O	S		
20	n	222	1703	1100	277	321	5	0	0
			Total	C	N	O	S		
20	N1	222	1703	1100	277	321	5	0	0
			Total	C	N	O	S		
20	n1	222	1703	1100	277	321	5	0	0

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	G	221	1680	1085	271	321	3	0	0
			Total	C	N	O	S		
21	g	221	1680	1085	271	321	3	0	0
			Total	C	N	O	S		
21	G1	221	1680	1085	271	321	3	0	0
			Total	C	N	O	S		
21	g1	221	1680	1085	271	321	3	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	180	ALA	PRO	conflict	UNP A1XKU7
g	180	ALA	PRO	conflict	UNP A1XKU7
G1	180	ALA	PRO	conflict	UNP A1XKU7
g1	180	ALA	PRO	conflict	UNP A1XKU7

- Molecule 22 is a protein called CP29.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	R	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	r	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	R1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	r1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	S1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

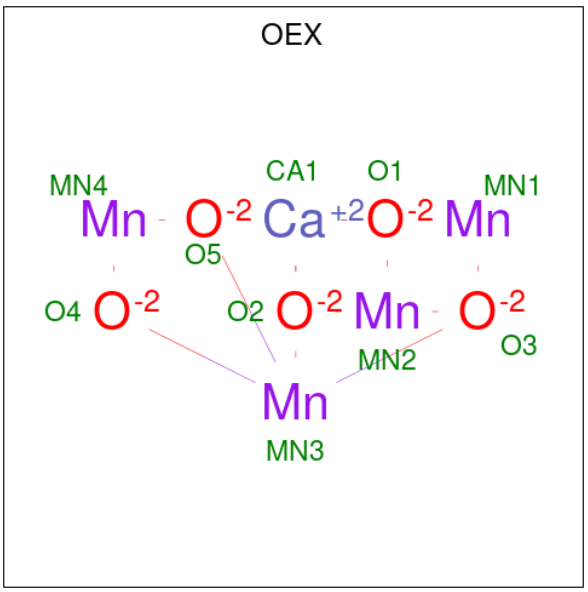
- Molecule 24 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	Y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

- Molecule 25 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	27	Total 224	C 134	N 42	O 47	S 1	0	0
25	u	27	Total 224	C 134	N 42	O 47	S 1	0	0
25	U1	27	Total 224	C 134	N 42	O 47	S 1	0	0
25	u1	27	Total 224	C 134	N 42	O 47	S 1	0	0

- Molecule 26 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total 10	Ca 1	Mn 4	O 5	0
26	a	1	Total 10	Ca 1	Mn 4	O 5	0
26	A1	1	Total 10	Ca 1	Mn 4	O 5	0
26	a1	1	Total 10	Ca 1	Mn 4	O 5	0

- Molecule 27 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total 1	Fe 1	0
27	a	1	Total 1	Fe 1	0

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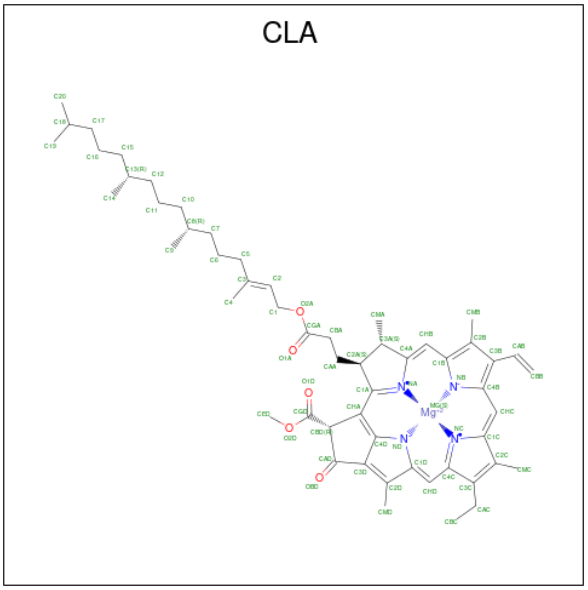
Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
27	A1	1	1	1	0
27	a1	1	1	1	0

- Molecule 28 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
28	A	2	2	2	0
28	a	2	2	2	0
28	A1	2	2	2	0
28	a1	2	2	2	0

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	A	1	65	55	1	4	5	0
29	A	1	65	55	1	4	5	0
29	A	1	50	40	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	D	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	D	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	N	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	N	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
29	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	N	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	G	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	G	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	G	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
29	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	G	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	R	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	S	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	S	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
29	S	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
29	S	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	S	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	S	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
29	S	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
29	S	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
29	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	Y	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
29	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	a	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	a	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	d	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	d	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	n	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	n	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
29	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	n	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	g	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	g	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
29	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	g	1	49	39	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	r	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	r	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	r	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	r	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	r	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	r	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	r	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	s	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	s	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	s	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
29	s	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
29	s	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	s	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	s	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	s	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
29	s	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
29	s	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
29	s	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
29	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	y	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	y	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
29	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	A1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	A1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	A1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
29	A1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	C1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	D1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	D1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	N1	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	N1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	N1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	N1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	N1	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	N1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
29	N1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	N1	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	G1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	G1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	G1	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	G1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	G1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	G1	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
29	G1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	G1	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	R1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	R1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	R1	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	R1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	R1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	R1	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	R1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	S1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	S1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	S1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
29	S1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
29	S1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	S1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	S1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	S1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
29	S1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
29	S1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
29	S1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
29	Y1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	Y1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	Y1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	Y1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
29	Y1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	Y1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	Y1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	Y1	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	a1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	a1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	a1	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	a1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	b1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	b1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	d1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	d1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	n1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	n1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	n1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	n1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	n1	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	n1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
29	n1	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	n1	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	g1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	g1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	g1	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	g1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	g1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	g1	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
29	g1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	g1	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	r1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	r1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	r1	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
29	r1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	r1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	r1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	r1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	s1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
29	s1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	s1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
29	s1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
29	s1	1	60	50	1	4	5	0

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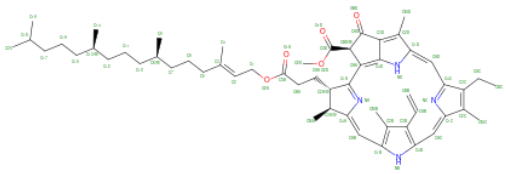
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	s1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	s1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	s1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
29	s1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
29	s1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
29	s1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
29	y1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	y1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	y1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	y1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
29	y1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	y1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	y1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	y1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
29	y1	1	65	55	1	4	5	0

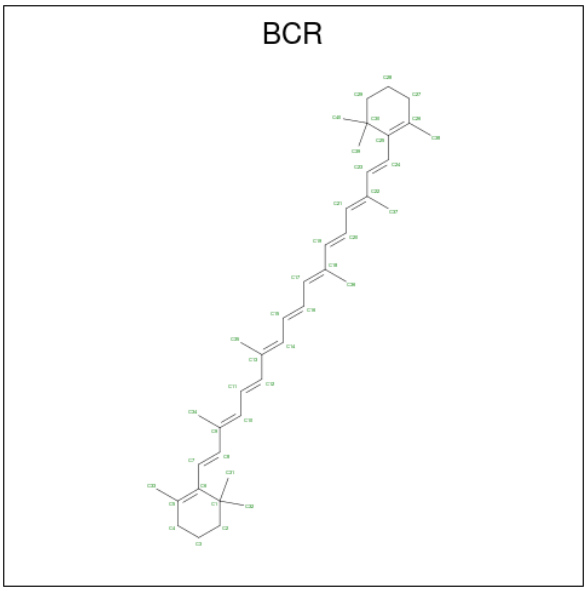
- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).

PHO



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
30	A	1	64	55	4	5	0
30	A	1	64	55	4	5	0
30	a	1	64	55	4	5	0
30	a	1	64	55	4	5	0
30	A1	1	64	55	4	5	0
30	A1	1	64	55	4	5	0
30	a1	1	64	55	4	5	0
30	a1	1	64	55	4	5	0

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
31	A	1	40	40	0
31	B	1	40	40	0
31	B	1	40	40	0
31	C	1	40	40	0
31	C	1	40	40	0
31	C	1	40	40	0
31	C	1	40	40	0
31	D	1	40	40	0
31	a	1	40	40	0
31	b	1	40	40	0
31	b	1	40	40	0
31	c	1	40	40	0
31	c	1	40	40	0
31	c	1	40	40	0

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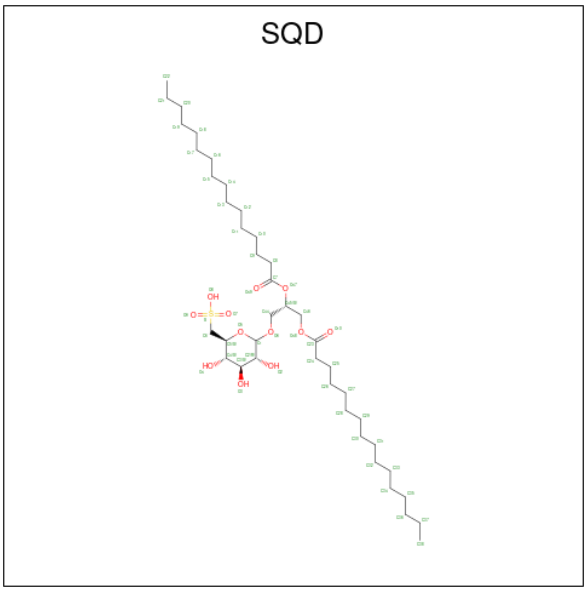
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
31	c	1	40	40	0
31	d	1	40	40	0
31	A1	1	40	40	0
31	B1	1	40	40	0
31	B1	1	40	40	0
31	C1	1	40	40	0
31	C1	1	40	40	0
31	C1	1	40	40	0
31	C1	1	40	40	0
31	D1	1	40	40	0
31	a1	1	40	40	0
31	b1	1	40	40	0
31	b1	1	40	40	0
31	c1	1	40	40	0
31	c1	1	40	40	0
31	c1	1	40	40	0
31	c1	1	40	40	0
31	d1	1	40	40	0

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
32	A	1	51	38	12	1	0
32	B	1	42	29	12	1	0
32	B	1	54	41	12	1	0
32	C	1	54	41	12	1	0
32	M	1	42	29	12	1	0
32	a	1	51	38	12	1	0
32	b	1	42	29	12	1	0
32	b	1	54	41	12	1	0
32	c	1	54	41	12	1	0
32	m	1	42	29	12	1	0
32	A1	1	51	38	12	1	0
32	B1	1	42	29	12	1	0
32	B1	1	54	41	12	1	0
32	C1	1	54	41	12	1	0

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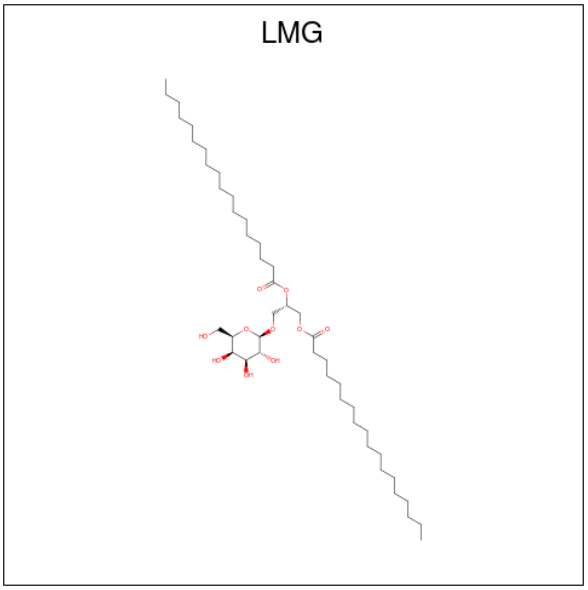
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
32	M1	1	42	29	12	1	0
32	a1	1	51	38	12	1	0
32	b1	1	42	29	12	1	0
32	b1	1	54	41	12	1	0
32	c1	1	54	41	12	1	0
32	m1	1	42	29	12	1	0

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	A	1	48	38	10	0
33	B	1	44	34	10	0
33	C	1	51	41	10	0
33	C	1	55	45	10	0
33	D	1	46	36	10	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	H	1	48	38	10	0
33	W	1	39	29	10	0
33	a	1	48	38	10	0
33	b	1	44	34	10	0
33	c	1	51	41	10	0
33	c	1	55	45	10	0
33	d	1	46	36	10	0
33	h	1	48	38	10	0
33	w	1	39	29	10	0
33	A1	1	48	38	10	0
33	B1	1	44	34	10	0
33	C1	1	51	41	10	0
33	C1	1	55	45	10	0
33	D1	1	46	36	10	0
33	H1	1	48	38	10	0
33	W1	1	39	29	10	0
33	a1	1	48	38	10	0
33	b1	1	44	34	10	0
33	c1	1	51	41	10	0
33	c1	1	55	45	10	0
33	d1	1	46	36	10	0

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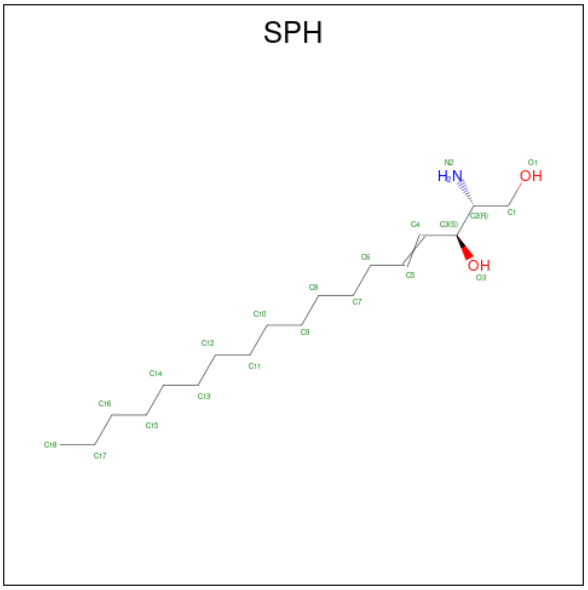
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	h1	1	48	38	10	0
			Total	C	O	
33	w1	1	39	29	10	0

- Molecule 34 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).

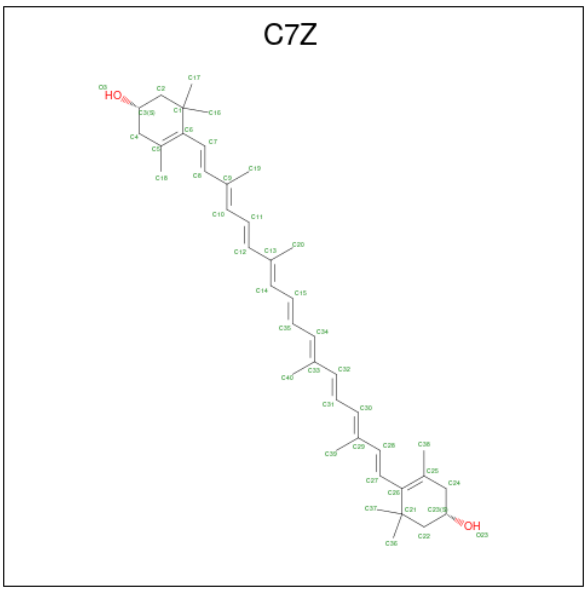


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
34	A	1	21	18	1	2	0
			Total	C	N	O	
34	Y	1	21	18	1	2	0
			Total	C	N	O	
34	a	1	21	18	1	2	0
			Total	C	N	O	
34	y	1	21	18	1	2	0
			Total	C	N	O	
34	A1	1	21	18	1	2	0
			Total	C	N	O	
34	Y1	1	21	18	1	2	0
			Total	C	N	O	
34	a1	1	21	18	1	2	0
			Total	C	N	O	
34	y1	1	21	18	1	2	0

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms			AltConf
			Total	Na		
35	A	1	1	1		0
35	a	1	1	1		0
35	A1	1	1	1		0
35	a1	1	1	1		0

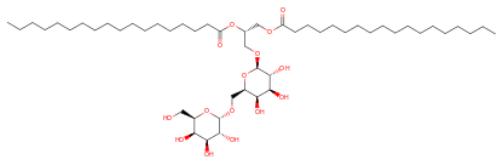
- Molecule 36 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	B	1	42	40	2	0
36	b	1	42	40	2	0
36	B1	1	42	40	2	0
36	b1	1	42	40	2	0

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

DGD



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
37	B	1	43	28	15	0
37	C	1	55	40	15	0
37	C	1	62	47	15	0
37	C	1	59	44	15	0
37	b	1	43	28	15	0
37	c	1	55	40	15	0
37	c	1	62	47	15	0
37	c	1	59	44	15	0
37	B1	1	43	28	15	0
37	C1	1	55	40	15	0
37	C1	1	62	47	15	0
37	C1	1	59	44	15	0
37	b1	1	43	28	15	0
37	c1	1	55	40	15	0

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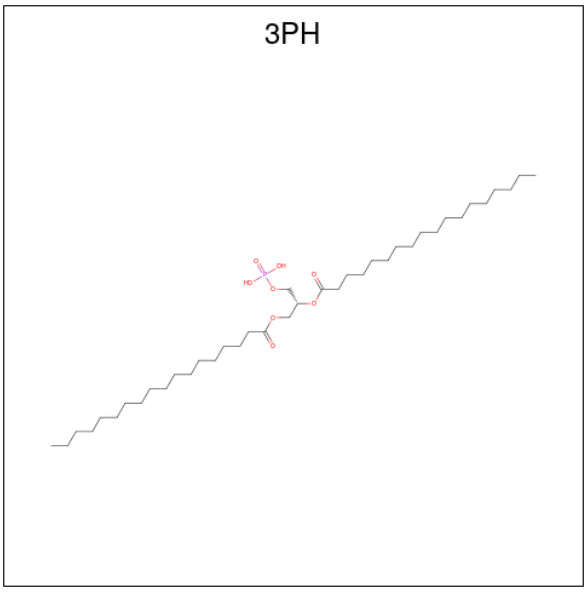
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
37	c1	1	62	47	15	0
			Total	C	O	
37	c1	1	59	44	15	0

- Molecule 38 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
38	B	1	48	39	8	1	0
			Total	C	O	P	
38	T	1	48	39	8	1	0
			Total	C	O	P	
38	S	1	48	39	8	1	0
			Total	C	O	P	
38	b	1	48	39	8	1	0
			Total	C	O	P	
38	t	1	48	39	8	1	0
			Total	C	O	P	
38	s	1	48	39	8	1	0
			Total	C	O	P	
38	B1	1	48	39	8	1	0
			Total	C	O	P	
38	T1	1	48	39	8	1	0
			Total	C	O	P	
38	S1	1	48	39	8	1	0

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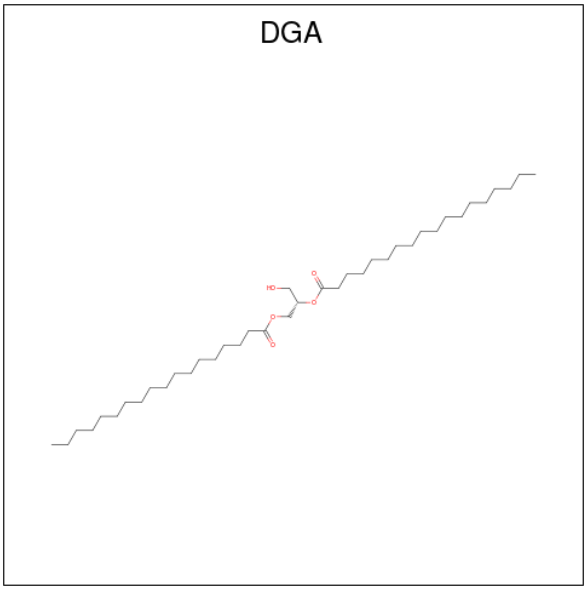
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
38	b1	1	48	39	8	1	0
38	t1	1	48	39	8	1	0
38	s1	1	48	39	8	1	0

- Molecule 39 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	B	1	44	39	5	0
39	C	1	44	39	5	0
39	J	1	29	24	5	0
39	b	1	44	39	5	0
39	c	1	44	39	5	0
39	j	1	29	24	5	0
39	B1	1	44	39	5	0
39	C1	1	44	39	5	0

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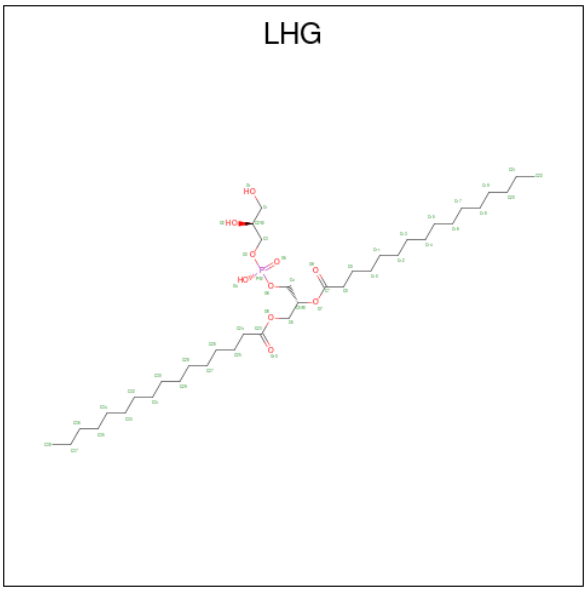
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	J1	1	29	24	5	0
			Total	C	O	
39	b1	1	44	39	5	0
			Total	C	O	
39	c1	1	44	39	5	0
			Total	C	O	
39	j1	1	29	24	5	0

- Molecule 40 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	
40	C	1	47	36	10	1	0
			Total	C	O	P	
40	D	1	44	33	10	1	0
			Total	C	O	P	
40	D	1	49	38	10	1	0
			Total	C	O	P	
40	D	1	39	28	10	1	0
			Total	C	O	P	
40	L	1	49	38	10	1	0
			Total	C	O	P	
40	N	1	49	38	10	1	0
			Total	C	O	P	
40	G	1	49	38	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
40	S	1	45	34	10	1	0
			Total	C	O	P	
40	Y	1	49	38	10	1	0
			Total	C	O	P	
40	c	1	47	36	10	1	0
			Total	C	O	P	
40	d	1	44	33	10	1	0
			Total	C	O	P	
40	d	1	49	38	10	1	0
			Total	C	O	P	
40	d	1	39	28	10	1	0
			Total	C	O	P	
40	l	1	49	38	10	1	0
			Total	C	O	P	
40	n	1	49	38	10	1	0
			Total	C	O	P	
40	g	1	49	38	10	1	0
			Total	C	O	P	
40	s	1	45	34	10	1	0
			Total	C	O	P	
40	y	1	49	38	10	1	0
			Total	C	O	P	
40	C1	1	47	36	10	1	0
			Total	C	O	P	
40	D1	1	44	33	10	1	0
			Total	C	O	P	
40	D1	1	49	38	10	1	0
			Total	C	O	P	
40	D1	1	39	28	10	1	0
			Total	C	O	P	
40	L1	1	49	38	10	1	0
			Total	C	O	P	
40	N1	1	49	38	10	1	0
			Total	C	O	P	
40	G1	1	49	38	10	1	0
			Total	C	O	P	
40	S1	1	45	34	10	1	0
			Total	C	O	P	
40	Y1	1	49	38	10	1	0
			Total	C	O	P	
40	c1	1	47	36	10	1	0

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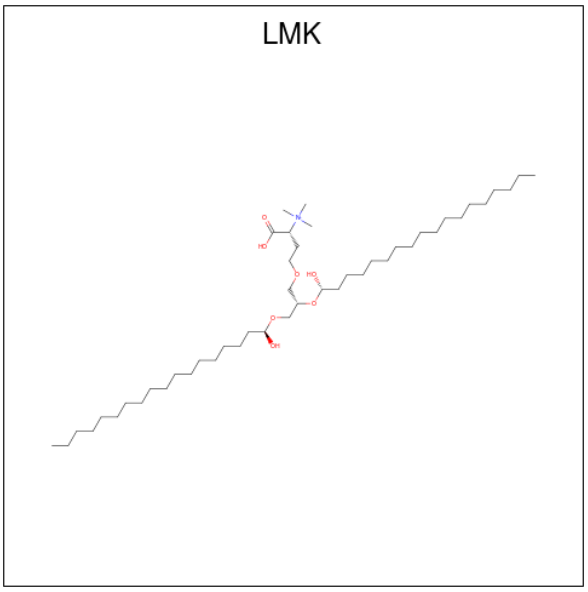
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
40	d1	1	44	33	10	1	0
40	d1	1	49	38	10	1	0
40	d1	1	39	28	10	1	0
40	n1	1	49	38	10	1	0
40	g1	1	49	38	10	1	0
40	s1	1	45	34	10	1	0
40	y1	1	49	38	10	1	0

- Molecule 41 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: $C_{46}H_{94}NO_7$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
41	C	1	40	32	1	7	0
41	c	1	40	32	1	7	0
41	C1	1	40	32	1	7	0

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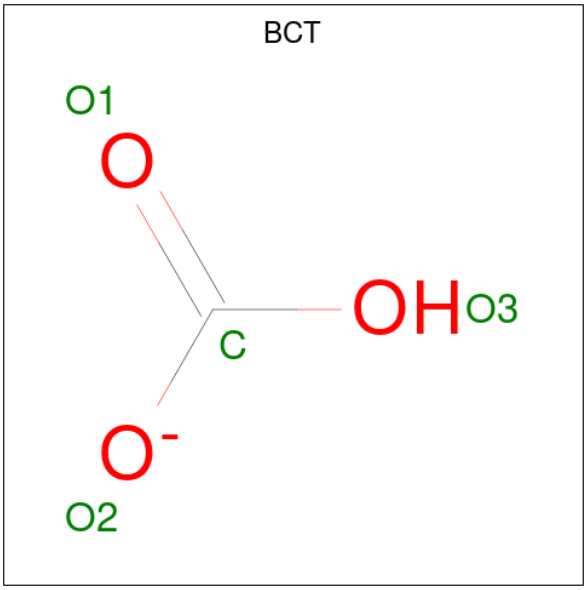
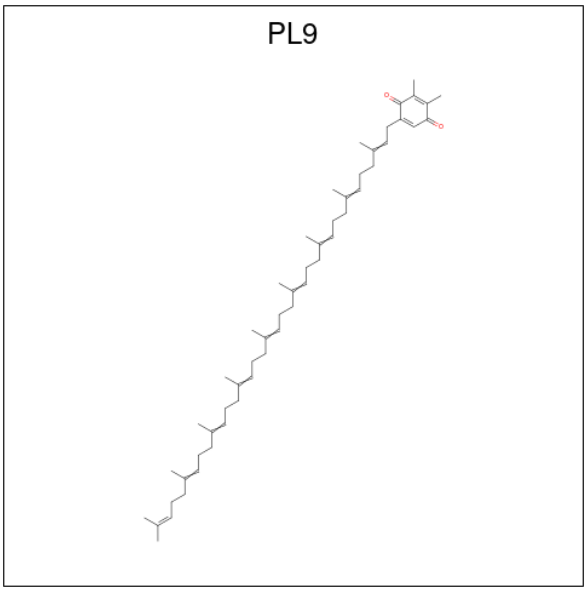
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
41	c1	1	40	32	1	7	0

- Molecule 42 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



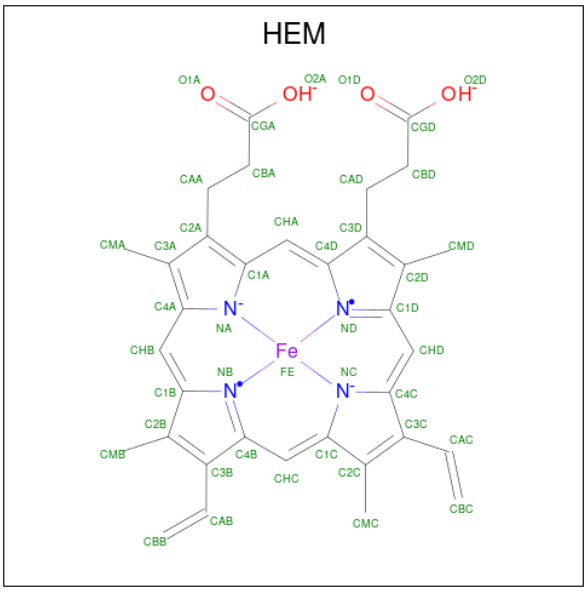
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
42	D	1	4	1	3		0
42	d	1	4	1	3		0
42	D1	1	4	1	3		0
42	d1	1	4	1	3		0

- Molecule 43 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: $C_{53}H_{80}O_2$).



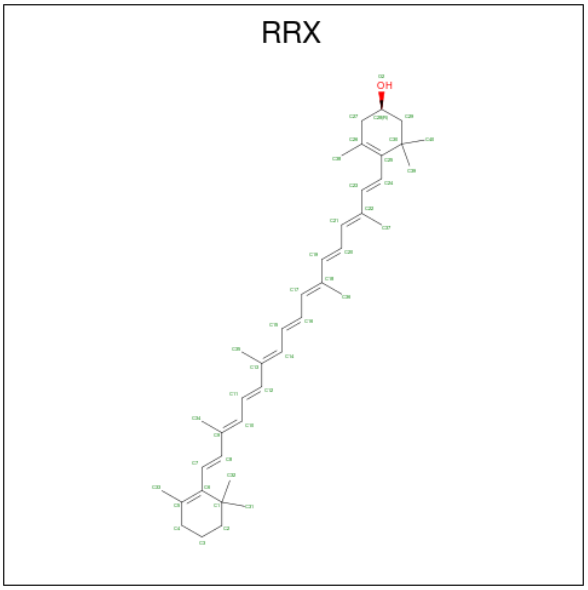
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
43	D	1	55	53	2	0
			Total	C	O	
43	d	1	55	53	2	0
			Total	C	O	
43	D1	1	55	53	2	0
			Total	C	O	
43	d1	1	55	53	2	0

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



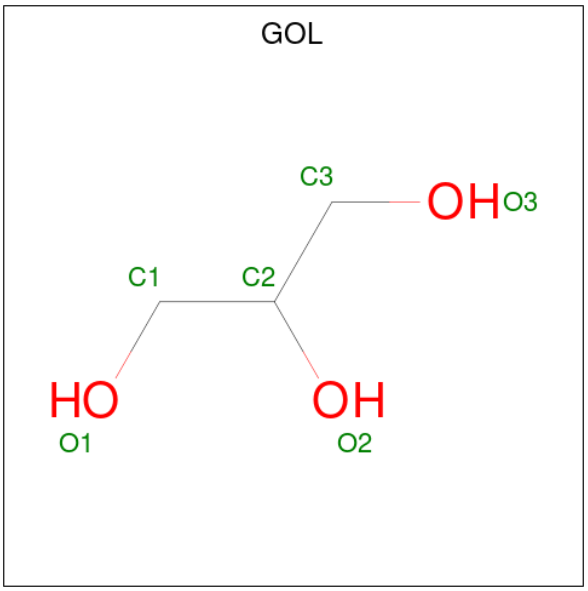
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
44	F	1	43	34	1	4	4	0
44	f	1	43	34	1	4	4	0
44	F1	1	43	34	1	4	4	0
44	f1	1	43	34	1	4	4	0

- Molecule 45 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



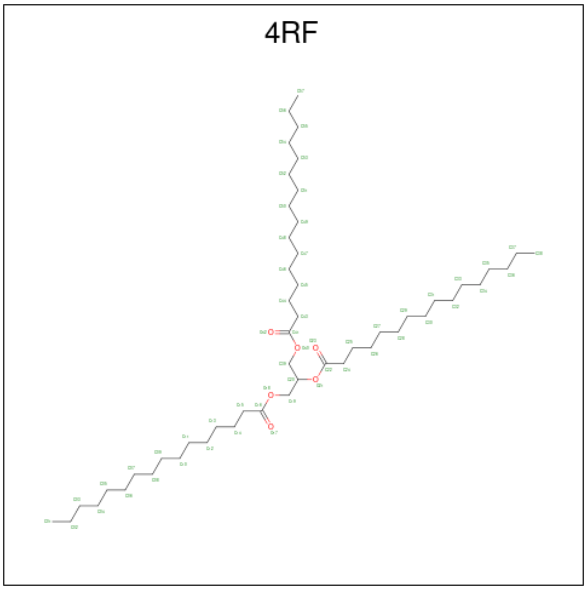
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	H	1	41	40	1	0
45	h	1	41	40	1	0
45	H1	1	41	40	1	0
45	h1	1	41	40	1	0

- Molecule 46 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
46	I	1	6	3	3	0
			Total	C	O	
46	I1	1	6	3	3	0

- Molecule 47 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: $C_{51}H_{98}O_6$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
47	I	1	57	51	6	0
			Total	C	O	
47	K	1	57	51	6	0

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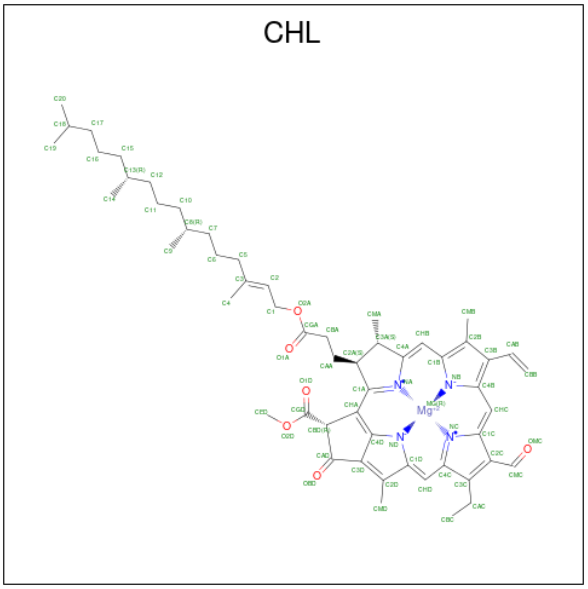
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
47	i	1	57	51	6	0
47	k	1	57	51	6	0
47	I1	1	57	51	6	0
47	K1	1	57	51	6	0
47	i1	1	57	51	6	0
47	k1	1	57	51	6	0

- Molecule 48 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
48	N	1	66	55	1	4	6	0
48	N	1	66	55	1	4	6	0
48	N	1	66	55	1	4	6	0
48	N	1	66	55	1	4	6	0
48	N	1	50	39	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
48	N	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	G	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
48	G	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
48	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	G	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
48	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	R	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
48	R	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
48	S	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
48	S	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
48	S	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
48	S	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
48	Y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	Y	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
48	Y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	Y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	Y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	n	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
48	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	n	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
48	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	g	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	g	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
48	g	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
48	g	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	g	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
48	g	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	r	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
48	r	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
48	s	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
48	s	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
48	s	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
48	s	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
48	y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	y	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
48	y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	N1	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
48	N1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	N1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	N1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	N1	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
48	N1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	G1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	G1	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
48	G1	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
48	G1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	G1	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
48	G1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	R1	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
48	R1	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
48	S1	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
48	S1	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
48	S1	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
48	S1	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
48	Y1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	Y1	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
48	Y1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	Y1	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
48	Y1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	n1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	n1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	n1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	n1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	n1	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
48	n1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	g1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	g1	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
48	g1	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
48	g1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	g1	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
48	g1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	r1	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
48	r1	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
48	s1	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
48	s1	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
48	s1	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
48	s1	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
48	y1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	y1	1	46	35	1	4	6	0

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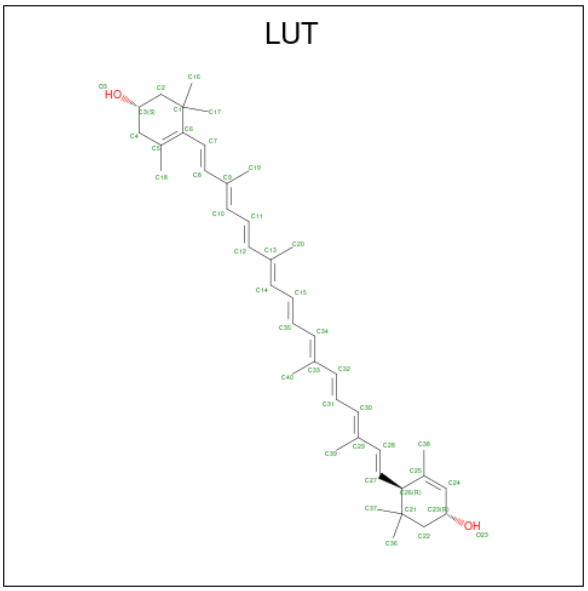
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
48	y1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	y1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
48	y1	1	66	55	1	4	6	0

- Molecule 49 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	
49	N	1	42	40	2	0
			Total	C	O	
49	N	1	42	40	2	0
			Total	C	O	
49	G	1	42	40	2	0
			Total	C	O	
49	G	1	42	40	2	0
			Total	C	O	
49	R	1	42	40	2	0
			Total	C	O	
49	S	1	42	40	2	0
			Total	C	O	
49	S	1	42	40	2	0
			Total	C	O	
49	Y	1	42	40	2	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
49	Y	1	42	40	2	0
49	n	1	42	40	2	0
49	n	1	42	40	2	0
49	g	1	42	40	2	0
49	g	1	42	40	2	0
49	r	1	42	40	2	0
49	s	1	42	40	2	0
49	s	1	42	40	2	0
49	y	1	42	40	2	0
49	y	1	42	40	2	0
49	N1	1	42	40	2	0
49	N1	1	42	40	2	0
49	G1	1	42	40	2	0
49	G1	1	42	40	2	0
49	R1	1	42	40	2	0
49	S1	1	42	40	2	0
49	S1	1	42	40	2	0
49	Y1	1	42	40	2	0
49	Y1	1	42	40	2	0
49	n1	1	42	40	2	0
49	n1	1	42	40	2	0

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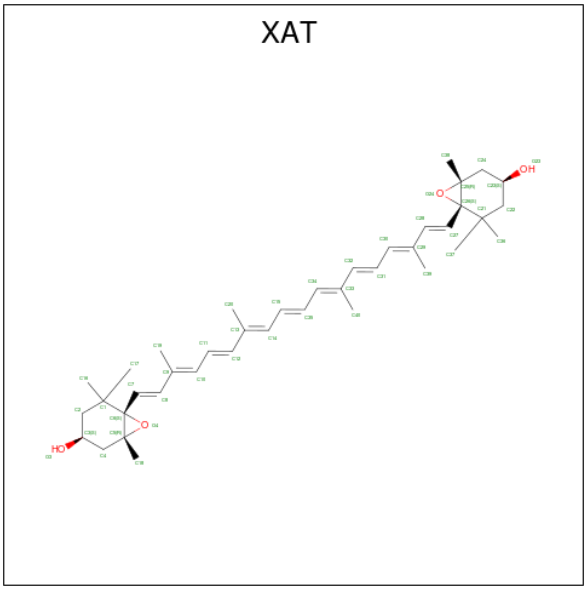
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
49	g1	1	42	40	2	0
49	g1	1	42	40	2	0
49	r1	1	42	40	2	0
49	s1	1	42	40	2	0
49	s1	1	42	40	2	0
49	y1	1	42	40	2	0
49	y1	1	42	40	2	0

- Molecule 50 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	
50	N	1	44	40	4	0
50	G	1	44	40	4	0
50	R	1	44	40	4	0
50	Y	1	44	40	4	0

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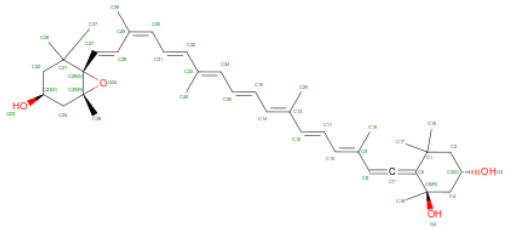
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
50	n	1	44	40	4	0
50	g	1	44	40	4	0
50	r	1	44	40	4	0
50	y	1	44	40	4	0
50	N1	1	44	40	4	0
50	G1	1	44	40	4	0
50	R1	1	44	40	4	0
50	Y1	1	44	40	4	0
50	n1	1	44	40	4	0
50	g1	1	44	40	4	0
50	r1	1	44	40	4	0
50	y1	1	44	40	4	0

- Molecule 51 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	
51	N	1	44	40	4	0
51	G	1	44	40	4	0
51	R	1	44	40	4	0
51	S	1	44	40	4	0
51	Y	1	44	40	4	0
51	n	1	44	40	4	0
51	g	1	44	40	4	0
51	r	1	44	40	4	0
51	s	1	44	40	4	0
51	y	1	44	40	4	0
51	N1	1	44	40	4	0
51	G1	1	44	40	4	0
51	R1	1	44	40	4	0
51	S1	1	44	40	4	0

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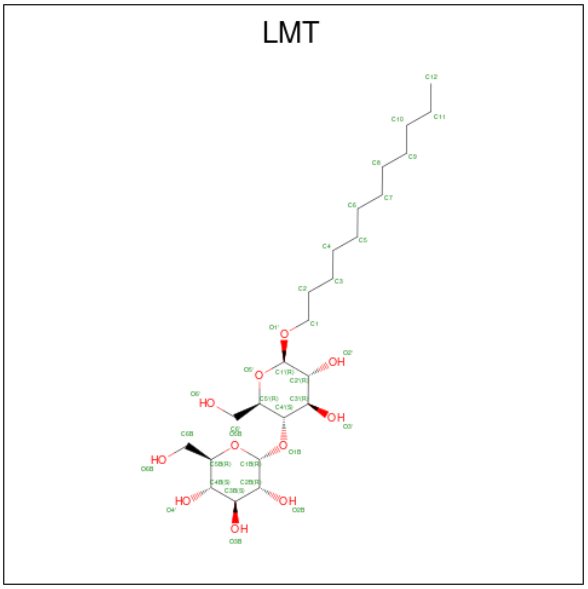
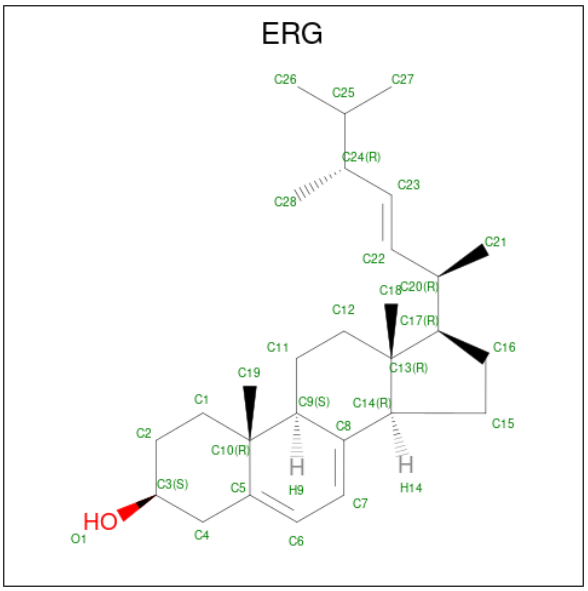
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
51	Y1	1	44	40	4	0
51	n1	1	44	40	4	0
51	g1	1	44	40	4	0
51	r1	1	44	40	4	0
51	s1	1	44	40	4	0
51	y1	1	44	40	4	0

- Molecule 52 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



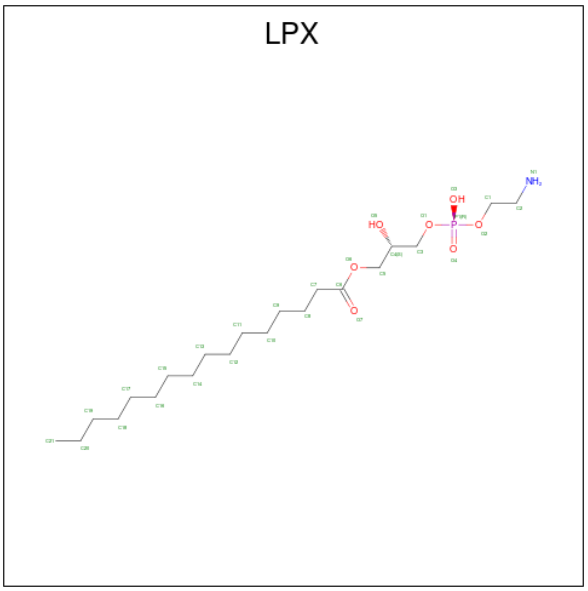
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
52	R	1	35	24	11	0
52	r	1	35	24	11	0
52	R1	1	35	24	11	0
52	r1	1	35	24	11	0

- Molecule 53 is ERGOSTEROL (CCD ID: ERG) (formula: $C_{28}H_{44}O$).



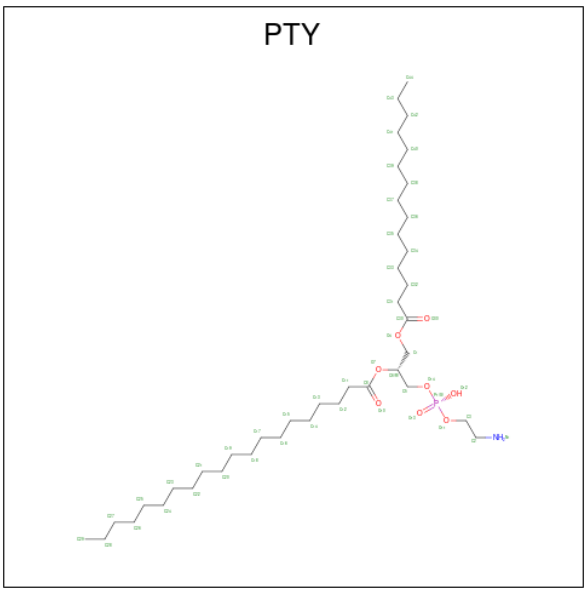
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
53	R	1	29	28	1	0
			Total	C	O	
53	r	1	29	28	1	0
			Total	C	O	
53	R1	1	29	28	1	0
			Total	C	O	
53	r1	1	29	28	1	0

- Molecule 54 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: $C_{21}H_{44}NO_7P$).



Mol	Chain	Residues	Atoms					AltConf
54	S	1	Total	C	N	O	P	0
			30	21	1	7	1	
54	s	1	Total	C	N	O	P	0
			30	21	1	7	1	
54	S1	1	Total	C	N	O	P	0
			30	21	1	7	1	
54	s1	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 55 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



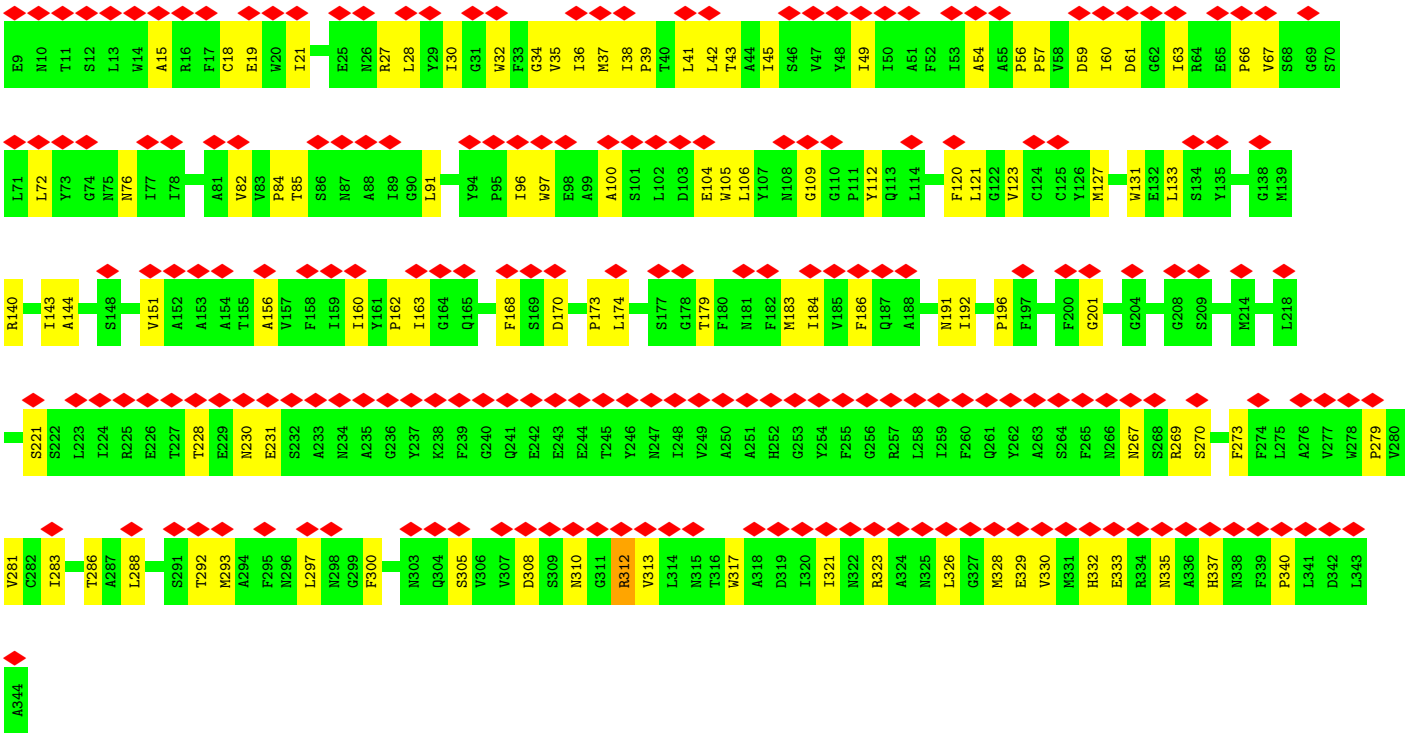
Mol	Chain	Residues	Atoms					AltConf
55	Y	1	Total	C	N	O	P	0
			50	40	1	8	1	
55	Y	1	Total	C	N	O	P	0
			19	9	1	8	1	
55	y	1	Total	C	N	O	P	0
			50	40	1	8	1	
55	y	1	Total	C	N	O	P	0
			19	9	1	8	1	
55	Y1	1	Total	C	N	O	P	0
			50	40	1	8	1	
55	Y1	1	Total	C	N	O	P	0
			19	9	1	8	1	
55	y1	1	Total	C	N	O	P	0
			50	40	1	8	1	
55	y1	1	Total	C	N	O	P	0
			19	9	1	8	1	

3 Residue-property plots (i)

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

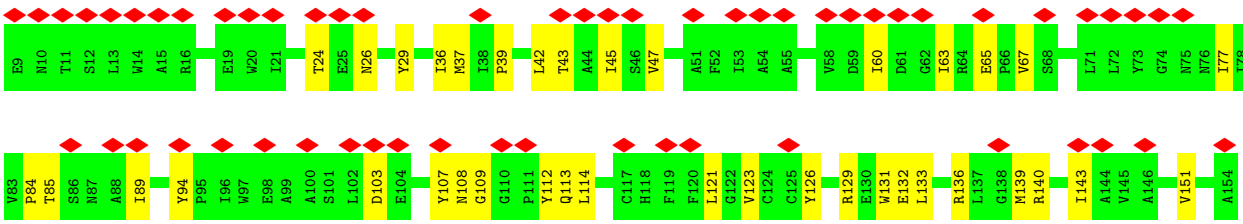
• Molecule 1: Photosystem II protein D1

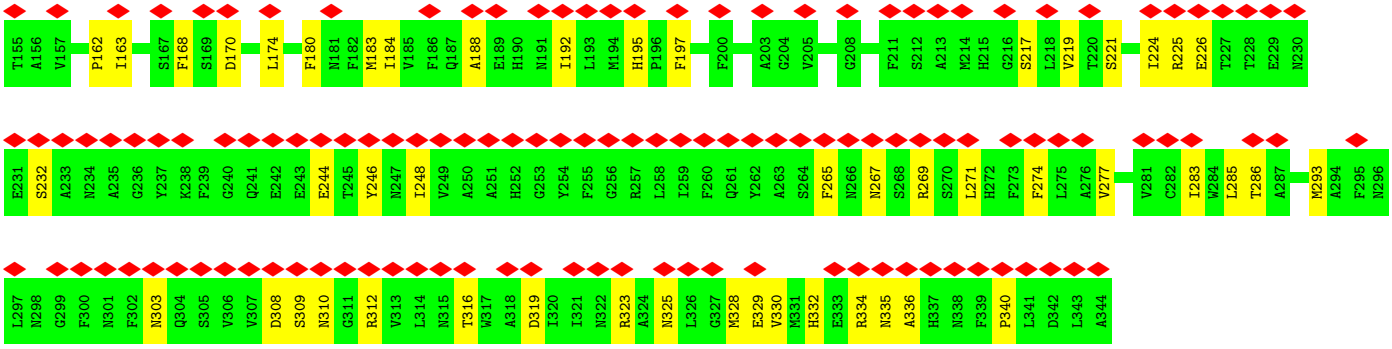
Chain A:



• Molecule 1: Photosystem II protein D1

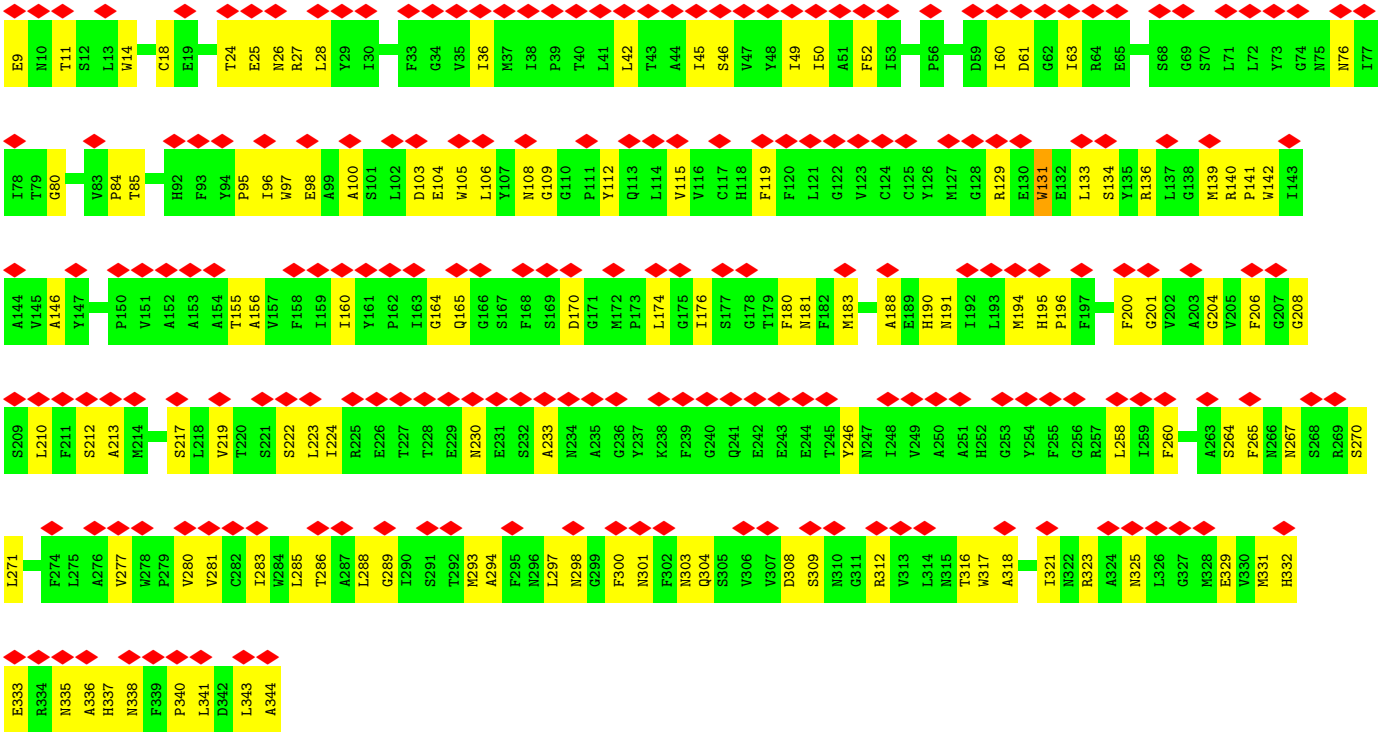
Chain a:





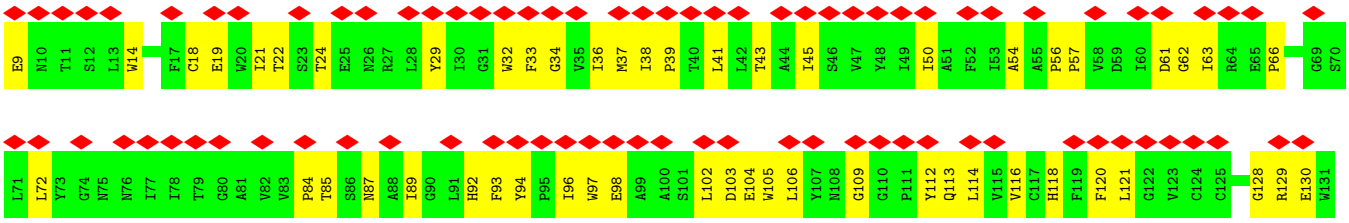
- Molecule 1: Photosystem II protein D1

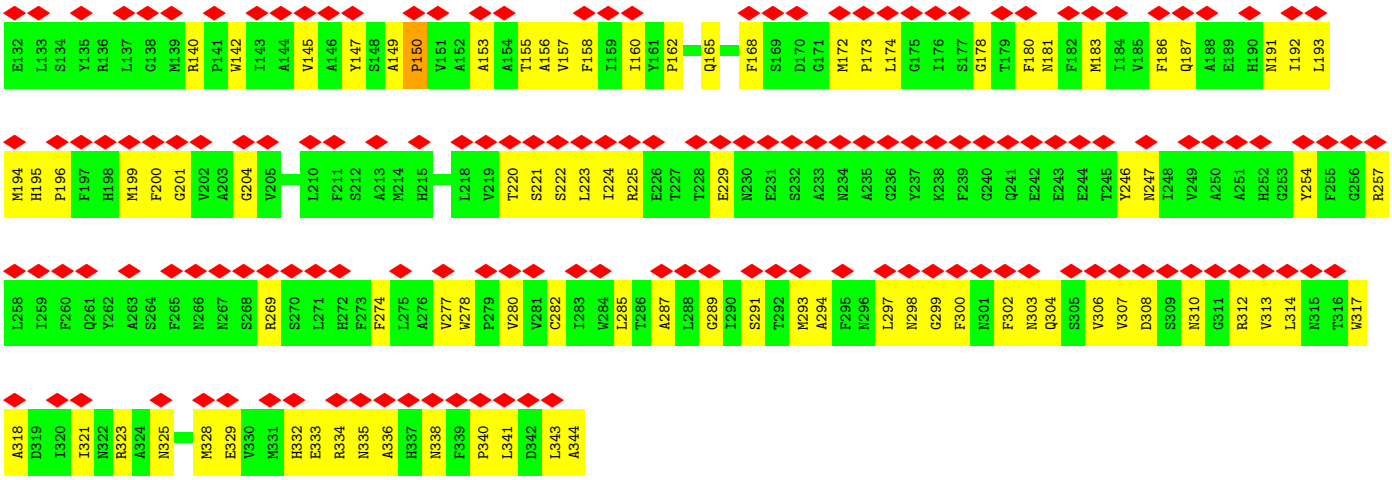
Chain A1:



- Molecule 1: Photosystem II protein D1

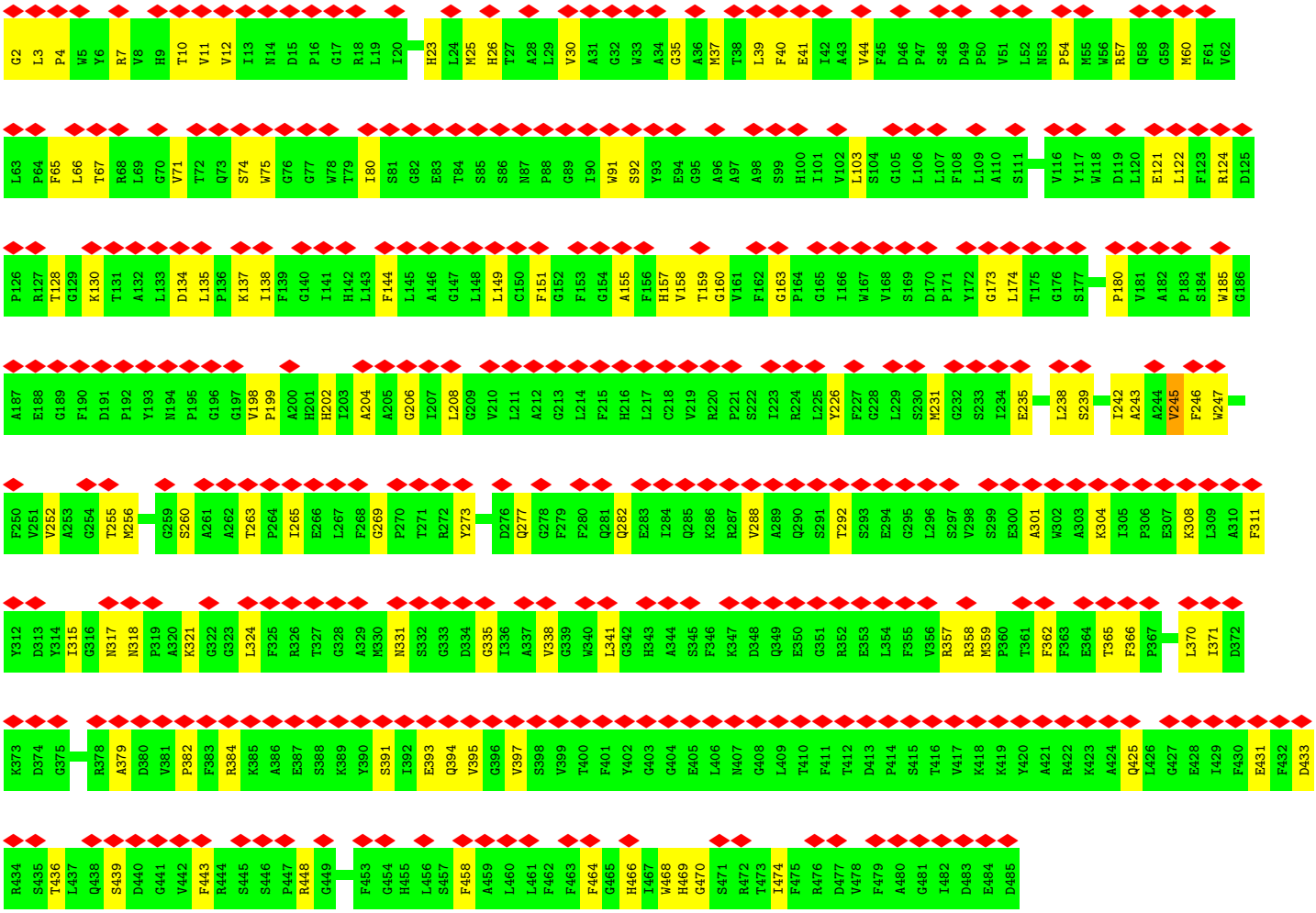
Chain a1:





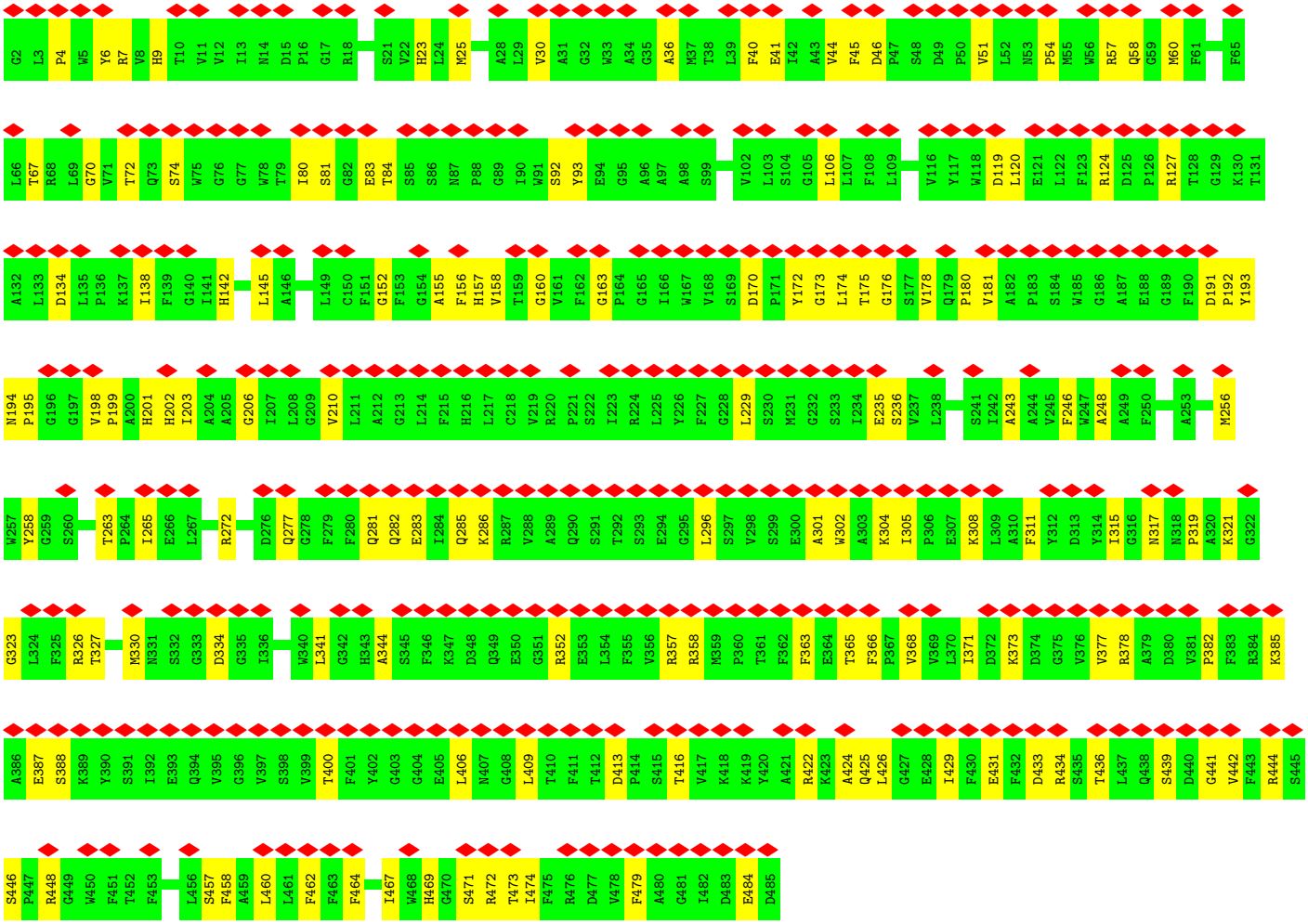
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



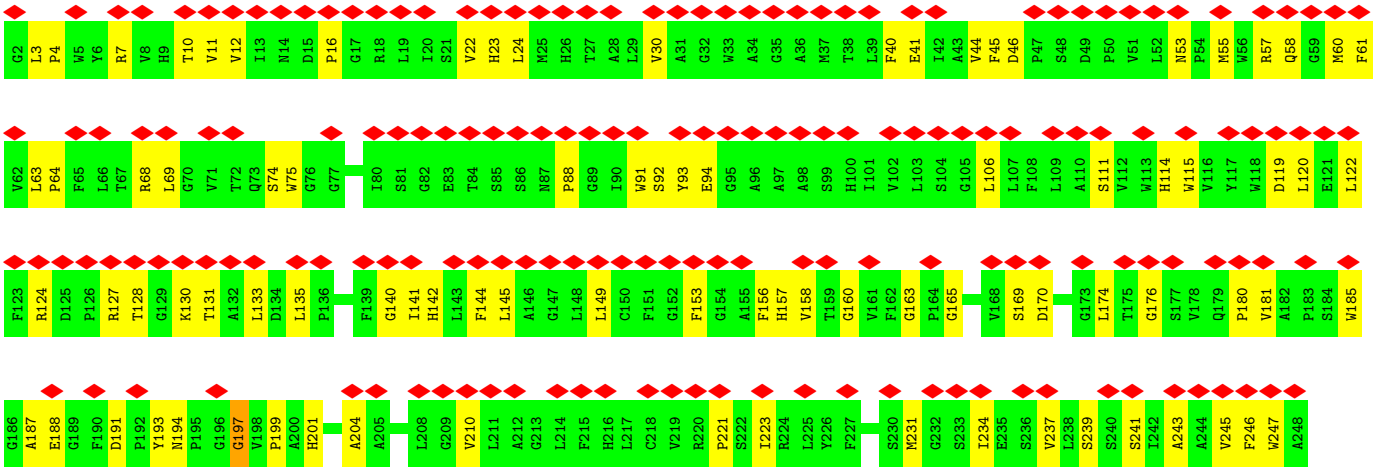
- Molecule 2: Photosystem II CP47 reaction center protein

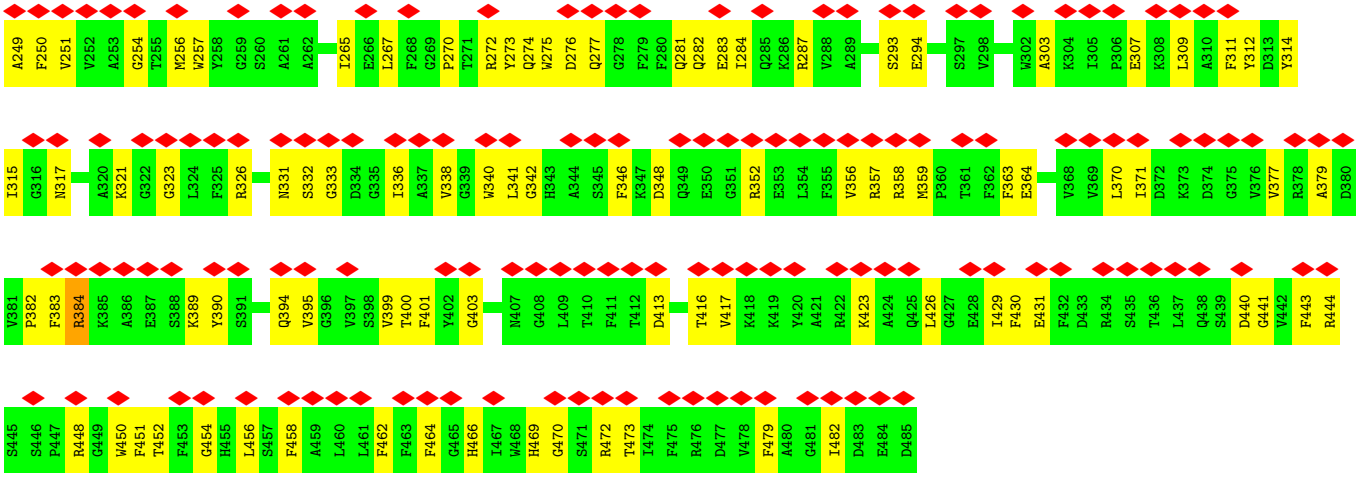
Chain b: 70% 69% 31%



- Molecule 2: Photosystem II CP47 reaction center protein

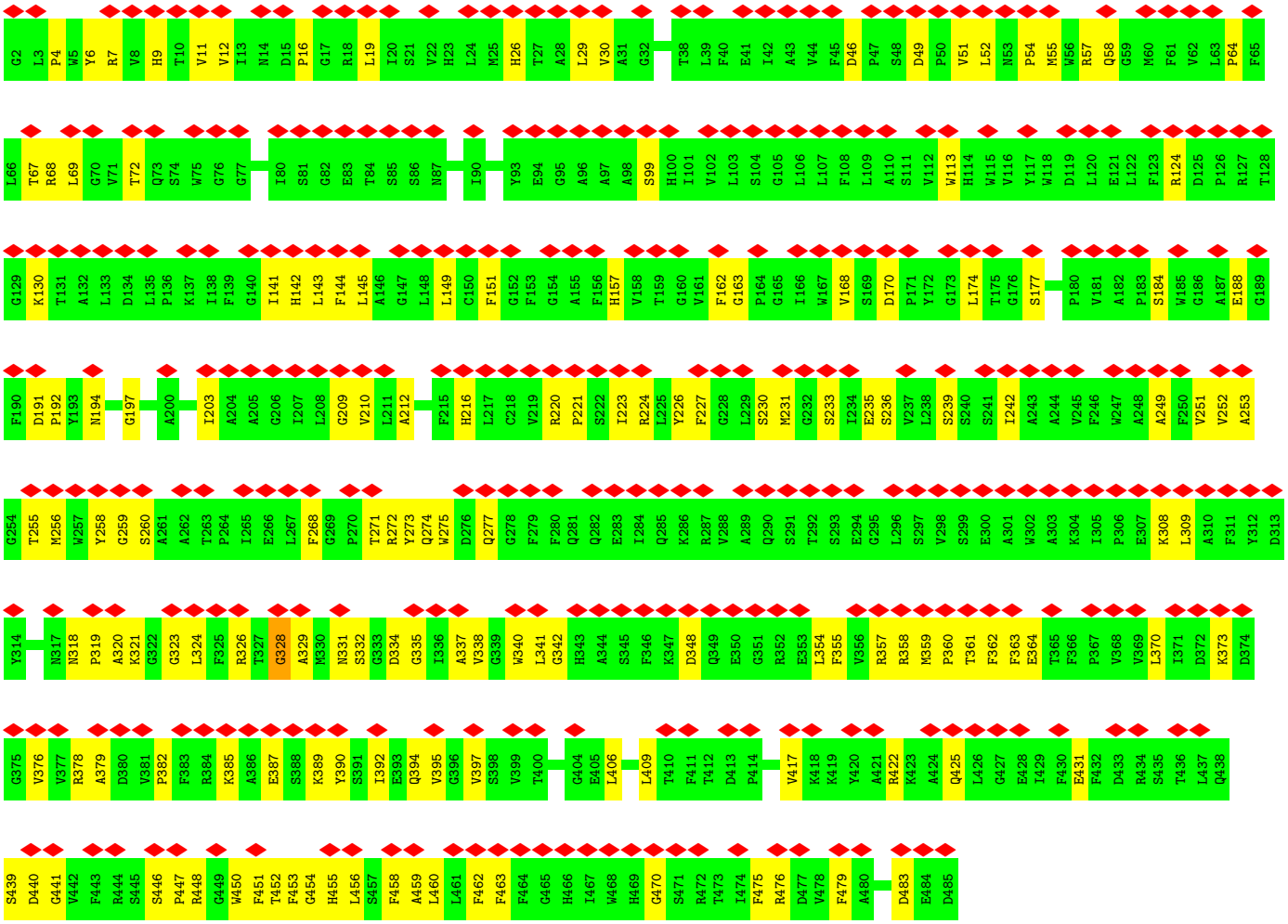
Chain B1: 66% 63% 37%





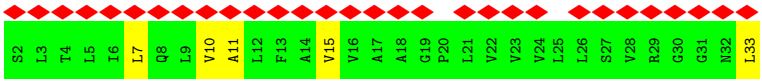
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b1: 71% 68% 32%



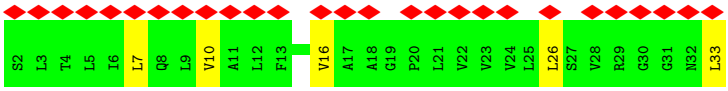
- Molecule 3: Photosystem II reaction center protein Ycf12

Chain V: 94% 84% 16%



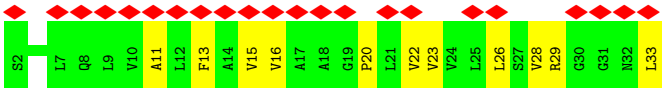
• Molecule 3: Photosystem II reaction center protein Ycf12

Chain v: 84% 84% 16%



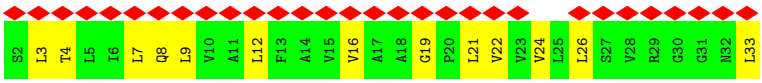
• Molecule 3: Photosystem II reaction center protein Ycf12

Chain V1: 69% 66% 34%



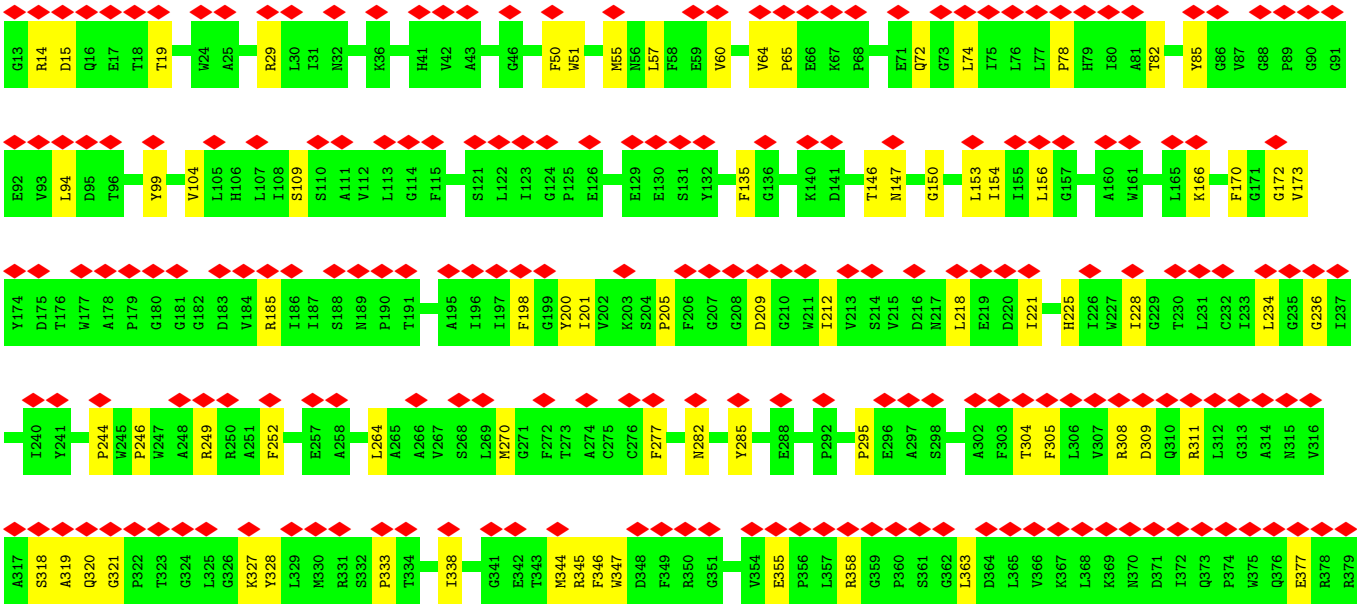
• Molecule 3: Photosystem II reaction center protein Ycf12

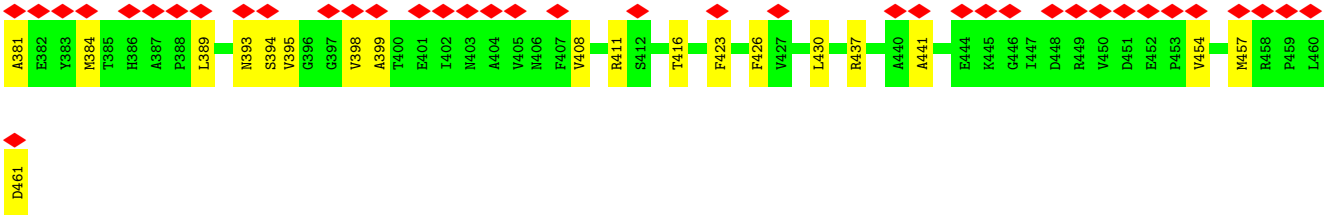
Chain v1: 94% 59% 41%



• Molecule 4: Photosystem II CP43 reaction center protein

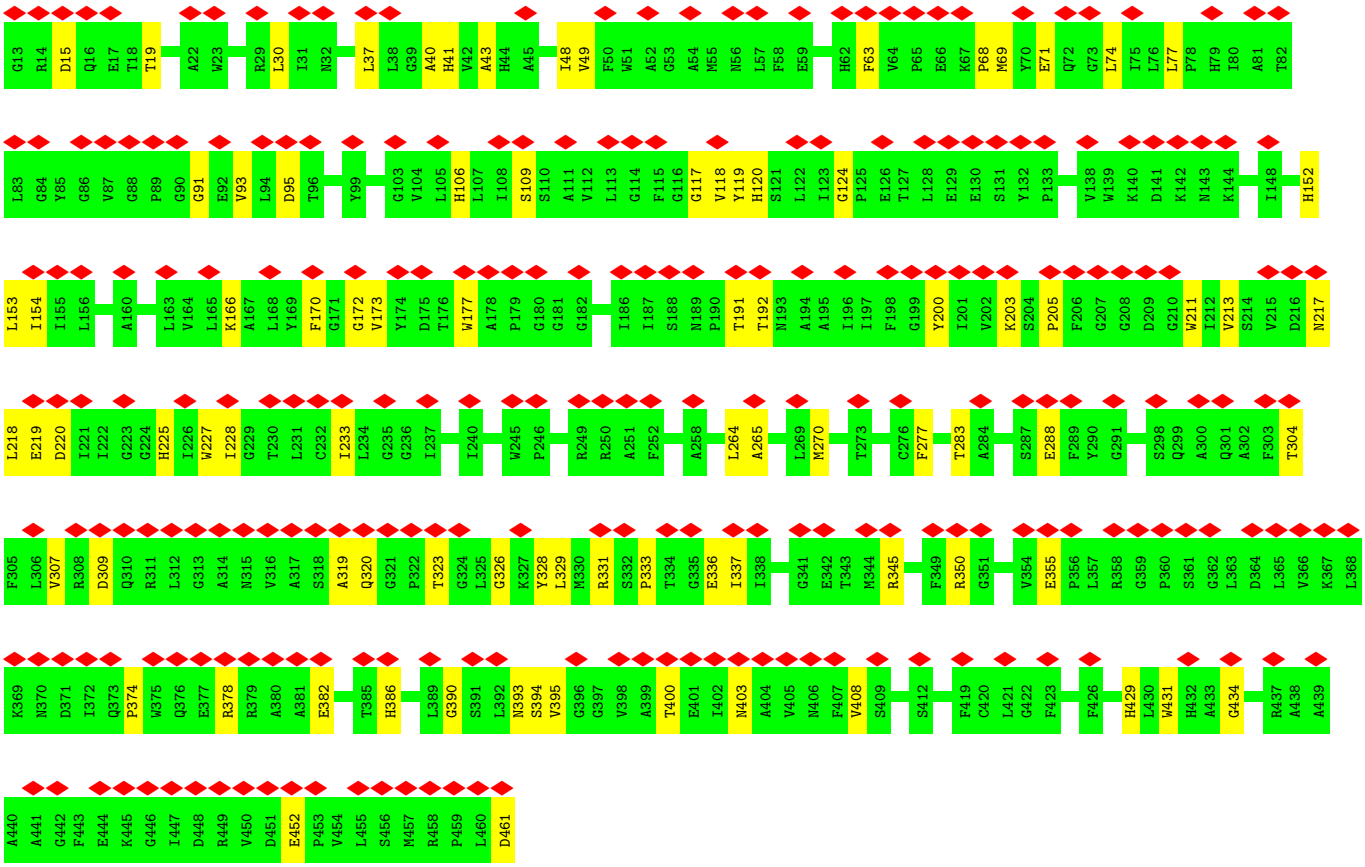
Chain C: 55% 79% 21%





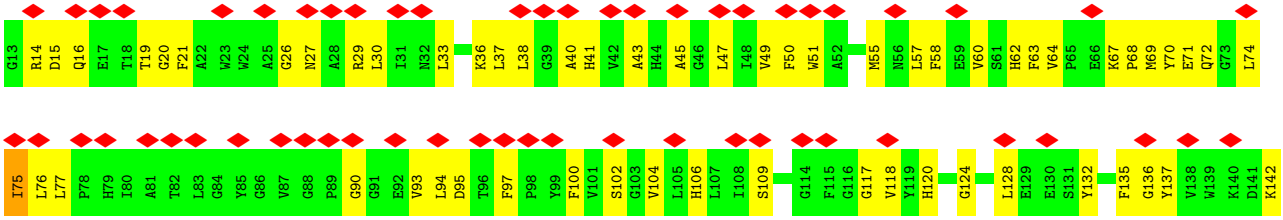
• Molecule 4: Photosystem II CP43 reaction center protein

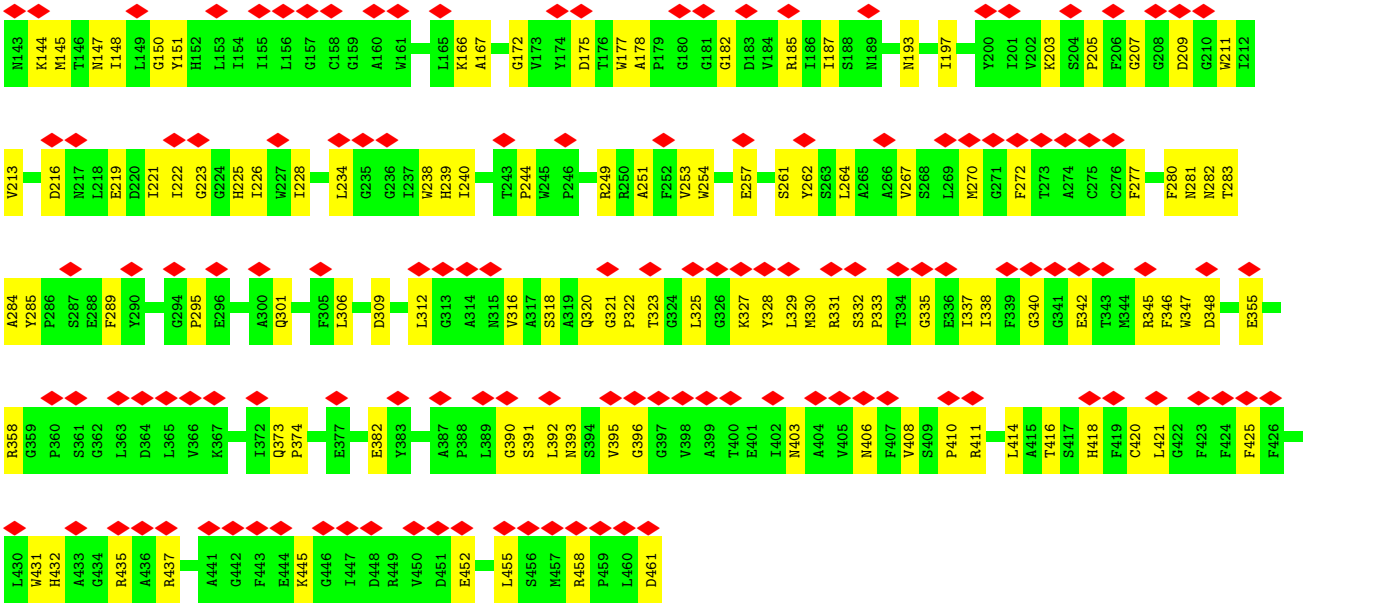
Chain c:



• Molecule 4: Photosystem II CP43 reaction center protein

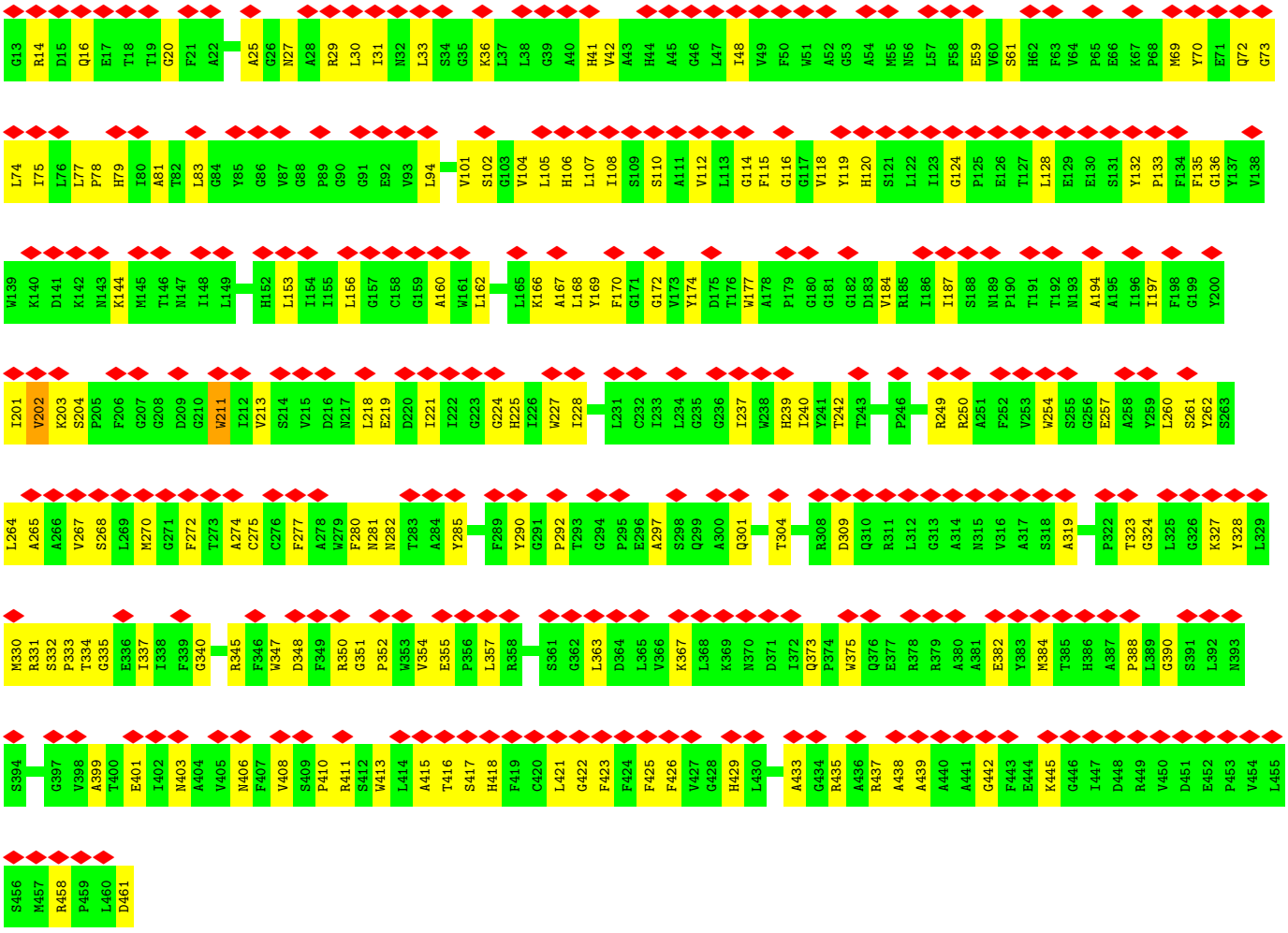
Chain C1:





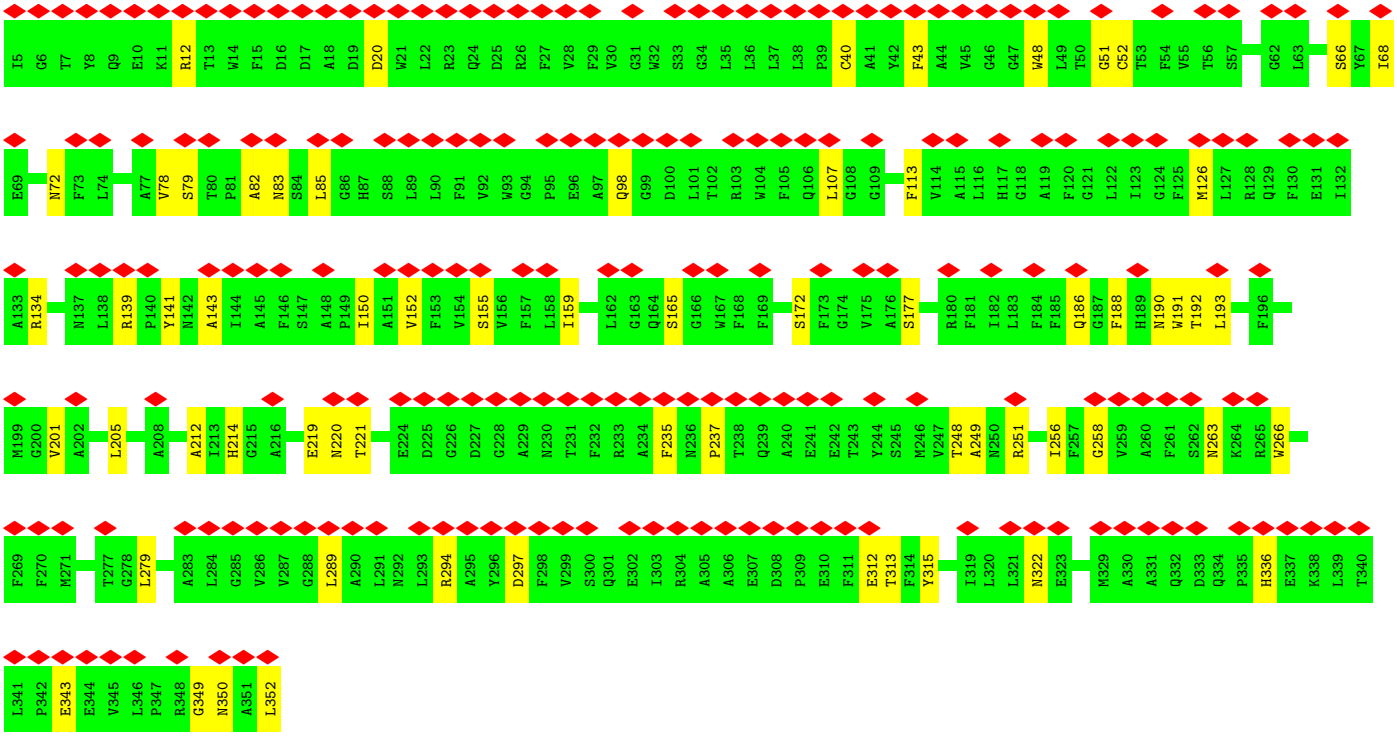
- Molecule 4: Photosystem II CP43 reaction center protein

Chain c1:



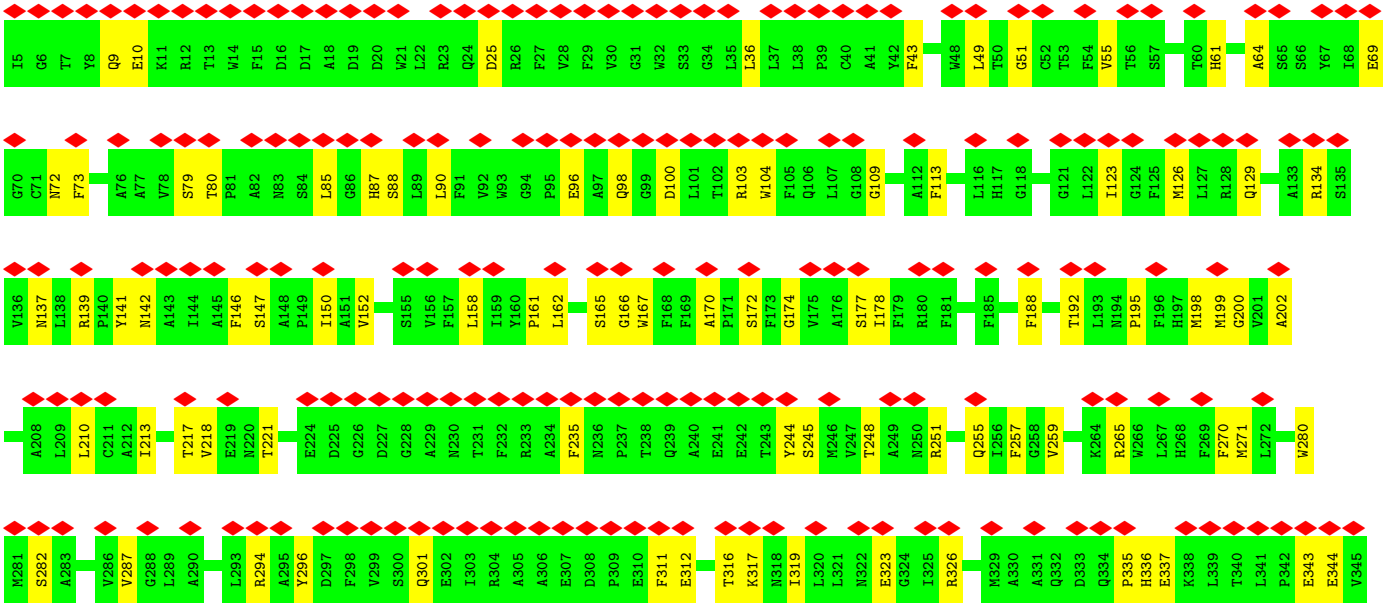
- Molecule 5: Photosystem II D2 protein

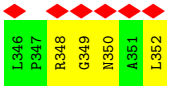
Chain D: 63% 81% 19%



- Molecule 5: Photosystem II D2 protein

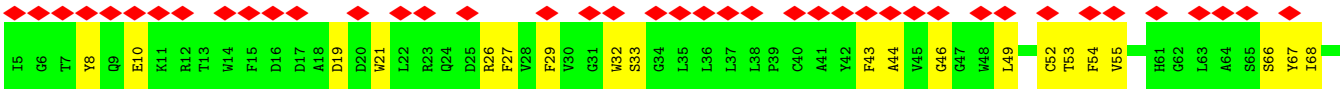
Chain d: 61% 73% 27%

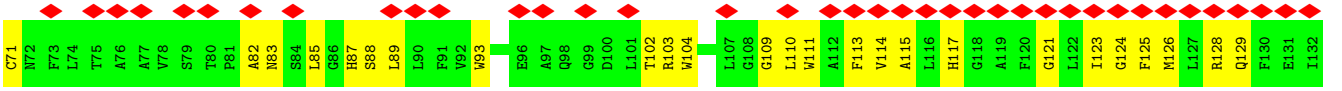


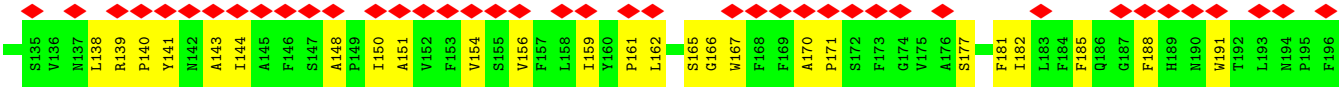


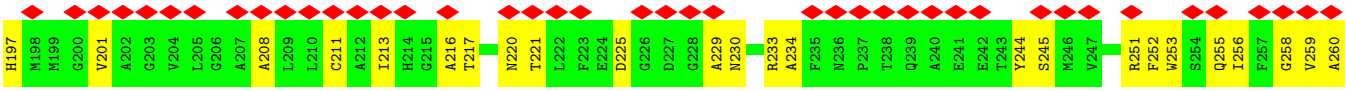
• Molecule 5: Photosystem II D2 protein

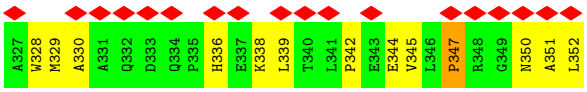
Chain D1:





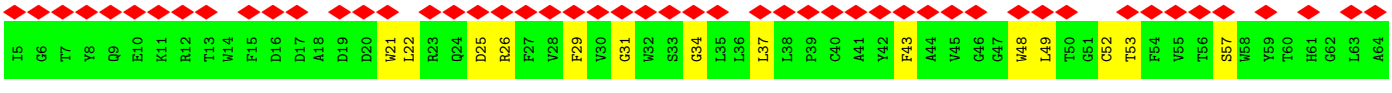


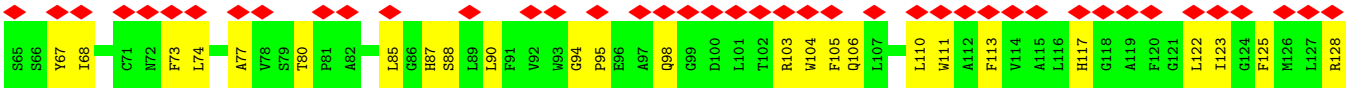


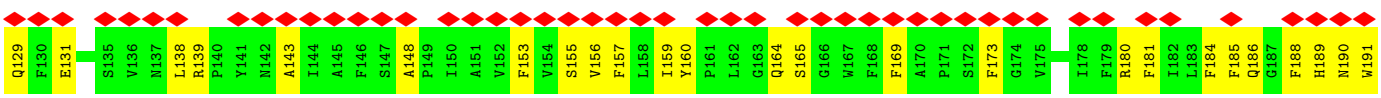


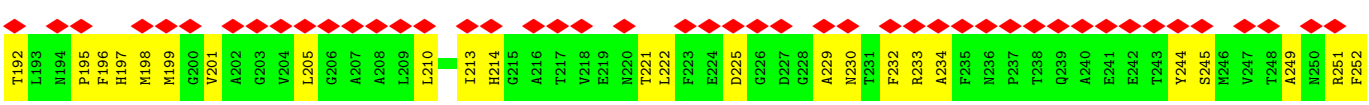
• Molecule 5: Photosystem II D2 protein

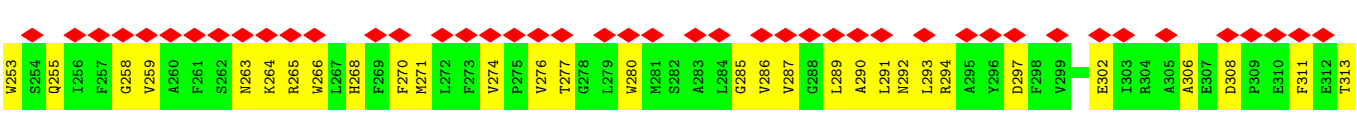
Chain d1:

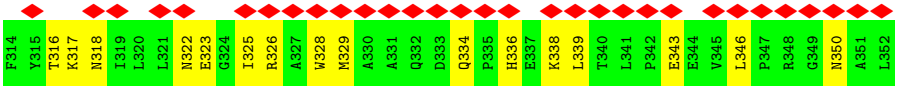






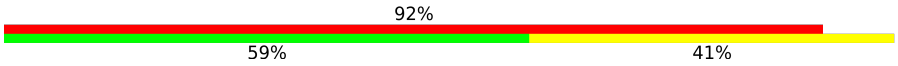


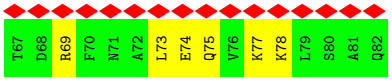




• Molecule 6: Cytochrome b559 subunit alpha

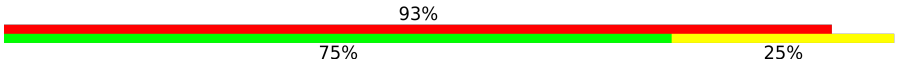
Chain E:

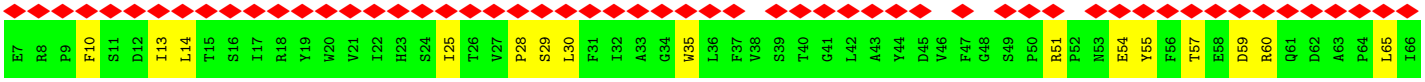


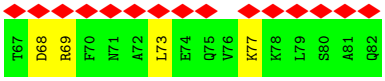


• Molecule 6: Cytochrome b559 subunit alpha

Chain e:

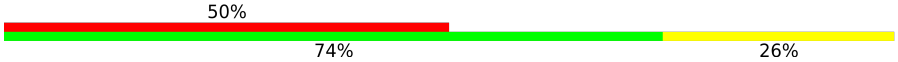


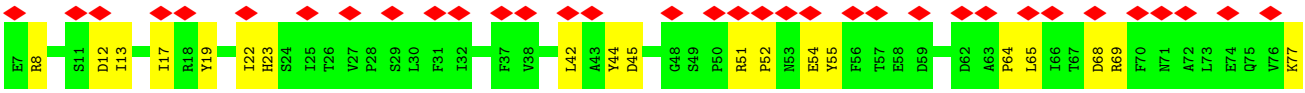


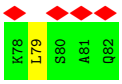


• Molecule 6: Cytochrome b559 subunit alpha

Chain E1:

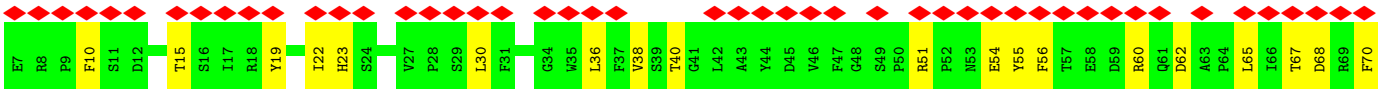


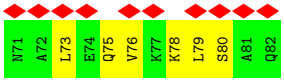




• Molecule 6: Cytochrome b559 subunit alpha

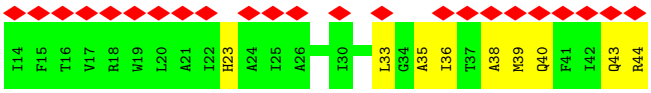
Chain e1:





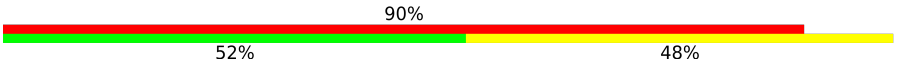
• Molecule 7: Cytochrome b559 subunit beta

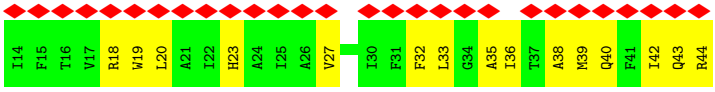
Chain F:



• Molecule 7: Cytochrome b559 subunit beta

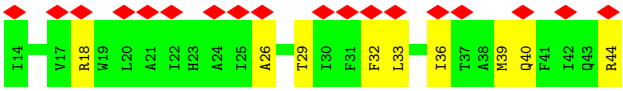
Chain f:





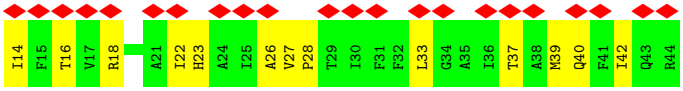
• Molecule 7: Cytochrome b559 subunit beta

Chain F1:



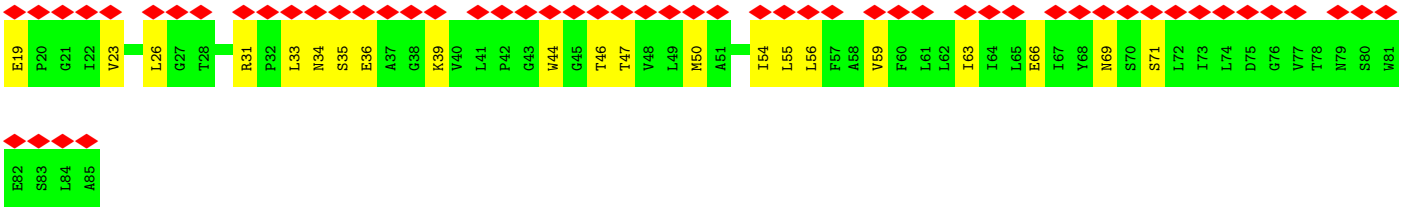
• Molecule 7: Cytochrome b559 subunit beta

Chain f1:



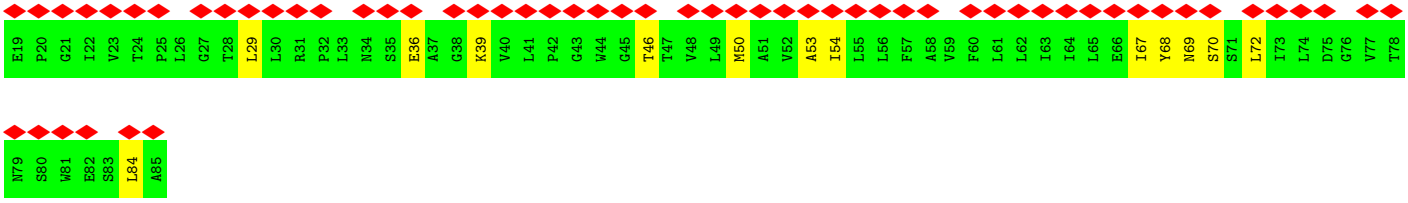
• Molecule 8: Photosystem II reaction center protein H

Chain H:



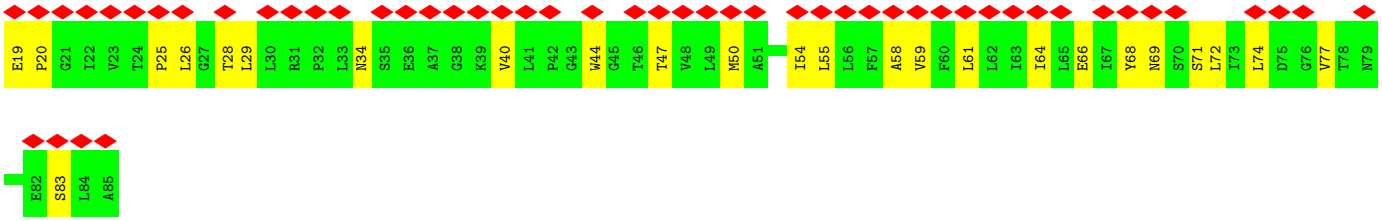
• Molecule 8: Photosystem II reaction center protein H

Chain h:



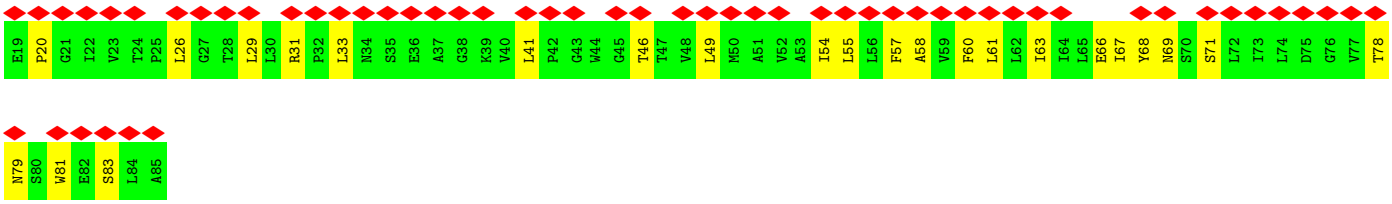
• Molecule 8: Photosystem II reaction center protein H

Chain H1:



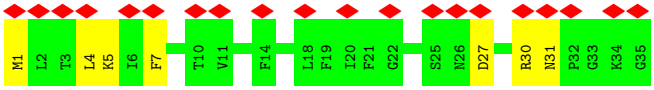
- Molecule 8: Photosystem II reaction center protein H

Chain h1:



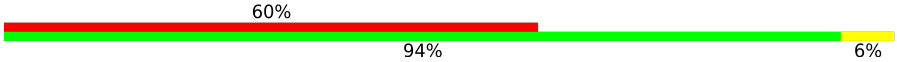
- Molecule 9: Photosystem II reaction center protein I

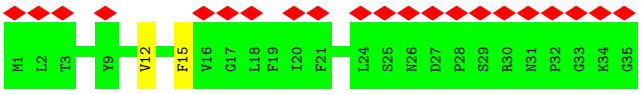
Chain I:



- Molecule 9: Photosystem II reaction center protein I

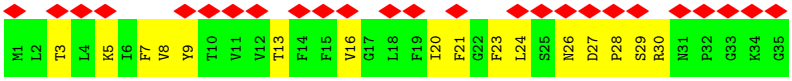
Chain i:





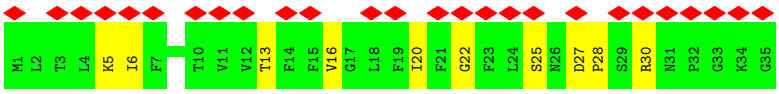
- Molecule 9: Photosystem II reaction center protein I

Chain I1:



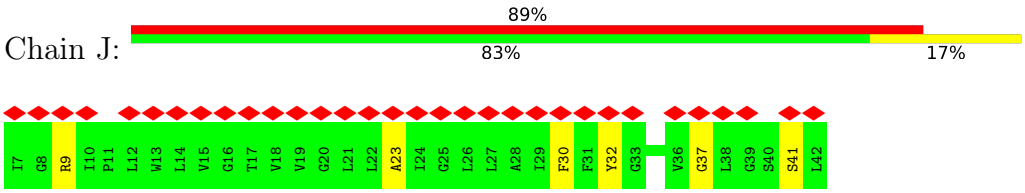
- Molecule 9: Photosystem II reaction center protein I

Chain i1:



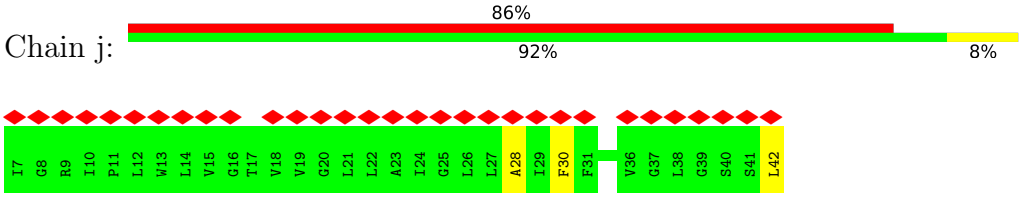
- Molecule 10: PsbJ

Chain J:



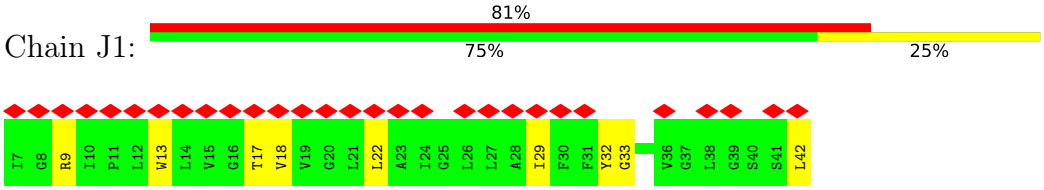
- Molecule 10: PsbJ

Chain j:



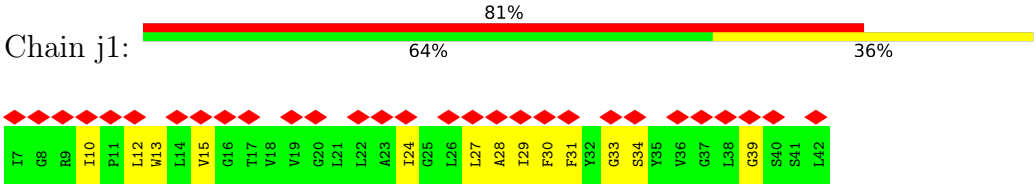
- Molecule 10: PsbJ

Chain J1:



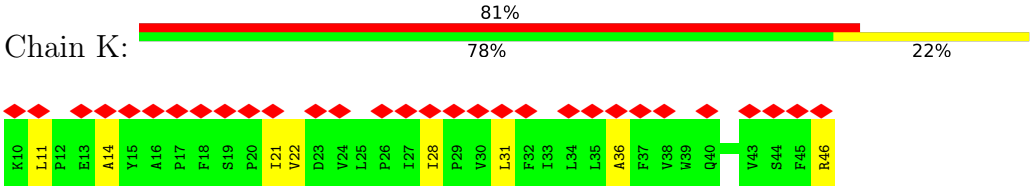
- Molecule 10: PsbJ

Chain j1:



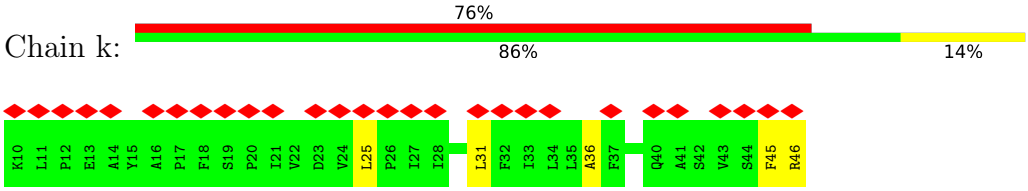
- Molecule 11: Photosystem II reaction center protein K

Chain K:



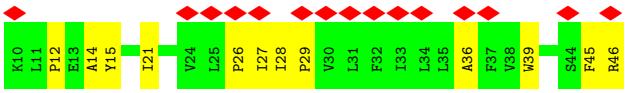
- Molecule 11: Photosystem II reaction center protein K

Chain k:



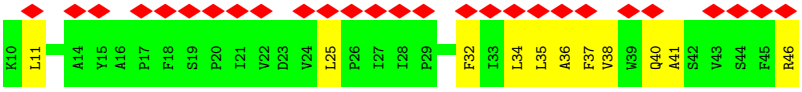
- Molecule 11: Photosystem II reaction center protein K

Chain K1:



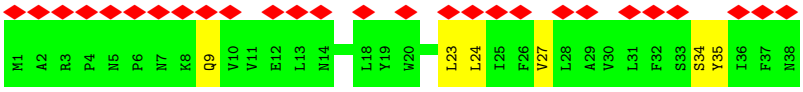
• Molecule 11: Photosystem II reaction center protein K

Chain k1:



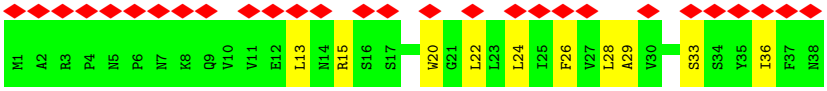
• Molecule 12: Photosystem II reaction center protein L

Chain L:



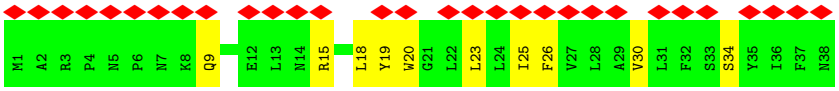
• Molecule 12: Photosystem II reaction center protein L

Chain l:



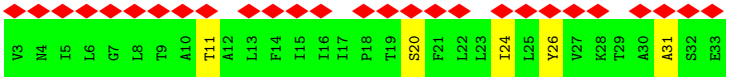
• Molecule 12: Photosystem II reaction center protein L

Chain L1:



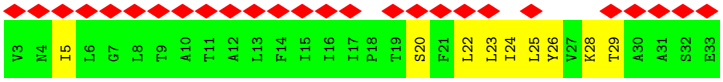
• Molecule 13: PsbM

Chain M:



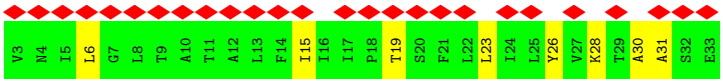
• Molecule 13: PsbM

Chain m:



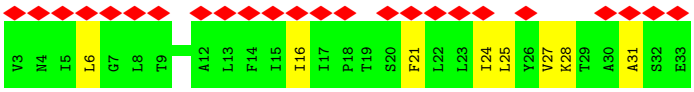
• Molecule 13: PsbM

Chain M1:



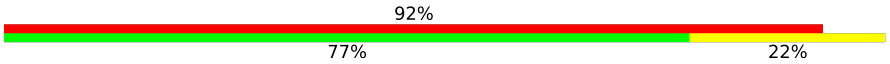
• Molecule 13: PsbM

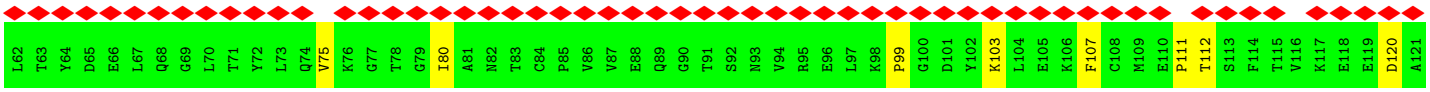
Chain m1:

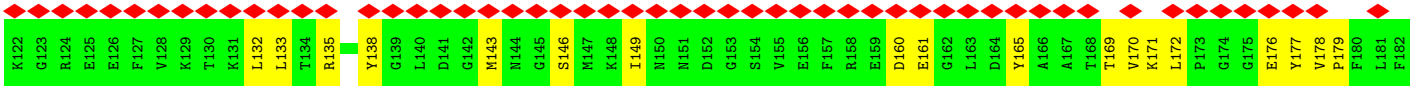


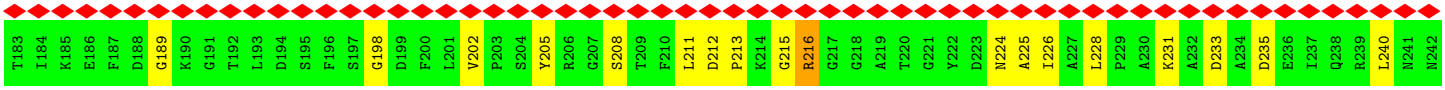
• Molecule 14: PsbO

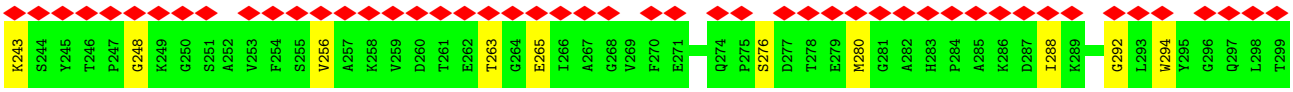
Chain O:





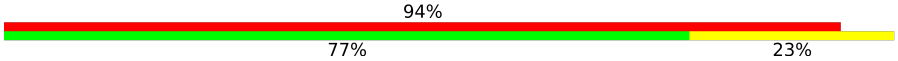


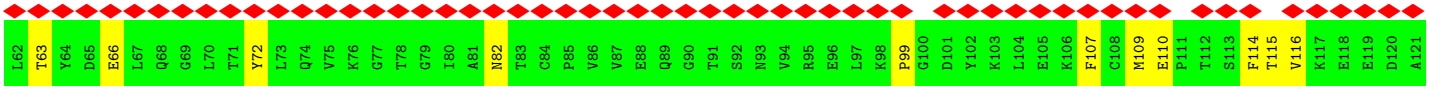


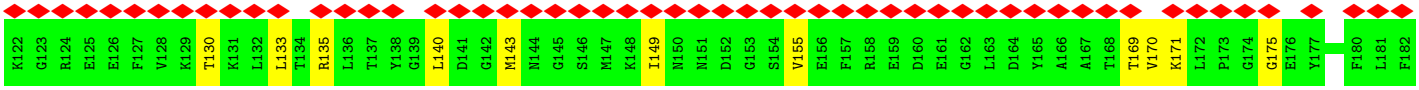


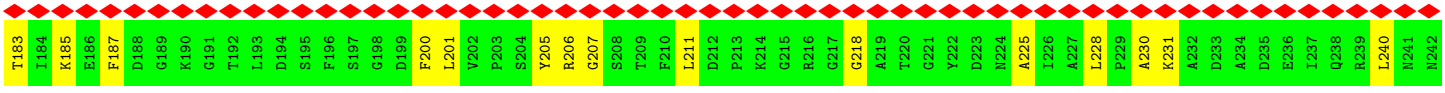
• Molecule 14: PsbO

Chain o:



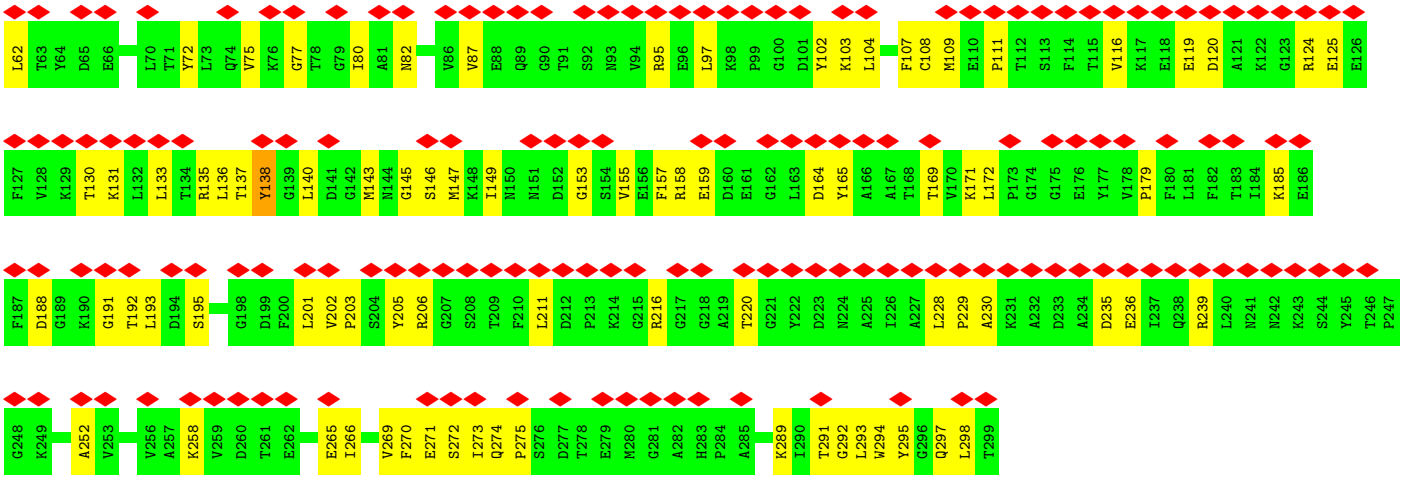






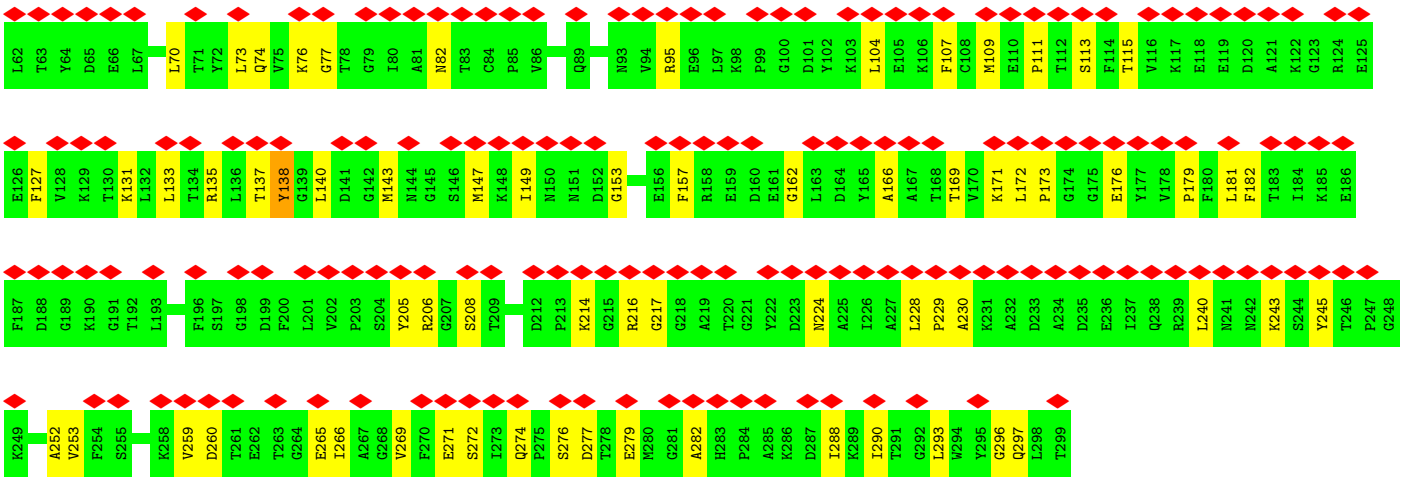
• Molecule 14: PsbO

Chain O1: 67% 65% 35%



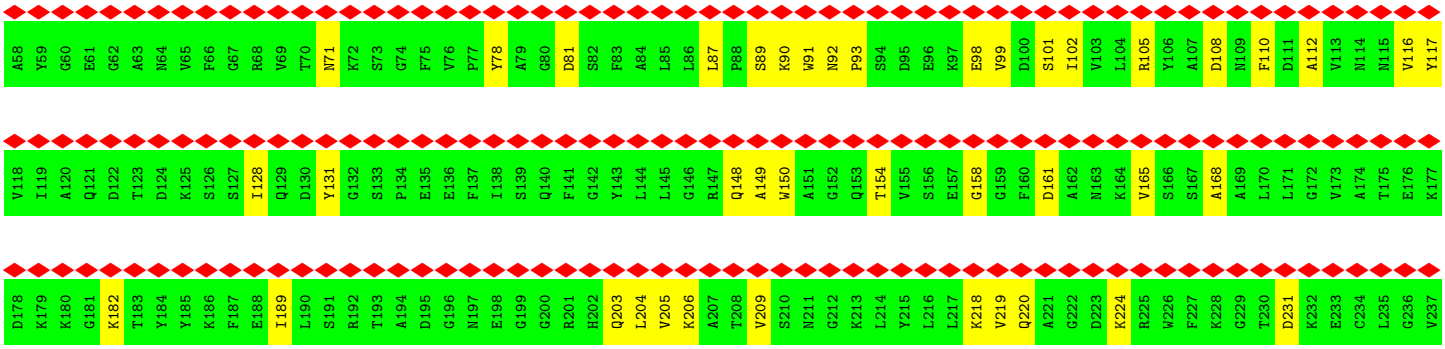
- Molecule 14: PsbO

Chain o1: 72% 72% 28%



- Molecule 15: PsbP

Chain P: 100% 77% 23%



L238 D239 S240 F241 T242 V243 V244

- Molecule 15: PsbP

Chain p: 100% 72% 28%

A58 Y59 G60 E61 G62 A63 N64 V65 F66 G67 R68 V69 T70 N71 K72 S73 G74 F75 V76 P77 Y78 A79 G80 D81 S82 F83 A84 L85 L86 L87 P88 S89 K90 W91 N92 P93 S94 D95 E96 K97 E98 V99 D100 S101 I102 V103 L104 R105 Y106 A107 D108 N109 F110 D111 A112 V113 N114 N115 V116 Y117

V118 I119 A120 Q121 D122 T123 D124 K125 S126 S127 I128 Q129 D130 Y131 G132 S133 P134 E135 E136 F137 I138 S139 Q140 F141 G142 Y143 L144 L145 G146 R147 Q148 A149 W150 A151 G152 Q153 T154 V155 S156 E157 G158 G159 F160 D161 A162 N163 K164 V165 S166 S167 A168 A169 L170 L171 G172 V173 A174 T175 E176 K177

D178 K179 K180 G181 K182 T183 Y184 Y185 K186 F187 E188 I189 L190 S191 R192 T193 A194 D195 G196 N197 E198 G199 G200 R201 H202 Q203 L204 V205 K206 A207 T208 V209 S210 N211 G212 K213 L214 Y215 L216 L217 K218 V219 Q220 A221 G222 D223 K224 R225 W226 F227 K228 G229 T230 D231 K232 E233 C234 L235 G236 V237

L238 D239 S240 F241 T242 V243 V244

- Molecule 15: PsbP

Chain P1: 98% 75% 25%

A58 Y59 G60 E61 G62 A63 N64 V65 F66 G67 R68 V69 T70 N71 K72 S73 G74 F75 V76 P77 Y78 A79 G80 D81 S82 F83 A84 L85 L86 L87 P88 S89 K90 W91 N92 P93 S94 D95 E96 K97 E98 V99 D100 S101 I102 V103 L104 R105 Y106 A107 D108 N109 F110 D111 A112 V113 N114 N115 V116 Y117

V118 I119 A120 Q121 D122 T123 D124 K125 S126 S127 I128 Q129 D130 Y131 G132 S133 P134 E135 E136 F137 I138 S139 Q140 F141 G142 Y143 L144 L145 G146 R147 Q148 A149 W150 A151 G152 Q153 T154 V155 S156 E157 G158 G159 F160 D161 A162 N163 K164 V165 S166 S167 A168 A169 L170 L171 G172 V173 A174 T175 E176 K177

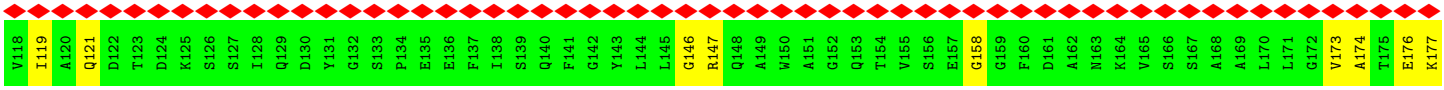
D178 K179 K180 G181 K182 T183 Y184 Y185 K186 F187 E188 I189 L190 S191 R192 T193 A194 D195 G196 N197 E198 G199 G200 R201 H202 Q203 L204 V205 K206 A207 T208 V209 S210 N211 G212 K213 L214 Y215 L216 L217 K218 V219 Q220 A221 G222 D223 K224 R225 W226 F227 K228 G229 T230 D231 K232 E233 C234 L235 G236 V237

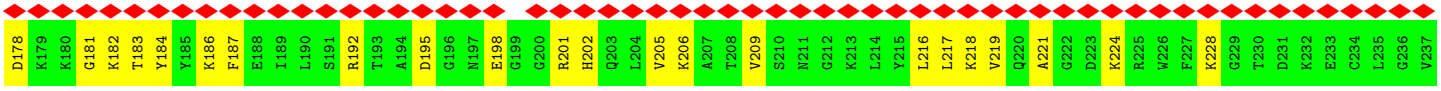
L238 D239 S240 F241 T242 V243 V244

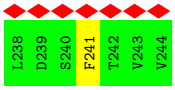
- Molecule 15: PsbP

Chain p1: 99% 73% 27%

A58 Y59 G60 E61 G62 A63 N64 V65 F66 G67 R68 V69 T70 N71 K72 S73 G74 F75 V76 P77 Y78 A79 G80 D81 S82 F83 A84 L85 L86 L87 P88 S89 K90 W91 N92 P93 S94 D95 E96 K97 E98 V99 D100 S101 I102 V103 L104 R105 Y106 A107 D108 N109 F110 D111 A112 V113 N114 N115 V116 Y117

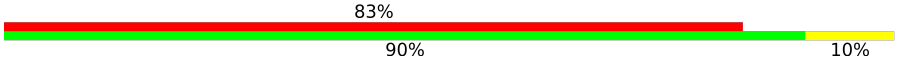


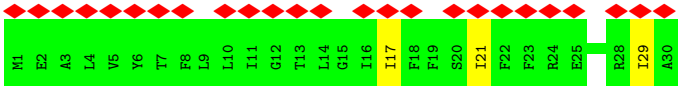




- Molecule 16: Photosystem II reaction center protein T

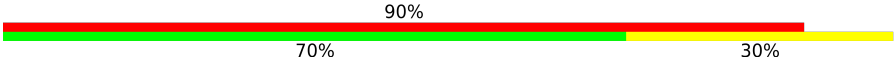
Chain T:

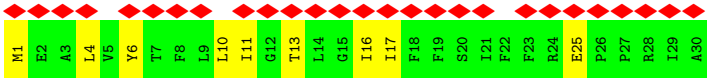




- Molecule 16: Photosystem II reaction center protein T

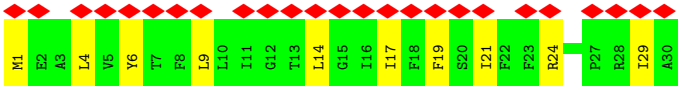
Chain t:





- Molecule 16: Photosystem II reaction center protein T

Chain T1:

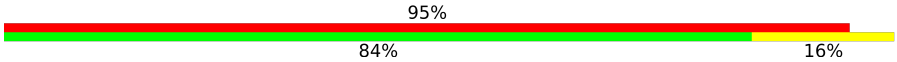


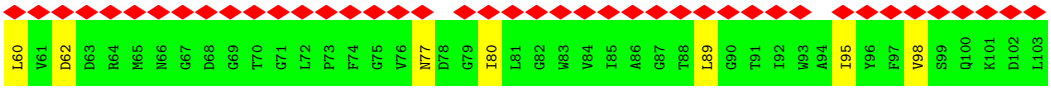
- Molecule 16: Photosystem II reaction center protein T

Chain t1:

- Molecule 17: PsbW

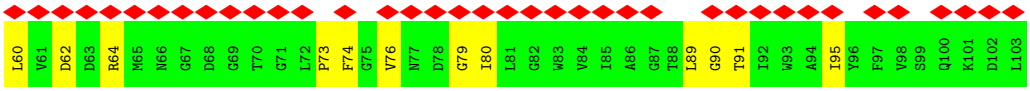
Chain W:





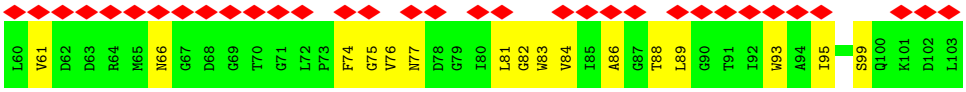
- Molecule 17: PsbW

Chain w:



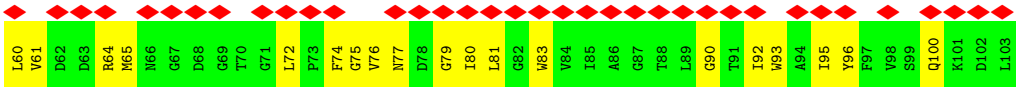
- Molecule 17: PsbW

Chain W1:



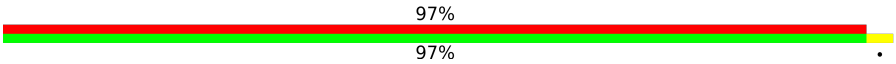
- Molecule 17: PsbW

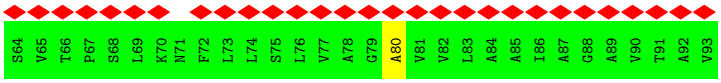
Chain w1:



- Molecule 18: PsbX

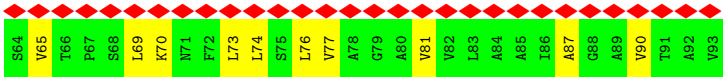
Chain X:





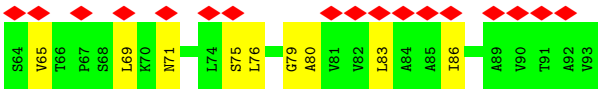
- Molecule 18: PsbX

Chain x:



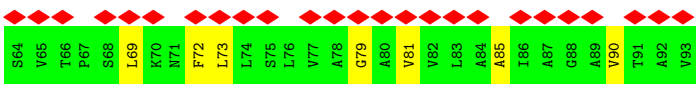
- Molecule 18: PsbX

Chain X1:



- Molecule 18: PsbX

Chain x1:



- Molecule 19: Photosystem II reaction center protein Z

Chain Z: 90% (90% / 10%)

M1 T2 S3 I4 L5 Q6 I7 A8 L9 L10 G11 L12 V13 L14 V15 S16 F17 A18 L19 V20 V21 G22 V25 V26 F27 A28 S29 P30 N31 G32 W33 T34 E35 N36 K37 G38 V39 V40 F41 S42 G43 L44 S45 V46 W47 F48 L49 L50 V51 F52 A53 V54 G55 V56 F57 N58 S59 F60 A61

- Molecule 19: Photosystem II reaction center protein Z

Chain z: 87% (87% / 13%)

M1 T2 S3 I4 L5 Q6 I7 A8 L9 L10 G11 L12 V13 L14 F17 A18 L19 V20 V21 G22 V23 P24 V25 V26 F27 A28 S29 P30 N31 G32 W33 T34 E35 N36 K37 G38 V39 V40 F41 S42 G43 L44 S45 V46 W47 F48 L49 L50 V51 F52 A53 V54 F57 N58 S59 F60 A61

- Molecule 19: Photosystem II reaction center protein Z

Chain Z1: 52% (77% / 23%)

M1 I4 L5 Q6 I7 A8 L9 L12 V13 L14 V15 S16 F17 A18 L19 V20 V21 G22 V23 P24 V25 V26 F27 N31 T34 E35 N36 K37 L44 S45 V46 W47 F48 L49 L50 V51 F52 A53 V54 G55 V56 F57 N58 S59 F60 A61

- Molecule 19: Photosystem II reaction center protein Z

Chain z1: 84% (80% / 20%)

M1 I4 L5 Q6 I7 A8 L9 L12 V13 L14 V15 S16 F17 A18 L19 V20 V21 G22 V23 P24 V25 V26 F27 A28 S29 P30 N31 G32 W33 T34 E35 N36 K37 G38 V39 V40 F41 S42 G43 L44 S45 V46 W47 F48 L49 L50 V51 F52 A53 V54 G55 V56 F57 N58 S59 F60 A61

- Molecule 20: LHCII M3

Chain N: 94% (75% / 25%)

T36 I37 N38 Q39 F40 Y41 G42 P43 D44 R45 N46 K47 W48 L49 G50 P51 Y52 S53 T54 N55 T56 P57 P58 Y59 L60 T61 G62 E63 F64 P65 G66 D67 Y68 G69 W70 D71 T72 A73 G74 L75 S76 A77 D78 P79 E80 T81 F82 K83 R84 Y85 R86 E87 L88 E89 L90 I91 H92 A93 R94 W95

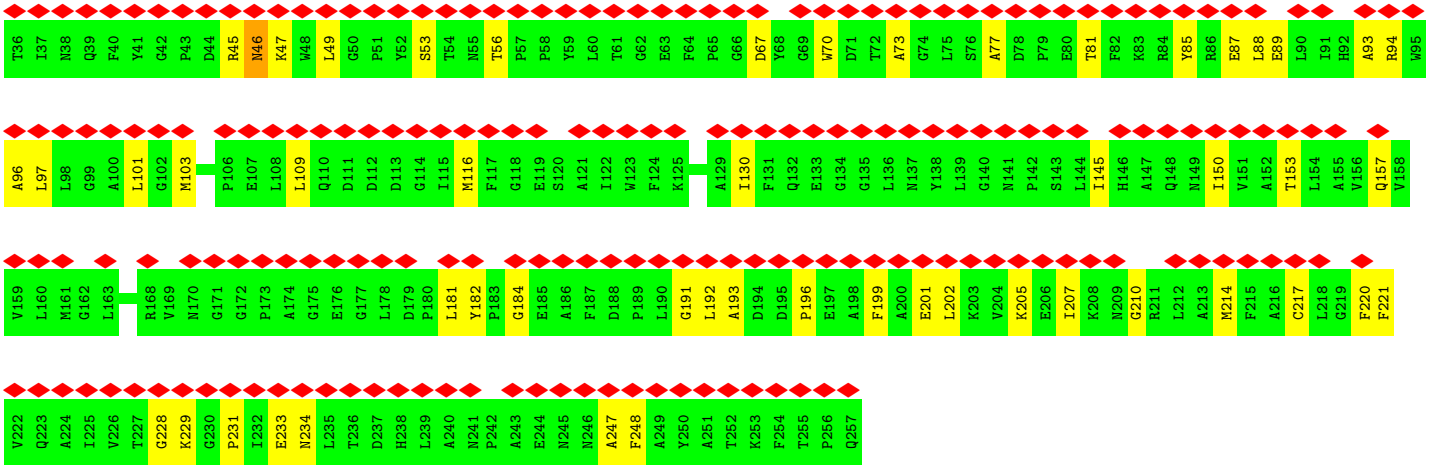
A96 L97 L98 G99 A100 L101 G102 M103 V104 T105 P106 E107 L108 L109 Q110 D111 D112 D113 G114 I115 M116 F117 G118 E119 S120 A121 I122 W123 F124 K125 A126 G127 A128 A129 I130 F131 Q132 E133 G134 G135 L136 N137 Y138 L139 G140 N141 P142 S143 L144 I145 H146 A147 Q148 N149 I150 V151 A152 T153 L154 A155

V156 Q157 V158 M161 G162 L163 V164 E165 G166 Y167 R168 V169 N170 G171 G172 P173 A174 G175 E176 G177 L178 D179 P180 L181 Y182 P183 G184 E185 A186 F187 D188 P189 L190 G191 L192 A193 D194 D195 P196 E197 A198 F199 A200 E201 L202 K203 V204 K205 E206 I207 K208 N209 G210 R211 L212 A213 M214 F215 A216

C217 L218 G219 F220 F221 V222 Q223 A224 I225 V226 T227 G228 K229 G230 P231 I232 E233 N234 L235 T236 D237 H238 L239 A240 N241 P242 A243 E244 N245 N246 A247 F248 A249 Y250 A251 T252 K253 F254 T255 P256 Q257

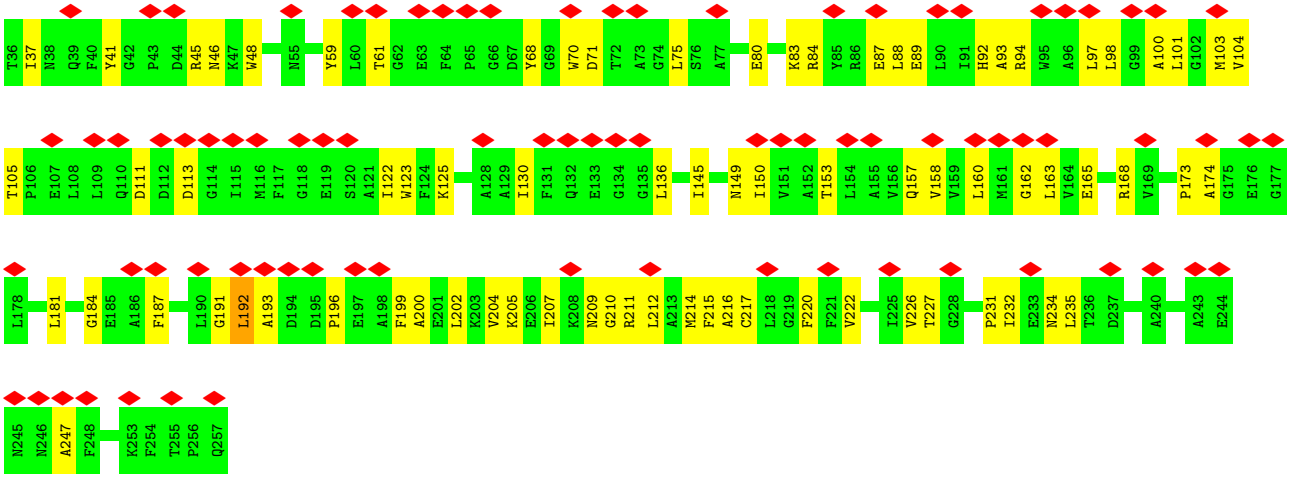
- Molecule 20: LHCII M3

Chain n: 89% (77% / 23%)



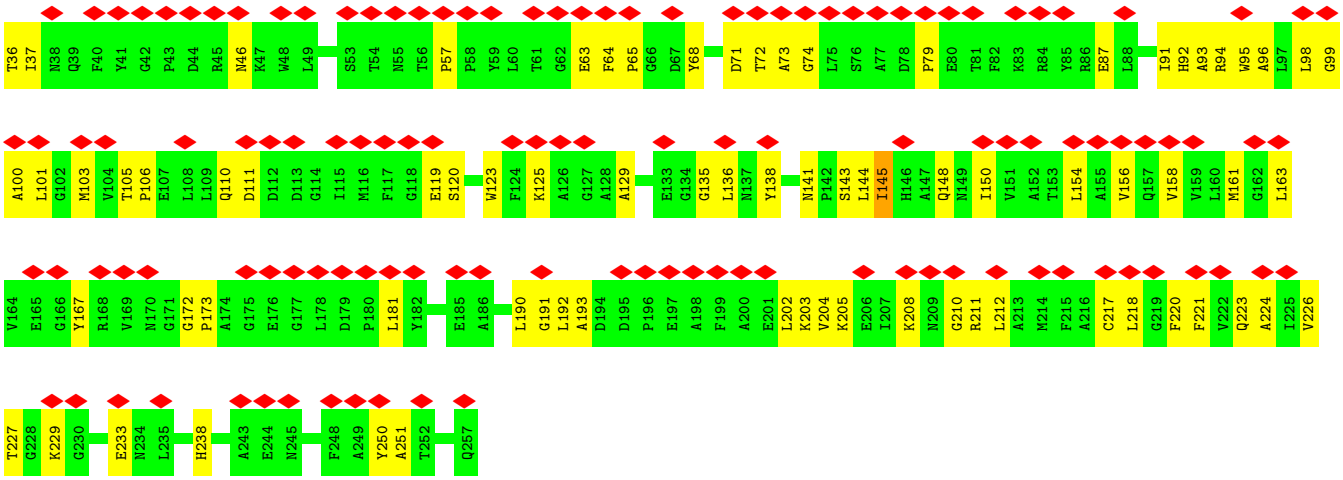
- Molecule 20: LHCII M3

Chain N1:



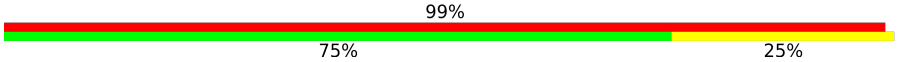
- Molecule 20: LHCII M3

Chain n1:



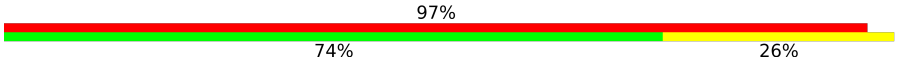
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain G:



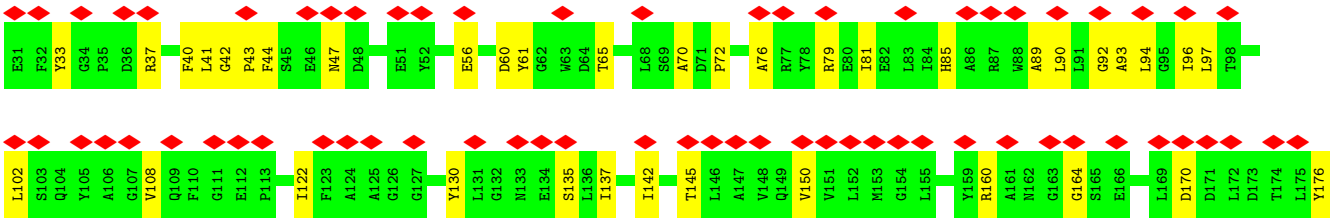
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

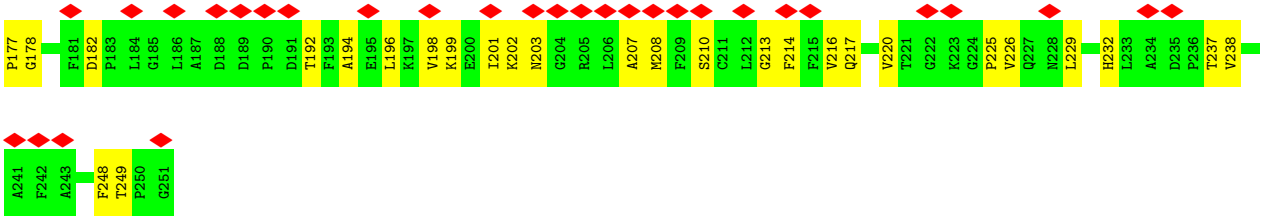
Chain g:



- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

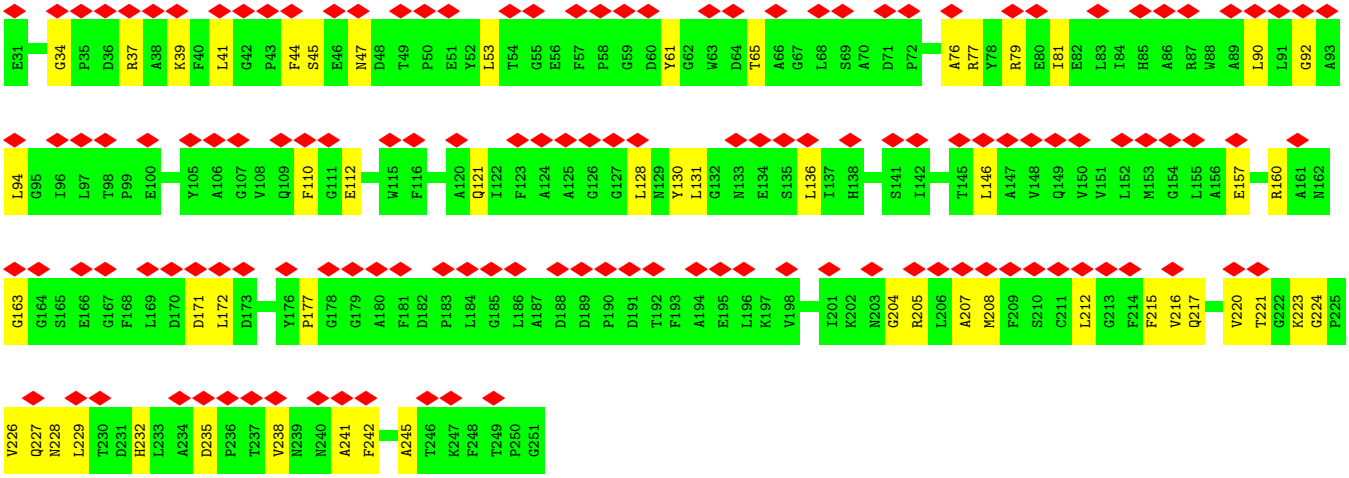
Chain G1:





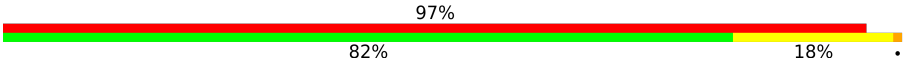
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

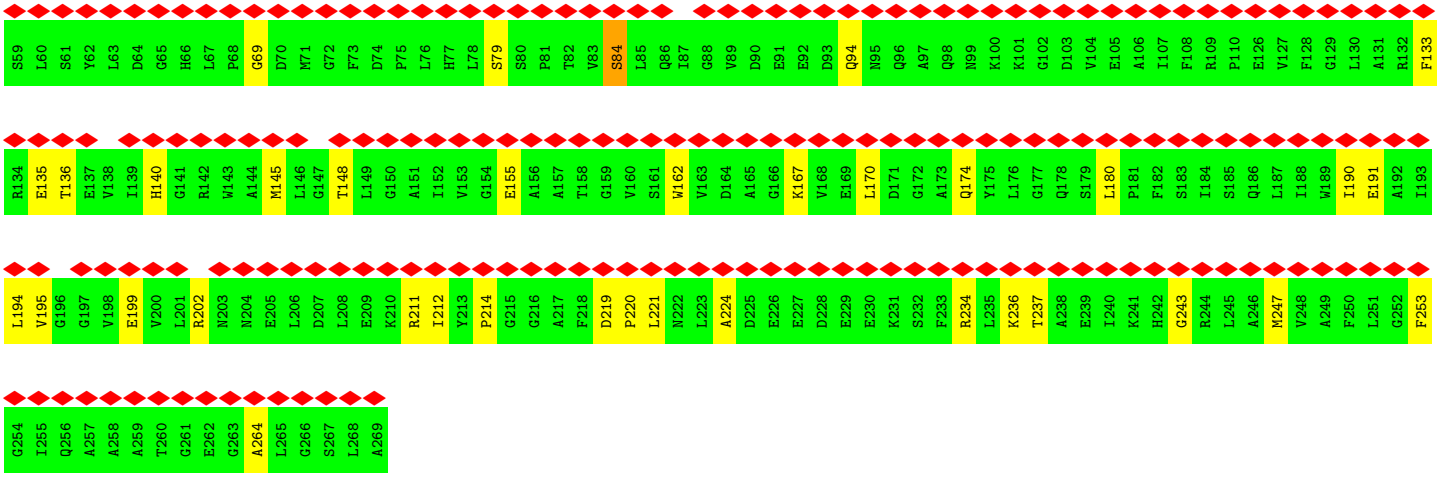
Chain g1:



• Molecule 22: CP29

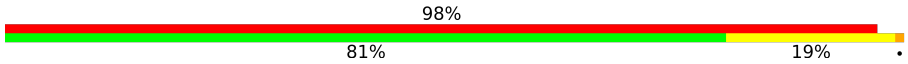
Chain R:





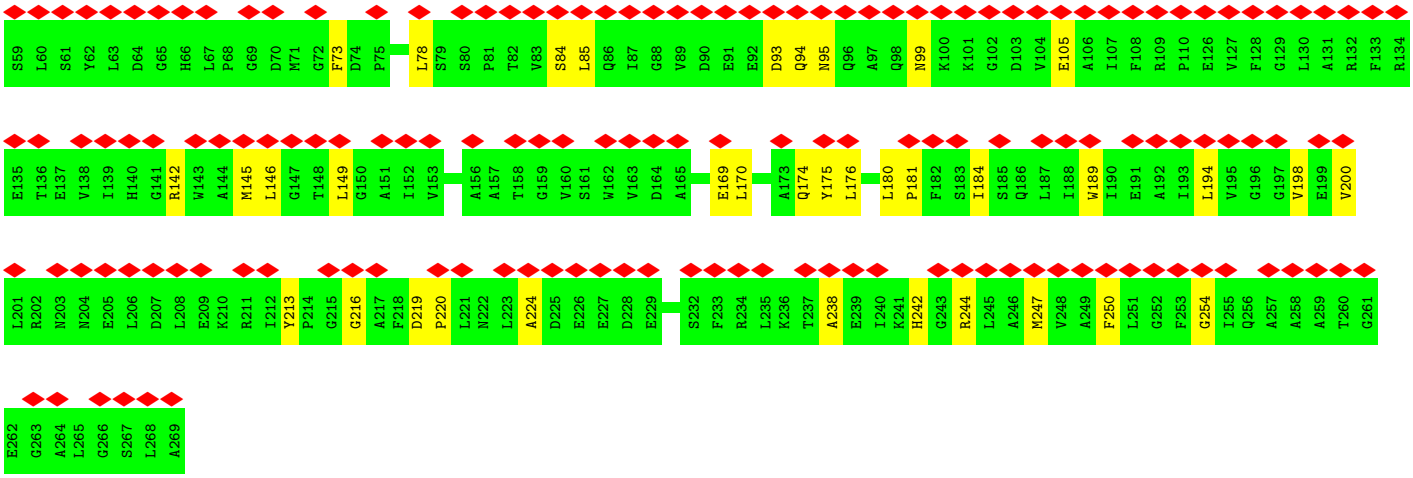
• Molecule 22: CP29

Chain r:



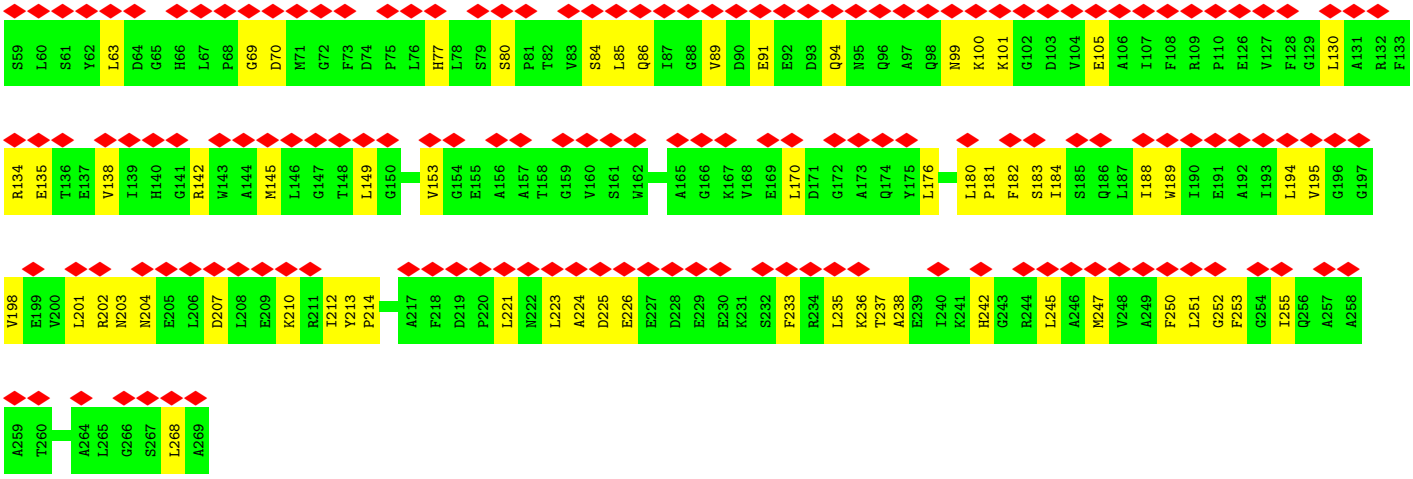
- Molecule 22: CP29

Chain R1:



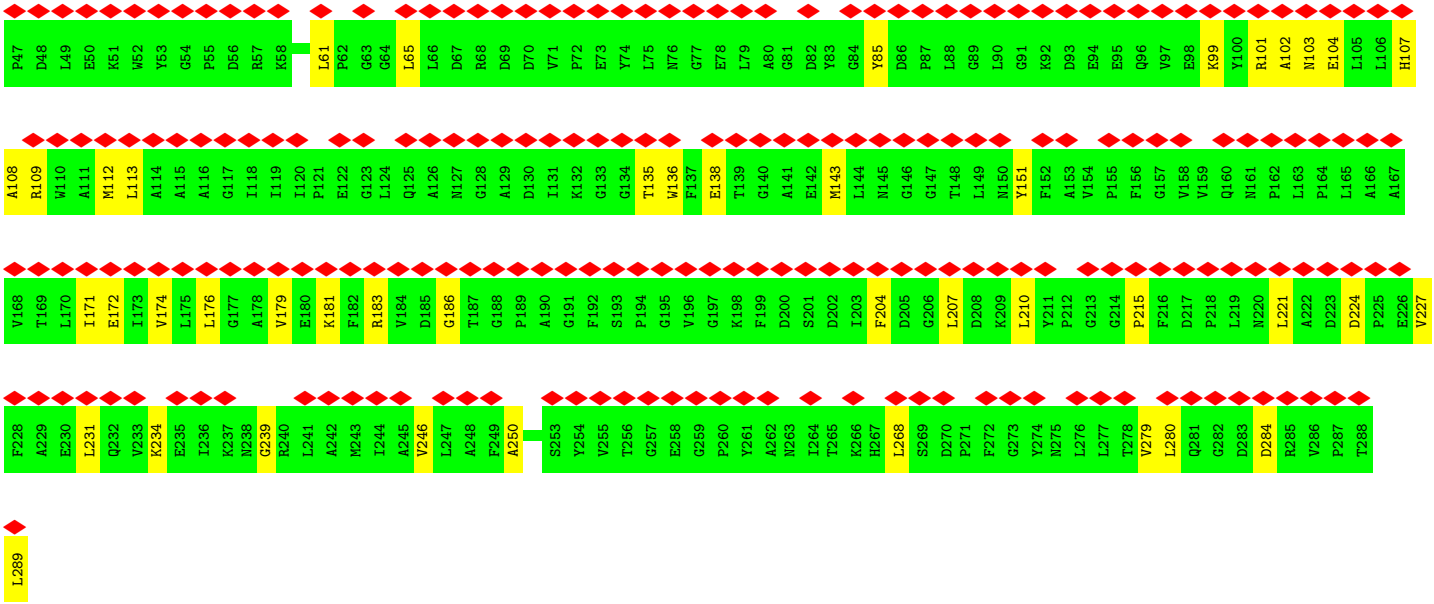
- Molecule 22: CP29

Chain r1:



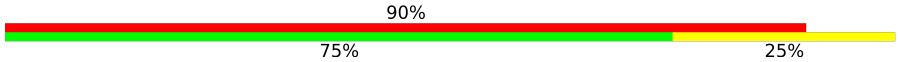
- Molecule 23: CP26

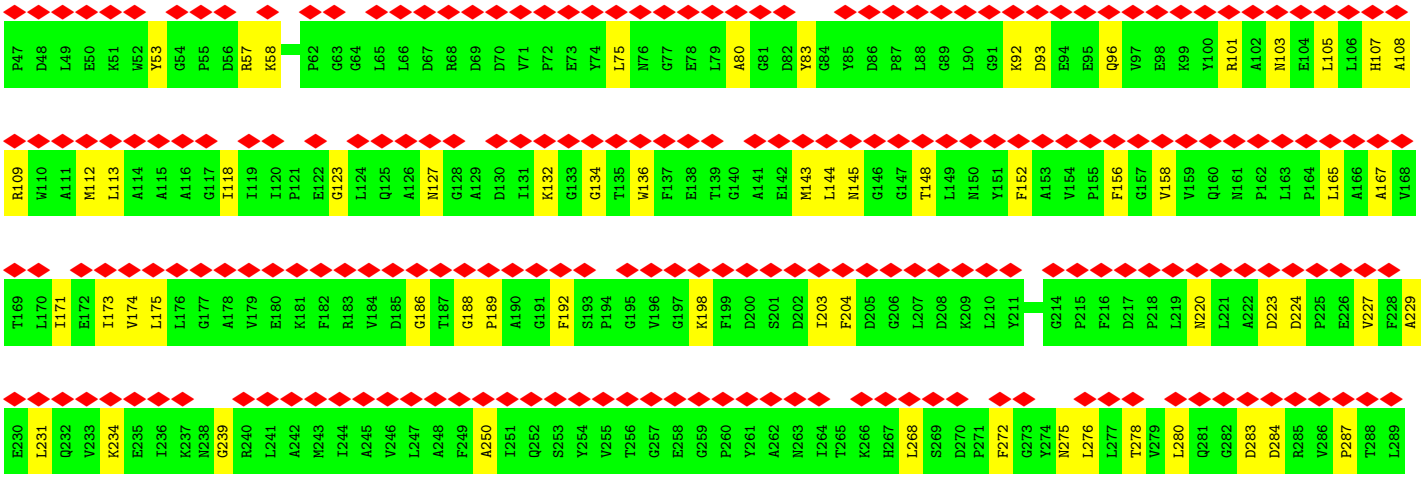
Chain S:



- Molecule 23: CP26

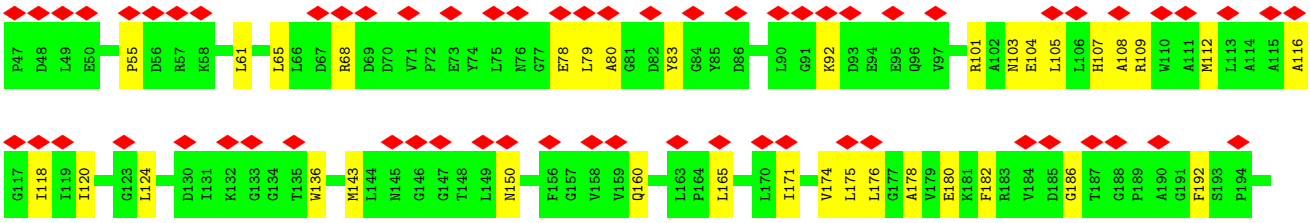
Chain s:

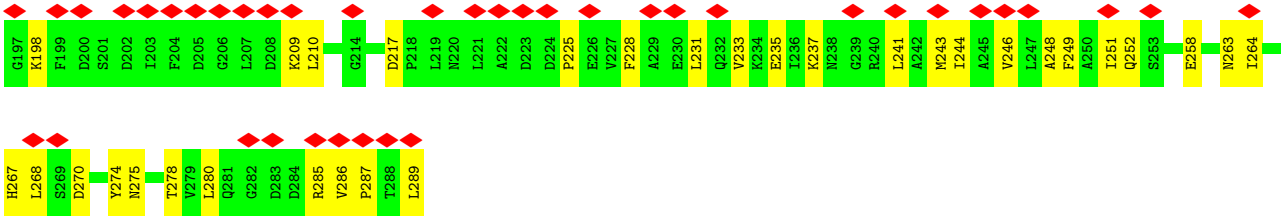




- Molecule 23: CP26

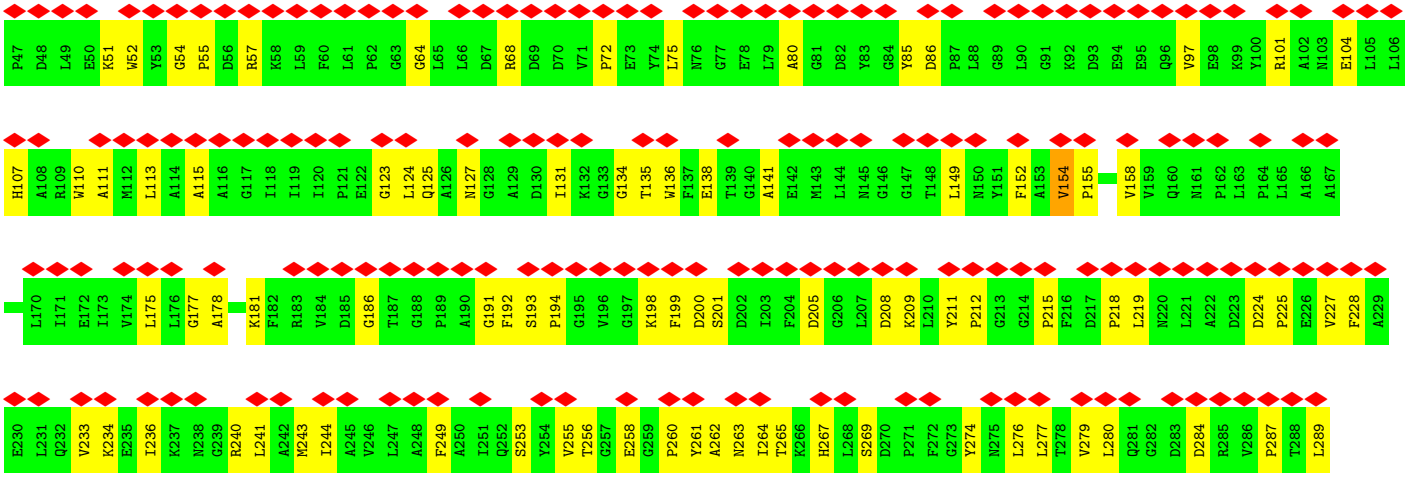
Chain S1:





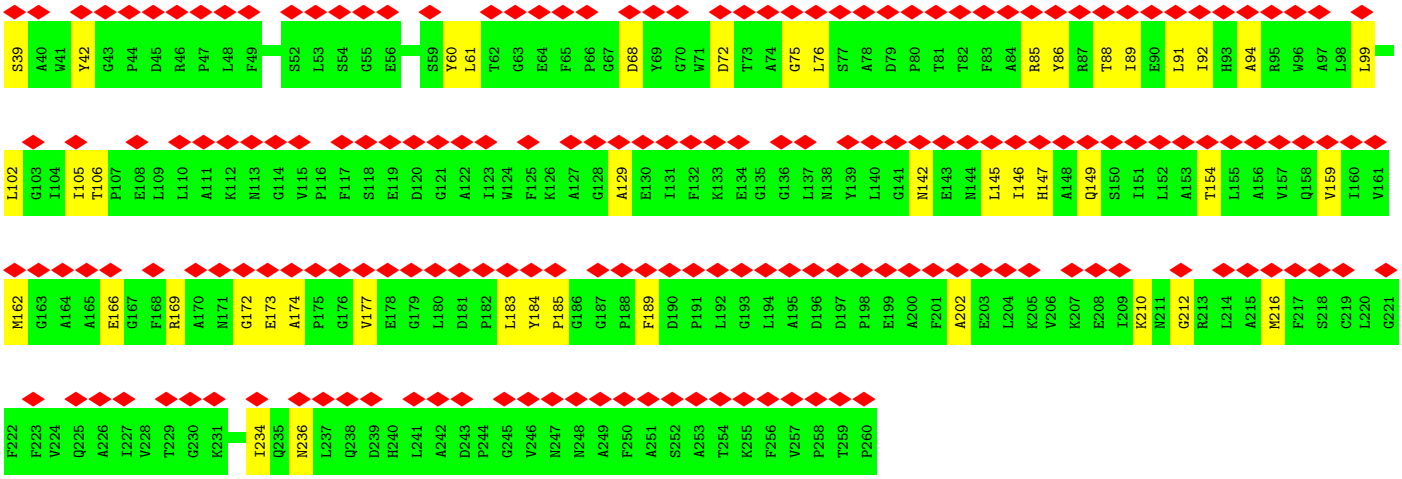
- Molecule 23: CP26

Chain s1:



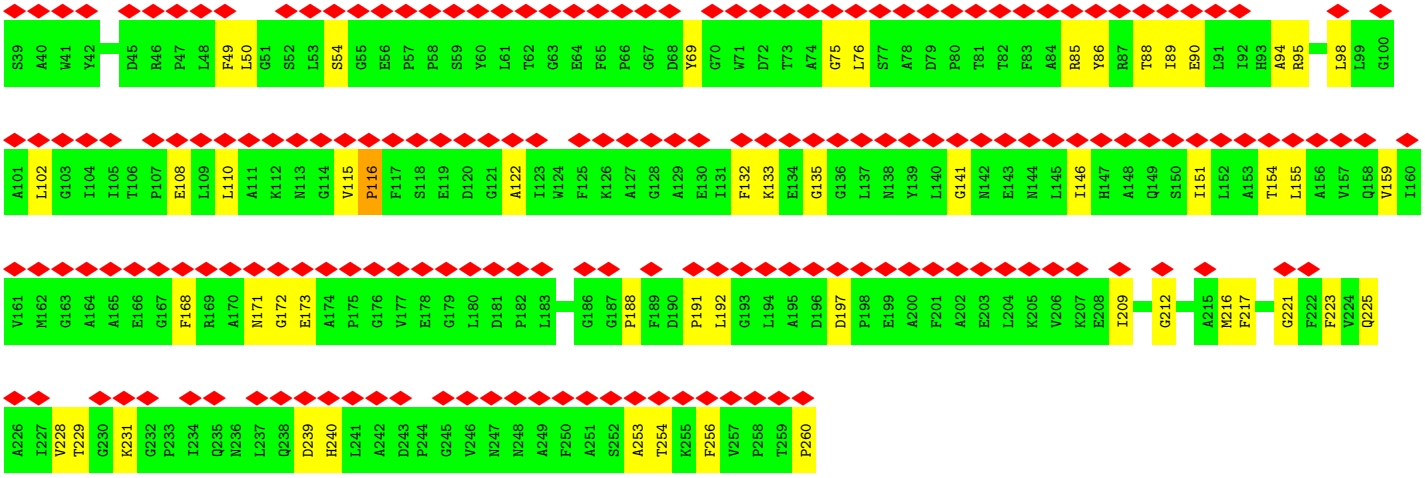
- Molecule 24: LHCII M1

Chain Y:



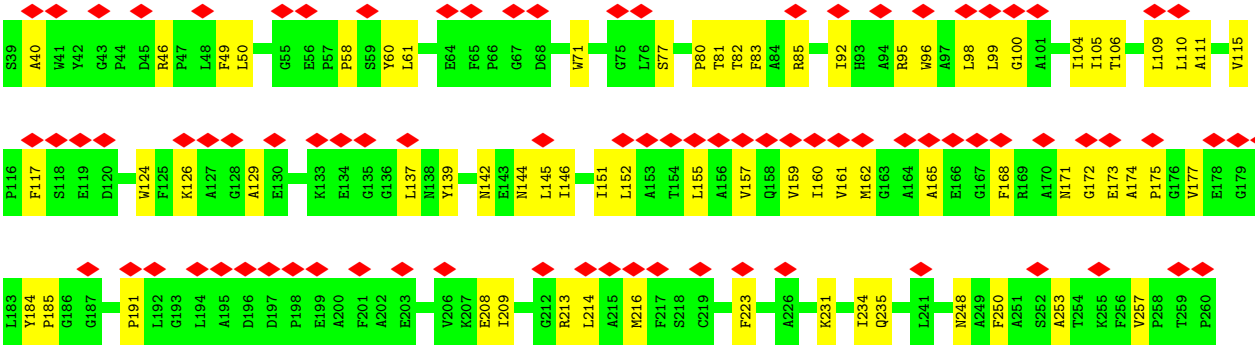
- Molecule 24: LHCII M1

Chain y:



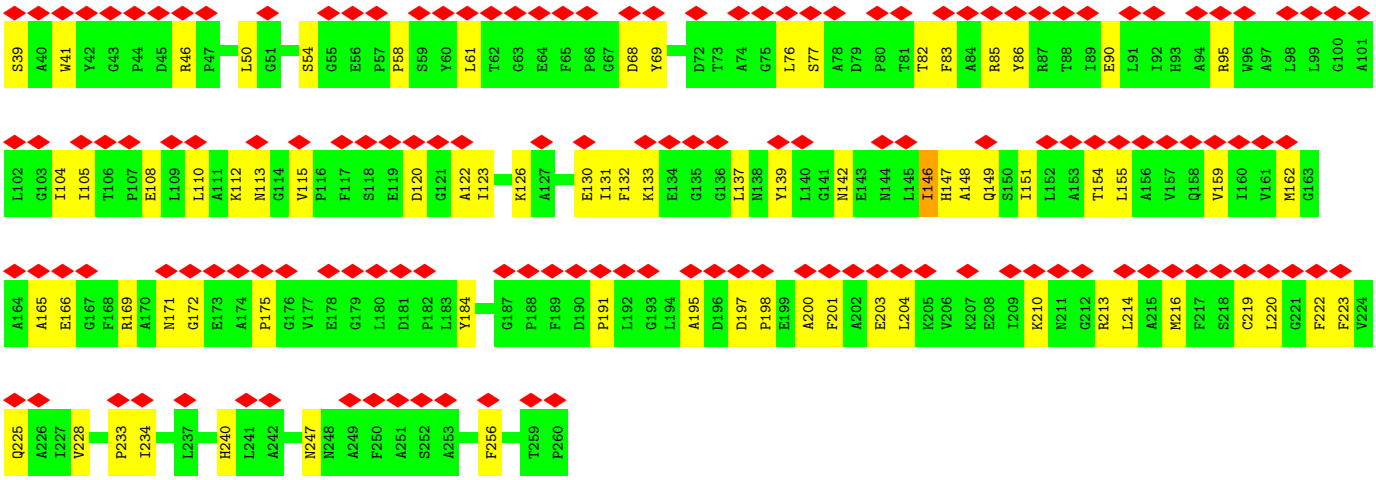
- Molecule 24: LHCII M1

Chain Y1:



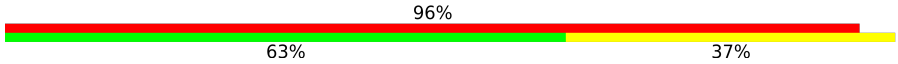
- Molecule 24: LHCII M1

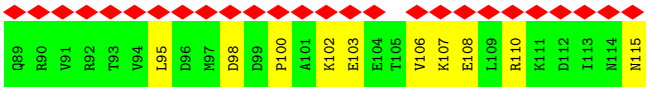
Chain y1:



- Molecule 25: PsbU

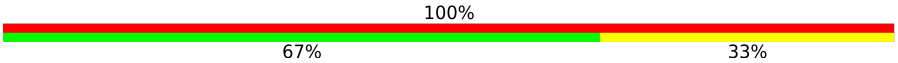
Chain U:

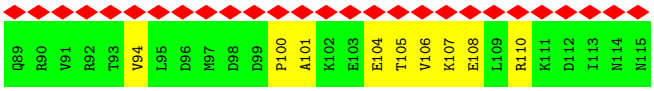




- Molecule 25: PsbU

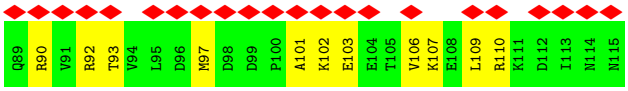
Chain u:





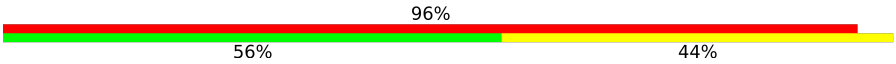
- Molecule 25: PsbU

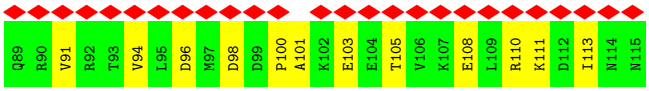
Chain U1:



- Molecule 25: PsbU

Chain u1:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9567	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.102	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	460.8, 460.8, 460.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	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, PL9, LUT, 3PH, LMK, RRX, XAT, SPH, ERG, LHG, BCT, CLA, LMT, SEP, CHL, DGD, OEX, PTY, FE2, 4RF, SQD, PHO, CL, GOL, LMG, NEX, BCR, LPX, C7Z, NA, DGA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.34	0/2723	0.57	0/3715
1	A1	0.27	0/2723	0.61	2/3715 (0.1%)
1	a	0.34	0/2723	0.57	0/3715
1	a1	0.28	0/2723	0.65	2/3715 (0.1%)
2	B	0.31	0/3912	0.59	2/5327 (0.0%)
2	B1	0.27	0/3912	0.60	2/5327 (0.0%)
2	b	0.31	0/3912	0.54	1/5327 (0.0%)
2	b1	0.25	0/3912	0.56	3/5327 (0.1%)
3	V	0.25	0/228	0.57	0/311
3	V1	0.19	0/228	0.47	0/311
3	v	0.24	0/228	0.55	0/311
3	v1	0.25	0/228	0.67	0/311
4	C	0.39	2/3602 (0.1%)	0.65	4/4913 (0.1%)
4	C1	0.26	0/3602	0.54	1/4913 (0.0%)
4	c	0.31	0/3602	0.51	0/4913
4	c1	0.32	2/3602 (0.1%)	0.66	4/4913 (0.1%)
5	D	0.36	0/2860	0.60	2/3899 (0.1%)
5	D1	0.28	0/2860	0.63	2/3899 (0.1%)
5	d	0.32	0/2860	0.57	0/3899
5	d1	0.29	0/2860	0.64	0/3899
6	E	0.26	0/639	0.60	0/870
6	E1	0.26	0/639	0.63	0/870
6	e	0.50	1/639 (0.2%)	0.84	3/870 (0.3%)
6	e1	0.23	0/639	0.62	0/870
7	F	0.29	0/259	0.56	0/351
7	F1	0.26	0/259	0.58	0/351
7	f	0.37	0/259	0.71	0/351
7	f1	0.26	0/259	0.71	0/351
8	H	0.34	0/513	0.68	0/703
8	H1	0.25	0/513	0.57	0/703
8	h	0.30	0/513	0.58	0/703

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	h1	0.24	0/513	0.57	0/703
9	I	0.35	0/287	0.52	0/386
9	I1	0.24	0/287	0.57	0/386
9	i	0.30	0/287	0.55	0/386
9	i1	0.26	0/287	0.63	0/386
10	J	0.24	0/272	0.46	0/369
10	J1	0.21	0/272	0.55	0/369
10	j	0.27	0/272	0.56	0/369
10	j1	0.21	0/272	0.59	0/369
11	K	0.36	0/308	0.73	0/423
11	K1	0.28	0/308	0.64	0/423
11	k	0.33	0/308	0.58	0/423
11	k1	0.32	0/308	0.70	0/423
12	L	0.27	0/321	0.46	0/435
12	L1	0.35	0/321	0.68	0/435
12	l	0.33	0/321	0.59	0/435
13	M	0.30	0/237	0.53	0/323
13	M1	0.23	0/237	0.57	0/323
13	m	0.35	0/237	0.78	1/323 (0.3%)
13	m1	0.26	0/237	0.60	0/323
14	O	0.28	0/1855	0.63	0/2505
14	O1	0.27	0/1855	0.62	0/2505
14	o	0.28	0/1855	0.58	0/2505
14	o1	0.43	1/1855 (0.1%)	0.78	4/2505 (0.2%)
15	P	0.21	0/1473	0.56	2/1988 (0.1%)
15	P1	0.21	0/1473	0.53	0/1988
15	p	0.23	0/1473	0.53	0/1988
15	p1	0.27	0/1473	0.58	0/1988
16	T	0.29	0/254	0.60	0/342
16	T1	0.32	0/254	0.65	0/342
16	t	0.26	0/254	0.42	0/342
16	t1	0.24	0/254	0.57	0/342
17	W	0.28	0/339	0.63	0/460
17	W1	0.26	0/339	0.54	0/460
17	w	0.27	0/339	0.53	0/460
17	w1	0.24	0/339	0.60	0/460
18	X	0.26	0/202	0.55	0/276
18	X1	0.24	0/202	0.52	0/276
18	x	0.28	0/202	0.62	0/276
18	x1	0.22	0/202	0.55	0/276
19	Z	0.23	0/469	0.45	0/641
19	Z1	0.22	0/469	0.59	1/641 (0.2%)
19	z	0.24	0/469	0.45	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	z1	0.19	0/469	0.49	0/641
20	N	0.28	0/1751	0.56	0/2386
20	N1	0.25	0/1751	0.54	0/2386
20	n	0.29	0/1750	0.55	0/2382
20	n1	0.39	2/1750 (0.1%)	0.71	5/2382 (0.2%)
21	G	0.26	0/1725	0.58	0/2348
21	G1	0.28	0/1725	0.61	2/2348 (0.1%)
21	g	0.27	0/1725	0.60	0/2348
21	g1	0.25	0/1725	0.58	0/2348
22	R	0.26	0/1506	0.56	0/2035
22	R1	0.21	0/1506	0.50	0/2035
22	r	0.24	0/1506	0.56	0/2035
22	r1	0.24	0/1506	0.59	0/2035
23	S	0.28	0/1903	0.60	0/2590
23	S1	0.25	0/1903	0.59	0/2590
23	s	0.28	0/1903	0.63	0/2590
23	s1	0.34	1/1903 (0.1%)	0.71	3/2590 (0.1%)
24	Y	0.30	0/1715	0.51	0/2338
24	Y1	0.26	0/1715	0.58	0/2338
24	y	0.29	0/1715	0.53	1/2338 (0.0%)
24	y1	0.23	0/1715	0.53	0/2338
25	U	0.32	0/224	0.63	0/298
25	U1	0.33	0/224	0.62	0/298
25	u	0.33	0/224	0.67	0/298
25	u1	0.30	0/224	0.67	0/298
All	All	0.29	9/117985 (0.0%)	0.59	47/160485 (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
1	A	0	1
1	A1	0	1
2	B1	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	o1	111	PRO	CG-CD	-13.88	1.03	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	65	PRO	CG-CD	-12.67	1.07	1.50
6	e	28	PRO	CG-CD	-10.34	1.15	1.50
4	c1	352	PRO	CG-CD	-8.86	1.20	1.50
20	n1	57	PRO	CG-CD	-8.42	1.22	1.50
23	s1	155	PRO	CG-CD	-8.36	1.29	1.51
20	n1	79	PRO	CG-CD	-7.42	1.25	1.50
4	c1	352	PRO	N-CD	5.16	1.54	1.47
4	C	65	PRO	CB-CG	-5.05	1.24	1.49

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	65	PRO	N-CD-CG	-18.59	75.32	103.20
14	o1	111	PRO	N-CD-CG	-18.29	75.77	103.20
23	s1	155	PRO	N-CD-CG	-12.66	88.60	103.80
6	e	28	PRO	N-CD-CG	-12.50	84.44	103.20
20	n1	57	PRO	N-CD-CG	-12.30	84.74	103.20
4	C	65	PRO	CB-CG-CD	11.89	144.16	106.10
4	C	65	PRO	CA-CB-CG	-11.84	82.00	104.50
5	D	237	PRO	CA-N-CD	-11.30	96.18	112.00
14	o1	111	PRO	CA-CB-CG	-11.26	83.11	104.50
4	c1	352	PRO	CA-N-CD	-11.07	96.50	112.00
23	s1	155	PRO	CA-N-CD	-10.81	96.37	111.50
4	c1	352	PRO	N-CD-CG	-10.76	87.06	103.20
20	n1	79	PRO	N-CD-CG	-10.33	87.70	103.20
6	e	28	PRO	CA-N-CD	-9.79	98.29	112.00
20	n1	57	PRO	CA-CB-CG	-9.46	86.53	104.50
14	o1	111	PRO	CB-CG-CD	8.44	133.09	106.10
2	B1	197	GLY	CA-C-N	8.08	125.33	120.24
2	B1	197	GLY	C-N-CA	8.08	125.33	120.24
1	a1	150	PRO	CA-N-CD	-7.55	101.43	112.00
14	o1	111	PRO	CA-N-CD	-7.40	101.65	112.00
5	D	237	PRO	N-CD-CG	-7.33	92.20	103.20
13	m	5	ILE	N-CA-C	-7.12	106.14	112.12
6	e	28	PRO	CA-CB-CG	-7.11	90.99	104.50
24	y	116	PRO	CA-N-CD	-6.76	102.53	112.00
20	n1	57	PRO	N-CA-CB	-6.76	95.57	103.00
4	C	65	PRO	CA-N-CD	-6.71	102.61	112.00
4	c1	352	PRO	CA-CB-CG	-6.38	92.38	104.50
20	n1	79	PRO	CA-N-CD	-6.16	103.38	112.00
1	a1	150	PRO	N-CD-CG	-6.12	94.02	103.20
19	Z1	24	PRO	CA-N-CD	-6.10	103.46	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	P	165	VAL	N-CA-C	-6.01	106.90	112.43
15	P	161	ASP	CB-CA-C	-5.93	109.17	117.23
4	c1	202	VAL	N-CA-C	-5.69	107.20	112.83
2	B	245	VAL	CA-C-N	-5.50	111.51	121.14
2	B	245	VAL	C-N-CA	-5.50	111.51	121.14
5	D1	347	PRO	CA-N-CD	-5.48	104.33	112.00
1	A1	141	PRO	CA-C-N	-5.43	113.94	122.95
1	A1	141	PRO	C-N-CA	-5.43	113.94	122.95
2	b1	197	GLY	CA-C-N	5.42	125.63	120.43
2	b1	197	GLY	C-N-CA	5.42	125.63	120.43
23	s1	154	VAL	C-N-CD	5.25	132.15	120.60
2	b1	328	GLY	N-CA-C	5.22	118.38	110.97
21	G1	56	GLU	CA-C-N	5.14	139.77	121.59
21	G1	56	GLU	C-N-CA	5.14	139.77	121.59
5	D1	347	PRO	N-CD-CG	-5.08	95.57	103.20
2	b	296	LEU	CA-CB-CG	5.03	133.91	116.30
4	C1	75	ILE	N-CA-C	-5.01	108.62	113.53

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	ARG	Sidechain
1	A1	131	TRP	Peptide
2	B1	384	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	A	2638	0	2541	95	0
1	A1	2638	0	2541	120	0
1	a	2638	0	2541	73	0
1	a1	2638	0	2541	128	0
2	B	3783	0	3663	99	0
2	B1	3783	0	3663	150	0
2	b	3783	0	3663	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b1	3783	0	3663	137	0
3	V	227	0	261	4	0
3	V1	227	0	261	12	0
3	v	227	0	261	4	0
3	v1	227	0	261	10	0
4	C	3483	0	3376	76	0
4	C1	3483	0	3376	151	0
4	c	3483	0	3376	68	0
4	c1	3483	0	3376	154	0
5	D	2766	0	2654	61	0
5	D1	2766	0	2654	123	0
5	d	2766	0	2655	80	0
5	d1	2766	0	2655	149	0
6	E	621	0	605	25	0
6	E1	621	0	605	20	0
6	e	621	0	605	17	0
6	e1	621	0	605	23	0
7	F	252	0	265	9	0
7	F1	252	0	265	11	0
7	f	252	0	265	16	0
7	f1	252	0	265	13	0
8	H	503	0	532	18	0
8	H1	503	0	532	25	0
8	h	503	0	532	13	0
8	h1	503	0	532	23	0
9	I	279	0	288	7	0
9	I1	279	0	288	18	0
9	i	279	0	288	3	0
9	i1	279	0	288	12	0
10	J	266	0	286	6	0
10	J1	266	0	286	8	0
10	j	266	0	286	3	0
10	j1	266	0	286	15	0
11	K	297	0	312	7	0
11	K1	297	0	312	14	0
11	k	297	0	312	5	0
11	k1	297	0	312	16	0
12	L	313	0	325	8	0
12	L1	313	0	325	12	0
12	l	313	0	325	10	0
13	M	234	0	258	6	0
13	M1	234	0	258	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	m	234	0	258	8	0
13	m1	234	0	258	7	0
14	O	1820	0	1776	42	0
14	O1	1820	0	1776	59	0
14	o	1820	0	1776	34	0
14	o1	1820	0	1776	50	0
15	P	1444	0	1403	32	0
15	P1	1444	0	1403	33	0
15	p	1444	0	1403	40	0
15	p1	1444	0	1403	40	0
16	T	247	0	260	2	0
16	T1	247	0	260	15	0
16	t	247	0	260	12	0
16	t1	247	0	260	7	0
17	W	332	0	323	7	0
17	W1	332	0	323	21	0
17	w	332	0	323	11	0
17	w1	332	0	323	18	0
18	X	201	0	224	2	0
18	X1	201	0	224	7	0
18	x	201	0	224	6	0
18	x1	201	0	224	5	0
19	Z	457	0	478	5	0
19	Z1	457	0	478	10	0
19	z	457	0	478	6	0
19	z1	457	0	478	11	0
20	N	1703	0	1641	46	0
20	N1	1703	0	1641	72	0
20	n	1703	0	1641	43	0
20	n1	1703	0	1641	69	0
21	G	1680	0	1614	45	0
21	G1	1680	0	1613	52	0
21	g	1680	0	1614	53	0
21	g1	1680	0	1614	43	0
22	R	1490	0	1454	32	0
22	R1	1490	0	1454	31	0
22	r	1490	0	1454	31	0
22	r1	1490	0	1454	54	0
23	S	1856	0	1816	31	0
23	S1	1856	0	1816	61	0
23	s	1856	0	1816	45	0
23	s1	1856	0	1816	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Y	1667	0	1624	44	0
24	Y1	1667	0	1624	62	0
24	y	1667	0	1624	45	0
24	y1	1667	0	1624	70	0
25	U	224	0	226	11	0
25	U1	224	0	226	11	0
25	u	224	0	226	7	0
25	u1	224	0	226	13	0
26	A	10	0	0	1	0
26	A1	10	0	0	0	0
26	a	10	0	0	0	0
26	a1	10	0	0	1	0
27	A	1	0	0	0	0
27	A1	1	0	0	0	0
27	a	1	0	0	0	0
27	a1	1	0	0	0	0
28	A	2	0	0	1	0
28	A1	2	0	0	1	0
28	a	2	0	0	1	0
28	a1	2	0	0	1	0
29	A	240	0	242	17	0
29	A1	240	0	240	18	0
29	B	1040	0	1149	71	0
29	B1	1040	0	1147	93	0
29	C	845	0	933	55	0
29	C1	845	0	930	67	0
29	D	130	0	144	10	0
29	D1	130	0	143	10	0
29	G	466	0	467	24	0
29	G1	466	0	467	35	0
29	N	468	0	469	27	0
29	N1	468	0	468	43	0
29	R	409	0	391	19	0
29	R1	409	0	391	26	0
29	S	625	0	588	21	0
29	S1	625	0	586	25	0
29	Y	570	0	613	51	0
29	Y1	570	0	612	48	0
29	a	239	0	242	14	0
29	a1	239	0	241	29	0
29	b	1040	0	1151	62	0
29	b1	1040	0	1146	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	c	845	0	934	43	0
29	c1	845	0	931	69	0
29	d	130	0	143	8	0
29	d1	130	0	143	13	0
29	g	466	0	468	20	0
29	g1	466	0	465	36	0
29	n	468	0	468	21	0
29	n1	468	0	469	38	0
29	r	409	0	392	18	0
29	r1	409	0	390	23	0
29	s	625	0	588	22	0
29	s1	625	0	586	34	0
29	y	570	0	614	38	0
29	y1	570	0	612	51	0
30	A	128	0	148	11	0
30	A1	128	0	148	13	0
30	a	128	0	148	7	0
30	a1	128	0	148	20	0
31	A	40	0	53	2	0
31	A1	40	0	53	4	0
31	B	80	0	106	3	0
31	B1	80	0	105	2	0
31	C	160	0	210	16	0
31	C1	160	0	209	22	0
31	D	40	0	53	3	0
31	D1	40	0	53	4	0
31	a	40	0	53	3	0
31	a1	40	0	53	4	0
31	b	80	0	106	6	0
31	b1	80	0	106	6	0
31	c	160	0	211	12	0
31	c1	160	0	211	30	0
31	d	40	0	53	3	0
31	d1	40	0	53	3	0
32	A	51	0	68	5	0
32	A1	51	0	68	6	0
32	B	96	0	124	6	0
32	B1	96	0	124	6	0
32	C	54	0	77	4	0
32	C1	54	0	77	3	0
32	M	42	0	47	4	0
32	M1	42	0	47	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	a	51	0	68	2	0
32	a1	51	0	68	3	0
32	b	96	0	124	7	0
32	b1	96	0	124	8	0
32	c	54	0	77	0	0
32	c1	54	0	77	4	0
32	m	42	0	47	6	0
32	m1	42	0	47	3	0
33	A	48	0	66	3	0
33	A1	48	0	66	10	0
33	B	44	0	58	2	0
33	B1	44	0	58	5	0
33	C	106	0	158	7	0
33	C1	106	0	158	13	0
33	D	46	0	62	2	0
33	D1	46	0	62	2	0
33	H	48	0	66	2	0
33	H1	48	0	66	15	0
33	W	39	0	48	2	0
33	W1	39	0	48	8	0
33	a	48	0	66	5	0
33	a1	48	0	66	8	0
33	b	44	0	58	5	0
33	b1	44	0	58	5	0
33	c	106	0	158	12	0
33	c1	106	0	158	7	0
33	d	46	0	62	2	0
33	d1	46	0	62	2	0
33	h	48	0	66	5	0
33	h1	48	0	66	4	0
33	w	39	0	48	6	0
33	w1	39	0	48	4	0
34	A	21	0	37	1	0
34	A1	21	0	37	4	0
34	Y	21	0	37	4	0
34	Y1	21	0	37	7	0
34	a	21	0	37	3	0
34	a1	21	0	37	1	0
34	y	21	0	37	4	0
34	y1	21	0	37	2	0
35	A	1	0	0	0	0
35	A1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	a	1	0	0	0	0
35	a1	1	0	0	0	0
36	B	42	0	0	0	0
36	B1	42	0	0	0	0
36	b	42	0	0	0	0
36	b1	42	0	0	0	0
37	B	43	0	44	3	0
37	B1	43	0	44	2	0
37	C	176	0	226	13	0
37	C1	176	0	226	31	0
37	b	43	0	44	3	0
37	b1	43	0	44	4	0
37	c	176	0	226	10	0
37	c1	176	0	226	26	0
38	B	48	0	75	7	0
38	B1	48	0	75	6	0
38	S	48	0	75	7	0
38	S1	48	0	75	4	0
38	T	48	0	75	2	0
38	T1	48	0	75	8	0
38	b	48	0	75	6	0
38	b1	48	0	75	8	0
38	s	48	0	75	6	0
38	s1	48	0	75	5	0
38	t	48	0	75	2	0
38	t1	48	0	75	5	0
39	B	44	0	76	1	0
39	B1	44	0	76	1	0
39	C	44	0	76	3	0
39	C1	44	0	76	6	0
39	J	29	0	40	2	0
39	J1	29	0	40	4	0
39	b	44	0	76	5	0
39	b1	44	0	76	4	0
39	c	44	0	76	9	0
39	c1	44	0	76	4	0
39	j	29	0	40	3	0
39	j1	29	0	40	4	0
40	C	47	0	67	7	0
40	C1	47	0	67	8	0
40	D	132	0	183	11	0
40	D1	132	0	183	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	G	49	0	74	4	0
40	G1	49	0	74	6	0
40	L	49	0	74	5	0
40	L1	49	0	74	6	0
40	N	49	0	74	4	0
40	N1	49	0	74	5	0
40	S	45	0	63	5	0
40	S1	45	0	63	5	0
40	Y	49	0	74	6	0
40	Y1	49	0	74	6	0
40	c	47	0	67	4	0
40	c1	47	0	67	11	0
40	d	132	0	183	12	0
40	d1	132	0	183	17	0
40	g	49	0	74	7	0
40	g1	49	0	74	7	0
40	l	49	0	74	4	0
40	n	49	0	74	3	0
40	n1	49	0	74	10	0
40	s	45	0	63	4	0
40	s1	45	0	63	7	0
40	y	49	0	74	5	0
40	y1	49	0	74	6	0
41	C	40	0	0	0	0
41	C1	40	0	0	0	0
41	c	40	0	0	0	0
41	c1	40	0	0	0	0
42	D	4	0	0	0	0
42	D1	4	0	0	1	0
42	d	4	0	0	0	0
42	d1	4	0	1	0	0
43	D	55	0	80	4	0
43	D1	55	0	80	11	0
43	d	55	0	80	7	0
43	d1	55	0	80	8	0
44	F	43	0	30	3	0
44	F1	43	0	30	3	0
44	f	43	0	30	1	0
44	f1	43	0	30	3	0
45	H	41	0	56	1	0
45	H1	41	0	56	3	0
45	h	41	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	h1	41	0	56	4	0
46	I	6	0	8	0	0
46	I1	6	0	8	0	0
47	I	57	0	98	2	0
47	I1	57	0	98	9	0
47	K	57	0	98	2	0
47	K1	57	0	98	5	0
47	i	57	0	98	6	0
47	i1	57	0	98	2	0
47	k	57	0	98	2	0
47	k1	57	0	98	2	0
48	G	340	0	306	18	0
48	G1	340	0	306	19	0
48	N	380	0	383	18	0
48	N1	380	0	383	37	0
48	R	94	0	67	4	0
48	R1	94	0	67	3	0
48	S	194	0	144	9	0
48	S1	194	0	144	12	0
48	Y	310	0	307	7	0
48	Y1	310	0	308	21	0
48	g	340	0	306	15	0
48	g1	340	0	306	19	0
48	n	380	0	385	18	0
48	n1	380	0	383	29	0
48	r	94	0	66	3	0
48	r1	94	0	67	6	0
48	s	194	0	146	9	0
48	s1	194	0	146	14	0
48	y	310	0	308	7	0
48	y1	310	0	308	15	0
49	G	84	0	110	13	0
49	G1	84	0	110	16	0
49	N	84	0	110	8	0
49	N1	84	0	110	12	0
49	R	42	0	55	6	0
49	R1	42	0	55	4	0
49	S	84	0	110	7	0
49	S1	84	0	110	13	0
49	Y	84	0	110	8	0
49	Y1	84	0	110	14	0
49	g	84	0	110	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	g1	84	0	110	22	0
49	n	84	0	110	5	0
49	n1	84	0	110	14	0
49	r	42	0	55	4	0
49	r1	42	0	55	7	0
49	s	84	0	110	4	0
49	s1	84	0	110	10	0
49	y	84	0	110	5	0
49	y1	84	0	110	13	0
50	G	44	0	56	6	0
50	G1	44	0	56	10	0
50	N	44	0	56	5	0
50	N1	44	0	56	9	0
50	R	44	0	56	4	0
50	R1	44	0	56	5	0
50	Y	44	0	56	6	0
50	Y1	44	0	56	4	0
50	g	44	0	56	9	0
50	g1	44	0	56	6	0
50	n	44	0	56	6	0
50	n1	44	0	56	5	0
50	r	44	0	56	2	0
50	r1	44	0	56	5	0
50	y	44	0	56	4	0
50	y1	44	0	56	9	0
51	G	44	0	54	0	0
51	G1	44	0	54	0	0
51	N	44	0	54	3	0
51	N1	44	0	55	6	0
51	R	44	0	54	2	0
51	R1	44	0	54	4	0
51	S	44	0	54	0	0
51	S1	44	0	55	4	0
51	Y	44	0	54	2	0
51	Y1	44	0	54	3	0
51	g	44	0	54	1	0
51	g1	44	0	54	0	0
51	n	44	0	54	3	0
51	n1	44	0	54	6	0
51	r	44	0	54	3	0
51	r1	44	0	54	5	0
51	s	44	0	54	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	s1	44	0	56	6	0
51	y	44	0	54	1	0
51	y1	44	0	55	2	0
52	R	35	0	44	4	0
52	R1	35	0	45	7	0
52	r	35	0	44	4	0
52	r1	35	0	45	2	0
53	R	29	0	38	7	0
53	R1	29	0	38	9	0
53	r	29	0	38	7	0
53	r1	29	0	38	5	0
54	S	30	0	43	4	0
54	S1	30	0	43	2	0
54	s	30	0	43	3	0
54	s1	30	0	43	3	0
55	Y	69	0	90	5	0
55	Y1	69	0	90	3	0
55	y	69	0	90	9	0
55	y1	69	0	90	9	0
All	All	152240	0	154365	4580	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 15.

All (4580) 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)
53:r:626:ERG:O1	53:r:626:ERG:C3	1.70	1.38
53:r1:626:ERG:O1	53:r1:626:ERG:C3	1.70	1.37
53:R:626:ERG:O1	53:R:626:ERG:C3	1.70	1.36
53:R1:626:ERG:O1	53:R1:626:ERG:C3	1.70	1.35
24:y1:76:LEU:CD1	29:y1:602:CLA:H42	1.79	1.10
24:y1:76:LEU:HD12	29:y1:602:CLA:H11	1.12	1.10
24:y1:76:LEU:CD1	29:y1:602:CLA:H11	1.86	1.04
24:y1:76:LEU:HD11	29:y1:602:CLA:H42	1.39	1.00
24:Y:76:LEU:HD22	29:Y:602:CLA:H11	1.45	0.98
24:y1:76:LEU:CD1	29:y1:602:CLA:C4	2.42	0.97
14:O:138:TYR:OH	17:W:60:LEU:HA	1.64	0.97
24:y1:76:LEU:HD13	29:y1:602:CLA:C4	1.98	0.93
22:r:195:VAL:HG23	29:r:609:CLA:HAB	1.51	0.92
24:y1:76:LEU:HD13	29:y1:602:CLA:H43	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:y:76:LEU:HD13	29:y:602:CLA:H42	1.55	0.88
22:r1:194:LEU:HD22	51:r1:622:NEX:H15	1.56	0.87
24:Y:76:LEU:CD2	29:Y:602:CLA:H43	2.05	0.85
29:B1:604:CLA:HAB	29:B1:606:CLA:H152	1.58	0.85
29:b1:609:CLA:HAB	5:d1:123:ILE:HG23	1.59	0.84
1:a:107:TYR:HB2	14:o:133:LEU:HD12	1.60	0.84
33:c1:523:LMG:H151	33:c1:523:LMG:H361	1.60	0.84
20:n:49:LEU:HB2	20:n:53:SER:HB3	1.62	0.82
24:Y:76:LEU:CD2	29:Y:602:CLA:C4	2.57	0.82
30:a1:409:PHO:H3A	29:d1:402:CLA:H121	1.61	0.81
40:C1:525:LHG:H142	29:S1:611:CLA:HBB2	1.62	0.81
29:Y1:602:CLA:H52	49:Y1:621:LUT:H28	1.63	0.81
29:N1:602:CLA:H52	49:N1:621:LUT:H28	1.62	0.81
22:r1:195:VAL:HG23	29:r1:609:CLA:HAB	1.63	0.80
24:y1:76:LEU:HD12	29:y1:602:CLA:C1	2.06	0.80
20:n1:119:GLU:HG3	20:n1:125:LYS:HD3	1.64	0.80
29:g1:610:CLA:H52	49:g1:620:LUT:H30	1.64	0.79
29:G1:602:CLA:H52	49:G1:621:LUT:H28	1.62	0.79
1:A1:333:GLU:O	1:A1:337:HIS:CE1	2.35	0.79
33:a1:413:LMG:H402	37:c1:518:DGD:HBT2	1.65	0.79
2:b:382:PRO:HG2	2:b:385:LYS:HG2	1.65	0.78
1:A:333:GLU:O	1:A:337:HIS:CE1	2.37	0.78
22:R:194:LEU:HD13	51:R:622:NEX:H34	1.65	0.78
22:R1:224:ALA:HB3	29:R1:610:CLA:HAA2	1.65	0.78
2:b:9:HIS:HB3	29:b:613:CLA:HAB	1.65	0.78
2:b:460:LEU:HD11	5:d:287:VAL:HG21	1.65	0.78
29:N1:604:CLA:HBB1	51:N1:623:NEX:H27	1.66	0.78
29:N1:613:CLA:H172	50:G1:622:XAT:H32	1.65	0.77
20:n:87:GLU:HG2	20:n:181:LEU:HD21	1.67	0.77
1:A:30:ILE:O	1:A:34:GLY:HA3	1.85	0.76
2:b:67:THR:HG1	2:b:93:TYR:HH	1.30	0.76
29:A1:410:CLA:HAC2	31:A1:411:BCR:H16C	1.67	0.76
29:A1:406:CLA:HAA2	43:D1:405:PL9:H371	1.67	0.76
29:b1:609:CLA:H2	39:b1:625:DGA:HA91	1.68	0.76
23:s:189:PRO:HD2	48:s:608:CHL:HBB2	1.67	0.76
29:s:603:CLA:HAB	29:s:609:CLA:HBC2	1.65	0.76
29:g:602:CLA:H52	49:g:621:LUT:H28	1.67	0.76
4:c1:437:ARG:NH2	9:i1:27:ASP:OD1	2.19	0.76
29:C:513:CLA:H101	31:C:514:BCR:H23C	1.67	0.75
14:O1:107:PHE:HB3	14:O1:143:MET:HB2	1.68	0.75
24:y:76:LEU:CD1	29:y:602:CLA:H42	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:68:ARG:HG3	2:b1:69:LEU:HG	1.66	0.75
15:P1:169:ALA:HB3	15:P1:190:LEU:HB3	1.68	0.75
13:M:24:ILE:HD13	13:m:24:ILE:HD13	1.67	0.75
24:Y1:95:ARG:NH1	29:Y1:608:CLA:OBD	2.18	0.75
2:B:37:MET:O	2:B:41:GLU:HB2	1.85	0.74
33:C:521:LMG:H242	33:C:521:LMG:H341	1.69	0.74
5:d1:258:GLY:HA3	16:t1:21:ILE:HD12	1.69	0.74
30:A1:409:PHO:HBD	5:D1:125:PHE:HE2	1.52	0.74
1:a1:37:MET:HE2	1:a1:129:ARG:HD3	1.69	0.74
23:s:112:MET:HE1	29:s:610:CLA:HAB	1.70	0.74
5:d:296:TYR:OH	5:d:326:ARG:NH1	2.21	0.74
21:G1:208:MET:HE1	29:G1:602:CLA:HAB	1.68	0.73
22:r1:180:LEU:HD11	48:r1:606:CHL:HMD1	1.70	0.73
21:g1:47:ASN:HB2	24:y1:171:ASN:HB2	1.69	0.73
2:b1:451:PHE:O	2:b1:455:HIS:ND1	2.20	0.73
5:d1:350:ASN:ND2	15:p1:195:ASP:OD1	2.20	0.73
23:S:246:VAL:HG11	49:S:621:LUT:H12	1.70	0.73
4:c1:292:PRO:HG2	4:c1:388:PRO:HD3	1.71	0.73
1:a1:225:ARG:NH2	2:b1:483:ASP:OD1	2.22	0.73
1:A:18:CYS:SG	9:I:30:ARG:NH1	2.60	0.73
2:B:474:ILE:O	5:D:134:ARG:NH1	2.22	0.72
8:h:54:ILE:HD13	45:h:101:RRX:H20	1.70	0.72
2:b1:476:ARG:NH2	22:r1:91:GLU:O	2.21	0.72
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.71	0.72
23:s:268:LEU:HD13	38:s:626:3PH:H271	1.72	0.72
1:A1:288:LEU:HD11	4:C1:420:CYS:HA	1.71	0.72
29:C1:513:CLA:H101	31:C1:514:BCR:H21C	1.71	0.72
21:G1:41:LEU:HB3	21:G1:44:PHE:HB2	1.72	0.72
14:O1:138:TYR:HE2	17:W1:61:VAL:HG13	1.53	0.72
19:z1:57:PHE:HA	19:z1:60:PHE:HB2	1.72	0.72
15:P:189:ILE:HG23	15:P:203:GLN:HB2	1.72	0.72
29:r:610:CLA:H52	49:r:620:LUT:H30	1.70	0.72
23:S:102:ALA:HA	23:S:210:LEU:HD21	1.72	0.71
2:b:44:VAL:HG23	2:b:60:MET:HE1	1.72	0.71
1:A1:344:ALA:HB3	4:C1:342:GLU:HG2	1.72	0.71
20:N:83:LYS:HG2	20:N:86:ARG:HH21	1.55	0.71
32:B:626:SQD:H352	32:B:626:SQD:H221	1.71	0.71
2:b1:224:ARG:HH12	39:b1:625:DGA:HB42	1.55	0.71
5:d:129:GLN:NE2	5:d:142:ASN:OD1	2.21	0.71
24:y1:120:ASP:HA	24:y1:126:LYS:HE3	1.72	0.71
8:h:36:GLU:HB2	8:h:39:LYS:HD3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:272:ARG:NH1	5:d1:164:GLN:OE1	2.24	0.71
20:N:49:LEU:HB2	20:N:53:SER:HB3	1.72	0.71
2:b:442:VAL:HG23	2:b:444:ARG:HH12	1.56	0.71
21:G1:76:ALA:HA	21:G1:79:ARG:HE	1.54	0.71
40:C:525:LHG:H251	29:S:611:CLA:HAB	1.72	0.71
8:h1:29:LEU:HD12	22:r1:203:ASN:HD22	1.53	0.71
23:s:103:ASN:O	23:s:107:HIS:ND1	2.24	0.70
4:c1:166:LYS:HA	4:c1:170:PHE:HB2	1.74	0.70
30:A1:409:PHO:HHB	29:D1:402:CLA:H121	1.73	0.70
33:C1:521:LMG:H192	39:J1:101:DGA:HA82	1.71	0.70
13:M1:28:LYS:HD3	13:m1:27:VAL:HB	1.72	0.70
1:a1:18:CYS:SG	9:i1:30:ARG:NH2	2.63	0.70
2:b1:394:GLN:HB3	15:p1:147:ARG:HE	1.56	0.70
2:b1:456:LEU:HD11	33:h1:102:LMG:H211	1.72	0.70
6:e:69:ARG:NH2	8:h:70:SER:OG	2.25	0.70
24:y:76:LEU:HD12	29:y:602:CLA:H11	1.72	0.70
20:N1:160:LEU:HD12	51:N1:623:NEX:H15	1.74	0.70
37:C:519:DGD:HA71	37:C:520:DGD:HB91	1.72	0.70
2:b1:145:LEU:HB3	29:b1:605:CLA:H162	1.73	0.70
4:c1:59:GLU:HG3	4:c1:74:LEU:HD22	1.72	0.70
5:d1:188:PHE:HA	5:d1:326:ARG:HE	1.56	0.70
2:B:235:GLU:OE2	2:B:469:HIS:ND1	2.24	0.70
14:o1:138:TYR:OH	17:w1:60:LEU:HA	1.91	0.70
21:G:34:GLY:O	21:G:37:ARG:HB3	1.90	0.70
1:a:192:ILE:HA	1:a:293:MET:HE1	1.74	0.70
29:A:406:CLA:HAA2	43:D:405:PL9:H371	1.74	0.70
12:L1:25:ILE:HD11	40:L1:101:LHG:H292	1.73	0.70
1:a1:140:ARG:HH12	40:d1:410:LHG:HC42	1.56	0.70
1:a:329:GLU:O	1:a:332:HIS:ND1	2.24	0.69
29:b:613:CLA:H171	29:b:614:CLA:HBB2	1.74	0.69
2:B1:338:VAL:HB	2:B1:431:GLU:HG3	1.74	0.69
37:C1:519:DGD:HB22	33:C1:521:LMG:H311	1.73	0.69
29:C1:503:CLA:H172	29:C1:510:CLA:HBB2	1.73	0.69
22:R1:176:LEU:O	24:y1:142:ASN:ND2	2.26	0.69
1:a1:114:LEU:O	1:a1:118:HIS:ND1	2.25	0.69
2:b1:355:PHE:HB2	25:u1:100:PRO:HB2	1.74	0.69
4:c1:237:ILE:HA	4:c1:240:ILE:HD12	1.73	0.69
29:C:501:CLA:HBB1	29:C:501:CLA:H71	1.73	0.69
21:G:199:LYS:HD3	29:G:611:CLA:HED2	1.72	0.69
4:c1:75:ILE:HG22	4:c1:410:PRO:HB3	1.73	0.69
7:F:36:ILE:O	7:F:40:GLN:HB2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:n:624:LHG:H191	50:g:622:XAT:H14	1.74	0.69
53:r:626:ERG:O1	53:r:626:ERG:C2	2.36	0.69
1:A1:14:TRP:HB2	17:W1:95:ILE:HG22	1.75	0.69
13:M1:19:THR:HG22	13:M1:23:LEU:HD23	1.74	0.69
2:B1:141:ILE:HD12	29:B1:616:CLA:HBB1	1.73	0.69
2:B1:357:ARG:NH1	25:U1:101:ALA:O	2.26	0.69
8:H1:69:ASN:ND2	33:H1:102:LMG:O10	2.26	0.69
24:y1:155:LEU:HD13	48:y1:607:CHL:HAC2	1.73	0.69
4:C:461:ASP:HA	5:D:251:ARG:HE	1.58	0.69
1:a:183:MET:HB3	29:a:405:CLA:HBC2	1.72	0.69
39:c:524:DGA:HAW2	33:w:201:LMG:H381	1.75	0.69
20:n1:158:VAL:HG13	48:n1:609:CHL:HBB2	1.75	0.69
29:r1:602:CLA:H72	50:r1:621:XAT:H28	1.75	0.69
23:S:186:GLY:HA2	48:S:608:CHL:HAC1	1.75	0.69
14:O1:109:MET:HE3	14:O1:140:LEU:HD23	1.74	0.69
7:f1:23:HIS:HA	7:f1:26:ALA:HB3	1.75	0.69
24:y:168:PHE:HD2	29:y:608:CLA:HAB	1.58	0.68
2:b1:454:GLY:HA2	33:b1:622:LMG:H192	1.75	0.68
1:a:303:ASN:O	4:c:403:ASN:ND2	2.26	0.68
29:c:513:CLA:H101	31:c:514:BCR:H21C	1.74	0.68
29:b1:605:CLA:C1C	29:b1:614:CLA:HAB	2.22	0.68
29:D1:403:CLA:H121	18:X1:80:ALA:HB2	1.75	0.68
2:b1:441:GLY:HA3	14:o1:228:LEU:HD12	1.75	0.68
29:y1:610:CLA:H2	49:y1:620:LUT:H28	1.76	0.68
23:s:80:ALA:O	23:s:101:ARG:NH2	2.26	0.68
1:A1:85:THR:HA	1:A1:109:GLY:HA3	1.74	0.68
29:Y1:602:CLA:HAB	49:Y1:621:LUT:H32	1.75	0.68
19:z1:5:LEU:HD13	19:z1:57:PHE:HB2	1.75	0.68
37:c1:519:DGD:HA32	39:j1:101:DGA:HA91	1.75	0.68
55:y1:626:PTY:H181	55:y1:626:PTY:H352	1.73	0.68
21:G:87:ARG:HA	21:G:90:LEU:HD12	1.74	0.68
1:a1:57:PRO:HB2	1:a1:66:PRO:HB2	1.74	0.68
4:c1:285:TYR:O	4:c1:411:ARG:NH2	2.27	0.68
4:c1:270:MET:HE1	29:c1:503:CLA:H142	1.74	0.68
22:R:69:GLY:H	22:R:237:THR:HG22	1.58	0.68
29:b:616:CLA:H2	29:b:617:CLA:HBB2	1.75	0.68
24:y:50:LEU:HB2	24:y:54:SER:HA	1.75	0.68
2:b:371:ILE:HG22	2:b:377:VAL:HA	1.76	0.68
29:N1:613:CLA:H13	50:G1:622:XAT:H34	1.75	0.68
29:n1:610:CLA:H51	49:n1:620:LUT:H30	1.74	0.67
29:a1:405:CLA:H141	29:a1:406:CLA:H121	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:362:PHE:O	5:d1:326:ARG:NH2	2.26	0.67
4:c1:257:GLU:HA	4:c1:260:LEU:HD13	1.76	0.67
39:c1:524:DGA:HB81	33:w1:201:LMG:H402	1.76	0.67
14:o1:172:LEU:HB3	14:o1:176:GLU:HB2	1.74	0.67
14:O:171:LYS:HE3	14:O:177:TYR:HE1	1.59	0.67
29:Y1:602:CLA:HAB	49:Y1:621:LUT:C32	2.25	0.67
4:c1:116:GLY:O	4:c1:120:HIS:ND1	2.24	0.67
4:C:437:ARG:NH2	9:I:27:ASP:OD2	2.28	0.67
48:N:606:CHL:H192	38:S:626:3PH:H281	1.77	0.67
23:S:108:ALA:HB1	23:S:239:GLY:HA3	1.75	0.67
4:C1:16:GLN:OE1	5:D1:233:ARG:NH1	2.28	0.67
14:o1:109:MET:HB2	14:o1:140:LEU:HB2	1.76	0.67
40:C:525:LHG:H311	40:S:624:LHG:H101	1.77	0.67
2:B1:142:HIS:HD2	2:B1:145:LEU:HD12	1.60	0.67
38:B1:624:3PH:H381	16:t1:4:LEU:HB2	1.75	0.67
4:c1:458:ARG:O	5:d1:251:ARG:NH1	2.21	0.67
1:a1:338:ASN:O	4:c1:327:LYS:NZ	2.27	0.67
23:s1:54:GLY:O	23:s1:57:ARG:NH1	2.28	0.67
1:A:121:LEU:HD21	29:C:505:CLA:H162	1.77	0.67
1:A1:329:GLU:O	1:A1:332:HIS:ND1	2.17	0.67
17:w1:79:GLY:HA2	33:w1:201:LMG:HC72	1.75	0.67
29:A1:405:CLA:H122	30:A1:408:PHO:H3A	1.77	0.67
29:g1:602:CLA:HBB2	49:g1:621:LUT:H34	1.76	0.67
14:O:138:TYR:OH	17:W:60:LEU:HD23	1.95	0.67
6:E1:17:ILE:HG12	10:J1:9:ARG:HG3	1.76	0.67
6:E:8:ARG:NH2	44:F:101:HEM:O2A	2.28	0.67
20:n:46:ASN:C	20:n:46:ASN:HD22	2.02	0.67
14:o1:138:TYR:HE2	17:w1:61:VAL:HG22	1.60	0.67
23:S:103:ASN:O	23:S:107:HIS:ND1	2.28	0.66
2:b:311:PHE:O	2:b:317:ASN:ND2	2.28	0.66
31:c:516:BCR:H271	47:k:101:4RF:H18	1.76	0.66
1:a1:192:ILE:HG22	1:a1:293:MET:HE2	1.76	0.66
29:b1:604:CLA:HAB	29:b1:606:CLA:H152	1.76	0.66
31:d:404:BCR:H373	7:f:33:LEU:HD21	1.76	0.66
5:D1:296:TYR:OH	5:D1:326:ARG:NH1	2.28	0.66
48:g:601:CHL:HED3	40:g:624:LHG:H131	1.77	0.66
33:C1:521:LMG:H321	33:C1:521:LMG:H201	1.77	0.66
1:a1:274:PHE:HA	1:a1:277:VAL:HG12	1.77	0.66
29:c1:505:CLA:H43	31:c1:515:BCR:HC7	1.78	0.66
1:A1:140:ARG:NH2	4:C1:445:LYS:O	2.29	0.66
31:d1:404:BCR:H14C	7:f1:28:PRO:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h1:67:ILE:O	8:h1:79:ASN:ND2	2.29	0.66
14:o1:214:LYS:HB2	14:o1:216:ARG:HH11	1.61	0.66
20:n1:68:TYR:OH	20:n1:208:LYS:NZ	2.28	0.66
24:y1:225:GLN:HE22	49:y1:620:LUT:H42	1.59	0.66
8:h:72:LEU:HD11	18:x:69:LEU:HD23	1.78	0.66
1:A:269:ARG:HD2	5:D:235:PHE:HB2	1.77	0.66
5:D:186:GLN:NE2	5:D:322:ASN:OD1	2.29	0.66
14:O1:82:ASN:HD22	14:O1:136:LEU:HD23	1.61	0.66
22:R:195:VAL:HG13	29:R:609:CLA:HAB	1.76	0.66
2:b:366:PHE:HB3	2:b:425:GLN:HE21	1.60	0.66
48:y:606:CHL:HBB2	48:y:607:CHL:HAB	1.77	0.66
5:d1:164:GLN:NE2	5:d1:290:ALA:O	2.29	0.66
29:b:608:CLA:H2	33:b:622:LMG:H151	1.77	0.66
37:c:520:DGD:O1A	5:d:72:ASN:ND2	2.28	0.66
5:D1:126:MET:HA	5:D1:129:GLN:HB3	1.77	0.66
2:b1:324:LEU:HA	5:d1:293:LEU:HD13	1.78	0.66
6:e1:70:PHE:H	25:u1:110:ARG:HH22	1.44	0.66
29:y1:610:CLA:H52	49:y1:620:LUT:H30	1.77	0.66
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.76	0.66
1:a:269:ARG:HD2	5:d:235:PHE:HB2	1.76	0.66
40:c:525:LHG:H311	40:s:624:LHG:H101	1.77	0.66
20:n:153:THR:HG22	48:n:605:CHL:HAC1	1.78	0.66
2:B1:30:VAL:HG12	29:B1:606:CLA:HHD	1.78	0.66
5:D1:252:PHE:O	5:D1:256:ILE:N	2.28	0.66
2:b1:460:LEU:HD11	5:d1:287:VAL:HG21	1.78	0.66
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.78	0.66
23:S1:109:ARG:NE	23:S1:235:GLU:OE2	2.28	0.66
2:b1:256:MET:HE1	2:b1:451:PHE:HB3	1.76	0.66
2:b1:357:ARG:HG2	5:d1:339:LEU:HD21	1.77	0.66
21:G:94:LEU:HB3	29:G:604:CLA:HMC2	1.78	0.65
22:R1:220:PRO:HB3	24:y1:191:PRO:HB3	1.76	0.65
2:b1:142:HIS:ND1	29:b1:611:CLA:OBD	2.23	0.65
29:d1:403:CLA:H91	8:h1:55:LEU:HD13	1.77	0.65
9:I:7:PHE:HB2	47:I:102:4RF:H71	1.77	0.65
21:g:94:LEU:HD22	29:g:604:CLA:HMC1	1.78	0.65
21:g:94:LEU:HB2	49:g:620:LUT:H35	1.78	0.65
23:s:224:ASP:HB3	23:s:227:VAL:HG22	1.78	0.65
1:A1:36:ILE:HG23	29:A1:410:CLA:HBB1	1.78	0.65
29:B1:608:CLA:H152	33:B1:622:LMG:H351	1.77	0.65
4:c1:282:ASN:ND2	4:c1:350:ARG:O	2.29	0.65
5:D:192:THR:HG23	29:D:402:CLA:HBC2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:103:MET:HE3	20:N:220:PHE:HD2	1.61	0.65
21:g:86:ALA:HB1	21:g:204:GLY:HA3	1.78	0.65
4:C1:102:SER:O	4:C1:106:HIS:ND1	2.23	0.65
1:a1:181:ASN:ND2	28:a1:403:CL:CL	2.66	0.65
4:c1:426:PHE:CZ	29:c1:505:CLA:HAB	2.32	0.65
22:r1:134:ARG:NH2	22:r1:213:TYR:OH	2.29	0.65
5:d:192:THR:HG23	29:d:402:CLA:HBC2	1.78	0.65
5:D1:82:ALA:HB3	5:D1:85:LEU:HD23	1.79	0.65
1:a1:302:PHE:HE2	5:d1:74:LEU:HD12	1.59	0.65
33:c1:523:LMG:HC72	29:y1:611:CLA:HBA1	1.78	0.65
23:s1:123:GLY:O	23:s1:127:ASN:ND2	2.29	0.65
48:y1:607:CHL:H92	48:y1:607:CHL:H142	1.78	0.65
21:G:211:CYS:HA	21:G:214:PHE:HD2	1.60	0.65
53:r:626:ERG:O1	53:r:626:ERG:C4	2.41	0.65
29:c1:507:CLA:H142	31:c1:515:BCR:H16C	1.76	0.65
1:A:85:THR:HA	1:A:109:GLY:HA3	1.78	0.65
4:C:319:ALA:HA	15:P:158:GLY:HA3	1.79	0.65
2:B1:265:ILE:HG21	2:B1:274:GLN:HE22	1.62	0.65
2:B1:283:GLU:OE2	2:B1:287:ARG:NH2	2.30	0.65
2:b1:212:ALA:O	2:b1:216:HIS:ND1	2.29	0.65
4:c1:445:LYS:HE3	5:d1:229:ALA:HA	1.79	0.65
37:c1:519:DGD:HB22	33:c1:521:LMG:H311	1.79	0.65
33:c:523:LMG:H171	29:y:612:CLA:HBC1	1.77	0.65
29:B1:616:CLA:H8	29:B1:617:CLA:HBB1	1.77	0.65
4:C1:137:TYR:HB2	4:C1:145:MET:HE1	1.77	0.65
1:a1:183:MET:HB3	29:a1:405:CLA:HBC2	1.78	0.65
5:d1:259:VAL:HG11	40:d1:409:LHG:H262	1.76	0.65
20:n1:205:LYS:HG3	29:n1:611:CLA:HED2	1.77	0.65
29:N:603:CLA:HMA1	29:N:603:CLA:H2	1.78	0.65
29:b:616:CLA:H8	29:b:617:CLA:HBB1	1.79	0.65
2:B1:247:TRP:HB2	29:B1:609:CLA:HBC1	1.78	0.65
2:B1:364:GLU:OE2	5:D1:294:ARG:NH1	2.30	0.65
4:c1:437:ARG:HH12	9:i1:28:PRO:HG3	1.61	0.65
29:c1:502:CLA:H42	29:c1:503:CLA:H112	1.79	0.65
15:p:165:VAL:HB	15:p:194:ALA:HB2	1.79	0.65
40:D1:409:LHG:H172	12:L1:23:LEU:HD21	1.79	0.65
13:M1:15:ILE:O	13:M1:19:THR:OG1	2.10	0.65
1:a1:54:ALA:HB2	1:a1:72:LEU:HD12	1.78	0.65
23:s:186:GLY:HA2	48:s:608:CHL:HAC1	1.78	0.65
4:c1:42:VAL:HA	29:c1:512:CLA:HED1	1.78	0.65
21:g1:220:VAL:HG13	21:g1:221:THR:HG23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:s1:55:PRO:O	23:s1:68:ARG:NH1	2.29	0.65
22:r:190:ILE:HG21	48:r:606:CHL:HED2	1.78	0.64
1:A1:308:ASP:OD1	1:A1:312:ARG:N	2.28	0.64
29:G1:613:CLA:H2	29:G1:614:CLA:HMD1	1.79	0.64
4:c1:166:LYS:HD3	29:c1:502:CLA:H161	1.79	0.64
24:Y:76:LEU:CD2	29:Y:602:CLA:H42	2.27	0.64
15:P1:205:VAL:HG22	15:P1:218:LYS:HG3	1.80	0.64
20:N1:94:ARG:HA	20:N1:97:LEU:HD12	1.77	0.64
23:S1:55:PRO:O	23:S1:68:ARG:NH1	2.30	0.64
1:a1:333:GLU:HB3	1:a1:336:ALA:HB3	1.78	0.64
23:s:171:ILE:HA	23:s:174:VAL:HG12	1.79	0.64
1:A1:233:ALA:O	5:D1:265:ARG:NH1	2.31	0.64
20:N1:235:LEU:HD13	49:N1:620:LUT:H163	1.79	0.64
29:g1:602:CLA:H52	49:g1:621:LUT:H30	1.79	0.64
23:s1:277:LEU:HA	23:s1:280:LEU:HB3	1.78	0.64
1:A:45:ILE:HD11	30:A:408:PHO:H51	1.80	0.64
21:G:112:GLU:O	21:G:121:GLN:NE2	2.30	0.64
2:b:365:THR:OG1	5:d:326:ARG:NH2	2.29	0.64
2:B1:383:PHE:H	5:D1:345:VAL:HA	1.62	0.64
4:C1:281:ASN:OD1	4:C1:284:ALA:N	2.31	0.64
2:b1:341:LEU:HD21	2:b1:431:GLU:HB2	1.80	0.64
22:r1:224:ALA:HB3	29:r1:610:CLA:HAA2	1.78	0.64
29:A:406:CLA:H43	40:L:101:LHG:H211	1.78	0.64
20:N:191:GLY:O	20:N:193:ALA:N	2.31	0.64
1:A1:95:PRO:HD2	1:A1:98:GLU:HB2	1.80	0.64
2:B1:273:TYR:HA	2:B1:276:ASP:HB2	1.80	0.64
33:a1:413:LMG:H392	37:c1:518:DGD:HB92	1.80	0.64
3:v1:4:THR:HG22	3:v1:8:GLN:HE22	1.62	0.64
2:B1:275:TRP:O	25:U1:102:LYS:NZ	2.24	0.64
2:B1:472:ARG:HH12	29:B1:612:CLA:HED3	1.62	0.64
7:F1:36:ILE:HA	7:F1:39:MET:HG2	1.79	0.64
17:W1:86:ALA:HB1	33:W1:201:LMG:H361	1.79	0.64
24:Y1:168:PHE:CD2	29:Y1:608:CLA:HAB	2.32	0.64
24:y:216:MET:HE1	29:y:602:CLA:HAB	1.78	0.64
4:C1:320:GLN:NE2	15:P1:156:SER:OG	2.31	0.64
31:b1:618:BCR:H382	32:b1:621:SQD:H282	1.80	0.64
21:g:81:ILE:O	21:g:85:HIS:HB2	1.96	0.64
24:y:231:LYS:NZ	24:y:239:ASP:OD2	2.30	0.64
20:N1:216:ALA:O	20:N1:220:PHE:N	2.30	0.64
29:B1:603:CLA:H161	33:H1:102:LMG:H362	1.80	0.64
16:T1:4:LEU:HD13	38:b1:624:3PH:H281	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S1:249:PHE:HE1	49:S1:620:LUT:H41	1.63	0.64
4:c1:406:ASN:ND2	37:c1:519:DGD:O5E	2.31	0.64
31:c1:517:BCR:H391	11:k1:36:ALA:HB2	1.78	0.64
15:p1:99:VAL:HB	15:p1:102:ILE:HG13	1.81	0.64
15:p1:198:GLU:HG2	15:p1:224:LYS:HG2	1.80	0.63
22:r1:250:PHE:HA	22:r1:253:PHE:HB2	1.80	0.63
30:A:409:PHO:HBC3	5:D:279:LEU:HD22	1.80	0.63
20:n:130:ILE:HG21	20:n:150:ILE:HD13	1.80	0.63
1:A1:24:THR:O	5:D1:251:ARG:NH2	2.31	0.63
7:f1:42:ILE:HG12	15:p1:65:VAL:HB	1.80	0.63
29:C:513:CLA:HAB	31:C:514:BCR:H24C	1.79	0.63
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.81	0.63
12:l:22:LEU:HB3	16:t:16:ILE:HD13	1.79	0.63
29:y:611:CLA:H193	29:y:612:CLA:HBB2	1.80	0.63
5:d1:148:ALA:HB2	5:d1:276:VAL:HG13	1.80	0.63
4:C:104:VAL:HG21	31:C:514:BCR:HC32	1.81	0.63
6:E1:65:LEU:H	6:E1:79:LEU:HD21	1.61	0.63
2:b1:253:ALA:HB1	2:b1:452:THR:HG23	1.80	0.63
29:b1:603:CLA:HBD	29:b1:603:CLA:H2	1.80	0.63
4:c1:102:SER:O	4:c1:106:HIS:ND1	2.31	0.63
29:n1:603:CLA:H52	29:y1:603:CLA:H51	1.80	0.63
15:p:127:SER:O	15:p:130:ASP:HB2	1.97	0.63
29:y:613:CLA:H12	29:y:614:CLA:HED2	1.79	0.63
1:A1:260:PHE:O	1:A1:264:SER:OG	2.16	0.63
29:Y1:610:CLA:H52	49:Y1:620:LUT:H30	1.81	0.63
20:n1:101:LEU:HB3	29:n1:604:CLA:HMC2	1.80	0.63
29:g1:602:CLA:H72	49:g1:621:LUT:H30	1.80	0.63
29:C:505:CLA:H172	37:C:518:DGD:HA71	1.81	0.63
29:y:602:CLA:H72	49:y:621:LUT:H30	1.80	0.63
32:b1:621:SQD:H271	32:m1:101:SQD:H131	1.81	0.63
13:m1:21:PHE:HA	13:m1:24:ILE:HD12	1.81	0.63
15:p1:205:VAL:HG22	15:p1:218:LYS:HG2	1.79	0.63
5:D:82:ALA:HB3	5:D:85:LEU:HD23	1.81	0.63
20:N:84:ARG:NH1	24:Y:72:ASP:O	2.32	0.63
24:Y:76:LEU:HD23	29:Y:602:CLA:H43	1.81	0.63
4:c:166:LYS:HA	4:c:170:PHE:HB2	1.79	0.63
29:c:505:CLA:H172	37:c:518:DGD:HA71	1.79	0.63
15:p1:119:ILE:HG22	15:p1:121:GLN:H	1.63	0.63
29:B1:612:CLA:H172	29:B1:614:CLA:H8	1.80	0.63
17:W1:82:GLY:HA3	33:W1:201:LMG:HC91	1.81	0.63
55:Y1:626:PTY:H182	55:Y1:626:PTY:H362	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c1:94:LEU:HA	23:s1:289:LEU:HD13	1.81	0.63
22:r1:194:LEU:HD13	51:r1:622:NEX:H34	1.81	0.63
22:R:224:ALA:HB3	29:R:610:CLA:HAA2	1.81	0.63
1:A1:18:CYS:SG	9:I1:30:ARG:NH2	2.67	0.63
1:A1:129:ARG:NH2	5:D1:256:ILE:O	2.32	0.63
29:N1:603:CLA:H2	29:N1:603:CLA:HMA3	1.80	0.63
24:Y1:139:TYR:CE1	29:Y1:604:CLA:H2	2.34	0.63
4:c1:107:LEU:HD13	31:c1:517:BCR:HC8	1.81	0.63
5:d1:302:GLU:OE1	14:o1:214:LYS:NZ	2.32	0.63
6:E:25:ILE:O	6:E:29:SER:HB3	1.99	0.62
2:B1:384:ARG:HA	14:O1:220:THR:HG22	1.81	0.62
39:C1:524:DGA:HBT1	33:W1:201:LMG:H372	1.81	0.62
1:a1:318:ALA:HA	1:a1:321:ILE:HD12	1.81	0.62
29:c1:502:CLA:HBB2	29:c1:510:CLA:H151	1.79	0.62
15:p1:182:LYS:NZ	15:p1:209:VAL:O	2.32	0.62
24:y1:214:LEU:HD23	40:y1:624:LHG:H272	1.79	0.62
5:D:190:ASN:OD1	5:D:322:ASN:ND2	2.32	0.62
48:N1:605:CHL:HAA1	38:S1:626:3PH:H3C2	1.81	0.62
29:R1:603:CLA:HAB	52:R1:625:LMT:H22	1.79	0.62
5:d1:98:GLN:HB2	6:e1:73:LEU:HD22	1.81	0.62
14:O:208:SER:HB3	15:P:154:THR:HG21	1.81	0.62
20:n:247:ALA:HB3	50:g:622:XAT:H193	1.81	0.62
29:g:611:CLA:HAC1	40:g:624:LHG:H292	1.82	0.62
22:r:194:LEU:HD22	51:r:622:NEX:H15	1.81	0.62
8:H1:47:THR:HA	8:H1:50:MET:HG2	1.82	0.62
1:a1:344:ALA:OXT	4:c1:345:ARG:NH1	2.32	0.62
29:c1:504:CLA:H62	37:c1:519:DGD:HB62	1.80	0.62
20:N:84:ARG:NH2	24:Y:60:TYR:OH	2.31	0.62
29:G:613:CLA:H101	40:G:624:LHG:H132	1.81	0.62
29:c:505:CLA:H43	31:c:515:BCR:HC7	1.81	0.62
29:B1:612:CLA:HBC2	40:D1:408:LHG:H341	1.81	0.62
14:O1:271:GLU:OE1	14:O1:291:THR:OG1	2.16	0.62
2:b1:46:ASP:H	2:b1:58:GLN:HE22	1.47	0.62
40:d1:409:LHG:H311	16:t1:17:ILE:HG23	1.81	0.62
1:A:61:ASP:HB3	1:A:63:ILE:HG12	1.82	0.62
29:G:602:CLA:H52	49:G:621:LUT:H28	1.80	0.62
1:A1:323:ARG:NH2	15:P1:110:PHE:O	2.32	0.62
1:A1:338:ASN:ND2	4:C1:327:LYS:O	2.33	0.62
24:Y1:80:PRO:HA	24:Y1:83:PHE:HB3	1.80	0.62
29:a1:405:CLA:H192	29:a1:406:CLA:H122	1.81	0.62
29:b1:614:CLA:HED3	29:b1:614:CLA:H2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:s1:603:CLA:HAB	29:s1:609:CLA:HBC2	1.81	0.62
5:D:141:TYR:OH	40:D:408:LHG:O4	2.17	0.62
15:P:148:GLN:NE2	15:P:150:TRP:O	2.33	0.62
4:C1:69:MET:SD	4:C1:69:MET:N	2.70	0.62
4:C1:145:MET:HA	4:C1:148:ILE:HD12	1.81	0.62
23:S1:241:LEU:HG	49:S1:620:LUT:H11	1.80	0.62
5:d1:268:HIS:HA	5:d1:271:MET:HE3	1.81	0.62
29:r1:610:CLA:H52	49:r1:620:LUT:H30	1.79	0.62
53:r1:626:ERG:O1	53:r1:626:ERG:C2	2.40	0.62
21:G:90:LEU:HD13	29:G:610:CLA:HAB	1.81	0.62
20:n:103:MET:HE3	49:n:621:LUT:H8	1.82	0.62
21:G1:177:PRO:HB3	48:G1:608:CHL:HBC2	1.82	0.62
23:s1:186:GLY:HA2	48:s1:608:CHL:HMC	1.80	0.62
1:A:335:ASN:HA	5:D:350:ASN:HD22	1.65	0.62
23:S:224:ASP:HB3	23:S:227:VAL:HG22	1.81	0.62
1:a1:223:LEU:HD23	1:a1:246:TYR:HB3	1.82	0.62
24:y1:105:ILE:HA	24:y1:234:ILE:HD11	1.81	0.62
38:B:624:3PH:H3A1	16:t:4:LEU:HD13	1.81	0.62
15:p:157:GLU:HG2	15:p:194:ALA:HB1	1.81	0.62
1:a1:306:VAL:HA	10:j1:39:GLY:HA2	1.82	0.62
23:s1:267:HIS:ND1	23:s1:274:TYR:O	2.28	0.62
2:B:384:ARG:NH2	5:D:343:GLU:OE1	2.32	0.62
23:S:183:ARG:NH2	29:S:609:CLA:O1D	2.33	0.62
29:b:603:CLA:H161	33:h:102:LMG:H382	1.82	0.62
14:o:183:THR:HG22	14:o:185:LYS:H	1.65	0.62
50:N1:622:XAT:H34	29:Y1:613:CLA:H111	1.81	0.62
23:S1:105:LEU:HD23	23:S1:210:LEU:HB3	1.80	0.62
4:c1:240:ILE:HD13	32:c1:526:SQD:H82	1.80	0.62
29:c1:511:CLA:HBC2	11:k1:40:GLN:HG3	1.81	0.62
29:y1:614:CLA:HAB	55:y1:626:PTY:H211	1.81	0.62
22:R1:142:ARG:NH1	29:R1:608:CLA:OBD	2.33	0.61
1:a1:200:PHE:O	1:a1:204:GLY:N	2.33	0.61
1:a1:335:ASN:ND2	5:d1:350:ASN:OD1	2.25	0.61
30:a1:409:PHO:HAB	29:d1:402:CLA:H11	1.82	0.61
4:c1:401:GLU:OE2	15:p1:228:LYS:NZ	2.33	0.61
5:d1:186:GLN:NE2	5:d1:322:ASN:OD1	2.33	0.61
4:c:319:ALA:HA	15:p:158:GLY:HA3	1.82	0.61
14:O1:103:LYS:HA	14:O1:146:SER:HA	1.82	0.61
50:N1:622:XAT:H363	40:Y1:624:LHG:HC41	1.82	0.61
23:S1:186:GLY:HA2	48:S1:608:CHL:HMC	1.82	0.61
1:a1:285:LEU:O	1:a1:289:GLY:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c1:373:GLN:OE1	4:c1:375:TRP:NE1	2.32	0.61
20:n1:223:GLN:O	20:n1:227:THR:OG1	2.16	0.61
2:B:311:PHE:O	2:B:317:ASN:ND2	2.33	0.61
29:Y:614:CLA:H2	55:Y:626:PTY:H361	1.81	0.61
4:c:390:GLY:HA3	4:c:408:VAL:HG22	1.82	0.61
29:g:613:CLA:H12	29:g:614:CLA:HED2	1.80	0.61
30:A1:409:PHO:H61	29:D1:402:CLA:H111	1.82	0.61
29:Y1:602:CLA:H72	49:Y1:621:LUT:H30	1.80	0.61
5:d1:104:TRP:HZ2	29:d1:403:CLA:HED2	1.64	0.61
5:d1:286:VAL:O	5:d1:290:ALA:N	2.34	0.61
24:y1:46:ARG:NH2	24:y1:61:LEU:O	2.33	0.61
1:A:133:LEU:HD23	5:D:256:ILE:HG12	1.82	0.61
1:A:292:THR:HG22	4:C:416:THR:HG23	1.83	0.61
21:G:52:TYR:OH	21:G:64:ASP:OD2	2.18	0.61
22:r:184:ILE:HD13	22:r:187:LEU:HD12	1.83	0.61
9:I1:5:LYS:NZ	17:W1:77:ASN:OD1	2.33	0.61
23:S1:244:ILE:HD11	29:S1:602:CLA:HAC1	1.81	0.61
2:b1:258:TYR:HB3	33:h1:102:LMG:HC61	1.81	0.61
48:n:606:CHL:H192	38:s:626:3PH:H2A1	1.82	0.61
6:e1:38:VAL:HG21	7:f1:39:MET:HE3	1.83	0.61
14:o:133:LEU:HD21	14:o:171:LYS:HB2	1.82	0.61
1:a1:41:LEU:HD22	30:a1:408:PHO:H92	1.82	0.61
4:c1:33:LEU:HD23	4:c1:36:LYS:HD2	1.81	0.61
5:d1:225:ASP:HB2	5:d1:234:ALA:HB1	1.82	0.61
6:e1:36:LEU:O	6:e1:40:THR:OG1	2.17	0.61
17:w1:65:MET:HG3	17:w1:77:ASN:HD22	1.65	0.61
14:O:225:ALA:H	14:O:240:LEU:HD22	1.64	0.61
4:C1:67:LYS:O	4:C1:72:GLN:NE2	2.34	0.61
4:C1:461:ASP:OD2	16:T1:24:ARG:NH2	2.34	0.61
23:S1:217:ASP:OD1	49:S1:620:LUT:O23	2.18	0.61
2:b1:392:ILE:HG21	2:b1:417:VAL:HG11	1.83	0.61
1:A:54:ALA:HB2	1:A:72:LEU:HD12	1.83	0.61
17:w:89:LEU:HB3	33:w:201:LMG:H401	1.83	0.61
22:r:207:ASP:HB3	22:r:210:LYS:HB2	1.81	0.61
2:B:384:ARG:NH2	5:D:343:GLU:O	2.33	0.61
15:p:189:ILE:HB	15:p:203:GLN:HB2	1.83	0.61
50:n:622:XAT:H372	29:y:611:CLA:HAB	1.83	0.61
23:s:112:MET:HE1	29:s:610:CLA:CAB	2.31	0.61
1:A1:344:ALA:OXT	4:C1:345:ARG:NH1	2.34	0.61
4:C1:437:ARG:HH12	9:I1:28:PRO:HA	1.66	0.61
29:R1:610:CLA:HBC3	49:R1:620:LUT:H392	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:s1:224:ASP:HB3	23:s1:227:VAL:HG22	1.83	0.61
32:B:626:SQD:O4	1:a:103:ASP:OD1	2.19	0.61
29:C:501:CLA:HMB2	31:C:515:BCR:H23C	1.83	0.61
23:S:112:MET:SD	29:S:610:CLA:HAB	2.40	0.61
1:a:285:LEU:HD21	29:c:504:CLA:H151	1.83	0.61
2:b:106:LEU:HD11	29:b:607:CLA:H122	1.83	0.61
6:e:30:LEU:HD11	7:f:27:VAL:HG13	1.81	0.61
1:A1:341:LEU:H	4:C1:301:GLN:HE22	1.47	0.61
5:D1:264:LYS:NZ	42:D1:401:BCT:O2	2.31	0.61
15:P1:174:ALA:HB3	15:P1:186:LYS:HB3	1.82	0.61
2:b1:390:TYR:OH	15:p1:96:GLU:OE2	2.16	0.61
22:r1:214:PRO:HB3	29:r1:608:CLA:HBC2	1.82	0.61
24:Y:76:LEU:HD22	29:Y:602:CLA:C4	2.31	0.60
24:Y:210:LYS:NZ	29:Y:611:CLA:O1D	2.34	0.60
1:a:45:ILE:HD11	30:a:408:PHO:H51	1.82	0.60
29:b:606:CLA:HMA3	29:b:607:CLA:H3A	1.83	0.60
29:n:603:CLA:H41	29:y:603:CLA:H51	1.83	0.60
4:C1:452:GLU:HB3	4:C1:455:LEU:HG	1.81	0.60
4:c1:221:ILE:HA	31:c1:515:BCR:H282	1.82	0.60
1:A:313:VAL:HG23	15:P:90:LYS:HD2	1.83	0.60
1:A:340:PRO:HD2	4:C:305:PHE:HE2	1.65	0.60
33:A:413:LMG:H191	29:C:505:CLA:H8	1.83	0.60
2:b:54:PRO:HD2	2:b:57:ARG:HG3	1.83	0.60
23:s:173:ILE:HG23	29:s:609:CLA:HBB2	1.83	0.60
5:D1:29:PHE:HB3	5:D1:128:ARG:HH21	1.65	0.60
20:N1:101:LEU:HB3	29:N1:604:CLA:HMC2	1.84	0.60
29:N1:603:CLA:H13	48:Y1:609:CHL:H18	1.82	0.60
23:S1:251:ILE:HG21	29:S1:613:CLA:HBC3	1.83	0.60
1:a1:186:PHE:HB3	1:a1:192:ILE:HG21	1.82	0.60
4:c1:250:ARG:HH21	9:i1:25:SER:HA	1.64	0.60
29:n:603:CLA:HAC1	48:n:607:CHL:HBB2	1.83	0.60
1:A1:335:ASN:HA	5:D1:350:ASN:HD22	1.67	0.60
29:C1:513:CLA:H41	40:C1:525:LHG:H292	1.82	0.60
39:C:524:DGA:HAF1	33:W:201:LMG:H352	1.84	0.60
29:A1:410:CLA:H111	33:A1:413:LMG:H132	1.84	0.60
2:B1:122:LEU:O	8:H1:34:ASN:ND2	2.35	0.60
4:C1:205:PRO:HD3	4:C1:211:TRP:HB2	1.84	0.60
23:S1:112:MET:SD	29:S1:610:CLA:HAB	2.41	0.60
29:Y1:602:CLA:H71	29:Y1:603:CLA:HHB	1.83	0.60
14:o1:253:VAL:HB	14:o1:271:GLU:HB3	1.84	0.60
20:n1:251:ALA:HA	50:g1:622:XAT:H22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:HG23	29:A:410:CLA:HBB1	1.83	0.60
29:A:405:CLA:H122	30:A:408:PHO:H3A	1.82	0.60
2:B:30:VAL:HG12	29:B:606:CLA:HHD	1.84	0.60
4:C:355:GLU:OE2	4:C:358:ARG:NH1	2.34	0.60
24:Y:172:GLY:HA2	29:Y:608:CLA:HAC1	1.81	0.60
1:A1:224:ILE:HG12	1:A1:246:TYR:HA	1.83	0.60
29:B1:609:CLA:H91	39:B1:625:DGA:HBF1	1.84	0.60
22:r1:134:ARG:NH1	22:r1:134:ARG:O	2.31	0.60
29:B:606:CLA:HMA3	29:B:607:CLA:H3A	1.83	0.60
29:C:502:CLA:H61	29:C:512:CLA:H42	1.82	0.60
21:G:86:ALA:HB1	21:G:204:GLY:HA3	1.84	0.60
29:R:609:CLA:H102	52:R:625:LMT:H122	1.82	0.60
23:S:151:TYR:CZ	29:S:604:CLA:H2	2.37	0.60
2:b:357:ARG:NH2	5:d:337:GLU:OE1	2.35	0.60
2:B1:193:TYR:HB2	8:H1:83:SER:HB2	1.82	0.60
2:B1:234:ILE:HG22	29:B1:613:CLA:HAC1	1.83	0.60
9:I1:13:THR:HA	9:I1:16:VAL:HG12	1.84	0.60
4:c1:309:ASP:OD1	15:p1:192:ARG:NH2	2.34	0.60
29:c1:505:CLA:H141	37:c1:518:DGD:HA82	1.82	0.60
21:G:87:ARG:NH1	48:G:608:CHL:OBD	2.27	0.60
11:k:45:PHE:HB2	47:k:101:4RF:H5	1.84	0.60
21:G1:81:ILE:O	21:G1:85:HIS:ND1	2.23	0.60
21:G1:249:THR:OG1	24:Y1:126:LYS:NZ	2.31	0.60
22:R1:146:LEU:HD11	29:R1:610:CLA:HAC1	1.84	0.60
4:c1:221:ILE:O	4:c1:225:HIS:ND1	2.34	0.60
20:n1:91:ILE:HD13	20:n1:94:ARG:HH12	1.67	0.60
29:n1:603:CLA:H93	29:g1:603:CLA:H72	1.83	0.60
29:r1:602:CLA:HBB1	29:r1:602:CLA:H51	1.84	0.60
53:r1:626:ERG:O1	53:r1:626:ERG:C4	2.41	0.60
1:A:312:ARG:NH2	15:P:93:PRO:HD2	2.17	0.60
24:Y:142:ASN:ND2	22:r:176:LEU:O	2.35	0.60
1:A1:340:PRO:HB2	15:P1:224:LYS:HD3	1.84	0.60
2:B1:157:HIS:HA	2:B1:163:GLY:HA3	1.82	0.60
5:D1:253:TRP:HA	5:D1:256:ILE:HB	1.83	0.60
20:N1:101:LEU:O	20:N1:105:THR:OG1	2.19	0.60
5:d1:195:PRO:HA	5:d1:198:MET:HE2	1.84	0.60
29:S:604:CLA:H43	48:S:606:CHL:HAA2	1.82	0.60
33:c:523:LMG:H411	34:y:625:SPH:H101	1.84	0.60
2:B1:10:THR:O	22:R1:94:GLN:NE2	2.35	0.60
4:C1:75:ILE:HG22	4:C1:410:PRO:HB3	1.84	0.60
20:N1:92:HIS:HB3	20:N1:214:MET:HE1	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U1:93:THR:HG22	25:U1:97:MET:HE2	1.83	0.60
4:c1:224:GLY:HA3	31:c1:515:BCR:H292	1.82	0.60
20:n1:202:LEU:HA	20:n1:205:LYS:HD2	1.83	0.60
4:C1:234:LEU:HB3	34:Y1:625:SPH:H141	1.84	0.59
29:C1:501:CLA:H172	29:C1:506:CLA:HBB1	1.83	0.59
29:C1:501:CLA:H191	29:C1:507:CLA:HBB1	1.84	0.59
50:N1:622:XAT:H162	24:Y1:253:ALA:HA	1.83	0.59
4:c1:270:MET:HG2	29:c1:501:CLA:H41	1.84	0.59
5:d1:292:ASN:OD1	5:d1:294:ARG:NH1	2.36	0.59
15:p1:119:ILE:HD13	15:p1:216:LEU:HB3	1.83	0.59
1:a:139:MET:HE3	5:d:221:THR:HG22	1.84	0.59
4:C1:150:GLY:HA3	4:C1:240:ILE:HG13	1.84	0.59
21:g1:229:LEU:HD21	49:g1:620:LUT:H163	1.83	0.59
48:y:607:CHL:H143	48:y:609:CHL:H101	1.83	0.59
1:A1:181:ASN:ND2	5:D1:314:PHE:O	2.29	0.59
32:A1:412:SQD:O8	5:D1:233:ARG:NE	2.34	0.59
2:B1:281:GLN:HA	2:B1:284:ILE:HG22	1.84	0.59
4:C1:221:ILE:O	4:C1:225:HIS:ND1	2.32	0.59
1:a1:103:ASP:HB2	14:o1:131:LYS:HE2	1.83	0.59
2:b1:476:ARG:NH2	22:r1:100:LYS:O	2.35	0.59
5:d1:264:LYS:O	5:d1:268:HIS:ND1	2.35	0.59
20:n1:65:PRO:HD3	20:n1:203:LYS:HE2	1.83	0.59
29:n1:604:CLA:HBA2	51:n1:623:NEX:H241	1.85	0.59
29:b:615:CLA:H8	32:m:101:SQD:H281	1.84	0.59
40:c:525:LHG:H141	29:s:611:CLA:HBB2	1.83	0.59
24:y:192:LEU:HD12	49:y:620:LUT:H222	1.84	0.59
2:B1:57:ARG:HE	2:B1:311:PHE:HZ	1.48	0.59
2:B1:270:PRO:HG3	2:B1:312:TYR:HD1	1.68	0.59
38:B1:624:3PH:H221	13:M1:6:LEU:HD11	1.83	0.59
6:E1:42:LEU:HD12	6:E1:45:ASP:HB2	1.83	0.59
4:c1:20:GLY:HA3	5:d1:229:ALA:H	1.66	0.59
29:y1:610:CLA:H101	29:y1:612:CLA:H121	1.84	0.59
9:I:5:LYS:NZ	17:W:77:ASN:OD1	2.29	0.59
24:Y:174:ALA:HB3	24:Y:177:VAL:HG12	1.85	0.59
20:n:217:CYS:HA	20:n:220:PHE:HD2	1.67	0.59
16:T1:1:MET:H1	38:b1:624:3PH:H361	1.66	0.59
23:S1:108:ALA:HA	23:S1:243:MET:HE1	1.85	0.59
23:S1:150:ASN:OD1	23:S1:160:GLN:NE2	2.36	0.59
23:S1:176:LEU:HD12	29:S1:609:CLA:HAB	1.84	0.59
14:o1:95:ARG:HH22	14:o1:153:GLY:HA2	1.67	0.59
17:w1:80:ILE:HA	17:w1:83:TRP:HD1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:n1:622:XAT:H221	29:y1:611:CLA:HAB	1.83	0.59
38:B:624:3PH:H321	16:t:1:MET:HE2	1.85	0.59
1:a:335:ASN:ND2	5:d:350:ASN:OD1	2.34	0.59
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.84	0.59
39:c:524:DGA:HBE2	33:w:201:LMG:H392	1.84	0.59
1:A1:340:PRO:HA	5:D1:352:LEU:H	1.67	0.59
29:A1:407:CLA:HMB2	29:D1:402:CLA:H122	1.85	0.59
2:B1:191:ASP:HB3	2:B1:194:ASN:HB2	1.84	0.59
2:B1:452:THR:HB	5:D1:291:LEU:HD21	1.83	0.59
29:C1:508:CLA:H162	33:C1:521:LMG:H412	1.84	0.59
29:Y1:612:CLA:HMB2	29:Y1:612:CLA:H143	1.85	0.59
4:c1:202:VAL:HG12	17:w1:74:PHE:HB2	1.83	0.59
29:c1:508:CLA:H43	29:c1:511:CLA:HAC1	1.85	0.59
14:O:107:PHE:HB3	14:O:143:MET:HB2	1.85	0.59
20:N:226:VAL:HG23	20:N:227:THR:HG23	1.84	0.59
21:G:189:ASP:HB3	21:G:192:THR:HG22	1.83	0.59
29:g:613:CLA:H2	29:g:614:CLA:HMD1	1.84	0.59
2:B1:197:GLY:O	2:B1:201:HIS:N	2.32	0.59
32:B1:626:SQD:H151	34:a1:414:SPH:H102	1.82	0.59
20:N1:184:GLY:HA3	29:N1:610:CLA:HED2	1.83	0.59
5:d1:185:PHE:HE2	5:d1:286:VAL:HG22	1.67	0.59
29:y1:602:CLA:H72	49:y1:621:LUT:H30	1.84	0.59
1:A:28:LEU:HB2	38:T:101:3PH:H222	1.84	0.59
2:B:357:ARG:NH1	2:B:358:ARG:O	2.36	0.59
14:O:133:LEU:HD21	14:O:171:LYS:HD2	1.84	0.59
1:a:267:ASN:HD22	5:d:235:PHE:HD2	1.49	0.59
1:a:310:ASN:O	15:p:89:SER:OG	2.20	0.59
4:c:91:GLY:HA3	4:c:288:GLU:HG2	1.84	0.59
6:e:25:ILE:O	6:e:29:SER:OG	2.18	0.59
21:g:153:MET:HE3	21:g:157:GLU:HG2	1.84	0.59
1:A1:155:THR:HG21	37:C1:518:DGD:HBW1	1.84	0.59
2:B1:128:THR:HG23	2:B1:130:LYS:H	1.68	0.59
48:R1:606:CHL:HBC2	48:R1:607:CHL:HAC2	1.85	0.59
7:F:23:HIS:NE2	44:F:101:HEM:NB	2.51	0.59
1:A1:285:LEU:O	1:A1:289:GLY:N	2.34	0.59
2:B1:64:PRO:HB3	2:B1:267:LEU:HB3	1.85	0.59
31:B1:618:BCR:H14C	31:B1:619:BCR:H341	1.84	0.59
22:R1:175:TYR:HB2	22:R1:180:LEU:HD11	1.85	0.59
1:a1:14:TRP:O	1:a1:18:CYS:N	2.35	0.59
6:e1:19:TYR:O	6:e1:23:HIS:ND1	2.27	0.59
23:s1:194:PRO:HB2	23:s1:218:PRO:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:406:LEU:HB3	2:b:409:LEU:HD12	1.85	0.59
20:n:247:ALA:HB1	50:g:622:XAT:H161	1.83	0.59
48:N1:601:CHL:H171	48:G1:607:CHL:H161	1.84	0.59
21:G1:47:ASN:HB2	24:Y1:171:ASN:HB2	1.84	0.59
1:a1:165:GLN:NE2	1:a1:294:ALA:O	2.36	0.59
1:a1:257:ARG:O	5:d1:128:ARG:NH2	2.34	0.59
30:a1:409:PHO:H11	5:d1:125:PHE:HB2	1.85	0.59
29:c1:513:CLA:H41	40:c1:525:LHG:H292	1.83	0.59
7:f1:40:GLN:NE2	10:j1:30:PHE:O	2.36	0.59
24:y1:139:TYR:CE1	29:y1:604:CLA:H2	2.38	0.59
24:y1:240:HIS:ND1	24:y1:247:ASN:O	2.28	0.59
2:B:301:ALA:HA	2:B:304:LYS:HD3	1.84	0.58
4:c:309:ASP:OD2	4:c:328:TYR:OH	2.17	0.58
14:o:133:LEU:HB2	14:o:169:THR:HG23	1.85	0.58
15:p:129:GLN:OE1	15:p:183:THR:OG1	2.20	0.58
22:r:223:LEU:O	22:r:231:LYS:NZ	2.33	0.58
4:C1:21:PHE:O	4:C1:29:ARG:NH2	2.35	0.58
5:D1:83:ASN:HB3	5:D1:336:HIS:HD2	1.68	0.58
20:N1:70:TRP:HZ3	48:N1:601:CHL:HAA2	1.68	0.58
1:a1:114:LEU:HD22	29:a1:410:CLA:HED2	1.84	0.58
2:b1:113:TRP:NE1	29:b1:617:CLA:O1A	2.36	0.58
48:g1:609:CHL:HHC	48:g1:609:CHL:HBB1	1.85	0.58
1:A:97:TRP:HA	9:I:1:MET:HE2	1.86	0.58
14:O:75:VAL:HG13	14:O:80:ILE:HB	1.84	0.58
24:Y:76:LEU:HD22	29:Y:602:CLA:C1	2.29	0.58
31:c:516:BCR:HC41	11:k:25:LEU:HD21	1.85	0.58
15:p:205:VAL:HG22	15:p:218:LYS:HG3	1.84	0.58
23:s:192:PHE:HA	23:s:198:LYS:H	1.66	0.58
2:B1:135:LEU:HD11	2:B1:234:ILE:HD13	1.85	0.58
29:N1:613:CLA:H102	40:N1:624:LHG:H311	1.84	0.58
2:b1:256:MET:O	2:b1:448:ARG:NH1	2.36	0.58
37:b1:623:DGD:HD61	22:r1:170:LEU:HD11	1.84	0.58
38:t1:101:3PH:H2A2	38:t1:101:3PH:H2H1	1.84	0.58
1:A:231:GLU:OE2	2:B:2:GLY:N	2.36	0.58
40:D:409:LHG:H261	12:L:23:LEU:HD22	1.84	0.58
4:c:153:LEU:HD21	29:c:506:CLA:HAB	1.85	0.58
4:c:452:GLU:OE2	5:d:245:SER:OG	2.17	0.58
2:B1:61:PHE:HE1	2:B1:451:PHE:HD1	1.51	0.58
5:D1:49:LEU:HA	5:D1:52:CYS:HB2	1.84	0.58
12:L1:30:VAL:HG22	16:T1:9:LEU:HD13	1.85	0.58
15:P1:204:LEU:HB2	15:P1:219:VAL:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a1:32:TRP:HZ3	9:i1:27:ASP:HB2	1.68	0.58
5:d:343:GLU:HB2	15:p:112:ALA:HB3	1.86	0.58
30:A1:409:PHO:H3A	29:D1:402:CLA:H142	1.85	0.58
53:R1:626:ERG:O1	53:R1:626:ERG:C4	2.44	0.58
29:c1:504:CLA:H51	37:c1:520:DGD:HB52	1.85	0.58
29:c1:511:CLA:H142	11:k1:32:PHE:HE1	1.68	0.58
29:B:616:CLA:H2	29:B:617:CLA:HBB2	1.85	0.58
53:R:626:ERG:O1	53:R:626:ERG:C2	2.42	0.58
1:a:140:ARG:HH22	40:d:410:LHG:HC42	1.68	0.58
2:B1:464:PHE:HD2	29:B1:612:CLA:HAC2	1.67	0.58
4:C1:403:ASN:OD1	37:C1:520:DGD:O2E	2.18	0.58
14:O1:77:GLY:O	17:W1:66:ASN:ND2	2.36	0.58
1:a1:120:PHE:HZ	37:c1:518:DGD:HBT1	1.69	0.58
4:c1:31:ILE:HG12	29:c1:509:CLA:HBC2	1.85	0.58
2:B:338:VAL:HB	2:B:431:GLU:HG3	1.86	0.58
6:E:35:TRP:HA	7:F:38:ALA:HB2	1.85	0.58
2:B1:23:HIS:ND1	29:B1:616:CLA:OBD	2.37	0.58
40:C1:525:LHG:H131	32:C1:526:SQD:H301	1.85	0.58
9:I1:26:ASN:OD1	9:I1:29:SER:OG	2.22	0.58
21:G1:164:GLY:HA3	21:G1:170:ASP:HA	1.85	0.58
29:G1:603:CLA:HAC2	48:G1:607:CHL:H18	1.86	0.58
23:S1:83:TYR:OH	23:S1:237:LYS:NZ	2.37	0.58
2:b1:360:PRO:HD2	2:b1:363:PHE:HD2	1.69	0.58
4:c1:242:THR:HG22	34:y1:625:SPH:H4	1.86	0.58
5:d1:122:LEU:HD21	29:d1:402:CLA:H8	1.86	0.58
20:n1:226:VAL:HG22	20:n1:250:TYR:HB3	1.86	0.58
4:C:234:LEU:HB3	34:Y:625:SPH:H151	1.85	0.58
11:K:11:LEU:HD11	11:K:22:VAL:HG21	1.85	0.58
48:G:601:CHL:H11	48:Y:609:CHL:H43	1.85	0.58
4:C1:221:ILE:HD12	31:C1:515:BCR:H282	1.85	0.58
4:C1:425:PHE:HE1	29:C1:508:CLA:HAB	1.67	0.58
14:O1:138:TYR:CE2	17:W1:61:VAL:HG22	2.39	0.58
5:d1:197:HIS:O	5:d1:201:VAL:N	2.36	0.58
29:y1:614:CLA:H3A	55:y1:626:PTY:H322	1.85	0.58
4:C:156:LEU:HD11	29:C:509:CLA:H61	1.85	0.58
1:a:170:ASP:OD1	4:c:345:ARG:NH1	2.36	0.58
3:v:33:LEU:HA	29:c:511:CLA:H42	1.85	0.58
4:c:205:PRO:HB2	37:c:518:DGD:HA21	1.85	0.58
2:B1:187:ALA:HB1	8:H1:74:LEU:HD13	1.86	0.58
29:C1:512:CLA:H12	29:C1:513:CLA:H201	1.85	0.58
33:C1:521:LMG:H301	33:C1:521:LMG:H171	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M1:28:LYS:HD2	13:m1:31:ALA:HB2	1.84	0.58
4:c1:324:GLY:HA3	14:o1:206:ARG:HH21	1.68	0.58
20:n1:154:LEU:HD13	48:n1:607:CHL:HAC2	1.85	0.58
29:B:604:CLA:HAB	29:B:606:CLA:H161	1.84	0.58
4:C:109:SER:HA	31:C:514:BCR:H16C	1.86	0.58
40:C:525:LHG:H142	29:S:611:CLA:HBB2	1.85	0.58
2:b:301:ALA:O	2:b:304:LYS:HB2	2.02	0.58
29:g:602:CLA:CAB	49:g:621:LUT:H32	2.33	0.58
1:A1:106:LEU:HD11	31:A1:411:BCR:H292	1.85	0.58
4:C1:285:TYR:O	4:C1:411:ARG:NH2	2.32	0.58
1:a1:34:GLY:HA2	1:a1:37:MET:HB2	1.86	0.58
29:a1:406:CLA:H72	30:a1:408:PHO:HMA1	1.85	0.58
39:c1:524:DGA:HBH2	17:w1:90:GLY:HA3	1.85	0.58
29:N:613:CLA:H152	40:N:624:LHG:H331	1.85	0.58
21:G:150:VAL:HG23	48:G:609:CHL:HBB2	1.86	0.58
23:S:221:LEU:HD11	29:S:610:CLA:H42	1.85	0.58
29:Y:602:CLA:H72	49:Y:621:LUT:H30	1.85	0.58
21:g:66:ALA:HA	24:y:89:ILE:HD11	1.86	0.58
29:S1:602:CLA:H72	49:S1:621:LUT:H28	1.84	0.58
2:b1:192:PRO:O	2:b1:260:SER:OG	2.21	0.58
4:c1:167:ALA:HA	4:c1:172:GLY:HA2	1.85	0.58
43:d1:405:PL9:H401	40:d1:409:LHG:H211	1.84	0.58
20:n1:141:ASN:ND2	20:n1:143:SER:OG	2.36	0.58
53:R:626:ERG:O1	53:R:626:ERG:C4	2.44	0.57
29:B1:615:CLA:H193	13:m1:16:ILE:HD11	1.86	0.57
4:C1:14:ARG:HB2	4:C1:29:ARG:HD3	1.85	0.57
25:U1:90:ARG:HG3	25:U1:92:ARG:H	1.69	0.57
21:g1:157:GLU:OE1	21:g1:160:ARG:NH2	2.37	0.57
14:O:216:ARG:HH11	14:O:240:LEU:HB3	1.69	0.57
22:R:135:GLU:HG3	22:R:212:ILE:HG12	1.84	0.57
2:b:479:PHE:O	5:d:139:ARG:NH2	2.37	0.57
29:b:605:CLA:H143	29:b:616:CLA:HMA3	1.86	0.57
15:p:218:LYS:NZ	15:p:220:GLN:OE1	2.37	0.57
21:g:41:LEU:HB3	21:g:44:PHE:HB2	1.86	0.57
21:g:192:THR:O	21:g:196:LEU:HB2	2.04	0.57
4:C1:43:ALA:HB2	4:C1:117:GLY:HA3	1.85	0.57
8:H1:61:LEU:HA	8:H1:64:ILE:HG22	1.86	0.57
21:g1:90:LEU:HD21	21:g1:204:GLY:HA2	1.86	0.57
24:y1:210:LYS:NZ	40:y1:624:LHG:O4	2.37	0.57
48:y1:607:CHL:H71	48:y1:607:CHL:HMB2	1.85	0.57
34:a:414:SPH:H91	47:i:101:4RF:H40	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:341:LEU:HD12	2:b:429:ILE:HG22	1.85	0.57
2:b:458:PHE:HB3	29:b:605:CLA:HBC2	1.86	0.57
16:T1:1:MET:HG2	38:b1:624:3PH:H342	1.86	0.57
19:Z1:57:PHE:O	19:Z1:61:ALA:N	2.37	0.57
20:N:208:LYS:NZ	29:N:611:CLA:O1D	2.36	0.57
32:B1:626:SQD:H81	31:a1:411:BCR:H391	1.86	0.57
4:C1:358:ARG:HD2	14:O1:72:TYR:CD2	2.39	0.57
20:N1:217:CYS:SG	49:N1:621:LUT:H12	2.45	0.57
5:d1:160:TYR:HD1	5:d1:290:ALA:HA	1.69	0.57
15:p1:178:ASP:OD1	15:p1:181:GLY:N	2.37	0.57
25:u:105:THR:HB	25:u:108:GLU:HG3	1.86	0.57
29:b1:614:CLA:H202	29:b1:614:CLA:H141	1.87	0.57
29:D:403:CLA:H102	18:X:80:ALA:HB2	1.86	0.57
20:N:93:ALA:HB1	20:N:210:GLY:HA3	1.86	0.57
20:N:205:LYS:HD3	29:N:612:CLA:HAA2	1.86	0.57
24:y:76:LEU:CD1	29:y:602:CLA:H11	2.35	0.57
1:A1:136:ARG:HH12	9:I1:30:ARG:HD3	1.69	0.57
23:s1:110:TRP:HA	23:s1:113:LEU:HD12	1.85	0.57
1:A:228:THR:OG1	1:A:230:ASN:OD1	2.18	0.57
4:c:166:LYS:NZ	4:c:172:GLY:O	2.36	0.57
4:c:225:HIS:HA	4:c:228:ILE:HG22	1.85	0.57
4:C1:306:LEU:HG	4:C1:316:VAL:HG11	1.86	0.57
2:b1:318:ASN:HD21	2:b1:361:THR:HG23	1.69	0.57
4:c1:69:MET:N	4:c1:69:MET:SD	2.77	0.57
14:o1:143:MET:HA	14:o1:162:GLY:HA3	1.85	0.57
20:n1:36:THR:OG1	20:n1:37:ILE:N	2.37	0.57
29:n1:613:CLA:H13	40:n1:624:LHG:H361	1.85	0.57
21:g1:90:LEU:HD23	21:g1:207:ALA:HB3	1.85	0.57
22:r1:130:LEU:O	22:r1:134:ARG:N	2.34	0.57
48:s1:601:CHL:HMD3	40:s1:624:LHG:HC61	1.87	0.57
24:y1:204:LEU:HD11	29:y1:612:CLA:HBA2	1.87	0.57
2:B:365:THR:HG21	14:O:226:ILE:HD12	1.86	0.57
1:a:36:ILE:HG23	29:a:410:CLA:HBB1	1.86	0.57
4:C1:136:GLY:O	4:C1:144:LYS:NZ	2.37	0.57
7:F1:40:GLN:HE21	10:J1:33:GLY:HA3	1.69	0.57
29:N1:613:CLA:H152	40:N1:624:LHG:H331	1.87	0.57
1:a1:45:ILE:HD11	30:a1:408:PHO:H51	1.86	0.57
4:c1:332:SER:OG	4:c1:335:GLY:N	2.38	0.57
2:B1:127:ARG:HH22	22:R1:105:GLU:HB2	1.68	0.57
20:N1:83:LYS:NZ	20:N1:87:GLU:OE2	2.38	0.57
48:G1:606:CHL:HHC	48:G1:606:CHL:HBB1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d1:185:PHE:HA	5:d1:189:HIS:HB2	1.87	0.57
14:o1:70:LEU:HD23	14:o1:74:GLN:HB3	1.86	0.57
24:Y:154:THR:HG22	48:Y:605:CHL:HAC1	1.87	0.57
2:b:145:LEU:HD12	29:b:605:CLA:H162	1.86	0.57
33:c:523:LMG:H401	40:y:624:LHG:H381	1.85	0.57
5:d:61:HIS:NE2	5:d:80:THR:O	2.36	0.57
54:s:625:LPX:H10	38:s:626:3PH:H291	1.87	0.57
1:A1:309:SER:OG	7:F1:44:ARG:OXT	2.21	0.57
32:A1:412:SQD:H331	29:C1:508:CLA:H71	1.85	0.57
48:N1:608:CHL:HBB1	51:N1:623:NEX:H12	1.86	0.57
23:S1:101:ARG:HH21	29:S1:602:CLA:HED1	1.70	0.57
2:b1:251:VAL:O	2:b1:255:THR:N	2.38	0.57
20:n1:65:PRO:HB3	20:n1:203:LYS:HG3	1.87	0.57
29:s1:617:CLA:OBD	51:s1:623:NEX:H10	2.05	0.57
4:C:457:MET:SD	5:D:251:ARG:NH1	2.77	0.56
2:b:23:HIS:HB3	29:b:616:CLA:HED2	1.85	0.56
2:b:385:LYS:HB3	15:p:149:ALA:HB3	1.86	0.56
2:b:387:GLU:OE2	15:p:201:ARG:NH1	2.38	0.56
5:d:335:PRO:HB2	6:e:65:LEU:HD11	1.86	0.56
20:n:101:LEU:HD12	29:n:612:CLA:HAB	1.87	0.56
24:y:217:PHE:CD2	29:y:613:CLA:HAB	2.40	0.56
20:N1:193:ALA:HB2	29:N1:610:CLA:HAA2	1.86	0.56
24:Y1:172:GLY:HA2	29:Y1:608:CLA:HAC1	1.86	0.56
20:n1:93:ALA:HB1	20:n1:210:GLY:HA3	1.87	0.56
29:b:608:CLA:H203	12:l:36:ILE:HG13	1.87	0.56
4:c:191:THR:HG23	4:c:219:GLU:HB3	1.88	0.56
14:o:201:LEU:HD11	14:o:247:PRO:HB2	1.87	0.56
29:s:611:CLA:H91	29:s:611:CLA:H142	1.86	0.56
24:y:217:PHE:HD2	29:y:613:CLA:HAB	1.70	0.56
34:A1:414:SPH:H91	47:I1:102:4RF:H40	1.86	0.56
2:B1:57:ARG:NH1	2:B1:331:ASN:OD1	2.38	0.56
6:E1:13:ILE:HG21	44:F1:101:HEM:HAD2	1.87	0.56
2:b1:6:TYR:HB2	40:d1:408:LHG:H382	1.87	0.56
48:g1:601:CHL:H72	40:g1:624:LHG:H191	1.86	0.56
23:s1:51:LYS:HZ3	23:s1:52:TRP:HE1	1.53	0.56
14:O:99:PRO:HA	14:O:149:ILE:HG23	1.86	0.56
21:G:68:LEU:HD23	29:G:602:CLA:H42	1.88	0.56
24:Y:94:ALA:HB1	24:Y:212:GLY:HA3	1.88	0.56
30:a:409:PHO:H3A	29:d:402:CLA:H142	1.86	0.56
4:c:227:TRP:HH2	29:y:614:CLA:HAB	1.70	0.56
29:n:613:CLA:H101	40:n:624:LHG:H142	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:104:GLU:N	14:O1:131:LYS:HZ1	2.03	0.56
2:B1:277:GLN:HB3	25:U1:106:VAL:HG13	1.87	0.56
3:V1:13:PHE:HA	3:V1:16:VAL:HG12	1.87	0.56
4:C1:414:LEU:O	4:C1:418:HIS:ND1	2.37	0.56
5:D1:111:TRP:CZ3	5:D1:167:TRP:HB3	2.40	0.56
5:D1:253:TRP:HB2	5:D1:260:ALA:HB2	1.86	0.56
16:T1:14:LEU:HD23	16:T1:17:ILE:HD12	1.87	0.56
21:G1:70:ALA:HB2	24:Y1:82:THR:HB	1.88	0.56
22:R1:181:PRO:HD2	53:R1:626:ERG:H262	1.87	0.56
23:S1:285:ARG:NH1	23:S1:286:VAL:O	2.38	0.56
48:S1:606:CHL:HHC	48:S1:606:CHL:HBB1	1.87	0.56
29:S1:610:CLA:CAB	49:S1:620:LUT:H32	2.35	0.56
29:Y1:603:CLA:HBB1	48:Y1:609:CHL:H13	1.86	0.56
29:Y1:612:CLA:H12	29:Y1:612:CLA:HED2	1.88	0.56
1:a1:129:ARG:NH2	5:d1:255:GLN:O	2.39	0.56
30:a1:409:PHO:HBD	5:d1:125:PHE:HE2	1.71	0.56
39:c1:524:DGA:HA42	17:w1:93:TRP:HH2	1.70	0.56
7:f1:22:ILE:HG21	44:f1:101:HEM:HBD2	1.88	0.56
23:s1:192:PHE:HA	23:s1:198:LYS:H	1.69	0.56
20:N:122:ILE:HB	20:N:125:LYS:HG2	1.88	0.56
29:C1:512:CLA:H121	32:C1:526:SQD:H351	1.88	0.56
5:D1:230:ASN:OD1	40:D1:410:LHG:O1	2.24	0.56
29:N1:604:CLA:H121	51:N1:623:NEX:H402	1.88	0.56
31:c1:516:BCR:HC41	11:k1:25:LEU:HD21	1.86	0.56
22:r1:195:VAL:HA	22:r1:198:VAL:HB	1.88	0.56
2:B:44:VAL:HG23	2:B:60:MET:HE1	1.88	0.56
2:B:57:ARG:NH2	2:B:335:GLY:O	2.38	0.56
2:b:67:THR:HG21	2:b:80:ILE:HD11	1.87	0.56
4:c:304:THR:HA	4:c:307:VAL:HG22	1.87	0.56
14:o:107:PHE:HB3	14:o:143:MET:HB2	1.88	0.56
8:H1:54:ILE:HG12	45:H1:101:RRX:H20	1.88	0.56
9:I1:13:THR:HG23	17:W1:88:THR:HG21	1.87	0.56
4:c1:105:LEU:HD23	4:c1:108:ILE:HD11	1.87	0.56
4:c1:187:ILE:HD11	4:c1:219:GLU:HG3	1.87	0.56
14:o1:265:GLU:HA	14:o1:297:GLN:HA	1.87	0.56
1:a:24:THR:O	5:d:255:GLN:NE2	2.39	0.56
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.88	0.56
2:b:235:GLU:OE1	2:b:472:ARG:NH1	2.39	0.56
29:B1:615:CLA:H51	32:M1:101:SQD:H141	1.88	0.56
8:H1:44:TRP:O	8:H1:47:THR:OG1	2.23	0.56
14:O1:116:VAL:HG23	14:O1:130:THR:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:124:ARG:O	8:h1:31:ARG:NH1	2.38	0.56
4:c1:213:VAL:O	4:c1:281:ASN:ND2	2.39	0.56
5:d1:191:TRP:CE2	5:d1:197:HIS:HB2	2.41	0.56
1:A:84:PRO:HD3	1:A:173:PRO:HB3	1.87	0.56
32:b:621:SQD:H151	32:m:101:SQD:H122	1.87	0.56
8:h:29:LEU:HD22	22:r:200:VAL:HG12	1.87	0.56
2:B1:11:VAL:HG23	2:B1:12:VAL:HG13	1.86	0.56
4:C1:406:ASN:ND2	37:C1:520:DGD:O5E	2.39	0.56
48:N1:601:CHL:HHC	48:N1:601:CHL:HBB1	1.87	0.56
2:b1:321:LYS:O	5:d1:294:ARG:NH2	2.37	0.56
5:d1:88:SER:HA	8:h1:69:ASN:HD21	1.70	0.56
5:d1:274:VAL:HG22	43:d1:405:PL9:H253	1.88	0.56
15:p:186:LYS:HG2	15:p:206:LYS:HG3	1.88	0.56
4:C1:257:GLU:OE1	4:C1:435:ARG:NH1	2.36	0.56
20:N1:125:LYS:NZ	48:N1:607:CHL:O1A	2.38	0.56
21:G1:40:PHE:HB3	21:G1:61:TYR:HB3	1.88	0.56
1:a1:140:ARG:HH22	40:d1:410:LHG:HC61	1.70	0.56
1:a1:310:ASN:O	15:p1:89:SER:OG	2.24	0.56
2:b1:456:LEU:HD21	33:h1:102:LMG:H192	1.88	0.56
29:b1:605:CLA:HBA1	29:b1:613:CLA:H143	1.87	0.56
15:p1:206:LYS:HD3	15:p1:241:PHE:HB3	1.88	0.56
1:A:84:PRO:HA	1:A:112:TYR:CG	2.41	0.56
14:O:172:LEU:HD23	14:O:178:VAL:HG21	1.88	0.56
20:N:57:PRO:HB2	20:N:60:LEU:HD13	1.88	0.56
1:A1:104:GLU:O	1:A1:108:ASN:ND2	2.39	0.56
3:V1:33:LEU:O	11:K1:39:TRP:NE1	2.36	0.56
4:C1:166:LYS:HB2	29:C1:502:CLA:H203	1.88	0.56
7:F1:33:LEU:HA	7:F1:36:ILE:HG12	1.86	0.56
20:N1:45:ARG:NH1	20:N1:61:THR:O	2.38	0.56
20:N1:94:ARG:NH1	48:N1:608:CHL:OBD	2.31	0.56
20:n1:163:LEU:O	20:n1:167:TYR:N	2.31	0.56
21:g1:216:VAL:HG11	29:g1:613:CLA:HAC2	1.88	0.56
48:s1:601:CHL:HBB1	48:s1:601:CHL:HHC	1.88	0.56
21:G:231:ASP:HB3	21:G:239:ASN:HD21	1.70	0.56
1:a:180:PHE:O	1:a:184:ILE:HG12	2.06	0.56
4:C1:223:GLY:HA2	4:C1:226:ILE:HD12	1.88	0.56
29:a1:406:CLA:HED2	5:d1:198:MET:HG2	1.88	0.56
29:a1:406:CLA:HED1	43:d1:405:PL9:H38	1.88	0.56
2:b1:320:ALA:O	5:d1:292:ASN:ND2	2.39	0.56
2:b1:329:ALA:O	2:b1:332:SER:OG	2.20	0.56
4:c1:14:ARG:O	4:c1:29:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c1:350:ARG:HH21	14:o1:73:LEU:HD13	1.71	0.56
31:C:514:BCR:H17C	40:C:525:LHG:H382	1.88	0.55
4:c:200:TYR:HA	4:c:203:LYS:HE3	1.87	0.55
29:r:610:CLA:H61	49:r:620:LUT:H371	1.88	0.55
14:O1:138:TYR:CE2	17:W1:61:VAL:HG13	2.38	0.55
14:O1:236:GLU:HB2	14:O1:239:ARG:HB2	1.87	0.55
53:R1:626:ERG:O1	53:R1:626:ERG:C2	2.44	0.55
48:Y1:607:CHL:O1A	50:Y1:622:XAT:O3	2.20	0.55
5:d1:48:TRP:CD1	5:d1:52:CYS:HG	2.24	0.55
20:n1:92:HIS:ND1	49:n1:621:LUT:H15	2.21	0.55
29:a:405:CLA:H152	30:a:408:PHO:H3A	1.86	0.55
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.89	0.55
5:d:9:GLN:HG2	5:d:10:GLU:H	1.71	0.55
48:g:608:CHL:HHC	48:g:608:CHL:HBB1	1.88	0.55
2:B1:273:TYR:HE1	5:D1:165:SER:HA	1.71	0.55
29:B1:608:CLA:HBB1	33:B1:622:LMG:H182	1.88	0.55
29:B1:616:CLA:H2	29:B1:617:CLA:HBB2	1.88	0.55
23:S1:225:PRO:HA	23:S1:228:PHE:HB3	1.87	0.55
29:Y1:602:CLA:HBA1	49:Y1:621:LUT:H382	1.87	0.55
2:b1:479:PHE:HA	5:d1:139:ARG:HD3	1.88	0.55
5:d1:308:ASP:HB3	5:d1:311:PHE:HB2	1.88	0.55
14:o1:252:ALA:HA	14:o1:272:SER:HA	1.88	0.55
17:w1:96:TYR:O	17:w1:100:GLN:NE2	2.38	0.55
21:g1:217:GLN:HA	21:g1:220:VAL:HG12	1.87	0.55
22:r1:238:ALA:O	22:r1:242:HIS:ND1	2.39	0.55
29:s1:602:CLA:H72	49:s1:621:LUT:H30	1.88	0.55
5:D:12:ARG:NH2	5:D:20:ASP:OD2	2.39	0.55
15:P:78:TYR:HB3	15:P:87:LEU:HD23	1.87	0.55
2:b:45:PHE:HD1	2:b:60:MET:HE3	1.71	0.55
23:s:132:LYS:NZ	23:s:148:THR:O	2.31	0.55
32:B1:621:SQD:H271	32:M1:101:SQD:H152	1.89	0.55
5:D1:111:TRP:HZ3	5:D1:167:TRP:HB3	1.69	0.55
7:f1:14:ILE:HG22	7:f1:16:THR:HG23	1.88	0.55
48:n1:601:CHL:HED1	40:n1:624:LHG:H271	1.89	0.55
1:A:184:ILE:HG23	1:A:328:MET:HE3	1.89	0.55
4:C:311:ARG:NH2	4:C:377:GLU:OE1	2.40	0.55
33:C:523:LMG:H352	33:C:523:LMG:H152	1.87	0.55
2:b:6:TYR:HE1	2:b:7:ARG:HH21	1.52	0.55
40:l:101:LHG:H282	13:m:22:LEU:HD11	1.86	0.55
21:g:37:ARG:NH1	21:g:60:ASP:OD1	2.39	0.55
1:A1:301:ASN:HD21	4:C1:395:VAL:HB	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C1:501:CLA:H102	29:C1:507:CLA:H92	1.87	0.55
20:n1:143:SER:HB2	23:s1:124:LEU:HD22	1.89	0.55
20:n1:221:PHE:HB3	48:n1:607:CHL:H62	1.88	0.55
2:B:122:LEU:O	8:H:34:ASN:ND2	2.35	0.55
48:N:607:CHL:H191	48:Y:601:CHL:H102	1.89	0.55
2:b:366:PHE:O	2:b:425:GLN:NE2	2.36	0.55
43:d:405:PL9:H111	40:d:409:LHG:H102	1.88	0.55
22:r:79:SER:OG	29:r:602:CLA:O1A	2.25	0.55
1:A1:50:ILE:HD13	32:b1:626:SQD:H282	1.88	0.55
4:C1:95:ASP:OD2	23:S1:285:ARG:NH2	2.40	0.55
6:E1:22:ILE:HG13	6:E1:23:HIS:HD1	1.72	0.55
6:E1:22:ILE:HD11	44:F1:101:HEM:HBA2	1.88	0.55
14:O1:109:MET:CE	14:O1:140:LEU:HD23	2.37	0.55
14:O1:133:LEU:HD11	14:O1:171:LYS:HE3	1.89	0.55
21:G1:198:VAL:HA	21:G1:201:ILE:HG22	1.87	0.55
15:p1:105:ARG:HG3	15:p1:117:TYR:HB3	1.88	0.55
21:g1:130:TYR:HB3	21:g1:136:LEU:HD13	1.88	0.55
20:N:130:ILE:HB	20:N:136:LEU:HD23	1.88	0.55
2:b:152:GLY:O	2:b:156:PHE:HB2	2.06	0.55
6:e:57:THR:HG23	6:e:59:ASP:H	1.70	0.55
8:h:69:ASN:ND2	33:h:102:LMG:O10	2.39	0.55
15:p:201:ARG:HD3	15:p:220:GLN:HE21	1.72	0.55
23:s:83:TYR:OH	40:s:624:LHG:O5	2.19	0.55
6:E1:69:ARG:NH2	8:H1:69:ASN:O	2.27	0.55
21:G1:208:MET:CE	29:G1:602:CLA:HAB	2.36	0.55
29:G1:603:CLA:HBB1	48:G1:607:CHL:H112	1.88	0.55
1:a1:162:PRO:HB3	1:a1:168:PHE:HA	1.87	0.55
29:c1:512:CLA:HMA1	29:c1:513:CLA:H18	1.89	0.55
2:B:256:MET:HG3	2:B:448:ARG:HG3	1.88	0.55
20:N:157:GLN:NE2	48:N:609:CHL:OMC	2.36	0.55
21:G:91:LEU:HB3	29:G:604:CLA:HAB	1.89	0.55
21:G:112:GLU:HG2	21:G:117:LYS:HG3	1.87	0.55
22:r:67:LEU:HD23	22:r:134:ARG:HD2	1.88	0.55
22:r:173:ALA:O	22:r:180:LEU:N	2.37	0.55
24:y:172:GLY:HA2	29:y:608:CLA:HAC1	1.87	0.55
29:B1:603:CLA:H202	33:H1:102:LMG:H391	1.89	0.55
29:Y1:614:CLA:H93	34:Y1:625:SPH:H142	1.88	0.55
4:c1:156:LEU:HD11	29:c1:509:CLA:H61	1.89	0.55
5:d1:325:ILE:HG23	5:d1:329:MET:HE1	1.89	0.55
29:s1:602:CLA:H52	49:s1:621:LUT:H28	1.89	0.55
1:A:305:SER:HA	10:J:41:SER:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B:623:DGD:O5D	37:B:623:DGD:O4D	2.21	0.55
4:C:228:ILE:HG12	29:C:501:CLA:HAB	1.89	0.55
13:m:20:SER:O	13:m:24:ILE:HG12	2.07	0.55
24:Y1:142:ASN:ND2	22:r1:176:LEU:O	2.40	0.55
24:Y1:171:ASN:ND2	24:Y1:173:GLU:OE2	2.39	0.55
4:c1:297:ALA:O	4:c1:301:GLN:N	2.33	0.55
21:g1:128:LEU:HD22	48:g1:606:CHL:HMD2	1.88	0.55
2:B:3:LEU:HG	12:L:9:GLN:HE21	1.72	0.55
6:E:19:TYR:O	6:E:23:HIS:ND1	2.39	0.55
14:O:202:VAL:O	14:O:248:GLY:N	2.40	0.55
39:C1:524:DGA:HBN2	29:Y1:612:CLA:H13	1.89	0.55
14:O1:202:VAL:HG11	14:O1:274:GLN:HE21	1.72	0.55
18:X1:65:VAL:HG13	18:X1:69:LEU:HB2	1.89	0.55
48:N1:606:CHL:HED1	48:N1:606:CHL:H72	1.89	0.55
1:a1:24:THR:O	5:d1:255:GLN:NE2	2.37	0.55
4:c1:267:VAL:HA	4:c1:270:MET:HE3	1.88	0.55
23:s1:256:THR:HG22	23:s1:279:VAL:HG21	1.89	0.55
4:C:94:LEU:HA	23:S:289:LEU:HD13	1.88	0.55
39:C:524:DGA:HBF1	29:Y:612:CLA:H102	1.88	0.55
15:P:182:LYS:NZ	15:P:209:VAL:O	2.40	0.55
33:a:413:LMG:H392	37:c:518:DGD:HA62	1.88	0.55
2:b:358:ARG:HD3	25:u:101:ALA:HB1	1.89	0.55
5:d:195:PRO:HA	5:d:198:MET:HG2	1.88	0.55
2:B1:231:MET:HG2	29:B1:611:CLA:HMC1	1.89	0.55
33:C1:521:LMG:H172	11:K1:27:ILE:HD13	1.88	0.55
48:N1:601:CHL:H161	40:N1:624:LHG:H221	1.89	0.55
21:G1:81:ILE:HD11	29:G1:603:CLA:HBD	1.89	0.55
2:b1:370:LEU:HD12	2:b1:379:ALA:HB3	1.88	0.55
1:A:179:THR:O	1:A:183:MET:HG3	2.07	0.54
33:C:523:LMG:H382	29:Y:614:CLA:H92	1.89	0.54
23:S:135:THR:HB	23:S:138:GLU:HG2	1.89	0.54
2:b:142:HIS:HE1	29:b:611:CLA:H202	1.72	0.54
39:c:524:DGA:HBN1	17:w:90:GLY:HA3	1.89	0.54
5:d:126:MET:HE3	5:d:150:ILE:HD12	1.89	0.54
2:B1:158:VAL:HA	2:B1:165:GLY:HA2	1.89	0.54
2:B1:323:GLY:HA2	5:D1:294:ARG:H	1.71	0.54
4:C1:431:TRP:HD1	4:C1:432:HIS:CE1	2.25	0.54
5:D1:44:ALA:HA	5:D1:114:VAL:HG23	1.89	0.54
5:D1:259:VAL:HG13	16:T1:21:ILE:HD12	1.88	0.54
9:I1:7:PHE:HB2	47:I1:102:4RF:H71	1.88	0.54
21:G1:176:TYR:HB3	29:G1:610:CLA:HED3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y1:92:ILE:HG23	29:Y1:608:CLA:HED3	1.88	0.54
1:a1:142:TRP:HZ2	4:c1:435:ARG:HB2	1.71	0.54
29:b1:609:CLA:H193	29:d1:403:CLA:HAA2	1.89	0.54
33:c1:523:LMG:H351	34:y1:625:SPH:H172	1.89	0.54
20:n1:218:LEU:HD22	49:n1:621:LUT:H403	1.89	0.54
1:A:329:GLU:HG2	5:D:352:LEU:HD21	1.88	0.54
26:A:401:OEX:O2	4:C:345:ARG:NH2	2.40	0.54
4:C:318:SER:HA	14:O:165:TYR:HE1	1.73	0.54
39:C:524:DGA:HAS1	33:W:201:LMG:H361	1.89	0.54
1:a:330:VAL:HG12	5:d:349:GLY:H	1.73	0.54
23:s:113:LEU:HD23	49:s:620:LUT:H402	1.89	0.54
4:C1:309:ASP:OD2	4:C1:328:TYR:OH	2.24	0.54
4:C1:392:LEU:HD13	37:C1:520:DGD:HB51	1.89	0.54
20:N1:226:VAL:HG23	20:N1:227:THR:HG23	1.89	0.54
29:n1:603:CLA:HED1	29:y1:602:CLA:H121	1.89	0.54
22:r1:224:ALA:HB2	22:r1:235:LEU:HD21	1.89	0.54
24:y1:39:SER:OG	24:y1:41:TRP:NE1	2.40	0.54
2:B:149:LEU:HD13	29:B:605:CLA:H192	1.88	0.54
6:E:17:ILE:HG21	10:J:9:ARG:HD3	1.89	0.54
21:G:41:LEU:HB3	21:G:44:PHE:HB2	1.89	0.54
2:b:74:SER:HA	2:b:92:SER:HB2	1.89	0.54
5:d:126:MET:HE1	5:d:147:SER:HA	1.89	0.54
15:p:176:GLU:HB3	15:p:184:TYR:HB2	1.90	0.54
23:s:275:ASN:H	23:s:278:THR:HB	1.72	0.54
29:B1:609:CLA:HBB2	5:D1:150:ILE:HD13	1.89	0.54
20:N1:247:ALA:HB3	50:G1:622:XAT:H193	1.89	0.54
29:c1:501:CLA:HMB2	31:c1:515:BCR:H23C	1.89	0.54
5:d1:192:THR:HA	5:d1:197:HIS:HD1	1.73	0.54
47:i1:101:4RF:H22	47:i1:101:4RF:H77	1.88	0.54
1:A:308:ASP:OD1	1:A:312:ARG:N	2.40	0.54
34:A:414:SPH:H61	9:I:4:LEU:HD22	1.90	0.54
31:C:517:BCR:H391	11:K:36:ALA:HB2	1.88	0.54
7:F:44:ARG:NH2	15:P:71:ASN:O	2.40	0.54
8:H:69:ASN:ND2	33:H:102:LMG:O10	2.41	0.54
14:O:212:ASP:N	14:O:215:GLY:O	2.40	0.54
48:G:605:CHL:HHC	48:G:605:CHL:HBB1	1.90	0.54
24:Y:76:LEU:HD21	29:Y:602:CLA:C4	2.35	0.54
2:b:248:ALA:HB2	29:b:604:CLA:H61	1.89	0.54
2:b:464:PHE:HD2	29:b:612:CLA:HAC2	1.72	0.54
4:c:173:VAL:HG23	4:c:218:LEU:HD13	1.88	0.54
29:c:504:CLA:H202	29:c:508:CLA:H13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:g:609:CHL:HHC	48:g:609:CHL:HBB1	1.90	0.54
1:A1:298:ASN:HB2	4:C1:391:SER:HA	1.89	0.54
5:D1:21:TRP:O	5:D1:26:ARG:NH2	2.36	0.54
5:D1:159:ILE:HG21	5:D1:287:VAL:HG22	1.89	0.54
14:O1:72:TYR:HA	14:O1:75:VAL:HG22	1.90	0.54
20:N1:75:LEU:HD12	49:N1:621:LUT:H221	1.89	0.54
29:b1:615:CLA:H8	32:m1:101:SQD:H281	1.90	0.54
37:b1:623:DGD:O5D	37:b1:623:DGD:O4D	2.25	0.54
8:h1:54:ILE:HG22	45:h1:101:RRX:H20	1.89	0.54
30:A:409:PHO:H3A	29:D:402:CLA:H142	1.88	0.54
22:R:155:GLU:HG3	22:R:264:ALA:HB3	1.89	0.54
40:S:624:LHG:H281	40:S:624:LHG:H141	1.88	0.54
51:s:623:NEX:H193	51:s:623:NEX:H171	1.88	0.54
20:N1:212:LEU:HA	20:N1:215:PHE:HD2	1.71	0.54
4:c1:25:ALA:HA	29:c1:508:CLA:HAA1	1.89	0.54
54:s1:625:LPX:H8A	38:s1:626:3PH:H272	1.89	0.54
40:S:624:LHG:H281	40:S:624:LHG:H121	1.88	0.54
1:A1:63:ILE:HB	4:C1:323:THR:HG21	1.89	0.54
4:C1:318:SER:HA	14:O1:165:TYR:HE1	1.72	0.54
4:C1:437:ARG:NH2	9:I1:27:ASP:OD2	2.41	0.54
29:C1:504:CLA:H43	37:C1:520:DGD:HB32	1.89	0.54
22:R1:142:ARG:HA	22:R1:145:MET:HE2	1.88	0.54
23:S1:109:ARG:NH2	29:S1:610:CLA:O1D	2.35	0.54
1:A:283:ILE:HA	1:A:286:THR:HG22	1.89	0.54
29:B:611:CLA:HAB	45:H:101:RRX:O2	2.08	0.54
14:O:189:GLY:HA2	14:O:198:GLY:HA3	1.89	0.54
4:c:15:ASP:O	4:c:19:THR:OG1	2.25	0.54
17:w:62:ASP:OD1	17:w:64:ARG:NH1	2.40	0.54
21:g:146:LEU:HD21	50:g:622:XAT:H202	1.89	0.54
1:A1:27:ARG:NH2	16:T1:21:ILE:O	2.41	0.54
1:A1:52:PHE:HE1	1:A1:80:GLY:HA3	1.72	0.54
1:A1:208:GLY:HA3	5:D1:208:ALA:HA	1.88	0.54
1:a1:50:ILE:HD13	31:a1:411:BCR:H23C	1.88	0.54
1:a1:204:GLY:HA2	1:a1:278:TRP:HE1	1.72	0.54
5:d1:230:ASN:HD22	5:d1:233:ARG:HG2	1.72	0.54
20:n1:218:LEU:HD21	29:n1:602:CLA:H152	1.88	0.54
29:g1:602:CLA:H52	49:g1:621:LUT:H28	1.89	0.54
22:r1:145:MET:HE1	29:r1:610:CLA:HHC	1.89	0.54
23:s1:111:ALA:O	23:s1:115:ALA:N	2.39	0.54
2:b:474:ILE:O	5:d:134:ARG:NH1	2.41	0.54
5:d:51:GLY:HA2	5:d:55:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C1:27:ASN:HB2	29:C1:508:CLA:HBA1	1.90	0.54
6:E1:19:TYR:O	6:E1:23:HIS:ND1	2.39	0.54
14:O1:265:GLU:HA	14:O1:297:GLN:HA	1.90	0.54
48:S1:608:CHL:HHC	48:S1:608:CHL:HBB1	1.90	0.54
40:c1:525:LHG:H311	40:s1:624:LHG:H101	1.88	0.54
48:n1:606:CHL:HHC	48:n1:606:CHL:HBB1	1.90	0.54
24:y1:130:GLU:HA	24:y1:133:LYS:HD3	1.89	0.54
48:y1:609:CHL:HHC	48:y1:609:CHL:HBB1	1.89	0.54
20:N:88:LEU:O	20:N:92:HIS:ND1	2.37	0.54
24:Y:88:THR:O	24:Y:92:ILE:HG12	2.08	0.54
5:d:73:PHE:HE2	33:d:411:LMG:H321	1.72	0.54
5:d:134:ARG:NH2	5:d:137:ASN:OD1	2.40	0.54
21:g:130:TYR:HB3	21:g:136:LEU:HD13	1.89	0.54
24:y:90:GLU:HG2	24:y:209:ILE:HD11	1.90	0.54
29:y:602:CLA:H142	49:y:621:LUT:H361	1.90	0.54
1:A1:49:ILE:HG12	43:D1:405:PL9:H501	1.90	0.54
29:C1:510:CLA:H72	40:D1:410:LHG:H361	1.90	0.54
11:K1:45:PHE:HB2	47:K1:101:4RF:H70	1.90	0.54
22:R1:238:ALA:O	22:R1:242:HIS:ND1	2.41	0.54
2:b1:382:PRO:HG2	2:b1:385:LYS:HG2	1.90	0.54
29:b1:612:CLA:H92	40:d1:408:LHG:H351	1.90	0.54
29:c1:504:CLA:H43	37:c1:520:DGD:HB32	1.90	0.54
29:g1:602:CLA:HAB	49:g1:621:LUT:C31	2.38	0.54
2:B:371:ILE:HG23	25:U:100:PRO:HB2	1.90	0.54
29:B:608:CLA:H92	33:B:622:LMG:H201	1.90	0.54
24:Y:162:MET:HE1	51:Y:623:NEX:H30	1.91	0.54
1:a:123:VAL:HB	1:a:151:VAL:HG22	1.90	0.54
29:c:501:CLA:H202	31:c:515:BCR:H14C	1.90	0.54
22:r:199:GLU:OE1	22:r:202:ARG:NH2	2.39	0.54
1:A1:156:ALA:HA	1:A1:160:ILE:HB	1.88	0.54
15:P1:193:THR:OG1	15:P1:195:ASP:OD1	2.22	0.54
20:N1:187:PHE:HB3	48:N1:608:CHL:H11	1.89	0.54
21:G1:72:PRO:O	21:G1:76:ALA:N	2.40	0.54
1:a1:116:VAL:HG13	1:a1:158:PHE:HB3	1.90	0.54
37:C:519:DGD:HB22	33:C:521:LMG:H311	1.90	0.53
5:D:172:SER:O	5:D:177:SER:OG	2.22	0.53
14:O:103:LYS:HA	14:O:146:SER:HA	1.90	0.53
4:c:95:ASP:HB3	23:s:287:PRO:HB3	1.90	0.53
23:s:268:LEU:HD22	54:s:625:LPX:H8A	1.89	0.53
4:C1:390:GLY:HA2	4:C1:396:GLY:HA2	1.89	0.53
15:P1:204:LEU:HD23	15:P1:238:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Y1:606:CHL:H101	29:r1:610:CLA:H102	1.90	0.53
29:a1:410:CLA:H8	9:i1:16:VAL:HG11	1.89	0.53
4:c1:334:THR:HG21	14:o1:77:GLY:HA2	1.88	0.53
29:c1:503:CLA:H172	29:c1:510:CLA:HBB2	1.88	0.53
21:g1:65:THR:OG1	49:g1:621:LUT:O23	2.25	0.53
24:y1:139:TYR:HB2	24:y1:146:ILE:HD12	1.89	0.53
2:B:315:ILE:HG23	2:B:443:PHE:HE2	1.73	0.53
2:B:470:GLY:HA2	29:B:609:CLA:HED1	1.91	0.53
29:G:613:CLA:H12	29:G:614:CLA:HED2	1.90	0.53
6:e:68:ASP:OD1	6:e:69:ARG:N	2.39	0.53
15:p:206:LYS:HD3	15:p:241:PHE:HD2	1.73	0.53
1:A1:104:GLU:OE1	1:A1:108:ASN:ND2	2.41	0.53
1:A1:131:TRP:CZ3	29:C1:505:CLA:HAA2	2.43	0.53
4:C1:187:ILE:HG13	4:C1:222:ILE:HG13	1.90	0.53
1:a1:92:HIS:NE2	4:c1:348:ASP:OD2	2.42	0.53
5:d1:95:PRO:O	5:d1:98:GLN:NE2	2.37	0.53
24:y1:184:TYR:HB3	29:y1:610:CLA:HED3	1.89	0.53
15:P:99:VAL:HB	15:P:102:ILE:HG13	1.89	0.53
48:S:608:CHL:HHC	48:S:608:CHL:HBB1	1.90	0.53
1:a:274:PHE:HD1	32:a:412:SQD:H112	1.73	0.53
2:b:256:MET:HA	2:b:263:THR:HG21	1.90	0.53
38:t:101:3PH:H2D2	38:t:101:3PH:H371	1.91	0.53
29:g:603:CLA:H52	29:y:603:CLA:H52	1.90	0.53
2:B1:346:PHE:HE2	2:B1:356:VAL:HG23	1.72	0.53
5:D1:156:VAL:HA	5:D1:286:VAL:HG11	1.90	0.53
40:D1:410:LHG:O1	40:D1:410:LHG:O3	2.26	0.53
26:a1:401:OEX:O4	4:c1:345:ARG:NH2	2.41	0.53
29:b1:607:CLA:OBD	37:b1:623:DGD:O3D	2.26	0.53
29:b1:617:CLA:H202	22:r1:189:TRP:HA	1.88	0.53
3:v1:21:LEU:HA	3:v1:24:VAL:HB	1.91	0.53
5:d1:103:ARG:HH21	6:e1:76:VAL:HG22	1.73	0.53
48:y1:606:CHL:HHC	48:y1:606:CHL:HBB1	1.91	0.53
40:D:409:LHG:H182	16:T:17:ILE:HD11	1.90	0.53
22:R:220:PRO:HB3	24:y:191:PRO:HB3	1.89	0.53
2:b:23:HIS:ND1	29:b:616:CLA:OBD	2.42	0.53
22:r:238:ALA:O	22:r:242:HIS:ND1	2.42	0.53
29:y:614:CLA:H13	55:y:626:PTY:H221	1.91	0.53
40:G1:624:LHG:H272	40:G1:624:LHG:H112	1.89	0.53
1:a1:194:MET:HG2	1:a1:300:PHE:HB2	1.91	0.53
4:c1:304:THR:HG21	4:c1:384:MET:HE2	1.90	0.53
31:c1:516:BCR:H292	11:k1:37:PHE:HE2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:c1:520:DGD:HG31	10:j1:34:SER:HB2	1.90	0.53
6:e1:51:ARG:HB2	6:e1:54:GLU:HG2	1.91	0.53
6:e1:75:GLN:HG2	6:e1:79:LEU:HD13	1.90	0.53
22:r1:77:HIS:HB3	22:r1:80:SER:HB3	1.91	0.53
55:y1:626:PTY:H381	55:y1:626:PTY:H192	1.91	0.53
20:N:196:PRO:HA	20:N:199:PHE:HB3	1.90	0.53
23:S:204:PHE:HA	23:S:207:LEU:HD12	1.91	0.53
29:b:603:CLA:H191	5:d:158:LEU:HB3	1.89	0.53
29:b:615:CLA:H51	32:m:101:SQD:H141	1.91	0.53
20:n:228:GLY:HA3	24:y:260:PRO:HD3	1.90	0.53
23:s:220:ASN:ND2	23:s:223:ASP:OD2	2.36	0.53
32:a1:412:SQD:O8	5:d1:230:ASN:ND2	2.41	0.53
32:a1:412:SQD:H251	40:d1:410:LHG:H111	1.90	0.53
2:b1:174:LEU:HD21	2:b1:309:LEU:HD13	1.91	0.53
47:i1:101:4RF:H8	47:i1:101:4RF:H46	1.90	0.53
23:s1:260:PRO:HA	23:s1:263:ASN:HB2	1.91	0.53
14:O:172:LEU:HB2	14:O:176:GLU:HG2	1.91	0.53
2:b:256:MET:HG3	2:b:448:ARG:HG3	1.89	0.53
5:d:79:SER:HA	5:d:172:SER:HB3	1.90	0.53
5:d:161:PRO:HB3	5:d:170:ALA:HB2	1.91	0.53
29:A1:405:CLA:H201	40:D1:409:LHG:H161	1.91	0.53
9:I1:9:TYR:HD2	17:W1:81:LEU:HD11	1.73	0.53
20:N1:130:ILE:HG21	20:N1:150:ILE:HD13	1.91	0.53
48:G1:609:CHL:H193	29:Y1:603:CLA:H141	1.90	0.53
23:S1:275:ASN:ND2	23:S1:278:THR:OG1	2.42	0.53
24:Y1:213:ARG:NH2	29:Y1:602:CLA:O2D	2.38	0.53
30:a1:409:PHO:H161	5:d1:173:PHE:HD1	1.73	0.53
29:b1:608:CLA:H152	33:b1:622:LMG:H332	1.91	0.53
20:n1:103:MET:HG2	20:n1:220:PHE:CD2	2.44	0.53
21:g1:61:TYR:OH	40:g1:624:LHG:O5	2.21	0.53
48:g1:607:CHL:H202	48:g1:609:CHL:H62	1.89	0.53
29:g1:610:CLA:H2	49:g1:620:LUT:H28	1.90	0.53
5:D:336:HIS:HA	6:E:65:LEU:HD21	1.91	0.53
15:P:91:TRP:CD1	15:P:108:ASP:HA	2.43	0.53
1:a:334:ARG:HG3	14:o:211:LEU:HD11	1.91	0.53
15:p:88:PRO:HG3	15:p:237:VAL:HG21	1.90	0.53
4:C1:238:TRP:HB2	34:Y1:625:SPH:H131	1.91	0.53
40:D1:409:LHG:H162	40:D1:409:LHG:H292	1.89	0.53
15:P1:202:HIS:N	15:P1:221:ALA:O	2.32	0.53
23:S1:80:ALA:O	23:S1:101:ARG:NH2	2.41	0.53
29:S1:610:CLA:H51	49:S1:620:LUT:H373	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:441:GLY:HA2	14:o1:230:ALA:HB3	1.91	0.53
4:c1:335:GLY:HA3	14:o1:82:ASN:HB2	1.90	0.53
14:o1:279:GLU:HB3	14:o1:282:ALA:HB3	1.89	0.53
15:p1:95:ASP:OD1	15:p1:97:LYS:NZ	2.41	0.53
24:y1:240:HIS:CG	29:y1:613:CLA:HAA2	2.43	0.53
29:B:609:CLA:H193	29:D:403:CLA:HAA2	1.90	0.53
13:M:20:SER:O	13:M:24:ILE:HG12	2.09	0.53
21:G:121:GLN:HB2	21:G:128:LEU:HD12	1.91	0.53
2:b:341:LEU:HD21	2:b:431:GLU:HB2	1.90	0.53
5:d:152:VAL:HG22	29:d:402:CLA:HED1	1.90	0.53
24:y:240:HIS:CG	29:y:613:CLA:HAA2	2.44	0.53
2:B1:257:TRP:HB2	2:B1:452:THR:HG21	1.91	0.53
38:T1:101:3PH:H2F2	38:T1:101:3PH:H391	1.91	0.53
17:W1:89:LEU:HB3	33:W1:201:LMG:H401	1.91	0.53
20:N1:122:ILE:HG22	20:N1:125:LYS:H	1.72	0.53
22:R1:198:VAL:HG23	51:R1:622:NEX:H14	1.90	0.53
1:a1:174:LEU:HB3	30:a1:408:PHO:H171	1.90	0.53
4:c1:128:LEU:HD13	4:c1:135:PHE:HB3	1.91	0.53
40:c1:525:LHG:H122	29:s1:611:CLA:HBB2	1.90	0.53
6:e1:30:LEU:HD11	44:f1:101:HEM:HAB	1.90	0.53
24:y1:220:LEU:HD23	29:y1:613:CLA:HAC1	1.90	0.53
2:B:7:ARG:HG2	29:B:612:CLA:HED2	1.90	0.53
2:B:11:VAL:HG23	2:B:12:VAL:HG13	1.90	0.53
2:B:366:PHE:HB3	2:B:425:GLN:HE21	1.74	0.53
48:N:601:CHL:H202	48:G:607:CHL:H13	1.91	0.53
48:G:609:CHL:HBB1	48:G:609:CHL:HHC	1.90	0.53
24:Y:76:LEU:HD22	29:Y:602:CLA:H42	1.88	0.53
1:a:84:PRO:HA	1:a:112:TYR:CG	2.44	0.53
6:e:13:ILE:HG23	6:e:14:LEU:HD12	1.91	0.53
20:n:93:ALA:HB1	20:n:210:GLY:HA3	1.91	0.53
21:g:199:LYS:HE3	29:g:611:CLA:HED2	1.91	0.53
24:y:94:ALA:HB1	24:y:212:GLY:HA3	1.89	0.53
2:B1:115:TRP:CD2	31:B1:618:BCR:H291	2.44	0.53
2:B1:246:PHE:HB3	2:B1:462:PHE:HB2	1.91	0.53
29:B1:616:CLA:H171	29:R1:609:CLA:H71	1.91	0.53
5:D1:258:GLY:HA3	16:T1:21:ILE:HD11	1.91	0.53
17:W1:76:VAL:HG13	17:W1:81:LEU:HB3	1.91	0.53
29:G1:613:CLA:H101	40:G1:624:LHG:H132	1.91	0.53
1:a1:121:LEU:HD21	29:c1:505:CLA:H162	1.90	0.53
1:a1:314:LEU:HD22	6:e1:55:TYR:CE2	2.44	0.53
5:d1:22:LEU:HB3	5:d1:31:GLY:HA2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:n1:602:CLA:H52	49:n1:621:LUT:H30	1.90	0.53
22:r1:138:VAL:O	22:r1:142:ARG:N	2.39	0.53
23:s1:125:GLN:OE1	23:s1:134:GLY:N	2.40	0.53
24:y1:172:GLY:HA2	29:y1:608:CLA:HAC1	1.91	0.53
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.44	0.53
2:B:185:TRP:HB2	29:B:602:CLA:HED2	1.91	0.53
20:N:55:ASN:ND2	21:G:161:ALA:O	2.35	0.53
48:N:607:CHL:H121	48:N:609:CHL:H121	1.91	0.53
40:G:624:LHG:HC81	50:Y:622:XAT:H371	1.89	0.53
20:n:109:LEU:HD21	23:s:156:PHE:HE1	1.74	0.53
24:y:228:VAL:HG12	24:y:256:PHE:HE2	1.73	0.53
1:A1:42:LEU:HD23	1:A1:45:ILE:HD11	1.91	0.53
1:A1:219:VAL:HG22	1:A1:246:TYR:CZ	2.44	0.53
7:F1:26:ALA:O	7:F1:29:THR:OG1	2.27	0.53
12:L1:20:TRP:HZ3	40:L1:101:LHG:H172	1.73	0.53
21:G1:122:ILE:HG21	21:G1:142:ILE:HD12	1.91	0.53
29:R1:604:CLA:O1A	51:R1:622:NEX:O23	2.22	0.53
23:S1:209:LYS:HG3	23:S1:210:LEU:HG	1.91	0.53
48:S1:607:CHL:HHC	48:S1:607:CHL:HBB1	1.92	0.53
22:r1:245:LEU:HD22	49:r1:620:LUT:H202	1.90	0.53
23:s1:136:TRP:NE1	23:s1:253:SER:OG	2.39	0.53
4:C1:330:MET:HG2	4:C1:340:GLY:HA2	1.91	0.52
20:N1:92:HIS:HD2	49:N1:621:LUT:H201	1.73	0.52
29:N1:602:CLA:H92	29:N1:603:CLA:HMA1	1.91	0.52
1:a1:145:VAL:HG11	40:d1:410:LHG:H302	1.91	0.52
1:a1:340:PRO:HB2	15:p1:224:LYS:HD3	1.91	0.52
2:b1:54:PRO:HD2	2:b1:57:ARG:HG3	1.90	0.52
5:d1:103:ARG:NH1	5:d1:106:GLN:OE1	2.42	0.52
5:d1:230:ASN:HD21	5:d1:232:PHE:HB2	1.74	0.52
48:r1:607:CHL:HBB1	48:r1:607:CHL:HHC	1.90	0.52
24:y1:68:ASP:N	24:y1:68:ASP:OD1	2.40	0.52
24:y1:108:GLU:HG2	24:y1:112:LYS:HE2	1.91	0.52
4:C:393:ASN:HB2	4:C:395:VAL:HG23	1.90	0.52
48:N:606:CHL:HHC	48:N:606:CHL:HBB1	1.91	0.52
1:a:85:THR:HA	1:a:109:GLY:HA3	1.92	0.52
39:c:524:DGA:HBE2	33:w:201:LMG:H371	1.91	0.52
40:d:408:LHG:H352	40:d:408:LHG:H102	1.91	0.52
22:r:180:LEU:HD22	53:r:626:ERG:H273	1.91	0.52
4:C1:309:ASP:HA	4:C1:312:LEU:HB2	1.91	0.52
20:N1:191:GLY:O	20:N1:193:ALA:N	2.43	0.52
4:c1:30:LEU:HA	4:c1:33:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r1:86:GLN:O	22:r1:105:GLU:N	2.39	0.52
1:A:170:ASP:OD2	4:C:345:ARG:NH1	2.29	0.52
1:a:244:GLU:HG2	1:a:248:ILE:HD11	1.92	0.52
2:b:51:VAL:HG23	2:b:308:LYS:HG2	1.90	0.52
2:b:433:ASP:OD2	2:b:436:THR:OG1	2.26	0.52
4:c:452:GLU:OE2	5:d:248:THR:OG1	2.26	0.52
1:A1:170:ASP:OD2	4:C1:345:ARG:NH1	2.42	0.52
2:B1:160:GLY:HA3	2:B1:180:PRO:HB3	1.90	0.52
2:B1:340:TRP:CD1	2:B1:342:GLY:H	2.26	0.52
4:C1:109:SER:HA	31:C1:514:BCR:H16C	1.90	0.52
5:D1:148:ALA:HB2	5:D1:276:VAL:HG23	1.90	0.52
29:N1:612:CLA:HAB	49:N1:620:LUT:C35	2.39	0.52
21:G1:102:LEU:HB3	21:G1:108:VAL:HB	1.91	0.52
2:b1:57:ARG:NH2	2:b1:335:GLY:O	2.42	0.52
2:b1:460:LEU:HB3	5:d1:280:TRP:HZ3	1.74	0.52
3:v1:9:LEU:HD12	3:v1:12:LEU:HD12	1.92	0.52
5:D:343:GLU:HB3	15:P:112:ALA:HB3	1.92	0.52
29:R:609:CLA:H62	52:R:625:LMT:H101	1.91	0.52
2:b:442:VAL:O	2:b:444:ARG:NH1	2.43	0.52
1:A1:190:HIS:NE2	1:A1:293:MET:O	2.42	0.52
12:L1:15:ARG:HD3	32:b1:621:SQD:H101	1.90	0.52
29:Y1:604:CLA:H172	22:r1:153:VAL:HG21	1.90	0.52
48:Y1:605:CHL:HBB1	48:Y1:605:CHL:HHC	1.91	0.52
1:a1:325:ASN:O	1:a1:329:GLU:HG3	2.09	0.52
30:a1:409:PHO:H43	29:d1:402:CLA:H13	1.91	0.52
2:b1:69:LEU:HD21	29:b1:604:CLA:HED2	1.91	0.52
4:c1:461:ASP:HA	5:d1:251:ARG:HD2	1.90	0.52
29:c1:513:CLA:H101	31:c1:514:BCR:H21C	1.91	0.52
31:c1:516:BCR:H21C	11:k1:34:LEU:HD22	1.90	0.52
5:d1:213:ILE:HG21	43:d1:405:PL9:H121	1.92	0.52
17:w1:76:VAL:HG23	17:w1:81:LEU:HD23	1.91	0.52
20:n1:106:PRO:O	20:n1:110:GLN:NE2	2.35	0.52
1:A:37:MET:HE3	1:A:41:LEU:HD12	1.92	0.52
1:A:57:PRO:HB2	1:A:66:PRO:HB2	1.92	0.52
4:C:147:ASN:HD21	32:C:526:SQD:H3	1.75	0.52
4:C:244:PRO:HA	29:C:506:CLA:HED3	1.91	0.52
1:a:94:TYR:N	1:a:113:GLN:OE1	2.40	0.52
1:A1:176:ILE:HD11	43:D1:405:PL9:H452	1.90	0.52
20:N1:247:ALA:HB1	50:G1:622:XAT:H161	1.90	0.52
29:G1:613:CLA:H12	29:G1:614:CLA:HED2	1.90	0.52
48:n1:601:CHL:H202	48:g1:607:CHL:H152	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:y1:605:CHL:HHC	48:y1:605:CHL:HBB1	1.91	0.52
4:C:285:TYR:O	4:C:411:ARG:NH2	2.37	0.52
20:N:90:LEU:HD23	20:N:181:LEU:HB3	1.91	0.52
48:G:601:CHL:HHC	48:G:601:CHL:HBB1	1.92	0.52
23:S:176:LEU:HA	23:S:179:VAL:HG22	1.92	0.52
24:Y:86:TYR:HA	24:Y:89:ILE:HG22	1.92	0.52
1:a:226:GLU:OE1	5:d:265:ARG:NH2	2.41	0.52
15:p:113:VAL:HG22	15:p:201:ARG:HE	1.75	0.52
21:g:157:GLU:OE1	21:g:160:ARG:NH2	2.33	0.52
31:C1:514:BCR:H332	19:Z1:54:VAL:HG23	1.92	0.52
5:D1:102:THR:HG23	5:D1:103:ARG:HD3	1.91	0.52
14:O1:203:PRO:HB3	15:P1:156:SER:HB2	1.92	0.52
21:G1:237:THR:HG23	21:G1:238:VAL:HG13	1.90	0.52
24:Y1:106:THR:HA	24:Y1:109:LEU:HB3	1.92	0.52
29:a1:410:CLA:H62	9:i1:13:THR:HA	1.91	0.52
40:d1:408:LHG:H142	40:d1:408:LHG:H332	1.92	0.52
14:o1:166:ALA:HB3	14:o1:182:PHE:HB3	1.92	0.52
20:n1:136:LEU:HD22	48:n1:606:CHL:HMD1	1.91	0.52
1:A:140:ARG:HB2	5:D:220:ASN:HA	1.91	0.52
2:B:128:THR:HG23	2:B:130:LYS:H	1.75	0.52
4:C:166:LYS:HD3	29:C:502:CLA:H162	1.92	0.52
8:H:44:TRP:O	8:H:47:THR:OG1	2.22	0.52
1:a:195:HIS:CD2	1:a:197:PHE:HB2	2.43	0.52
4:c:270:MET:HE1	29:c:507:CLA:H11	1.90	0.52
48:g:606:CHL:HBB1	48:g:606:CHL:HHC	1.91	0.52
2:B1:156:PHE:O	2:B1:163:GLY:N	2.37	0.52
2:B1:413:ASP:OD2	2:B1:416:THR:OG1	2.28	0.52
4:C1:338:ILE:HG21	4:C1:347:TRP:HB2	1.91	0.52
21:G1:37:ARG:NH2	21:G1:60:ASP:OD1	2.42	0.52
29:R1:610:CLA:H52	49:R1:620:LUT:H30	1.91	0.52
29:b1:610:CLA:C3	29:b1:611:CLA:HBB2	2.39	0.52
21:g1:34:GLY:O	21:g1:37:ARG:NH1	2.43	0.52
2:B:137:LYS:HZ2	8:H:36:GLU:HB2	1.75	0.52
40:C:525:LHG:H302	40:S:624:LHG:HC81	1.91	0.52
33:c:521:LMG:O4	33:c:521:LMG:O5	2.26	0.52
5:d:301:GLN:HG3	5:d:311:PHE:HE2	1.74	0.52
31:d:404:BCR:H21C	33:d:411:LMG:H362	1.92	0.52
14:o:149:ILE:HA	14:o:155:VAL:HG12	1.92	0.52
15:p:78:TYR:HB3	15:p:87:LEU:HD23	1.91	0.52
29:R1:603:CLA:H71	52:R1:625:LMT:H72	1.91	0.52
23:S1:228:PHE:HA	23:S1:231:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:221:PRO:HD3	29:b1:610:CLA:HED3	1.91	0.52
4:c1:357:LEU:HD13	4:c1:367:LYS:HG2	1.92	0.52
31:c1:515:BCR:H332	9:i1:20:ILE:HG12	1.92	0.52
6:e1:60:ARG:HH12	6:e1:79:LEU:HA	1.75	0.52
7:F:43:GLN:HA	10:J:37:GLY:HA2	1.91	0.52
1:a:195:HIS:HD2	1:a:197:PHE:HB2	1.74	0.52
1:a:308:ASP:OD1	1:a:312:ARG:N	2.43	0.52
10:j:28:ALA:HA	39:j:101:DGA:HA71	1.91	0.52
22:r:160:VAL:HG21	22:r:168:VAL:HG21	1.92	0.52
2:B1:221:PRO:HG2	8:H1:40:VAL:HG12	1.92	0.52
2:B1:321:LYS:HB3	2:B1:443:PHE:HD2	1.75	0.52
29:B1:615:CLA:H2	32:B1:621:SQD:H261	1.92	0.52
5:D1:162:LEU:HD13	33:H1:102:LMG:H172	1.91	0.52
1:a1:329:GLU:O	1:a1:332:HIS:ND1	2.40	0.52
4:c1:438:ALA:O	4:c1:442:GLY:N	2.41	0.52
10:j1:28:ALA:HA	39:j1:101:DGA:HA71	1.92	0.52
21:g1:224:GLY:O	21:g1:228:ASN:N	2.43	0.52
25:u1:105:THR:HB	25:u1:108:GLU:HG3	1.91	0.52
29:B:616:CLA:H172	8:H:26:LEU:HD21	1.92	0.52
14:O:111:PRO:HD2	14:O:138:TYR:CD1	2.45	0.52
24:Y:99:LEU:HB3	29:Y:604:CLA:HAB	1.91	0.52
33:b:622:LMG:HC1	38:b:624:3PH:H11	1.92	0.52
3:v:7:LEU:HA	3:v:10:VAL:HG12	1.90	0.52
12:l:15:ARG:NH2	16:t:25:GLU:OE2	2.43	0.52
22:r:145:MET:SD	29:r:610:CLA:HAB	2.50	0.52
14:O1:116:VAL:HG11	14:O1:172:LEU:HD21	1.92	0.52
22:R1:169:GLU:OE2	22:R1:174:GLN:NE2	2.43	0.52
1:a1:303:ASN:O	4:c1:403:ASN:ND2	2.41	0.52
29:b1:604:CLA:H201	8:h1:58:ALA:HB2	1.91	0.52
29:b1:610:CLA:HMA2	29:b1:611:CLA:C2C	2.40	0.52
14:o1:266:ILE:O	14:o1:296:GLY:N	2.39	0.52
20:n1:65:PRO:HA	20:n1:204:VAL:HG22	1.92	0.52
20:n1:103:MET:HE1	20:n1:123:TRP:CG	2.45	0.52
48:n1:605:CHL:HED3	23:s1:124:LEU:HD21	1.92	0.52
48:n1:605:CHL:HHC	48:n1:605:CHL:HBB1	1.91	0.52
23:s1:141:ALA:HB2	48:s1:607:CHL:HED2	1.91	0.52
29:y1:614:CLA:HBA1	55:y1:626:PTY:H362	1.91	0.52
6:E:62:ASP:OD1	6:E:63:ALA:N	2.43	0.51
31:c:516:BCR:H10C	19:z:20:VAL:HG11	1.92	0.51
1:A1:61:ASP:HB3	1:A1:63:ILE:HG12	1.92	0.51
1:A1:100:ALA:N	1:A1:104:GLU:OE2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:283:ILE:HA	1:A1:286:THR:HG22	1.92	0.51
2:B1:456:LEU:HD11	33:H1:102:LMG:H211	1.91	0.51
31:C1:515:BCR:H332	9:I1:20:ILE:HG22	1.92	0.51
2:b1:363:PHE:HA	5:d1:326:ARG:HH12	1.75	0.51
4:c1:425:PHE:HE1	29:c1:508:CLA:HAB	1.73	0.51
40:c1:525:LHG:O8	40:s1:624:LHG:O2	2.28	0.51
5:d1:306:ALA:HA	14:o1:216:ARG:HH12	1.75	0.51
33:d1:411:LMG:H232	33:d1:411:LMG:H352	1.92	0.51
23:s1:219:LEU:HB2	49:s1:620:LUT:H222	1.91	0.51
14:O:120:ASP:OD1	2:b:84:THR:OG1	2.27	0.51
21:G:40:PHE:HB3	21:G:61:TYR:HB3	1.91	0.51
29:S:602:CLA:H71	29:S:603:CLA:HMD1	1.91	0.51
3:v:26:LEU:HG	19:z:25:VAL:HG12	1.91	0.51
15:p:119:ILE:HG12	15:p:121:GLN:HG3	1.92	0.51
18:x:65:VAL:HA	18:x:69:LEU:HD12	1.92	0.51
48:g:607:CHL:HMA2	48:g:607:CHL:H2	1.93	0.51
23:s:108:ALA:HB1	23:s:239:GLY:HA3	1.92	0.51
1:A1:139:MET:HE1	5:D1:221:THR:HG23	1.91	0.51
38:B1:624:3PH:H251	16:t1:1:MET:HE1	1.92	0.51
5:D1:33:SER:OG	5:D1:124:GLY:O	2.25	0.51
5:D1:225:ASP:HB2	5:D1:234:ALA:HB1	1.92	0.51
19:Z1:12:LEU:HA	19:Z1:15:VAL:HG12	1.92	0.51
23:S1:83:TYR:OH	40:S1:624:LHG:O5	2.25	0.51
4:c1:101:VAL:HG13	31:c1:514:BCR:H313	1.91	0.51
22:r1:149:LEU:HD21	49:r1:620:LUT:H35	1.92	0.51
2:B:135:LEU:HD23	2:B:138:ILE:HD12	1.92	0.51
5:D:85:LEU:HD13	6:E:69:ARG:HG3	1.92	0.51
29:c:505:CLA:H41	31:c:515:BCR:H343	1.93	0.51
5:d:88:SER:O	5:d:167:TRP:NE1	2.40	0.51
48:n:607:CHL:HED1	24:y:254:THR:HG23	1.92	0.51
29:n:613:CLA:H121	50:g:622:XAT:H34	1.92	0.51
21:g:85:HIS:CD2	49:g:621:LUT:H15	2.45	0.51
2:B1:307:GLU:OE2	2:B1:340:TRP:N	2.43	0.51
4:C1:38:LEU:HD11	29:C1:513:CLA:HBB1	1.91	0.51
5:D1:148:ALA:HB1	5:D1:279:LEU:HB2	1.92	0.51
2:b1:331:ASN:O	2:b1:439:SER:OG	2.27	0.51
4:c1:265:ALA:HB2	4:c1:429:HIS:ND1	2.25	0.51
8:h1:66:GLU:HB2	8:h1:71:SER:HB2	1.91	0.51
48:g1:601:CHL:HHC	48:g1:601:CHL:HBB1	1.91	0.51
29:r1:602:CLA:CAB	50:r1:621:XAT:H32	2.39	0.51
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:458:PHE:HB3	29:B:605:CLA:HBC2	1.92	0.51
4:C:198:PHE:HA	4:C:201:ILE:HG12	1.91	0.51
29:G:602:CLA:CAB	49:G:621:LUT:H32	2.39	0.51
2:b:272:ARG:HH21	5:d:165:SER:HB2	1.75	0.51
4:C1:50:PHE:HE2	11:K1:29:PRO:HD3	1.74	0.51
5:D1:161:PRO:HB3	5:D1:170:ALA:HB2	1.92	0.51
48:S1:601:CHL:HBB1	48:S1:601:CHL:HHC	1.92	0.51
48:g1:605:CHL:HBD	48:g1:605:CHL:HBA1	1.91	0.51
24:y1:82:THR:O	24:y1:86:TYR:N	2.42	0.51
3:V:7:LEU:HA	3:V:10:VAL:HG12	1.91	0.51
1:a:163:ILE:HD11	37:c:518:DGD:HA31	1.91	0.51
1:a:330:VAL:HG11	5:d:348:ARG:HG3	1.92	0.51
20:n:202:LEU:HD12	20:n:205:LYS:HD2	1.93	0.51
48:n:606:CHL:HBB2	48:n:607:CHL:HAB	1.92	0.51
5:D1:141:TYR:HA	5:D1:144:ILE:HD12	1.92	0.51
29:S1:602:CLA:CAB	49:S1:621:LUT:H32	2.41	0.51
1:a1:310:ASN:HD22	6:e1:56:PHE:HZ	1.59	0.51
4:C:441:ALA:HA	9:I:31:ASN:HD22	1.75	0.51
29:b:615:CLA:H2	32:b:621:SQD:H262	1.93	0.51
29:b:616:CLA:H2	29:b:617:CLA:CBB	2.41	0.51
1:A1:174:LEU:HD22	30:A1:408:PHO:H151	1.92	0.51
1:A1:335:ASN:HA	5:D1:350:ASN:ND2	2.25	0.51
4:C1:193:ASN:O	4:C1:197:ILE:HG12	2.11	0.51
4:C1:203:LYS:HD2	4:C1:209:ASP:HB3	1.92	0.51
4:C1:282:ASN:OD1	37:C1:518:DGD:O5E	2.24	0.51
5:D1:306:ALA:O	14:O1:239:ARG:NE	2.43	0.51
31:D1:404:BCR:H21C	33:D1:411:LMG:H371	1.93	0.51
13:M1:31:ALA:HB2	13:m1:28:LYS:HE2	1.93	0.51
1:a1:173:PRO:HB2	1:a1:178:GLY:HA3	1.92	0.51
14:o1:172:LEU:HD12	14:o1:173:PRO:HD2	1.92	0.51
24:y1:95:ARG:NH1	29:y1:608:CLA:OBD	2.41	0.51
1:A:297:LEU:HD22	4:C:416:THR:HG21	1.92	0.51
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.46	0.51
4:C:304:THR:O	4:C:308:ARG:HG2	2.10	0.51
29:R:602:CLA:CBB	50:R:621:XAT:H32	2.41	0.51
5:d:88:SER:OG	6:e:69:ARG:NH1	2.43	0.51
14:o:99:PRO:HA	14:o:149:ILE:HB	1.92	0.51
20:n:196:PRO:HA	20:n:199:PHE:HB3	1.93	0.51
29:n:613:CLA:H91	40:n:624:LHG:H311	1.92	0.51
29:B1:603:CLA:H203	5:D1:154:VAL:HG13	1.92	0.51
29:B1:608:CLA:H92	33:B1:622:LMG:H201	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D1:276:VAL:HG13	40:D1:408:LHG:H261	1.93	0.51
40:S1:624:LHG:H292	40:S1:624:LHG:HC91	1.92	0.51
1:a1:85:THR:HA	1:a1:109:GLY:HA3	1.92	0.51
1:a1:204:GLY:HA2	1:a1:278:TRP:NE1	2.26	0.51
2:b1:389:LYS:HE2	15:p1:146:GLY:HA2	1.93	0.51
20:n1:211:ARG:NH2	29:n1:602:CLA:O2D	2.44	0.51
29:n1:610:CLA:H2	49:n1:620:LUT:H28	1.92	0.51
29:g1:602:CLA:H91	29:y1:603:CLA:H102	1.93	0.51
22:r1:188:ILE:HG12	48:r1:607:CHL:HBC1	1.92	0.51
23:s1:101:ARG:HA	23:s1:104:GLU:HB3	1.93	0.51
29:G:603:CLA:HMC2	48:G:607:CHL:H122	1.91	0.51
48:Y:609:CHL:HHC	48:Y:609:CHL:HBB1	1.93	0.51
1:a:63:ILE:HB	4:c:323:THR:HG21	1.93	0.51
2:b:30:VAL:HG12	29:b:606:CLA:HHD	1.92	0.51
2:b:36:ALA:HB1	38:b:624:3PH:H2C1	1.92	0.51
4:c:461:ASP:OD1	5:d:251:ARG:NE	2.38	0.51
31:c:517:BCR:H391	11:k:36:ALA:HB2	1.93	0.51
33:c:523:LMG:HC5	29:y:611:CLA:HMA3	1.92	0.51
20:n:46:ASN:C	20:n:46:ASN:ND2	2.68	0.51
48:n:606:CHL:HED1	48:n:606:CHL:H72	1.93	0.51
24:y:116:PRO:HD2	24:y:141:GLY:HA3	1.93	0.51
1:A1:103:ASP:OD1	32:b1:626:SQD:O2	2.29	0.51
2:B1:119:ASP:OD1	2:B1:124:ARG:NH2	2.43	0.51
48:N1:607:CHL:H171	48:N1:609:CHL:H71	1.93	0.51
23:S1:267:HIS:ND1	23:S1:274:TYR:O	2.37	0.51
29:c1:506:CLA:H101	29:c1:507:CLA:H172	1.91	0.51
31:c1:517:BCR:H342	19:z1:12:LEU:HG	1.92	0.51
10:j1:24:ILE:O	10:j1:28:ALA:N	2.39	0.51
48:g1:605:CHL:HHC	48:g1:605:CHL:HBB1	1.91	0.51
29:y1:614:CLA:H71	55:y1:626:PTY:H391	1.93	0.51
29:C:501:CLA:H201	29:C:506:CLA:H12	1.92	0.51
21:G:77:ARG:O	21:G:81:ILE:HG12	2.10	0.51
29:G:603:CLA:H52	29:Y:603:CLA:H52	1.92	0.51
1:a:60:ILE:HD12	1:a:84:PRO:HD2	1.93	0.51
29:s:614:CLA:HBB2	54:s:625:LPX:H7	1.91	0.51
1:A1:200:PHE:HE1	37:C1:520:DGD:HAW1	1.76	0.51
2:B1:149:LEU:O	2:B1:153:PHE:N	2.38	0.51
4:C1:205:PRO:HB2	37:C1:518:DGD:HA22	1.93	0.51
29:C1:513:CLA:H101	31:C1:514:BCR:H23C	1.93	0.51
8:H1:66:GLU:HB3	8:H1:72:LEU:HB2	1.93	0.51
12:L1:15:ARG:NH2	32:b1:621:SQD:O3	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P1:93:PRO:HA	15:P1:106:TYR:HA	1.93	0.51
15:P1:116:VAL:HG23	15:P1:219:VAL:HG22	1.93	0.51
50:N1:622:XAT:C34	29:Y1:613:CLA:H111	2.40	0.51
21:G1:232:HIS:CG	29:G1:613:CLA:HAA2	2.46	0.51
29:a1:406:CLA:OBD	5:d1:198:MET:HG3	2.11	0.51
14:o1:115:THR:HB	14:o1:127:PHE:HB3	1.92	0.51
15:p1:102:ILE:HD13	15:p1:105:ARG:HD2	1.93	0.51
40:C:525:LHG:H131	32:C:526:SQD:H291	1.92	0.51
21:G:102:LEU:HD23	21:G:108:VAL:HG21	1.93	0.51
48:G:608:CHL:HBB1	48:G:608:CHL:HHC	1.93	0.51
29:Y:610:CLA:H52	49:Y:620:LUT:H30	1.93	0.51
4:c:264:LEU:HD21	29:c:508:CLA:HAB	1.92	0.51
22:r:78:LEU:HD22	50:r:621:XAT:H23	1.92	0.51
2:B1:441:GLY:HA2	14:O1:230:ALA:HB3	1.93	0.51
4:C1:57:LEU:HA	4:C1:60:VAL:HG22	1.93	0.51
15:P1:235:LEU:O	15:P1:239:ASP:N	2.40	0.51
20:N1:123:TRP:CZ2	20:N1:220:PHE:HB3	2.46	0.51
4:c1:418:HIS:HA	4:c1:421:LEU:HD12	1.92	0.51
43:d1:405:PL9:H101	40:d1:409:LHG:H102	1.93	0.51
4:C:173:VAL:HG23	4:C:218:LEU:HD13	1.91	0.50
20:N:247:ALA:HB3	50:G:622:XAT:H193	1.93	0.50
4:c:109:SER:HA	31:c:514:BCR:H16C	1.93	0.50
14:o:116:VAL:HG22	14:o:288:ILE:HD12	1.93	0.50
18:x:73:LEU:HA	18:x:76:LEU:HD12	1.93	0.50
48:g:605:CHL:HBB1	48:g:605:CHL:HHC	1.93	0.50
22:r:201:LEU:HD13	29:r:608:CLA:HAB	1.93	0.50
1:A1:165:GLN:NE2	1:A1:294:ALA:O	2.44	0.50
1:A1:188:ALA:HB1	1:A1:329:GLU:HB3	1.93	0.50
2:B1:379:ALA:HB2	2:B1:395:VAL:HG21	1.93	0.50
4:C1:213:VAL:HG12	37:C1:518:DGD:HD61	1.93	0.50
4:C1:348:ASP:OD2	37:C1:518:DGD:O3D	2.28	0.50
29:C1:504:CLA:H61	37:C1:519:DGD:HB62	1.93	0.50
14:O1:169:THR:HA	14:O1:179:PRO:HA	1.92	0.50
29:G1:602:CLA:CBB	49:G1:621:LUT:H32	2.41	0.50
29:G1:603:CLA:H151	48:G1:609:CHL:H121	1.93	0.50
29:Y1:611:CLA:HBB2	34:Y1:625:SPH:H82	1.92	0.50
20:n1:208:LYS:HE3	40:n1:624:LHG:HC61	1.94	0.50
29:n1:613:CLA:H122	29:n1:614:CLA:HMD2	1.93	0.50
2:B:91:TRP:CD2	29:B:607:CLA:HBA2	2.47	0.50
5:D:79:SER:HA	5:D:172:SER:HB3	1.92	0.50
15:P:204:LEU:HB2	15:P:219:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:87:ARG:HA	21:g:90:LEU:HD12	1.94	0.50
1:A1:304:GLN:NE2	4:C1:403:ASN:O	2.45	0.50
2:B1:170:ASP:CG	2:B1:174:LEU:H	2.19	0.50
5:D1:139:ARG:HH12	5:D1:269:PHE:HZ	1.59	0.50
20:N1:196:PRO:HA	20:N1:199:PHE:HB3	1.92	0.50
48:N1:605:CHL:HED3	23:S1:124:LEU:HD21	1.92	0.50
1:a1:142:TRP:CZ2	4:c1:435:ARG:HB2	2.46	0.50
48:r1:606:CHL:HHC	48:r1:606:CHL:HBB1	1.94	0.50
1:A:329:GLU:O	1:A:332:HIS:ND1	2.44	0.50
33:A:413:LMG:O5	4:C:209:ASP:OD2	2.26	0.50
2:B:124:ARG:O	8:H:31:ARG:NH2	2.44	0.50
29:B:612:CLA:H52	29:B:614:CLA:HED3	1.93	0.50
29:B:616:CLA:HBB1	29:B:616:CLA:HHC	1.93	0.50
4:C:14:ARG:O	11:K:46:ARG:NH1	2.45	0.50
24:Y:184:TYR:HB3	29:Y:610:CLA:HED3	1.93	0.50
2:b:229:LEU:HD11	29:b:610:CLA:H12	1.94	0.50
39:b:625:DGA:HAT2	39:b:625:DGA:HB91	1.93	0.50
48:y:606:CHL:HHC	48:y:606:CHL:HBB1	1.92	0.50
4:C1:15:ASP:HB3	11:K1:46:ARG:HD2	1.93	0.50
29:C1:513:CLA:H121	31:C1:514:BCR:H392	1.93	0.50
21:G1:225:PRO:HB2	49:G1:620:LUT:H21	1.93	0.50
22:r1:207:ASP:H	22:r1:210:LYS:HE2	1.75	0.50
23:s1:72:PRO:HG2	23:s1:86:ASP:HB2	1.93	0.50
23:s1:276:LEU:N	29:s1:613:CLA:O1A	2.44	0.50
23:S:279:VAL:HG13	23:S:280:LEU:HD12	1.93	0.50
24:Y:159:VAL:HA	48:Y:609:CHL:HBB2	1.94	0.50
1:a:283:ILE:HA	1:a:286:THR:HG22	1.92	0.50
34:a:414:SPH:HN22	47:i:101:4RF:H41	1.75	0.50
2:b:192:PRO:HG2	8:h:68:TYR:CD1	2.46	0.50
29:y:614:CLA:H61	34:y:625:SPH:H152	1.94	0.50
1:A1:26:ASN:O	5:D1:255:GLN:NE2	2.44	0.50
2:B1:311:PHE:O	2:B1:317:ASN:ND2	2.45	0.50
29:C1:501:CLA:HMB2	31:C1:515:BCR:H23C	1.93	0.50
37:C1:520:DGD:HE4	10:J1:42:LEU:HD21	1.92	0.50
5:D1:27:PHE:HD2	7:F1:18:ARG:HG3	1.76	0.50
48:Y1:609:CHL:HHC	48:Y1:609:CHL:HBB1	1.93	0.50
1:a1:341:LEU:HB3	1:a1:343:LEU:HG	1.93	0.50
4:c1:133:PRO:O	4:c1:144:LYS:NZ	2.45	0.50
4:c1:319:ALA:HA	15:p1:158:GLY:HA3	1.93	0.50
5:d1:94:GLY:HA2	18:x1:72:PHE:HE1	1.76	0.50
14:o1:269:VAL:HG12	14:o1:293:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:s1:625:LPX:H10	38:s1:626:3PH:H2A2	1.93	0.50
2:B:37:MET:O	2:B:41:GLU:CB	2.57	0.50
29:B:612:CLA:H71	40:L:101:LHG:H322	1.94	0.50
29:C:504:CLA:H203	37:C:519:DGD:HAW1	1.92	0.50
6:E:36:LEU:HA	6:E:39:SER:HB3	1.93	0.50
14:O:276:SER:HB2	14:O:288:ILE:HD11	1.93	0.50
21:G:91:LEU:HG	29:G:610:CLA:HMC3	1.93	0.50
22:R:155:GLU:OE2	22:R:162:TRP:N	2.44	0.50
24:Y:129:ALA:HB2	48:Y:607:CHL:HED2	1.93	0.50
21:g:92:GLY:HA2	49:g:621:LUT:H181	1.92	0.50
24:y:76:LEU:HD12	29:y:602:CLA:C1	2.41	0.50
5:D1:342:PRO:HB2	5:D1:344:GLU:HG2	1.94	0.50
18:X1:65:VAL:HA	18:X1:69:LEU:HD12	1.93	0.50
23:S1:80:ALA:HB1	23:S1:233:VAL:HA	1.92	0.50
1:a1:112:TYR:OH	1:a1:172:MET:O	2.22	0.50
4:c1:61:SER:HA	11:k1:11:LEU:HG	1.93	0.50
29:n1:603:CLA:H72	29:n1:603:CLA:HMA3	1.93	0.50
21:g1:92:GLY:HA2	49:g1:621:LUT:H181	1.92	0.50
1:A:340:PRO:HB2	15:P:224:LYS:HD3	1.93	0.50
2:B:395:VAL:HG23	2:B:397:VAL:HG23	1.94	0.50
38:B:624:3PH:H381	16:t:4:LEU:HD22	1.93	0.50
6:E:74:GLU:HA	6:E:77:LYS:HB2	1.93	0.50
2:b:243:ALA:HA	2:b:246:PHE:CE1	2.46	0.50
29:s:613:CLA:HBB1	49:s:620:LUT:H181	1.94	0.50
5:D1:93:TRP:HB2	18:X1:71:ASN:HB3	1.94	0.50
14:O1:62:LEU:HD21	14:O1:80:ILE:HG23	1.94	0.50
1:a1:308:ASP:HB3	1:a1:314:LEU:HD11	1.94	0.50
1:a1:328:MET:HE3	5:d1:325:ILE:HG13	1.94	0.50
2:b1:11:VAL:HG23	2:b1:12:VAL:HG13	1.93	0.50
29:b1:611:CLA:H102	29:b1:616:CLA:HAA1	1.94	0.50
29:c1:512:CLA:HMB1	40:c1:525:LHG:H112	1.94	0.50
33:c1:521:LMG:H182	39:j1:101:DGA:HB81	1.93	0.50
29:B:613:CLA:H171	29:B:614:CLA:HBB2	1.94	0.50
29:N:613:CLA:H162	40:N:624:LHG:H361	1.93	0.50
29:b:609:CLA:H93	39:b:625:DGA:HBF1	1.94	0.50
33:A1:413:LMG:H362	37:C1:518:DGD:HA62	1.94	0.50
2:B1:24:LEU:HD23	2:B1:111:SER:HB2	1.92	0.50
1:a1:62:GLY:HA3	1:a1:87:ASN:HB3	1.94	0.50
2:b1:124:ARG:NH1	8:h1:20:PRO:HA	2.27	0.50
3:v1:16:VAL:HA	31:c1:516:BCR:H16C	1.93	0.50
5:d1:155:SER:HA	5:d1:159:ILE:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e1:65:LEU:HG	6:e1:67:THR:HB	1.94	0.50
20:n1:46:ASN:ND2	20:n1:68:TYR:OH	2.45	0.50
22:r1:170:LEU:HD12	22:r1:184:ILE:HG13	1.93	0.50
24:y1:223:PHE:HE2	48:y1:609:CHL:H172	1.77	0.50
29:y1:610:CLA:H71	29:y1:612:CLA:H112	1.94	0.50
4:C:72:GLN:HB2	4:C:74:LEU:HD13	1.92	0.50
6:E:35:TRP:HD1	7:F:38:ALA:HB2	1.77	0.50
29:R:603:CLA:O1A	52:R:625:LMT:O2'	2.29	0.50
29:a:410:CLA:H12	33:a:413:LMG:H112	1.94	0.50
48:g:606:CHL:HBA2	48:g:606:CHL:HBD	1.93	0.50
4:C1:185:ARG:NH2	4:C1:219:GLU:OE2	2.33	0.50
29:C1:511:CLA:H13	31:C1:517:BCR:H21C	1.93	0.50
20:N1:222:VAL:HG11	29:N1:613:CLA:HAC2	1.94	0.50
40:N1:624:LHG:H223	50:G1:622:XAT:H10	1.94	0.50
23:S1:287:PRO:HB2	23:S1:289:LEU:HD22	1.93	0.50
1:a1:103:ASP:HA	1:a1:106:LEU:HB2	1.94	0.50
5:d1:169:PHE:HA	5:d1:180:ARG:HH22	1.76	0.50
5:d1:199:MET:HG2	43:d1:405:PL9:H321	1.94	0.50
40:d1:410:LHG:H242	40:d1:410:LHG:H301	1.94	0.50
20:n1:87:GLU:O	20:n1:91:ILE:HG12	2.12	0.50
21:g1:223:LYS:HE2	21:g1:227:GLN:HG2	1.93	0.50
14:O:256:VAL:HG22	14:O:294:TRP:HZ2	1.76	0.50
30:a:409:PHO:HHB	29:d:402:CLA:H121	1.94	0.50
2:b:285:GLN:OE1	25:u:94:VAL:HG23	2.12	0.50
2:b:368:VAL:HG21	2:b:422:ARG:HG2	1.93	0.50
48:r:607:CHL:HBB1	48:r:607:CHL:HHC	1.94	0.50
24:y:228:VAL:HG21	29:y:613:CLA:HMD2	1.93	0.50
1:A1:341:LEU:HD13	1:A1:343:LEU:HD21	1.93	0.50
4:C1:33:LEU:HD23	4:C1:36:LYS:HD2	1.94	0.50
16:T1:1:MET:HA	16:T1:4:LEU:HD12	1.93	0.50
20:N1:153:THR:HG23	48:N1:605:CHL:HAC1	1.94	0.50
2:b1:141:ILE:HD11	8:h1:33:LEU:HD12	1.94	0.50
2:b1:168:VAL:N	2:b1:177:SER:O	2.40	0.50
2:b1:392:ILE:HD12	2:b1:397:VAL:HB	1.93	0.50
4:c1:27:ASN:N	29:c1:508:CLA:O1A	2.39	0.50
4:c1:118:VAL:HG21	29:c1:511:CLA:H161	1.93	0.50
4:c1:422:GLY:O	4:c1:426:PHE:N	2.45	0.50
10:j1:31:PHE:O	10:j1:34:SER:OG	2.25	0.50
21:g1:39:LYS:HB3	21:g1:45:SER:HB2	1.93	0.50
24:y1:131:ILE:HD13	24:y1:151:ILE:HB	1.94	0.50
4:C:221:ILE:O	4:C:225:HIS:ND1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:36:LEU:HD12	29:d:403:CLA:HBB1	1.92	0.49
15:p:178:ASP:OD1	15:p:182:LYS:N	2.36	0.49
2:B1:30:VAL:HG13	29:B1:614:CLA:HAC2	1.93	0.49
29:C1:512:CLA:H193	32:C1:526:SQD:H251	1.94	0.49
53:R1:626:ERG:H152	17:w1:80:ILE:HG21	1.93	0.49
14:o1:138:TYR:HE2	17:w1:61:VAL:CG2	2.23	0.49
22:r1:268:LEU:HD23	49:r1:620:LUT:H21	1.94	0.49
24:y1:198:PRO:HA	24:y1:201:PHE:HB3	1.93	0.49
4:C:78:PRO:O	4:C:82:THR:HG23	2.13	0.49
29:C:513:CLA:H2	31:C:514:BCR:H381	1.94	0.49
37:C:519:DGD:HA82	37:C:520:DGD:HBE2	1.93	0.49
23:S:61:LEU:HD22	23:S:65:LEU:HD12	1.93	0.49
31:c:516:BCR:H363	11:k:31:LEU:HD22	1.94	0.49
21:g:204:GLY:O	21:g:208:MET:HG3	2.11	0.49
2:B1:272:ARG:O	2:B1:276:ASP:N	2.41	0.49
29:C1:506:CLA:H42	31:C1:515:BCR:H323	1.93	0.49
15:P1:145:LEU:HD21	15:P1:168:ALA:HB2	1.94	0.49
21:G1:199:LYS:O	21:G1:203:ASN:ND2	2.44	0.49
30:a1:409:PHO:HBA1	29:d1:402:CLA:H121	1.92	0.49
2:b1:364:GLU:HG2	5:d1:294:ARG:HH21	1.78	0.49
20:n1:71:ASP:HB3	20:n1:74:GLY:HA2	1.95	0.49
20:n1:191:GLY:O	20:n1:193:ALA:N	2.45	0.49
48:n1:606:CHL:H192	38:s1:626:3PH:H292	1.92	0.49
23:s1:152:PHE:CE2	23:s1:154:VAL:HG12	2.47	0.49
2:B:67:THR:HG21	2:B:80:ILE:HD11	1.95	0.49
2:B:158:VAL:HG13	2:B:199:PRO:HB3	1.94	0.49
6:E:75:GLN:HA	6:E:78:LYS:HG2	1.93	0.49
29:G:611:CLA:HAC1	40:G:624:LHG:H292	1.94	0.49
22:R:191:GLU:O	22:R:195:VAL:HG12	2.12	0.49
53:R:626:ERG:H152	17:w:80:ILE:HG21	1.93	0.49
24:Y:236:ASN:ND2	29:Y:613:CLA:O1D	2.31	0.49
1:a:63:ILE:HG13	1:a:65:GLU:HG3	1.94	0.49
1:a:77:ILE:HD11	16:t:6:TYR:HB3	1.93	0.49
29:g:611:CLA:H72	29:g:611:CLA:H142	1.95	0.49
2:B1:357:ARG:HG2	2:B1:371:ILE:HD13	1.92	0.49
14:O1:155:VAL:N	14:O1:191:GLY:O	2.40	0.49
14:O1:235:ASP:N	14:O1:235:ASP:OD1	2.45	0.49
48:N1:606:CHL:HBB2	48:N1:607:CHL:HAB	1.93	0.49
1:a1:298:ASN:HB3	4:c1:399:ALA:HB2	1.94	0.49
29:c1:513:CLA:C1B	31:c1:514:BCR:H383	2.42	0.49
8:H:59:VAL:O	8:H:63:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:613:CLA:H102	40:Y:624:LHG:H132	1.95	0.49
2:b:373:LYS:H	2:b:373:LYS:HD2	1.77	0.49
5:d:98:GLN:HB2	6:e:73:LEU:HD22	1.94	0.49
21:g:118:ALA:O	21:g:121:GLN:HB2	2.12	0.49
23:s:143:MET:HE3	48:s:606:CHL:HAC1	1.92	0.49
2:B1:91:TRP:HB2	29:B1:607:CLA:HAA1	1.94	0.49
2:B1:254:GLY:HA3	33:H1:102:LMG:H132	1.93	0.49
29:B1:609:CLA:H143	29:D1:403:CLA:HMA3	1.94	0.49
4:C1:64:VAL:HG12	4:C1:67:LYS:H	1.78	0.49
4:C1:270:MET:HE3	29:C1:507:CLA:H11	1.94	0.49
5:D1:216:ALA:O	5:D1:220:ASN:ND2	2.32	0.49
7:F1:40:GLN:NE2	10:J1:29:ILE:O	2.31	0.49
14:O1:104:LEU:N	14:O1:145:GLY:O	2.45	0.49
29:G1:602:CLA:HED2	29:G1:602:CLA:H2A	1.95	0.49
2:b1:373:LYS:HE3	25:u1:96:ASP:HB3	1.95	0.49
4:c1:203:LYS:HB3	4:c1:211:TRP:HA	1.93	0.49
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.94	0.49
1:A:312:ARG:HH21	15:P:92:ASN:HA	1.77	0.49
2:B:65:PHE:HE1	29:B:605:CLA:HED2	1.77	0.49
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.95	0.49
31:C:516:BCR:H363	11:K:31:LEU:HD22	1.94	0.49
22:R:135:GLU:OE2	22:R:211:ARG:NH2	2.45	0.49
22:r:127:VAL:HG23	22:r:128:PHE:HD1	1.77	0.49
48:r:606:CHL:HBB1	48:r:606:CHL:HHC	1.94	0.49
23:s:93:ASP:OD1	23:s:93:ASP:N	2.45	0.49
48:y:605:CHL:HHC	48:y:605:CHL:HBB1	1.93	0.49
5:D1:68:ILE:HG12	6:E1:44:TYR:HE1	1.77	0.49
7:F1:44:ARG:NH2	15:P1:71:ASN:O	2.45	0.49
8:H1:25:PRO:HG2	51:R1:622:NEX:H42	1.93	0.49
1:a1:102:LEU:O	1:a1:106:LEU:N	2.32	0.49
2:b1:151:PHE:HD1	2:b1:203:ILE:HG23	1.77	0.49
40:c1:525:LHG:H251	29:s1:611:CLA:CAB	2.43	0.49
53:r1:626:ERG:C3	53:r1:626:ERG:HO1	2.13	0.49
23:s1:244:ILE:HG13	40:s1:624:LHG:H271	1.94	0.49
24:y1:126:LYS:HA	48:y1:607:CHL:HED3	1.94	0.49
4:C:153:LEU:HD11	29:C:506:CLA:HAB	1.95	0.49
29:C:512:CLA:H18	29:C:512:CLA:HBB1	1.94	0.49
21:G:211:CYS:SG	49:G:621:LUT:H14	2.52	0.49
2:b:25:MET:HG2	31:b:618:BCR:H23C	1.95	0.49
5:d:64:ALA:HB1	5:d:69:GLU:HG2	1.94	0.49
48:g:606:CHL:HAA2	51:g:623:NEX:H28	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:y:626:PTY:H401	55:y:626:PTY:H212	1.93	0.49
4:C1:207:GLY:HA2	37:C1:518:DGD:HD2	1.94	0.49
14:O1:102:TYR:HB3	14:O1:298:LEU:HD12	1.93	0.49
17:W1:76:VAL:HA	17:W1:81:LEU:HD23	1.95	0.49
21:G1:65:THR:N	49:G1:621:LUT:O23	2.45	0.49
48:G1:601:CHL:H171	48:Y1:607:CHL:H141	1.94	0.49
48:G1:601:CHL:HHC	48:G1:601:CHL:HBB1	1.93	0.49
23:S1:101:ARG:HA	23:S1:104:GLU:HB3	1.94	0.49
24:Y1:174:ALA:HB3	24:Y1:177:VAL:HG12	1.95	0.49
29:c1:501:CLA:C1B	29:c1:501:CLA:H2	2.42	0.49
20:n1:111:ASP:OD1	20:n1:111:ASP:N	2.44	0.49
23:s1:249:PHE:HE1	49:s1:620:LUT:H41	1.77	0.49
48:s1:608:CHL:HBD	29:s1:610:CLA:HAC2	1.94	0.49
1:A:43:THR:HG23	31:A:411:BCR:H362	1.95	0.49
32:A:412:SQD:H312	29:C:508:CLA:H71	1.94	0.49
38:B:624:3PH:H361	16:t:1:MET:HA	1.95	0.49
5:D:312:GLU:HB3	14:O:213:PRO:HG3	1.95	0.49
29:Y:614:CLA:HAB	55:Y:626:PTY:C23	2.42	0.49
2:b:134:ASP:O	2:b:138:ILE:HG12	2.13	0.49
2:b:323:GLY:HA3	2:b:326:ARG:HG3	1.95	0.49
29:b:606:CLA:H143	29:b:611:CLA:HMA1	1.95	0.49
48:n:606:CHL:HHC	48:n:606:CHL:HBB1	1.94	0.49
21:g:182:ASP:OD1	29:g:610:CLA:HBA2	2.12	0.49
2:B1:256:MET:O	2:B1:448:ARG:NH2	2.33	0.49
4:C1:70:TYR:OH	4:C1:382:GLU:OE2	2.22	0.49
47:I1:102:4RF:H60	47:I1:102:4RF:H38	1.94	0.49
13:M1:26:TYR:O	13:M1:30:ALA:N	2.40	0.49
21:G1:65:THR:HG21	48:Y1:609:CHL:HAA2	1.95	0.49
48:S1:608:CHL:H61	51:S1:623:NEX:H401	1.93	0.49
2:b1:275:TRP:NE1	2:b1:359:MET:O	2.41	0.49
2:b1:459:ALA:O	2:b1:463:PHE:N	2.41	0.49
7:f1:40:GLN:HG3	10:j1:33:GLY:HA3	1.94	0.49
2:B:134:ASP:OD2	8:H:35:SER:N	2.46	0.49
12:L:24:LEU:HD13	40:L:101:LHG:H142	1.95	0.49
20:N:88:LEU:HD12	48:N:609:CHL:HED3	1.94	0.49
29:N:604:CLA:H121	51:N:623:NEX:H402	1.94	0.49
2:b:321:LYS:NZ	2:b:363:PHE:O	2.39	0.49
48:n:601:CHL:HBB1	48:n:601:CHL:HHC	1.94	0.49
5:D1:185:PHE:HB3	5:D1:191:TRP:HB2	1.93	0.49
19:Z1:12:LEU:HD21	19:Z1:50:LEU:HB2	1.94	0.49
19:Z1:31:ASN:OD1	19:Z1:34:THR:OG1	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N1:160:LEU:HD13	20:N1:163:LEU:HD21	1.95	0.49
29:G1:603:CLA:H192	48:G1:609:CHL:H151	1.93	0.49
54:S1:625:LPX:H8	38:S1:626:3PH:H292	1.94	0.49
29:Y1:610:CLA:H2	49:Y1:620:LUT:H28	1.95	0.49
55:Y1:626:PTY:H182	55:Y1:626:PTY:H381	1.94	0.49
2:b1:364:GLU:OE2	5:d1:294:ARG:NE	2.38	0.49
29:c1:511:CLA:H171	19:z1:20:VAL:HA	1.94	0.49
5:d1:34:GLY:HA2	5:d1:37:LEU:HB3	1.94	0.49
5:d1:222:LEU:HD23	5:d1:244:TYR:HB3	1.93	0.49
14:o1:82:ASN:HD21	14:o1:138:TYR:H	1.61	0.49
22:r1:134:ARG:HH12	22:r1:138:VAL:HG23	1.77	0.49
1:A:156:ALA:HA	1:A:160:ILE:HB	1.94	0.49
1:A:273:PHE:N	5:D:219:GLU:OE2	2.46	0.49
29:N:602:CLA:H191	40:N:624:LHG:H152	1.94	0.49
22:R:199:GLU:OE1	22:R:202:ARG:NH2	2.36	0.49
2:b:258:TYR:HB3	33:h:102:LMG:HC61	1.95	0.49
29:b:604:CLA:H192	29:b:610:CLA:H91	1.94	0.49
5:d:319:ILE:O	5:d:323:GLU:HG3	2.13	0.49
31:C1:517:BCR:H391	11:K1:36:ALA:HB2	1.94	0.49
37:C1:519:DGD:HB72	33:C1:521:LMG:H401	1.94	0.49
22:R1:220:PRO:HD2	49:R1:620:LUT:H23	1.95	0.49
29:R1:610:CLA:H122	29:R1:612:CLA:HBB2	1.95	0.49
24:Y1:100:GLY:HA2	29:Y1:604:CLA:HAB	1.94	0.49
29:Y1:603:CLA:HAC2	48:Y1:607:CHL:H171	1.94	0.49
2:b1:273:TYR:HE1	5:d1:165:SER:HA	1.77	0.49
2:b1:379:ALA:HB2	2:b1:395:VAL:HG11	1.94	0.49
29:c1:511:CLA:HBA1	31:c1:517:BCR:H271	1.95	0.49
5:d1:210:LEU:HA	5:d1:213:ILE:HG22	1.94	0.49
15:p1:174:ALA:HB3	15:p1:186:LYS:HB2	1.95	0.49
20:n1:101:LEU:O	20:n1:105:THR:OG1	2.25	0.49
20:n1:138:TYR:HB3	20:n1:144:LEU:HD13	1.94	0.49
21:g1:242:PHE:HB3	24:y1:132:PHE:HZ	1.77	0.49
2:B:40:PHE:HD1	38:B:624:3PH:H362	1.76	0.49
5:D:297:ASP:HA	5:D:315:TYR:OH	2.13	0.49
33:D:411:LMG:H112	10:J:30:PHE:HB3	1.95	0.49
48:R:606:CHL:HHC	48:R:606:CHL:HBB1	1.95	0.49
2:b:81:SER:OG	2:b:83:GLU:OE1	2.26	0.49
2:b:371:ILE:HG13	25:u:100:PRO:HB3	1.95	0.49
4:c:350:ARG:NH1	4:c:355:GLU:OE2	2.46	0.49
29:c:506:CLA:H51	39:c:524:DGA:HA51	1.95	0.49
7:f:43:GLN:HE22	15:p:67:GLY:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:140:GLY:O	2:B1:144:PHE:N	2.43	0.49
29:B1:603:CLA:H18	33:H1:102:LMG:H342	1.95	0.49
5:D1:253:TRP:O	5:D1:258:GLY:N	2.46	0.49
5:D1:296:TYR:O	5:D1:315:TYR:OH	2.29	0.49
14:O1:185:LYS:O	14:O1:201:LEU:N	2.46	0.49
48:R1:607:CHL:HHC	48:R1:607:CHL:HBB1	1.95	0.49
1:a1:29:TYR:HB2	5:d1:255:GLN:HG2	1.95	0.49
4:c1:390:GLY:HA3	4:c1:408:VAL:HG22	1.93	0.49
5:d1:57:SER:O	5:d1:57:SER:OG	2.30	0.49
5:d1:323:GLU:HA	5:d1:326:ARG:HG3	1.95	0.49
1:A:100:ALA:N	1:A:104:GLU:OE2	2.42	0.48
2:B:204:ALA:CB	29:B:603:CLA:HAB	2.43	0.48
2:B:247:TRP:HH2	29:B:610:CLA:H18	1.78	0.48
10:J:32:TYR:HA	39:J:101:DGA:HA31	1.94	0.48
15:P:99:VAL:HG12	15:P:101:SER:H	1.78	0.48
29:G:602:CLA:H13	29:Y:603:CLA:H151	1.95	0.48
2:b:256:MET:O	2:b:448:ARG:NH1	2.43	0.48
12:l:26:PHE:HB3	16:t:13:THR:HG22	1.93	0.48
14:o:63:THR:OG1	14:o:66:GLU:OE1	2.23	0.48
15:p:121:GLN:O	15:p:214:LEU:N	2.42	0.48
3:V1:15:VAL:HG11	11:K1:28:ILE:HD12	1.95	0.48
38:T1:101:3PH:H381	38:T1:101:3PH:H2I3	1.95	0.48
29:N1:613:CLA:H18	50:G1:622:XAT:H30	1.94	0.48
21:G1:70:ALA:HB1	24:Y1:81:THR:HG23	1.95	0.48
3:v1:19:GLY:HA2	11:k1:35:LEU:HD21	1.94	0.48
4:c1:41:HIS:CE1	29:c1:509:CLA:H141	2.48	0.48
5:d1:198:MET:HB3	43:d1:405:PL9:H352	1.94	0.48
10:j1:13:TRP:NE1	11:k1:38:VAL:O	2.46	0.48
20:n1:120:SER:HB3	20:n1:129:ALA:HB2	1.95	0.48
20:n1:220:PHE:HZ	49:n1:620:LUT:H8	1.78	0.48
29:r1:612:CLA:H101	29:r1:612:CLA:HED3	1.95	0.48
29:s1:602:CLA:HBB2	49:s1:621:LUT:H34	1.94	0.48
24:y1:110:LEU:HB3	24:y1:115:VAL:HG21	1.95	0.48
1:A:191:ASN:HB2	4:C:399:ALA:HB1	1.95	0.48
1:A:288:LEU:O	1:A:292:THR:HG23	2.13	0.48
1:A:317:TRP:O	1:A:321:ILE:HG13	2.13	0.48
22:R:219:ASP:OD1	49:R:620:LUT:O23	2.23	0.48
6:e:35:TRP:HA	7:f:38:ALA:HB2	1.95	0.48
21:G1:142:ILE:HA	21:G1:145:THR:HG22	1.94	0.48
23:S1:186:GLY:HA2	48:S1:608:CHL:HAC1	1.95	0.48
23:S1:248:ALA:O	23:S1:252:GLN:N	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a1:405:CLA:H18	40:d1:409:LHG:H332	1.95	0.48
33:a1:413:LMG:H392	37:c1:518:DGD:HB61	1.94	0.48
31:c1:516:BCR:HC7	31:c1:517:BCR:H353	1.95	0.48
14:o1:104:LEU:HD11	14:o1:157:PHE:HE1	1.78	0.48
23:s1:264:ILE:HD13	49:s1:620:LUT:H22	1.94	0.48
48:s1:608:CHL:H91	29:s1:610:CLA:H162	1.95	0.48
1:A:91:LEU:HD11	1:A:163:ILE:HA	1.94	0.48
14:O:107:PHE:CD2	14:O:143:MET:HE3	2.47	0.48
23:S:101:ARG:NE	23:S:104:GLU:OE1	2.46	0.48
29:S:610:CLA:H143	49:S:620:LUT:H361	1.94	0.48
29:Y:604:CLA:H12	51:Y:623:NEX:H241	1.94	0.48
29:b:605:CLA:HBB1	29:b:614:CLA:C2C	2.43	0.48
29:b:611:CLA:H102	29:b:616:CLA:HAA1	1.94	0.48
21:g:225:PRO:O	49:g:620:LUT:O3	2.23	0.48
1:A1:164:GLY:HA3	1:A1:294:ALA:HB1	1.96	0.48
2:B1:331:ASN:CG	2:B1:336:ILE:HG13	2.38	0.48
29:B1:602:CLA:H8	29:B1:602:CLA:H51	1.60	0.48
23:S1:78:GLU:HG2	23:S1:79:LEU:HD12	1.95	0.48
2:b1:354:LEU:HD11	2:b1:378:ARG:HB3	1.95	0.48
2:b1:357:ARG:NH1	2:b1:358:ARG:O	2.46	0.48
4:c1:435:ARG:O	4:c1:439:ALA:N	2.36	0.48
5:d1:49:LEU:HD21	31:d1:404:BCR:H362	1.95	0.48
29:n1:603:CLA:HBB1	48:n1:607:CHL:H121	1.95	0.48
2:B:464:PHE:HD2	29:B:612:CLA:HAC2	1.79	0.48
29:C:504:CLA:H72	37:C:519:DGD:HBF2	1.96	0.48
21:G:37:ARG:HE	21:G:39:LYS:HG2	1.79	0.48
48:G:607:CHL:H2	48:G:607:CHL:HMA3	1.96	0.48
1:a:329:GLU:HG3	4:c:400:THR:HG21	1.95	0.48
5:d:188:PHE:O	5:d:294:ARG:NH1	2.47	0.48
34:A1:414:SPH:H132	47:I1:102:4RF:H4	1.95	0.48
2:B1:379:ALA:HA	2:B1:390:TYR:HB3	1.95	0.48
20:N1:87:GLU:HA	20:N1:181:LEU:HD21	1.95	0.48
48:N1:605:CHL:HHC	48:N1:605:CHL:HBB1	1.95	0.48
29:a1:410:CLA:H41	29:a1:410:CLA:H61	1.49	0.48
4:c1:275:CYS:SG	4:c1:415:ALA:HA	2.53	0.48
24:y1:147:HIS:CE1	24:y1:149:GLN:HE22	2.32	0.48
29:B:616:CLA:H2	29:B:617:CLA:CBB	2.43	0.48
21:G:100:GLU:CD	21:G:226:VAL:HG22	2.38	0.48
2:b:175:THR:OG1	2:b:176:GLY:N	2.47	0.48
7:f:40:GLN:NE2	10:j:30:PHE:O	2.46	0.48
22:r:221:LEU:HD23	49:r:620:LUT:H222	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:s:188:GLY:HA3	23:s:204:PHE:CE2	2.49	0.48
40:C1:525:LHG:H112	29:S1:611:CLA:HBB2	1.94	0.48
29:N1:612:CLA:HAB	49:N1:620:LUT:C15	2.43	0.48
21:G1:160:ARG:HH22	48:G1:609:CHL:CGD	2.27	0.48
23:S1:83:TYR:HE2	48:S1:601:CHL:HMD1	1.79	0.48
23:S1:175:LEU:HD23	48:S1:606:CHL:HMA2	1.96	0.48
4:c1:16:GLN:N	11:k1:46:ARG:OXT	2.46	0.48
4:c1:290:TYR:O	4:c1:411:ARG:HG3	2.14	0.48
17:w1:76:VAL:HG21	33:w1:201:LMG:HC71	1.95	0.48
4:C:146:THR:HG21	4:C:244:PRO:HD3	1.95	0.48
14:O:111:PRO:HD2	14:O:138:TYR:HD1	1.79	0.48
29:S:602:CLA:H2	49:S:621:LUT:H24	1.96	0.48
40:S:624:LHG:H271	40:S:624:LHG:HC91	1.96	0.48
29:Y:602:CLA:HBA1	49:Y:621:LUT:H382	1.95	0.48
33:a:413:LMG:H401	37:c:518:DGD:HBT2	1.96	0.48
40:y:624:LHG:H272	40:y:624:LHG:H242	1.64	0.48
1:A1:136:ARG:NH1	9:I1:30:ARG:HD3	2.28	0.48
30:A1:409:PHO:HMC2	5:D1:279:LEU:HD11	1.95	0.48
2:B1:45:PHE:HD1	2:B1:60:MET:HE3	1.79	0.48
5:D1:338:LYS:HB2	25:U1:103:GLU:OE2	2.14	0.48
24:Y1:157:VAL:HG11	48:Y1:605:CHL:HBC1	1.94	0.48
6:e1:70:PHE:H	25:u1:110:ARG:NH2	2.09	0.48
10:j1:12:LEU:HA	10:j1:15:VAL:HB	1.95	0.48
48:n1:605:CHL:H121	29:s1:612:CLA:HMB1	1.94	0.48
1:A:340:PRO:HB2	15:P:224:LYS:HB2	1.96	0.48
17:W:62:ASP:N	17:W:62:ASP:OD1	2.46	0.48
29:G:611:CLA:HAB	50:Y:622:XAT:H221	1.96	0.48
2:b:40:PHE:HA	38:b:624:3PH:H382	1.95	0.48
5:d:141:TYR:OH	40:d:408:LHG:O4	2.25	0.48
7:f:35:ALA:O	7:f:39:MET:HG2	2.13	0.48
14:o:109:MET:HE1	14:o:254:PHE:HZ	1.78	0.48
29:n:604:CLA:HBC3	29:n:610:CLA:H172	1.94	0.48
21:g:68:LEU:HD22	29:g:602:CLA:H42	1.94	0.48
21:g:85:HIS:CD2	49:g:621:LUT:H201	2.48	0.48
48:g:601:CHL:HMA3	40:g:624:LHG:H122	1.95	0.48
29:A1:406:CLA:HMA1	43:D1:405:PL9:H422	1.95	0.48
2:B1:458:PHE:HE2	29:B1:614:CLA:H102	1.78	0.48
4:C1:253:VAL:O	4:C1:262:TYR:OH	2.25	0.48
39:C1:524:DGA:HAF1	33:W1:201:LMG:H352	1.95	0.48
20:N1:165:GLU:HG3	48:N1:609:CHL:NB	2.28	0.48
48:G1:605:CHL:HHC	48:G1:605:CHL:HBB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:141:ILE:O	2:b1:145:LEU:HG	2.13	0.48
5:d1:25:ASP:HA	5:d1:29:PHE:HE2	1.77	0.48
5:d1:221:THR:HB	5:d1:245:SER:H	1.78	0.48
29:g1:611:CLA:H112	29:g1:611:CLA:H72	1.50	0.48
23:s1:152:PHE:HD1	23:s1:158:VAL:H	1.61	0.48
2:B:260:SER:H	2:B:263:THR:HG1	1.61	0.48
20:N:235:LEU:HD13	29:N:614:CLA:HBC2	1.95	0.48
2:b:70:GLY:HA2	2:b:178:VAL:HG11	1.95	0.48
29:b:607:CLA:OBD	37:b:623:DGD:O3D	2.30	0.48
4:c:74:LEU:HD13	4:c:77:LEU:HD12	1.95	0.48
2:B1:237:VAL:O	2:B1:241:SER:N	2.44	0.48
4:C1:90:GLY:N	4:C1:182:GLY:O	2.35	0.48
20:N1:100:ALA:HA	20:N1:103:MET:HE2	1.95	0.48
50:N1:622:XAT:H12	40:Y1:624:LHG:H192	1.95	0.48
2:b1:363:PHE:HA	5:d1:326:ARG:HH22	1.79	0.48
29:b1:611:CLA:HHC	29:b1:611:CLA:HBB1	1.94	0.48
4:c1:79:HIS:ND1	4:c1:290:TYR:OH	2.46	0.48
40:d1:410:LHG:H291	40:d1:410:LHG:H322	1.57	0.48
10:j1:13:TRP:HD1	11:k1:41:ALA:HB3	1.79	0.48
38:t1:101:3PH:H2B2	38:t1:101:3PH:H382	1.94	0.48
24:y1:166:GLU:HA	24:y1:169:ARG:HG2	1.95	0.48
29:A:406:CLA:H121	29:A:406:CLA:HMA1	1.96	0.48
4:C:166:LYS:NZ	4:C:170:PHE:O	2.38	0.48
29:N:603:CLA:H193	48:N:607:CHL:H142	1.95	0.48
24:Y:147:HIS:CE1	24:Y:149:GLN:HE22	2.31	0.48
39:c:524:DGA:HB81	33:w:201:LMG:H372	1.96	0.48
15:p:174:ALA:HB3	15:p:186:LYS:HB2	1.96	0.48
50:n:622:XAT:H34	29:y:613:CLA:H203	1.96	0.48
21:g:83:LEU:HD23	21:g:175:LEU:HG	1.95	0.48
2:B1:74:SER:HA	2:B1:92:SER:HB2	1.95	0.48
4:C1:14:ARG:O	11:K1:46:ARG:NH1	2.47	0.48
14:O1:87:VAL:HG23	14:O1:258:LYS:HD3	1.96	0.48
15:P1:81:ASP:OD1	15:P1:81:ASP:N	2.46	0.48
20:N1:89:GLU:OE2	20:N1:211:ARG:NH2	2.32	0.48
21:G1:150:VAL:HA	48:G1:609:CHL:HBB2	1.95	0.48
48:G1:608:CHL:HBB1	48:G1:608:CHL:HHC	1.95	0.48
53:R1:626:ERG:C3	53:R1:626:ERG:HO1	2.13	0.48
29:b1:604:CLA:HAB	29:b1:606:CLA:C15	2.44	0.48
29:g1:603:CLA:HMA3	29:g1:603:CLA:H12	1.94	0.48
29:y1:602:CLA:HBA1	49:y1:621:LUT:H382	1.95	0.48
1:A:330:VAL:O	5:D:349:GLY:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:ARG:NH1	8:H:19:GLU:O	2.45	0.48
4:C:218:LEU:HA	4:C:221:ILE:HB	1.96	0.48
15:P:231:ASP:OD1	15:P:231:ASP:N	2.46	0.48
29:N:610:CLA:H41	29:N:610:CLA:H61	1.52	0.48
1:a:39:PRO:HG3	9:i:15:PHE:CD2	2.49	0.48
20:n:191:GLY:O	20:n:193:ALA:N	2.46	0.48
48:y:609:CHL:HHC	48:y:609:CHL:HBB1	1.96	0.48
1:A1:344:ALA:HB1	4:C1:345:ARG:HD2	1.96	0.48
29:A1:405:CLA:HAB	29:D1:402:CLA:NC	2.29	0.48
5:D1:191:TRP:CE2	5:D1:197:HIS:HB2	2.49	0.48
38:T1:101:3PH:H3H2	31:b1:619:BCR:H373	1.96	0.48
21:G1:226:VAL:HA	21:G1:229:LEU:HB3	1.95	0.48
29:G1:611:CLA:H112	29:G1:611:CLA:H72	1.50	0.48
29:a1:410:CLA:CGA	33:a1:413:LMG:H112	2.44	0.48
29:b1:610:CLA:H92	29:b1:610:CLA:H61	1.70	0.48
29:b1:613:CLA:H61	29:b1:613:CLA:H102	1.69	0.48
14:o1:135:ARG:O	14:o1:137:THR:N	2.43	0.48
15:p1:217:LEU:HD22	15:p1:241:PHE:HB2	1.96	0.48
50:n1:622:XAT:H10	40:y1:624:LHG:H211	1.95	0.48
40:g1:624:LHG:H383	50:y1:622:XAT:H363	1.96	0.48
30:A:409:PHO:H3A	30:A:409:PHO:HBA1	1.46	0.47
4:C:338:ILE:HG21	4:C:347:TRP:HB2	1.95	0.47
40:c:525:LHG:H281	40:s:624:LHG:HC81	1.96	0.47
47:i:101:4RF:H67	47:i:101:4RF:H34	1.95	0.47
14:o:114:PHE:HD1	14:o:290:ILE:HG12	1.79	0.47
1:A1:42:LEU:O	1:A1:46:SER:OG	2.24	0.47
2:B1:174:LEU:HD21	2:B1:309:LEU:HD13	1.95	0.47
29:C1:511:CLA:H101	31:C1:517:BCR:H24C	1.96	0.47
33:C1:521:LMG:H121	39:J1:101:DGA:HB52	1.95	0.47
53:R1:626:ERG:H213	9:i1:6:ILE:HD13	1.95	0.47
4:c1:153:LEU:HD12	4:c1:239:HIS:HD2	1.78	0.47
37:c1:520:DGD:HA61	37:c1:520:DGD:HBT1	1.96	0.47
29:n1:613:CLA:H191	21:g1:146:LEU:HD13	1.96	0.47
4:C:295:PRO:HB3	4:C:346:PHE:HB3	1.96	0.47
29:C:501:CLA:H72	29:C:501:CLA:H111	1.56	0.47
29:a:406:CLA:HAA2	43:d:405:PL9:H371	1.96	0.47
2:b:127:ARG:NH1	22:r:105:GLU:OE1	2.47	0.47
14:o:253:VAL:O	14:o:271:GLU:N	2.46	0.47
1:A1:146:ALA:HA	1:A1:280:VAL:HG11	1.96	0.47
4:C1:41:HIS:O	4:C1:45:ALA:N	2.36	0.47
8:H1:25:PRO:O	8:H1:28:THR:OG1	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O1:273:ILE:HG22	14:O1:289:LYS:HB2	1.95	0.47
38:T1:101:3PH:H2B2	38:T1:101:3PH:H382	1.96	0.47
20:N1:136:LEU:HD11	48:N1:606:CHL:HMD2	1.95	0.47
29:N1:603:CLA:HED2	48:N1:609:CHL:H93	1.96	0.47
24:Y1:175:PRO:HB2	51:Y1:623:NEX:H183	1.96	0.47
33:a1:413:LMG:H142	29:c1:505:CLA:H161	1.96	0.47
2:b1:220:ARG:HB2	8:h1:41:LEU:HG	1.96	0.47
2:b1:452:THR:HB	5:d1:291:LEU:HD21	1.97	0.47
4:c1:429:HIS:CD2	4:c1:433:ALA:HB2	2.50	0.47
14:o1:169:THR:HA	14:o1:179:PRO:HA	1.96	0.47
21:g1:172:LEU:HB3	21:g1:177:PRO:HA	1.96	0.47
24:y1:191:PRO:HD2	49:y1:620:LUT:H23	1.94	0.47
29:B:606:CLA:H8	29:B:613:CLA:H203	1.96	0.47
29:B:609:CLA:H43	29:B:610:CLA:H101	1.96	0.47
5:D:152:VAL:HG22	29:D:402:CLA:HED1	1.95	0.47
20:N:84:ARG:HH21	24:Y:75:GLY:HA2	1.79	0.47
53:R:626:ERG:C3	53:R:626:ERG:HO1	2.13	0.47
29:S:610:CLA:H141	29:S:610:CLA:H161	1.71	0.47
25:U:95:LEU:HA	25:U:107:LYS:NZ	2.29	0.47
29:b:609:CLA:H62	29:b:609:CLA:H41	1.59	0.47
5:d:85:LEU:HD22	5:d:96:GLU:HG2	1.96	0.47
24:y:133:LYS:HG3	24:y:135:GLY:H	1.78	0.47
37:B1:623:DGD:O5D	37:B1:623:DGD:O4D	2.32	0.47
1:a1:201:GLY:HA2	1:a1:282:CYS:HB3	1.96	0.47
1:A:123:VAL:HB	1:A:151:VAL:HG22	1.96	0.47
2:B:35:GLY:O	2:B:39:LEU:HG	2.15	0.47
2:B:239:SER:O	2:B:466:HIS:ND1	2.44	0.47
2:B:252:VAL:HA	2:B:255:THR:HG22	1.95	0.47
14:O:132:LEU:HA	14:O:170:VAL:HG12	1.96	0.47
14:O:224:ASN:HA	14:O:240:LEU:HD13	1.95	0.47
20:N:59:TYR:OH	20:N:71:ASP:OD2	2.26	0.47
29:N:610:CLA:H3A	29:N:610:CLA:HBA2	1.70	0.47
29:Y:613:CLA:H143	40:Y:624:LHG:H361	1.96	0.47
2:b:9:HIS:CB	29:b:613:CLA:HAB	2.40	0.47
2:b:67:THR:HG23	2:b:72:THR:HG22	1.97	0.47
2:b:206:GLY:O	2:b:210:VAL:HG23	2.15	0.47
2:b:473:THR:O	22:r:101:LYS:NZ	2.45	0.47
29:c:503:CLA:H61	29:c:503:CLA:H41	1.65	0.47
38:t:101:3PH:H381	38:t:101:3PH:H352	1.75	0.47
21:g:212:LEU:HD13	49:g:621:LUT:H401	1.95	0.47
53:r:626:ERG:H212	53:r:626:ERG:H162	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:y:155:LEU:HD13	48:y:607:CHL:HAC2	1.96	0.47
24:y:223:PHE:HD2	29:y:603:CLA:HBB2	1.80	0.47
1:A1:316:THR:HG23	1:A1:318:ALA:H	1.80	0.47
2:B1:204:ALA:CB	29:B1:603:CLA:HAB	2.45	0.47
29:B1:616:CLA:H52	29:B1:617:CLA:HBB1	1.95	0.47
38:B1:624:3PH:H2B1	38:B1:624:3PH:H281	1.62	0.47
29:C1:501:CLA:H41	29:C1:501:CLA:H61	1.61	0.47
5:D1:87:HIS:CD2	5:D1:166:GLY:HA2	2.49	0.47
48:N1:609:CHL:H192	29:G1:603:CLA:H141	1.97	0.47
29:G1:602:CLA:H3A	29:G1:602:CLA:HBA2	1.47	0.47
23:S1:118:ILE:HG23	23:S1:136:TRP:HB3	1.95	0.47
1:a1:224:ILE:O	5:d1:265:ARG:NH2	2.33	0.47
33:a1:413:LMG:HC72	4:c1:204:SER:HB3	1.97	0.47
38:b1:624:3PH:H321	38:b1:624:3PH:H32	1.80	0.47
3:v1:22:VAL:HG13	19:z1:25:VAL:HG23	1.95	0.47
21:g1:94:LEU:HG	29:g1:604:CLA:HAC1	1.95	0.47
21:g1:212:LEU:HA	21:g1:215:PHE:HB2	1.96	0.47
48:g1:601:CHL:H62	48:y1:607:CHL:H203	1.96	0.47
29:g1:610:CLA:H71	29:g1:612:CLA:HHB	1.97	0.47
29:r1:608:CLA:HBA2	29:r1:608:CLA:H3A	1.58	0.47
24:y1:195:ALA:HB2	29:y1:610:CLA:HAA1	1.96	0.47
1:A:76:ASN:ND2	12:L:34:SER:HB3	2.29	0.47
30:A:409:PHO:HHB	29:D:402:CLA:H121	1.96	0.47
32:A:412:SQD:H181	29:C:504:CLA:H193	1.97	0.47
2:B:66:LEU:HB3	2:B:71:VAL:HB	1.96	0.47
29:B:603:CLA:H41	29:B:603:CLA:H61	1.66	0.47
4:C:270:MET:HE1	29:C:507:CLA:H42	1.95	0.47
29:C:506:CLA:H62	29:C:507:CLA:H171	1.96	0.47
29:C:513:CLA:H43	40:C:525:LHG:H241	1.97	0.47
29:N:602:CLA:HBA1	49:N:621:LUT:H382	1.96	0.47
22:R:194:LEU:HD21	48:R:606:CHL:HMA2	1.95	0.47
48:S:606:CHL:HHC	48:S:606:CHL:HBB1	1.96	0.47
1:a:143:ILE:HD11	5:d:217:THR:HA	1.97	0.47
29:c:501:CLA:H162	29:c:507:CLA:HMB2	1.95	0.47
15:p:203:GLN:OE1	15:p:218:LYS:NZ	2.37	0.47
2:B1:470:GLY:HA2	29:B1:609:CLA:HED1	1.97	0.47
4:C1:238:TRP:HZ3	4:C1:239:HIS:CE1	2.32	0.47
29:C1:501:CLA:C1D	29:C1:503:CLA:H51	2.44	0.47
20:N1:88:LEU:HD12	48:N1:609:CHL:HED3	1.95	0.47
20:N1:214:MET:HB3	49:N1:621:LUT:H402	1.95	0.47
20:N1:231:PRO:O	20:N1:235:LEU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:G1:609:CHL:HBB1	48:G1:609:CHL:HHC	1.96	0.47
23:S1:246:VAL:HG11	49:S1:621:LUT:H12	1.96	0.47
29:S1:610:CLA:H71	49:S1:620:LUT:H30	1.96	0.47
24:Y1:223:PHE:HE2	48:Y1:609:CHL:H172	1.79	0.47
37:c1:518:DGD:HA61	37:c1:518:DGD:HB72	1.95	0.47
47:k1:101:4RF:H62	47:k1:101:4RF:H19	1.95	0.47
20:n1:167:TYR:HE2	51:n1:623:NEX:H202	1.79	0.47
21:g1:41:LEU:HB3	21:g1:44:PHE:HB2	1.96	0.47
24:y1:69:TYR:HD2	29:y1:602:CLA:HMD2	1.80	0.47
29:y1:614:CLA:H152	29:y1:614:CLA:H18	1.61	0.47
1:A:230:ASN:HD22	12:L:9:GLN:HE22	1.62	0.47
29:D:403:CLA:H121	18:X:80:ALA:HB2	1.95	0.47
19:Z:16:SER:OG	19:Z:47:TRP:NE1	2.35	0.47
21:G:47:ASN:ND2	24:Y:173:GLU:OE2	2.47	0.47
21:G:85:HIS:HD2	49:G:621:LUT:H201	1.78	0.47
21:G:217:GLN:O	21:G:221:THR:OG1	2.28	0.47
1:a:219:VAL:HG13	1:a:246:TYR:CD2	2.50	0.47
1:a:316:THR:H	1:a:319:ASP:HB3	1.78	0.47
12:l:20:TRP:HE3	40:l:101:LHG:H141	1.79	0.47
14:o:171:LYS:HE3	14:o:175:GLY:HA2	1.95	0.47
17:w:73:PRO:O	17:w:76:VAL:HG22	2.14	0.47
17:w:91:THR:O	17:w:95:ILE:HG13	2.14	0.47
18:x:87:ALA:HA	18:x:90:VAL:HG12	1.96	0.47
29:n:613:CLA:H151	29:n:613:CLA:H18	1.70	0.47
24:y:85:ARG:O	24:y:89:ILE:HG13	2.14	0.47
1:A1:25:GLU:OE1	4:C1:458:ARG:NH2	2.43	0.47
2:B1:250:PHE:HE2	29:B1:603:CLA:H172	1.78	0.47
4:C1:20:GLY:HA3	5:D1:229:ALA:H	1.80	0.47
37:C1:520:DGD:HA81	37:C1:520:DGD:HBT1	1.97	0.47
8:H1:66:GLU:OE1	8:H1:71:SER:HB2	2.14	0.47
47:I1:102:4RF:H45	22:r1:183:SER:HB3	1.96	0.47
29:N1:602:CLA:CBB	49:N1:621:LUT:H32	2.44	0.47
48:N1:608:CHL:CBB	51:N1:623:NEX:H12	2.43	0.47
1:a1:89:ILE:HD11	14:o1:135:ARG:HH22	1.80	0.47
1:a1:130:GLU:HG3	5:d1:252:PHE:HZ	1.79	0.47
2:b1:67:THR:HG23	2:b1:72:THR:HG22	1.96	0.47
5:d1:48:TRP:NE1	5:d1:52:CYS:SG	2.88	0.47
10:j1:27:LEU:HA	10:j1:30:PHE:CD2	2.50	0.47
20:n1:190:LEU:HD13	23:s1:194:PRO:HA	1.96	0.47
23:s1:205:ASP:OD1	23:s1:205:ASP:N	2.46	0.47
1:A:67:VAL:HG13	5:D:313:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:LYS:H	2:B:308:LYS:HG2	1.47	0.47
29:B:610:CLA:HBA2	29:B:610:CLA:H3A	1.48	0.47
40:D:410:LHG:O3	40:D:410:LHG:O1	2.29	0.47
20:N:165:GLU:HG3	48:N:609:CHL:NB	2.30	0.47
21:G:214:PHE:CZ	49:G:620:LUT:H8	2.49	0.47
53:R:626:ERG:H212	53:R:626:ERG:H162	1.77	0.47
48:Y:605:CHL:HHC	48:Y:605:CHL:HBB1	1.95	0.47
50:Y:622:XAT:H31	50:Y:622:XAT:H391	1.61	0.47
1:a:43:THR:HG23	31:a:411:BCR:H362	1.97	0.47
2:b:46:ASP:HB2	2:b:58:GLN:HE22	1.80	0.47
4:c:63:PHE:HE1	4:c:69:MET:HG2	1.80	0.47
4:c:213:VAL:HG13	4:c:277:PHE:HA	1.96	0.47
29:c:502:CLA:HBB2	29:c:510:CLA:H151	1.96	0.47
48:n:605:CHL:H51	29:s:611:CLA:H171	1.96	0.47
21:g:142:ILE:HA	21:g:145:THR:HG22	1.97	0.47
50:g:622:XAT:H31	50:g:622:XAT:H391	1.72	0.47
50:y:622:XAT:H31	50:y:622:XAT:H391	1.72	0.47
1:A1:50:ILE:HG13	31:A1:411:BCR:H271	1.96	0.47
1:A1:200:PHE:CE1	37:C1:520:DGD:HAW1	2.50	0.47
29:A1:410:CLA:H2	33:A1:413:LMG:H131	1.96	0.47
2:B1:40:PHE:HB2	38:B1:624:3PH:H2A1	1.97	0.47
2:B1:185:TRP:HB2	29:B1:602:CLA:HED2	1.97	0.47
2:B1:383:PHE:CD2	5:D1:347:PRO:HA	2.49	0.47
37:B1:623:DGD:HE1	22:R1:170:LEU:HD21	1.96	0.47
9:I1:5:LYS:HA	9:I1:8:VAL:HG12	1.95	0.47
20:N1:104:VAL:HG23	20:N1:232:ILE:HD11	1.97	0.47
29:Y1:611:CLA:H41	29:Y1:611:CLA:H61	1.55	0.47
1:a1:221:SER:HB3	5:d1:138:LEU:HD12	1.96	0.47
1:a1:323:ARG:NH2	15:p1:109:ASN:O	2.47	0.47
2:b1:52:LEU:HB3	2:b1:337:ALA:HB3	1.97	0.47
29:b1:602:CLA:HHC	29:b1:602:CLA:HBB1	1.97	0.47
29:b1:605:CLA:H141	29:b1:605:CLA:H161	1.75	0.47
10:j1:13:TRP:HE1	11:k1:38:VAL:HG13	1.80	0.47
29:n1:602:CLA:HBA1	49:n1:621:LUT:H382	1.96	0.47
21:g1:208:MET:HG3	29:g1:602:CLA:HMC3	1.96	0.47
23:s1:177:GLY:CA	29:s1:609:CLA:HAB	2.44	0.47
24:y1:175:PRO:HG2	51:y1:623:NEX:H8	1.96	0.47
29:A:405:CLA:H102	30:A:408:PHO:HAA1	1.96	0.47
6:E:12:ASP:O	6:E:16:SER:OG	2.19	0.47
11:K:14:ALA:HB1	19:Z:5:LEU:HD22	1.97	0.47
19:Z:15:VAL:HG12	19:Z:47:TRP:HD1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N:605:CHL:H52	38:S:626:3PH:H3I2	1.97	0.47
23:S:215:PRO:HB2	29:S:617:CLA:HBC2	1.97	0.47
29:Y:613:CLA:H151	55:Y:626:PTY:H441	1.97	0.47
40:Y:624:LHG:H331	40:Y:624:LHG:H301	1.71	0.47
25:U:102:LYS:HE2	25:U:102:LYS:HB2	1.70	0.47
1:a:79:THR:HG21	5:d:301:GLN:HE22	1.80	0.47
29:c:502:CLA:H193	23:s:272:PHE:HE1	1.79	0.47
14:o:278:THR:HG22	14:o:285:ALA:HB2	1.96	0.47
20:n:85:TYR:HD1	20:n:88:LEU:HD12	1.80	0.47
21:g:143:ILE:H	21:g:143:ILE:HD12	1.79	0.47
48:g:601:CHL:HHC	48:g:601:CHL:HBB1	1.97	0.47
22:r:191:GLU:O	22:r:195:VAL:HG22	2.14	0.47
23:s:231:LEU:HD13	29:s:610:CLA:H12	1.95	0.47
1:A1:60:ILE:HD12	1:A1:84:PRO:HD2	1.97	0.47
1:A1:289:GLY:O	1:A1:293:MET:HG2	2.15	0.47
29:A1:406:CLA:H2	30:A1:408:PHO:HMB2	1.97	0.47
4:C1:216:ASP:N	4:C1:216:ASP:OD1	2.47	0.47
5:D1:140:PRO:HB2	5:D1:143:ALA:HB3	1.96	0.47
5:D1:302:GLU:O	5:D1:306:ALA:N	2.48	0.47
31:D1:404:BCR:H16C	7:F1:32:PHE:HB2	1.97	0.47
15:P1:148:GLN:HE22	15:P1:150:TRP:HB3	1.79	0.47
21:G1:216:VAL:HG21	29:G1:613:CLA:HAC2	1.96	0.47
23:S1:143:MET:HG3	23:S1:165:LEU:HB2	1.96	0.47
29:S1:602:CLA:H51	49:S1:621:LUT:H28	1.96	0.47
1:a1:84:PRO:HA	1:a1:112:TYR:CG	2.49	0.47
4:c1:194:ALA:HB2	29:y1:614:CLA:HBB2	1.96	0.47
5:d1:105:PHE:HA	5:d1:110:LEU:HD22	1.96	0.47
5:d1:192:THR:HG22	5:d1:197:HIS:CE1	2.50	0.47
20:n1:98:LEU:HG	29:n1:610:CLA:HMC3	1.96	0.47
48:n1:601:CHL:HBB1	48:n1:601:CHL:HHC	1.96	0.47
29:n1:604:CLA:H71	48:n1:606:CHL:CGA	2.44	0.47
23:s1:287:PRO:HB2	23:s1:289:LEU:HD22	1.97	0.47
29:A:405:CLA:H201	40:D:409:LHG:H161	1.96	0.47
2:B:174:LEU:HD22	2:B:308:LYS:HG3	1.96	0.47
4:C:85:TYR:O	4:C:99:TYR:OH	2.28	0.47
14:O:263:THR:HG23	14:O:265:GLU:HG2	1.97	0.47
22:R:145:MET:HE1	29:R:610:CLA:HHC	1.97	0.47
29:a:407:CLA:HMB2	29:d:402:CLA:H122	1.96	0.47
2:b:277:GLN:HB3	25:u:106:VAL:HG23	1.95	0.47
20:n:45:ARG:HG3	20:n:46:ASN:O	2.15	0.47
52:r:625:LMT:H91	52:r:625:LMT:H61	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N1:601:CHL:H143	48:G1:607:CHL:C1C	2.45	0.47
50:G1:622:XAT:H28	50:G1:622:XAT:H371	1.97	0.47
1:a1:36:ILE:HA	29:a1:410:CLA:HBB2	1.96	0.47
4:c1:337:ILE:HB	4:c1:363:LEU:H	1.80	0.47
5:d1:185:PHE:O	5:d1:190:ASN:N	2.47	0.47
6:e1:78:LYS:NZ	25:u1:113:ILE:O	2.48	0.47
47:k1:101:4RF:H78	47:k1:101:4RF:H84	1.72	0.47
29:y1:603:CLA:HMA3	29:y1:603:CLA:H61	1.97	0.47
1:A:30:ILE:HG23	1:A:38:ILE:HD12	1.97	0.47
1:A:131:TRP:CH2	29:C:505:CLA:HAA2	2.50	0.47
32:B:626:SQD:H352	32:B:626:SQD:H321	1.75	0.47
20:N:237:ASP:OD1	20:N:245:ASN:ND2	2.48	0.47
29:G:610:CLA:CAB	49:G:620:LUT:H32	2.44	0.47
22:R:234:ARG:O	22:R:237:THR:OG1	2.33	0.47
29:c:503:CLA:H172	29:c:510:CLA:HBB2	1.97	0.47
33:c:523:LMG:H291	29:y:611:CLA:H42	1.96	0.47
5:d:100:ASP:OD2	5:d:103:ARG:HG2	2.15	0.47
14:o:225:ALA:H	14:o:240:LEU:HD22	1.80	0.47
20:n:73:ALA:HA	21:g:81:ILE:HD11	1.97	0.47
20:n:89:GLU:HG2	20:n:207:ILE:HD11	1.96	0.47
40:y:624:LHG:H301	40:y:624:LHG:H331	1.67	0.47
1:A1:340:PRO:HB2	15:P1:224:LYS:HB2	1.97	0.47
2:B1:169:SER:HB3	2:B1:176:GLY:HA2	1.97	0.47
2:B1:251:VAL:HG13	29:B1:603:CLA:H51	1.96	0.47
29:B1:612:CLA:H8	29:B1:614:CLA:H51	1.96	0.47
4:C1:26:GLY:HA3	29:C1:511:CLA:C2D	2.45	0.47
4:C1:264:LEU:HD21	29:C1:508:CLA:HAB	1.96	0.47
37:C1:520:DGD:HE61	10:J1:42:LEU:HD11	1.96	0.47
5:D1:113:PHE:CE1	5:D1:117:HIS:CE1	3.03	0.47
5:D1:162:LEU:HD11	33:H1:102:LMG:H311	1.96	0.47
5:D1:201:VAL:HG13	29:D1:402:CLA:HMB1	1.97	0.47
29:G1:604:CLA:HED2	29:G1:604:CLA:H2A	1.97	0.47
1:a1:56:PRO:HG2	1:a1:106:LEU:HB3	1.97	0.47
29:a1:407:CLA:HBB1	30:a1:409:PHO:H91	1.97	0.47
2:b1:230:SER:O	2:b1:233:SER:OG	2.29	0.47
4:c1:132:TYR:HB3	4:c1:135:PHE:HD2	1.79	0.47
4:c1:261:SER:HB2	4:c1:429:HIS:CD2	2.50	0.47
32:m1:101:SQD:H132	32:m1:101:SQD:H252	1.96	0.47
14:o1:169:THR:HG23	14:o1:179:PRO:HG3	1.96	0.47
23:s1:107:HIS:HD2	49:s1:621:LUT:H15	1.80	0.47
49:s1:621:LUT:H35	49:s1:621:LUT:H401	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C:513:CLA:H122	29:C:513:CLA:H162	1.56	0.46
29:R:603:CLA:H92	29:R:603:CLA:H62	1.72	0.46
48:R:607:CHL:HBB1	48:R:607:CHL:HHC	1.96	0.46
28:a:403:CL:CL	5:d:317:LYS:HD3	2.52	0.46
2:b:155:ALA:HB2	2:b:203:ILE:HG12	1.97	0.46
2:b:181:VAL:HG21	2:b:195:PRO:HB2	1.95	0.46
29:b:608:CLA:H92	33:b:622:LMG:H202	1.96	0.46
29:b:608:CLA:HBA2	29:b:608:CLA:H3A	1.55	0.46
29:b:611:CLA:HAB	45:h:101:RRX:O2	2.15	0.46
4:c:192:THR:HG21	55:y:626:PTY:H122	1.97	0.46
4:c:217:ASN:ND2	4:c:220:ASP:OD2	2.39	0.46
1:A1:115:VAL:O	1:A1:119:PHE:N	2.44	0.46
2:B1:41:GLU:HA	2:B1:44:VAL:HG12	1.97	0.46
2:B1:246:PHE:HA	2:B1:249:ALA:HB3	1.97	0.46
29:B1:610:CLA:H112	29:B1:610:CLA:H151	1.49	0.46
29:C1:512:CLA:H61	29:C1:512:CLA:H92	1.72	0.46
8:H1:29:LEU:HD21	22:R1:200:VAL:HA	1.96	0.46
14:O1:108:CYS:HB2	14:O1:295:TYR:HB3	1.98	0.46
14:O1:157:PHE:CZ	14:O1:159:GLU:HB2	2.51	0.46
21:G1:96:ILE:HD11	21:G1:214:PHE:CD2	2.50	0.46
22:R1:93:ASP:O	22:R1:99:ASN:ND2	2.43	0.46
1:a1:155:THR:HG22	1:a1:160:ILE:HG12	1.96	0.46
1:a1:335:ASN:O	4:c1:323:THR:OG1	2.32	0.46
1:a1:344:ALA:HB1	4:c1:345:ARG:HH11	1.78	0.46
30:a1:408:PHO:HAB	5:d1:205:LEU:HD13	1.98	0.46
2:b1:319:PRO:HA	2:b1:446:SER:H	1.81	0.46
4:c1:70:TYR:OH	4:c1:382:GLU:OE1	2.27	0.46
18:x1:81:VAL:O	18:x1:85:ALA:N	2.45	0.46
48:y1:607:CHL:HBB2	48:y1:609:CHL:HBC1	1.96	0.46
29:C:501:CLA:H142	29:C:501:CLA:H112	1.80	0.46
20:N:87:GLU:HA	20:N:181:LEU:HD21	1.96	0.46
21:G:229:LEU:HD22	49:G:620:LUT:H172	1.96	0.46
24:Y:105:ILE:HG23	24:Y:234:ILE:HD11	1.98	0.46
25:U:95:LEU:HA	25:U:107:LYS:HZ3	1.80	0.46
29:a:405:CLA:H112	29:a:406:CLA:HBB1	1.96	0.46
47:i:101:4RF:H16	47:i:101:4RF:H84	1.97	0.46
50:n:622:XAT:H31	50:n:622:XAT:H391	1.64	0.46
21:g:149:GLN:NE2	48:g:607:CHL:OMC	2.45	0.46
21:g:217:GLN:O	21:g:221:THR:OG1	2.27	0.46
1:A1:331:MET:HE3	5:D1:321:LEU:HA	1.98	0.46
1:A1:333:GLU:HB3	1:A1:336:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D1:213:ILE:HB	5:D1:253:TRP:HH2	1.81	0.46
6:E1:52:PRO:HA	6:E1:55:TYR:CE2	2.50	0.46
20:N1:158:VAL:O	20:N1:162:GLY:N	2.47	0.46
21:G1:97:LEU:HD21	21:G1:214:PHE:CZ	2.49	0.46
48:G1:601:CHL:HED3	40:G1:624:LHG:H142	1.98	0.46
29:R1:609:CLA:H102	29:R1:609:CLA:H62	1.62	0.46
24:Y1:104:ILE:HG23	24:Y1:124:TRP:CD1	2.51	0.46
29:Y1:613:CLA:CHB	29:Y1:614:CLA:HMD3	2.44	0.46
2:b1:184:SER:HB3	2:b1:188:GLU:HG2	1.98	0.46
4:c1:237:ILE:HG22	32:c1:526:SQD:H101	1.98	0.46
5:d1:25:ASP:N	5:d1:25:ASP:OD1	2.44	0.46
23:s1:85:TYR:HE1	48:s1:601:CHL:HAA2	1.79	0.46
24:y1:108:GLU:HB3	24:y1:234:ILE:HD13	1.97	0.46
29:y1:602:CLA:H61	49:y1:621:LUT:H371	1.96	0.46
1:A:279:PRO:HG2	5:D:212:ALA:HB2	1.97	0.46
33:C:523:LMG:H442	34:Y:625:SPH:H92	1.97	0.46
6:E:11:SER:O	6:E:15:THR:OG1	2.25	0.46
6:E:38:VAL:HG11	7:F:39:MET:HB3	1.97	0.46
20:N:235:LEU:HD22	49:N:620:LUT:H163	1.97	0.46
48:N:605:CHL:HAA1	38:S:626:3PH:H3C2	1.96	0.46
29:N:610:CLA:H52	49:N:620:LUT:H28	1.97	0.46
29:a:406:CLA:H52	43:d:405:PL9:H151	1.98	0.46
29:b:608:CLA:H112	29:b:608:CLA:H152	1.51	0.46
31:b:618:BCR:HC32	33:b:622:LMG:H342	1.98	0.46
43:d:405:PL9:H513	16:t:10:LEU:HD22	1.97	0.46
15:p:91:TRP:CZ2	15:p:114:ASN:HB3	2.50	0.46
20:n:229:LYS:HB3	20:n:233:GLU:HG3	1.96	0.46
4:C1:373:GLN:OE1	4:C1:374:PRO:HD2	2.15	0.46
5:D1:188:PHE:HA	5:D1:326:ARG:HD3	1.97	0.46
20:N1:212:LEU:HD21	29:N1:611:CLA:HAC2	1.97	0.46
29:a1:406:CLA:HMD3	5:d1:201:VAL:HG21	1.98	0.46
4:c1:77:LEU:O	4:c1:81:ALA:N	2.41	0.46
5:d1:29:PHE:O	5:d1:128:ARG:NH1	2.48	0.46
20:n1:96:ALA:O	20:n1:100:ALA:N	2.46	0.46
21:g1:232:HIS:CG	29:g1:613:CLA:HAA2	2.50	0.46
29:y1:612:CLA:HED2	29:y1:612:CLA:H12	1.98	0.46
2:B:103:LEU:HD21	29:B:606:CLA:HMC3	1.97	0.46
37:C:519:DGD:HB72	33:C:521:LMG:H401	1.97	0.46
20:N:201:GLU:OE1	20:N:205:LYS:NZ	2.48	0.46
5:d:129:GLN:HE22	5:d:146:PHE:HB2	1.80	0.46
14:o:109:MET:HB3	14:o:140:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:258:LEU:O	5:D1:128:ARG:NH1	2.42	0.46
29:A1:410:CLA:H142	33:A1:413:LMG:H141	1.98	0.46
4:C1:63:PHE:HZ	4:C1:93:VAL:HG21	1.79	0.46
29:C1:506:CLA:H152	29:C1:506:CLA:H111	1.66	0.46
43:D1:405:PL9:H302	40:L1:101:LHG:H162	1.96	0.46
6:E1:51:ARG:HG2	6:E1:54:GLU:CD	2.41	0.46
33:H1:102:LMG:H182	33:H1:102:LMG:H152	1.62	0.46
47:I1:102:4RF:H38	47:I1:102:4RF:H54	1.98	0.46
20:N1:160:LEU:CD1	51:N1:623:NEX:H15	2.42	0.46
2:b1:258:TYR:HB2	8:h1:68:TYR:OH	2.15	0.46
2:b1:273:TYR:OH	5:d1:164:GLN:O	2.30	0.46
29:b1:604:CLA:H18	8:h1:61:LEU:HD12	1.98	0.46
29:c1:503:CLA:H61	29:c1:503:CLA:H41	1.54	0.46
15:p1:99:VAL:HG12	15:p1:101:SER:H	1.80	0.46
15:p1:176:GLU:O	15:p1:184:TYR:N	2.46	0.46
20:n1:101:LEU:HG	29:n1:604:CLA:HAC1	1.98	0.46
23:s1:52:TRP:CD2	23:s1:233:VAL:HG11	2.51	0.46
1:A:143:ILE:HG13	5:D:220:ASN:OD1	2.15	0.46
2:B:26:HIS:CE1	29:B:613:CLA:HMA3	2.51	0.46
29:C:510:CLA:H61	29:C:510:CLA:H102	1.70	0.46
5:D:172:SER:HB2	5:D:177:SER:HB2	1.96	0.46
5:D:191:TRP:CE3	5:D:289:LEU:HD11	2.50	0.46
21:G:171:ASP:OD1	21:G:171:ASP:N	2.49	0.46
55:Y:626:PTY:H391	55:Y:626:PTY:H443	1.97	0.46
25:U:95:LEU:HD21	25:U:115:ASN:HD21	1.80	0.46
4:c:177:TRP:HE1	4:c:283:THR:HB	1.80	0.46
33:c:521:LMG:H121	39:j:101:DGA:HB31	1.98	0.46
50:g:622:XAT:H15	50:g:622:XAT:H201	1.66	0.46
29:r:609:CLA:H93	29:r:609:CLA:HBB1	1.97	0.46
48:y:601:CHL:H62	40:y:624:LHG:H162	1.97	0.46
1:A1:297:LEU:HD22	4:C1:416:THR:HG21	1.98	0.46
30:A1:408:PHO:H192	30:A1:408:PHO:H162	1.80	0.46
4:C1:267:VAL:HA	4:C1:270:MET:HE2	1.97	0.46
4:C1:321:GLY:HA2	4:C1:327:LYS:HB2	1.96	0.46
20:N1:157:GLN:HE22	48:N1:606:CHL:HMA2	1.81	0.46
1:a1:93:PHE:HZ	29:a1:410:CLA:HAA1	1.80	0.46
29:a1:405:CLA:H141	29:a1:405:CLA:H162	1.81	0.46
2:b1:143:LEU:HD11	29:b1:606:CLA:H192	1.97	0.46
4:c1:120:HIS:HA	4:c1:124:GLY:HA3	1.96	0.46
29:n1:602:CLA:CBB	49:n1:621:LUT:H32	2.45	0.46
24:y1:58:PRO:HG2	24:y1:61:LEU:HD12	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:y1:200:ALA:HA	24:y1:203:GLU:HB3	1.98	0.46
4:C:50:PHE:HE2	11:K:28:ILE:HB	1.80	0.46
4:C:150:GLY:O	4:C:154:ILE:HG13	2.15	0.46
8:H:55:LEU:HD12	8:H:56:LEU:HD23	1.97	0.46
15:P:128:ILE:HA	15:P:131:TYR:HD2	1.79	0.46
29:c:504:CLA:HMD2	33:c:521:LMG:H292	1.98	0.46
29:s:613:CLA:H52	29:s:613:CLA:H11	1.73	0.46
29:y:612:CLA:H193	29:y:612:CLA:H162	1.73	0.46
1:A1:134:SER:HA	5:D1:252:PHE:CZ	2.51	0.46
1:A1:212:SER:HB2	5:D1:211:CYS:HB2	1.97	0.46
1:A1:303:ASN:OD1	4:C1:403:ASN:N	2.48	0.46
29:B1:610:CLA:HBA2	29:B1:610:CLA:H3A	1.40	0.46
5:D1:230:ASN:HD22	5:D1:233:ARG:HD3	1.81	0.46
40:L1:101:LHG:H241	40:L1:101:LHG:HC81	1.98	0.46
29:G1:613:CLA:HMB2	49:G1:620:LUT:H7	1.97	0.46
22:R1:73:PHE:HB3	29:R1:602:CLA:HMD3	1.97	0.46
38:S1:626:3PH:H351	38:S1:626:3PH:H321	1.76	0.46
24:Y1:162:MET:HA	24:Y1:165:ALA:HB3	1.97	0.46
2:b1:406:LEU:HD22	2:b1:409:LEU:HD12	1.98	0.46
4:c1:201:ILE:O	4:c1:211:TRP:NE1	2.48	0.46
5:d1:43:PHE:HD2	5:d1:117:HIS:CE1	2.34	0.46
21:g1:65:THR:OG1	48:y1:609:CHL:O1A	2.25	0.46
49:g1:621:LUT:H401	49:g1:621:LUT:H35	1.66	0.46
24:y1:197:ASP:OD1	24:y1:197:ASP:N	2.48	0.46
1:A:38:ILE:O	1:A:42:LEU:HG	2.16	0.46
1:A:127:MET:SD	4:C:430:LEU:HD11	2.56	0.46
2:B:23:HIS:ND1	29:B:616:CLA:OBD	2.47	0.46
2:B:134:ASP:OD2	8:H:36:GLU:N	2.49	0.46
29:B:603:CLA:H151	29:B:603:CLA:H112	1.80	0.46
29:B:609:CLA:H3A	29:B:609:CLA:HBA2	1.63	0.46
31:D:404:BCR:H373	7:F:33:LEU:HD21	1.96	0.46
14:O:171:LYS:HE3	14:O:177:TYR:CE1	2.45	0.46
48:N:601:CHL:HBB1	48:N:601:CHL:HHC	1.96	0.46
50:G:622:XAT:H191	50:G:622:XAT:H11	1.79	0.46
22:R:243:GLY:O	22:R:247:MET:HG3	2.16	0.46
29:R:608:CLA:H61	29:R:608:CLA:H41	1.74	0.46
49:Y:621:LUT:H35	49:Y:621:LUT:H401	1.79	0.46
33:c:521:LMG:H162	39:j:101:DGA:HB81	1.98	0.46
21:g:96:ILE:HD11	21:g:214:PHE:CD2	2.50	0.46
21:g:208:MET:HB2	29:g:602:CLA:HMC2	1.98	0.46
21:g:212:LEU:HD11	29:g:603:CLA:HAB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:231:ASP:O	21:g:239:ASN:ND2	2.48	0.46
33:C1:523:LMG:HC5	29:Y1:611:CLA:H3A	1.97	0.46
24:Y1:95:ARG:NH2	24:Y1:208:GLU:OE2	2.42	0.46
1:a1:317:TRP:HE1	5:d1:77:ALA:HB3	1.80	0.46
2:b1:162:PHE:O	37:b1:623:DGD:O2E	2.30	0.46
31:b1:618:BCR:H15C	31:b1:618:BCR:H351	1.58	0.46
4:c1:72:GLN:HG3	4:c1:74:LEU:HD21	1.98	0.46
4:c1:83:LEU:HD13	4:c1:166:LYS:NZ	2.31	0.46
49:n1:621:LUT:H11	49:n1:621:LUT:H191	1.80	0.46
2:B:370:LEU:HB2	2:B:379:ALA:HB3	1.98	0.46
15:P:203:GLN:NE2	15:P:220:GLN:OE1	2.38	0.46
29:a:406:CLA:HBA2	29:a:406:CLA:H3A	1.61	0.46
2:b:344:ALA:HA	2:b:400:THR:O	2.15	0.46
4:c:41:HIS:ND1	29:c:509:CLA:H141	2.31	0.46
29:c:505:CLA:H91	29:c:505:CLA:H111	1.79	0.46
21:g:84:ILE:HD11	48:g:609:CHL:CGD	2.45	0.46
29:B1:611:CLA:H112	29:B1:611:CLA:H72	1.65	0.46
4:C1:175:ASP:HB3	4:C1:178:ALA:HB2	1.97	0.46
4:C1:332:SER:OG	4:C1:335:GLY:N	2.49	0.46
29:C1:513:CLA:H72	31:C1:514:BCR:H23C	1.97	0.46
5:D1:88:SER:O	5:D1:167:TRP:NE1	2.49	0.46
18:X1:76:LEU:O	18:X1:80:ALA:N	2.45	0.46
22:R1:250:PHE:O	22:R1:254:GLY:N	2.45	0.46
29:S1:604:CLA:HBB1	49:S1:621:LUT:H181	1.98	0.46
29:S1:610:CLA:HBA2	29:S1:610:CLA:H3A	1.45	0.46
24:Y1:142:ASN:OD1	24:Y1:144:ASN:ND2	2.49	0.46
1:a1:254:TYR:CD2	5:d1:138:LEU:HD13	2.51	0.46
4:c1:107:LEU:HD11	31:c1:517:BCR:HC41	1.98	0.46
7:f1:23:HIS:HB3	7:f1:27:VAL:HG23	1.98	0.46
20:n1:123:TRP:HE1	20:n1:224:ALA:HB2	1.81	0.46
21:g1:163:GLY:HA2	48:g1:608:CHL:HAC1	1.97	0.46
50:g1:622:XAT:H15	50:g1:622:XAT:H201	1.77	0.46
53:r1:626:ERG:H212	53:r1:626:ERG:H162	1.79	0.46
23:s1:208:ASP:HB3	23:s1:211:TYR:HB2	1.98	0.46
23:s1:241:LEU:HA	40:s1:624:LHG:H252	1.98	0.46
25:u1:98:ASP:OD2	25:u1:105:THR:OG1	2.27	0.46
29:B:612:CLA:H112	29:B:612:CLA:H72	1.66	0.46
4:C:264:LEU:HD21	29:C:508:CLA:CAB	2.46	0.46
6:E:13:ILE:HG21	44:F:101:HEM:HAD2	1.97	0.46
49:R:620:LUT:H11	49:R:620:LUT:H191	1.76	0.46
24:Y:216:MET:SD	29:Y:602:CLA:HAB	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:107:LYS:HD2	25:U:108:GLU:HG3	1.98	0.46
2:b:441:GLY:HA2	14:o:230:ALA:HB3	1.97	0.46
29:b:602:CLA:H2	29:b:602:CLA:H8	1.97	0.46
29:b:607:CLA:H92	29:b:607:CLA:H61	1.74	0.46
29:c:501:CLA:C1D	29:c:503:CLA:H51	2.46	0.46
14:o:274:GLN:HE21	14:o:290:ILE:HD12	1.80	0.46
22:r:252:GLY:HA2	22:r:255:ILE:HG12	1.98	0.46
23:s:58:LYS:HE3	40:s:624:LHG:HC11	1.97	0.46
1:A1:204:GLY:O	1:A1:208:GLY:N	2.46	0.46
33:A1:413:LMG:H422	29:C1:505:CLA:H142	1.98	0.46
2:B1:223:ILE:HD11	22:R1:85:LEU:HB2	1.98	0.46
31:C1:514:BCR:H351	31:C1:514:BCR:H15C	1.68	0.46
29:N1:603:CLA:H61	29:Y1:602:CLA:H91	1.98	0.46
23:S1:178:ALA:O	23:S1:182:PHE:N	2.39	0.46
24:Y1:159:VAL:HA	48:Y1:609:CHL:HBB2	1.97	0.46
48:Y1:606:CHL:H71	29:r1:610:CLA:H121	1.98	0.46
1:a1:61:ASP:HB2	1:a1:63:ILE:HG12	1.98	0.46
2:b1:453:PHE:CZ	5:d1:293:LEU:HG	2.51	0.46
29:b1:608:CLA:H101	29:b1:608:CLA:H61	1.60	0.46
4:c1:333:PRO:HB3	14:o1:135:ARG:HD2	1.97	0.46
37:c1:519:DGD:HB72	33:c1:521:LMG:H401	1.97	0.46
20:n1:212:LEU:HD13	29:n1:611:CLA:HBC1	1.97	0.46
21:g1:226:VAL:HA	21:g1:229:LEU:HG	1.98	0.46
48:s1:606:CHL:HBA1	48:s1:606:CHL:H3A	1.78	0.46
1:A:15:ALA:O	1:A:19:GLU:HG3	2.16	0.46
30:A:409:PHO:HMC2	5:D:279:LEU:HD21	1.98	0.46
29:B:603:CLA:H61	29:B:603:CLA:H92	1.75	0.46
29:B:603:CLA:H202	33:H:102:LMG:H371	1.98	0.46
4:C:333:PRO:HB3	14:O:135:ARG:HG3	1.97	0.46
40:Y:624:LHG:HC12	34:Y:625:SPH:HN21	1.81	0.46
33:a:413:LMG:H291	4:c:205:PRO:HD3	1.98	0.46
4:c:320:GLN:HA	4:c:326:GLY:HA2	1.97	0.46
40:g:624:LHG:H202	50:y:622:XAT:H12	1.98	0.46
29:y:614:CLA:H62	29:y:614:CLA:H2	1.66	0.46
1:A1:200:PHE:HZ	37:C1:520:DGD:HBN2	1.81	0.46
29:B1:602:CLA:H142	29:B1:602:CLA:H111	1.75	0.46
29:C1:511:CLA:H162	31:C1:517:BCR:H19C	1.96	0.46
33:H1:102:LMG:H112	33:H1:102:LMG:H141	1.80	0.46
20:N1:103:MET:SD	49:N1:621:LUT:H8	2.56	0.46
21:G1:93:ALA:O	21:G1:97:LEU:HD23	2.16	0.46
29:G1:611:CLA:H141	29:G1:611:CLA:H162	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y1:604:CLA:NB	51:Y1:623:NEX:H242	2.31	0.46
1:a1:334:ARG:NH2	5:d1:317:LYS:HA	2.30	0.46
1:a1:343:LEU:HD12	4:c1:301:GLN:HG3	1.98	0.46
2:b1:9:HIS:HB2	29:b1:612:CLA:HAA2	1.98	0.46
29:c1:505:CLA:HBA2	29:c1:505:CLA:H3A	1.54	0.46
50:n1:622:XAT:H391	50:n1:622:XAT:H31	1.63	0.46
29:r1:612:CLA:H3A	29:r1:612:CLA:HBA1	1.67	0.46
49:s1:621:LUT:H11	49:s1:621:LUT:H191	1.74	0.46
29:y1:602:CLA:CBB	49:y1:621:LUT:H32	2.46	0.46
2:B:74:SER:HA	2:B:92:SER:HB2	1.98	0.45
2:B:273:TYR:O	2:B:277:GLN:HG2	2.15	0.45
2:B:331:ASN:O	2:B:439:SER:OG	2.34	0.45
20:N:190:LEU:HD13	49:N:620:LUT:H222	1.98	0.45
21:G:164:GLY:HA3	21:G:170:ASP:HA	1.99	0.45
22:R:167:LYS:HD2	48:R:607:CHL:HED2	1.97	0.45
29:S:603:CLA:O2A	29:S:609:CLA:H2	2.15	0.45
29:S:604:CLA:HBB1	49:S:621:LUT:H181	1.97	0.45
29:a:410:CLA:H2	9:i:12:VAL:HG11	1.96	0.45
29:b:614:CLA:H62	29:b:614:CLA:H41	1.83	0.45
4:c:393:ASN:HB2	4:c:395:VAL:HG23	1.97	0.45
29:d:403:CLA:H61	29:d:403:CLA:H41	1.48	0.45
1:A1:96:ILE:HG13	1:A1:105:TRP:CE2	2.52	0.45
29:B1:603:CLA:H42	8:H1:68:TYR:HD2	1.80	0.45
29:B1:614:CLA:H142	29:B1:614:CLA:H112	1.72	0.45
15:P1:101:SER:HB3	15:P1:121:GLN:H	1.81	0.45
49:G1:621:LUT:H362	48:Y1:609:CHL:H11	1.99	0.45
24:Y1:77:SER:HB2	24:Y1:83:PHE:CD1	2.51	0.45
1:a1:196:PRO:HA	1:a1:199:MET:HB2	1.98	0.45
29:a1:405:CLA:H2	30:a1:408:PHO:CHC	2.45	0.45
5:d1:213:ILE:HD13	43:d1:405:PL9:H121	1.97	0.45
18:x1:69:LEU:HD23	18:x1:73:LEU:HD23	1.98	0.45
29:g1:603:CLA:HAC1	48:g1:607:CHL:HBB2	1.97	0.45
48:g1:606:CHL:HBB1	48:g1:606:CHL:HHC	1.97	0.45
29:s1:604:CLA:NB	51:s1:623:NEX:H242	2.32	0.45
30:A:408:PHO:H2	30:A:408:PHO:H61	1.60	0.45
14:O:133:LEU:HD12	14:O:169:THR:HG22	1.97	0.45
48:G:607:CHL:H13	48:G:607:CHL:H102	1.81	0.45
29:S:611:CLA:H192	29:S:611:CLA:H162	1.76	0.45
18:x:70:LYS:O	18:x:74:LEU:HG	2.15	0.45
20:n:248:PHE:CE2	21:g:142:ILE:HG12	2.51	0.45
48:n:606:CHL:HMB1	48:n:609:CHL:HMC	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:s:607:CHL:HHC	48:s:607:CHL:HBB1	1.98	0.45
1:A1:321:ILE:O	1:A1:325:ASN:N	2.50	0.45
2:B1:53:ASN:ND2	2:B1:58:GLN:HE21	2.13	0.45
2:B1:326:ARG:HB3	2:B1:444:ARG:HG2	1.97	0.45
29:B1:608:CLA:H41	29:B1:608:CLA:H62	1.52	0.45
5:D1:328:TRP:C	5:D1:329:MET:HE2	2.42	0.45
48:N1:601:CHL:C4D	40:N1:624:LHG:HC91	2.47	0.45
29:N1:610:CLA:H51	49:N1:620:LUT:H30	1.97	0.45
2:b1:357:ARG:NH1	25:u1:101:ALA:O	2.48	0.45
29:b1:609:CLA:HMD2	29:b1:610:CLA:H51	1.97	0.45
29:b1:614:CLA:H71	29:b1:614:CLA:H112	1.83	0.45
32:b1:626:SQD:H131	32:b1:626:SQD:H162	1.72	0.45
4:c1:110:SER:O	4:c1:114:GLY:N	2.50	0.45
5:d1:286:VAL:HA	5:d1:289:LEU:HB2	1.98	0.45
33:h1:102:LMG:H182	33:h1:102:LMG:H152	1.71	0.45
20:n1:150:ILE:HD11	48:n1:607:CHL:HAC1	1.98	0.45
48:g1:601:CHL:H13	50:y1:622:XAT:H10	1.98	0.45
29:g1:613:CLA:H2	29:g1:614:CLA:HMD2	1.98	0.45
1:A:36:ILE:HA	29:A:410:CLA:HBB2	1.98	0.45
32:A:412:SQD:H321	29:C:504:CLA:H201	1.97	0.45
29:B:610:CLA:H62	29:B:610:CLA:H41	1.72	0.45
15:P:98:GLU:HG3	15:P:99:VAL:HG23	1.98	0.45
23:S:85:TYR:OH	48:S:601:CHL:O2A	2.33	0.45
24:Y:166:GLU:OE1	24:Y:169:ARG:NH2	2.34	0.45
1:a:232:SER:HB2	2:b:4:PRO:HG3	1.98	0.45
29:b:604:CLA:H91	29:b:604:CLA:H112	1.77	0.45
7:f:23:HIS:HE1	44:f:101:HEM:NB	2.14	0.45
23:s:188:GLY:HA3	23:s:204:PHE:HE2	1.81	0.45
24:y:171:ASN:OD1	24:y:173:GLU:HB3	2.16	0.45
29:y:614:CLA:H8	55:y:626:PTY:H411	1.99	0.45
1:A1:28:LEU:HB2	38:T1:101:3PH:H222	1.98	0.45
1:A1:341:LEU:HD23	15:P1:224:LYS:HD2	1.99	0.45
2:B1:281:GLN:OE1	25:U1:102:LYS:HE2	2.17	0.45
2:B1:281:GLN:HE22	25:U1:102:LYS:HG3	1.81	0.45
5:D1:221:THR:HB	5:D1:244:TYR:HB2	1.97	0.45
29:N1:602:CLA:H152	29:N1:602:CLA:H112	1.68	0.45
21:G1:33:TYR:CZ	21:G1:194:ALA:HB1	2.51	0.45
21:G1:213:GLY:O	21:G1:217:GLN:HG2	2.16	0.45
23:S1:280:LEU:HA	23:S1:280:LEU:HD23	1.84	0.45
30:a1:409:PHO:HAB	29:d1:402:CLA:H43	1.98	0.45
4:c1:177:TRP:CD1	4:c1:355:GLU:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c1:514:BCR:HC7	19:z1:55:GLY:HA3	1.98	0.45
5:d1:22:LEU:HA	5:d1:26:ARG:HH22	1.82	0.45
5:d1:210:LEU:HD13	5:d1:271:MET:HA	1.98	0.45
29:d1:403:CLA:H52	18:x1:79:GLY:HA3	1.97	0.45
49:n1:621:LUT:H35	49:n1:621:LUT:H401	1.75	0.45
48:g1:601:CHL:HHB	48:y1:609:CHL:HMB3	1.97	0.45
49:g1:620:LUT:H401	49:g1:620:LUT:H35	1.68	0.45
49:r1:620:LUT:H11	49:r1:620:LUT:H191	1.69	0.45
1:A:332:HIS:HA	28:A:403:CL:CL	2.53	0.45
29:A:406:CLA:HBA1	40:L:101:LHG:H221	1.99	0.45
37:B:623:DGD:O5E	37:B:623:DGD:O4E	2.27	0.45
29:C:513:CLA:H42	48:S:601:CHL:HHC	1.99	0.45
8:H:39:LYS:NZ	22:R:84:SEP:O1P	2.49	0.45
48:G:601:CHL:H92	50:Y:622:XAT:H14	1.98	0.45
29:b:615:CLA:H141	29:b:615:CLA:H161	1.80	0.45
12:l:20:TRP:CE3	40:l:101:LHG:H141	2.51	0.45
14:o:228:LEU:HG	14:o:231:LYS:HB2	1.98	0.45
14:o:259:VAL:HG12	14:o:266:ILE:HG22	1.97	0.45
49:g:620:LUT:H31	49:g:620:LUT:H391	1.76	0.45
23:s:186:GLY:HA2	48:s:608:CHL:HMC	1.99	0.45
29:A1:405:CLA:H3A	29:A1:405:CLA:HBA1	1.56	0.45
4:C1:51:TRP:HE1	29:C1:504:CLA:C2C	2.29	0.45
4:C1:55:MET:HA	4:C1:58:PHE:HB3	1.98	0.45
10:J1:18:VAL:O	10:J1:22:LEU:HG	2.16	0.45
19:Z1:12:LEU:O	19:Z1:16:SER:OG	2.33	0.45
23:S1:258:GLU:OE2	23:S1:274:TYR:OH	2.28	0.45
1:a1:180:PHE:CE1	5:d1:192:THR:HG21	2.50	0.45
1:a1:199:MET:HB3	37:c1:520:DGD:HAE1	1.98	0.45
2:b1:51:VAL:HG23	2:b1:52:LEU:HD12	1.99	0.45
2:b1:249:ALA:HA	2:b1:252:VAL:HG12	1.98	0.45
2:b1:323:GLY:N	2:b1:326:ARG:HD2	2.31	0.45
29:b1:617:CLA:H61	51:r1:622:NEX:H163	1.98	0.45
32:b1:626:SQD:H151	32:b1:626:SQD:H182	1.66	0.45
4:c1:119:TYR:OH	23:s1:64:GLY:HA3	2.15	0.45
48:n1:607:CHL:H8	48:n1:609:CHL:H202	1.97	0.45
24:y1:228:VAL:HG22	24:y1:256:PHE:HE2	1.81	0.45
2:B:341:LEU:HD21	2:B:431:GLU:HB3	1.98	0.45
29:B:608:CLA:H201	13:M:11:THR:HA	1.98	0.45
29:B:614:CLA:H43	40:D:408:LHG:H383	1.97	0.45
29:C:508:CLA:HMD2	40:D:410:LHG:H101	1.99	0.45
21:G:142:ILE:HA	21:G:145:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:G:620:LUT:H15	49:G:620:LUT:H201	1.85	0.45
22:R:236:LYS:HG3	29:R:610:CLA:HMA3	1.98	0.45
24:Y:91:LEU:HB3	24:Y:183:LEU:HD11	1.99	0.45
1:a:265:PHE:HB3	1:a:271:LEU:HB2	1.99	0.45
1:a:323:ARG:NH1	15:p:110:PHE:O	2.50	0.45
40:y:624:LHG:H351	40:y:624:LHG:H383	1.74	0.45
29:A1:410:CLA:H102	17:W1:74:PHE:HE2	1.82	0.45
2:B1:469:HIS:O	2:B1:473:THR:OG1	2.28	0.45
3:V1:22:VAL:HG13	19:Z1:25:VAL:HG23	1.98	0.45
39:C1:524:DGA:HAH1	39:C1:524:DGA:HAT2	1.48	0.45
29:R1:610:CLA:H92	29:R1:610:CLA:H61	1.83	0.45
4:c1:132:TYR:O	4:c1:136:GLY:N	2.50	0.45
38:t1:101:3PH:H2H1	38:t1:101:3PH:H2C1	1.97	0.45
29:n1:602:CLA:H72	49:n1:621:LUT:H30	1.98	0.45
40:n1:624:LHG:HC82	50:g1:622:XAT:H361	1.98	0.45
2:B:242:ILE:HA	2:B:245:VAL:HG12	1.99	0.45
5:D:193:LEU:O	12:L:35:TYR:OH	2.27	0.45
2:b:327:THR:HG22	29:b:608:CLA:H11	1.98	0.45
2:b:434:ARG:HG2	2:b:439:SER:HB2	1.99	0.45
29:b:603:CLA:H41	29:b:603:CLA:H61	1.67	0.45
29:b:608:CLA:H62	29:b:608:CLA:H41	1.55	0.45
31:b:619:BCR:H391	32:b:626:SQD:H321	1.99	0.45
4:c:152:HIS:ND1	29:c:507:CLA:OBD	2.35	0.45
4:c:329:LEU:HD12	4:c:337:ILE:HG22	1.98	0.45
33:c:523:LMG:HC91	29:y:611:CLA:H11	1.97	0.45
5:d:213:ILE:HA	5:d:213:ILE:HD12	1.83	0.45
8:h:67:ILE:HG13	8:h:72:LEU:HD23	1.98	0.45
12:l:13:LEU:N	13:m:29:THR:OG1	2.46	0.45
15:p:116:VAL:HG23	15:p:219:VAL:HG22	1.99	0.45
15:p:128:ILE:HD12	15:p:185:TYR:CD2	2.51	0.45
15:p:231:ASP:OD1	15:p:231:ASP:N	2.49	0.45
22:r:103:ASP:OD1	22:r:103:ASP:N	2.50	0.45
29:r:608:CLA:H93	29:r:608:CLA:H111	1.80	0.45
29:r:610:CLA:H92	49:r:620:LUT:H371	1.99	0.45
29:s:610:CLA:HBA2	29:s:610:CLA:H3A	1.61	0.45
24:y:95:ARG:HA	24:y:98:LEU:HD12	1.99	0.45
1:A1:9:GLU:OE1	1:A1:11:THR:OG1	2.31	0.45
11:K1:26:PRO:O	11:K1:29:PRO:HD2	2.16	0.45
49:G1:621:LUT:H15	49:G1:621:LUT:H201	1.77	0.45
24:Y1:191:PRO:HD2	49:Y1:620:LUT:H23	1.98	0.45
2:b1:29:LEU:HD21	29:b1:615:CLA:HBB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:239:SER:HA	2:b1:242:ILE:HB	1.99	0.45
2:b1:387:GLU:HA	15:p1:146:GLY:HA3	1.98	0.45
29:b1:606:CLA:H162	29:b1:606:CLA:H141	1.80	0.45
31:c1:516:BCR:HC21	19:z1:13:VAL:HG13	1.99	0.45
5:d1:277:THR:HG23	40:d1:408:LHG:H282	1.98	0.45
20:n1:148:GLN:O	55:y1:626:PTY:N1	2.49	0.45
50:g1:622:XAT:H391	50:g1:622:XAT:H31	1.64	0.45
51:s1:623:NEX:H11	51:s1:623:NEX:H191	1.76	0.45
29:B:605:CLA:HBB1	29:B:614:CLA:C2C	2.47	0.45
5:D:98:GLN:HB2	6:E:73:LEU:HD22	1.99	0.45
5:D:266:TRP:CD1	40:D:409:LHG:HC32	2.52	0.45
20:N:119:GLU:O	20:N:125:LYS:HG3	2.17	0.45
29:G:602:CLA:H122	29:Y:603:CLA:H143	1.99	0.45
23:S:112:MET:CE	29:S:610:CLA:HAB	2.46	0.45
2:b:464:PHE:HB2	5:d:280:TRP:CZ2	2.52	0.45
31:b:618:BCR:H342	38:b:624:3PH:H271	1.99	0.45
29:c:507:CLA:H91	29:c:507:CLA:H112	1.82	0.45
15:p:136:GLU:O	15:p:139:SER:OG	2.32	0.45
29:r:603:CLA:H102	52:r:625:LMT:H51	1.98	0.45
23:s:167:ALA:O	23:s:171:ILE:HG12	2.17	0.45
48:s:608:CHL:H91	29:s:610:CLA:H162	1.99	0.45
24:y:110:LEU:HD23	24:y:115:VAL:HG21	1.99	0.45
1:A1:142:TRP:N	5:D1:220:ASN:OD1	2.49	0.45
29:B1:609:CLA:H161	29:B1:609:CLA:H193	1.74	0.45
3:V1:16:VAL:HG22	31:C1:516:BCR:H363	1.98	0.45
4:C1:47:LEU:HD11	11:K1:29:PRO:HB3	1.98	0.45
4:C1:244:PRO:HB2	4:C1:249:ARG:HH11	1.82	0.45
4:C1:318:SER:OG	14:O1:164:ASP:OD1	2.28	0.45
5:D1:103:ARG:HG2	6:E1:77:LYS:NZ	2.31	0.45
5:D1:156:VAL:HG22	5:D1:286:VAL:HG21	1.98	0.45
15:P1:191:SER:O	15:P1:201:ARG:N	2.46	0.45
20:N1:204:VAL:HA	20:N1:207:ILE:HG22	1.99	0.45
23:S1:103:ASN:O	23:S1:107:HIS:ND1	2.32	0.45
23:S1:171:ILE:HA	23:S1:174:VAL:HG22	1.98	0.45
24:Y1:160:ILE:HG13	24:Y1:161:VAL:HG13	1.99	0.45
50:Y1:622:XAT:H15	50:Y1:622:XAT:H201	1.73	0.45
2:b1:376:VAL:HG11	15:p1:97:LYS:HB2	1.99	0.45
29:b1:617:CLA:H142	29:b1:617:CLA:H112	1.82	0.45
4:c1:29:ARG:NH1	29:c1:511:CLA:OBD	2.47	0.45
29:c1:502:CLA:C1C	29:c1:510:CLA:HAB	2.47	0.45
29:n1:613:CLA:HBD	29:n1:613:CLA:HBA1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g1:245:ALA:HA	50:y1:622:XAT:H22	1.98	0.45
29:g1:613:CLA:HBB1	49:g1:620:LUT:H181	1.97	0.45
23:s1:175:LEU:HD23	48:s1:606:CHL:HMA2	1.97	0.45
23:s1:265:THR:O	23:s1:269:SER:OG	2.21	0.45
32:C:526:SQD:H311	54:S:625:LPX:H20A	1.98	0.45
15:P:206:LYS:HD3	15:P:241:PHE:HB3	1.99	0.45
29:G:602:CLA:H72	49:G:621:LUT:H30	1.99	0.45
29:R:602:CLA:H72	50:R:621:XAT:H28	1.99	0.45
23:S:231:LEU:HD23	23:S:234:LYS:HD2	1.98	0.45
24:Y:105:ILE:HD12	24:Y:234:ILE:HD11	1.99	0.45
2:b:319:PRO:HB3	2:b:446:SER:HB2	1.98	0.45
4:c:205:PRO:HA	4:c:211:TRP:HB2	1.99	0.45
4:c:431:TRP:HZ3	40:d:410:LHG:H281	1.82	0.45
21:g:85:HIS:NE2	49:g:621:LUT:H15	2.31	0.45
23:s:123:GLY:O	23:s:127:ASN:ND2	2.49	0.45
23:s:144:LEU:HD12	23:s:145:ASN:HB2	1.99	0.45
23:s:203:ILE:HG23	23:s:204:PHE:CD1	2.52	0.45
2:B1:243:ALA:HA	2:B1:246:PHE:CE1	2.52	0.45
29:B1:604:CLA:H141	29:B1:604:CLA:H161	1.69	0.45
21:G1:130:TYR:CD1	29:G1:604:CLA:H2	2.52	0.45
49:G1:621:LUT:H35	49:G1:621:LUT:H401	1.78	0.45
22:R1:149:LEU:HD23	29:R1:604:CLA:HMC2	1.98	0.45
24:Y1:139:TYR:HB3	24:Y1:145:LEU:HD23	1.99	0.45
1:a1:63:ILE:HB	4:c1:323:THR:HG21	1.99	0.45
1:a1:312:ARG:NE	15:p1:92:ASN:OD1	2.42	0.45
2:b1:378:ARG:NH1	15:p1:100:ASP:OD1	2.50	0.45
14:o1:113:SER:O	14:o1:290:ILE:HD12	2.17	0.45
50:n1:622:XAT:H34	29:y1:613:CLA:H111	1.97	0.45
29:r1:603:CLA:H102	52:r1:625:LMT:H32	1.98	0.45
1:A:49:ILE:HG12	43:D:405:PL9:H501	1.99	0.45
4:C:172:GLY:HA3	4:C:185:ARG:O	2.17	0.45
29:C:513:CLA:C4B	31:C:514:BCR:H383	2.46	0.45
5:D:201:VAL:HG22	29:D:402:CLA:C2B	2.47	0.45
6:E:14:LEU:HD12	47:K:101:4RF:H53	1.98	0.45
8:H:33:LEU:HD23	8:H:33:LEU:HA	1.81	0.45
14:O:111:PRO:HA	14:O:292:GLY:HA3	1.99	0.45
20:N:205:LYS:HG3	29:N:611:CLA:HED2	1.98	0.45
2:b:388:SER:HB2	5:d:344:GLU:CD	2.42	0.45
29:b:609:CLA:H121	39:b:625:DGA:HAG2	1.99	0.45
29:b:615:CLA:H91	32:m:101:SQD:H301	1.98	0.45
14:o:115:THR:OG1	14:o:289:LYS:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:191:ASN:OD1	1:A1:325:ASN:ND2	2.49	0.45
1:A1:206:PHE:O	1:A1:210:LEU:N	2.37	0.45
2:B1:7:ARG:HH22	2:B1:479:PHE:HE2	1.64	0.45
29:B1:602:CLA:H111	29:B1:602:CLA:H72	1.56	0.45
29:B1:603:CLA:H18	33:H1:102:LMG:H362	1.99	0.45
29:B1:617:CLA:H112	29:B1:617:CLA:H91	1.82	0.45
21:G1:44:PHE:HA	24:Y1:171:ASN:ND2	2.32	0.45
29:G1:610:CLA:H171	49:G1:620:LUT:H393	1.97	0.45
24:Y1:185:PRO:HD2	29:Y1:610:CLA:CAD	2.47	0.45
24:Y1:216:MET:HG3	29:Y1:602:CLA:HMC3	1.98	0.45
1:a1:195:HIS:CD2	1:a1:299:GLY:HA2	2.52	0.45
2:b1:370:LEU:N	2:b1:379:ALA:O	2.48	0.45
13:m1:24:ILE:HG22	13:m1:25:LEU:HD23	1.99	0.45
29:g1:603:CLA:HMD3	48:g1:609:CHL:HBA2	1.99	0.45
23:s1:80:ALA:HB1	23:s1:233:VAL:HA	1.99	0.45
23:s1:135:THR:HB	23:s1:138:GLU:HG3	1.98	0.45
2:B:134:ASP:O	2:B:138:ILE:HG13	2.16	0.45
29:B:609:CLA:H162	29:B:609:CLA:H122	1.68	0.45
29:B:610:CLA:OBD	8:H:46:THR:OG1	2.27	0.45
37:B:623:DGD:HD61	22:R:170:LEU:HD11	1.98	0.45
32:C:526:SQD:H322	32:C:526:SQD:H351	1.70	0.45
5:D:126:MET:SD	5:D:150:ILE:HD12	2.57	0.45
8:H:50:MET:HE2	8:H:54:ILE:HD11	1.99	0.45
38:T:101:3PH:H3B1	38:T:101:3PH:H2F1	1.97	0.45
29:G:603:CLA:H91	29:G:603:CLA:H111	1.82	0.45
22:R:190:ILE:HD11	47:i:101:4RF:H29	1.99	0.45
29:S:610:CLA:HBA2	29:S:610:CLA:H3A	1.49	0.45
1:a:39:PRO:HG3	9:i:15:PHE:CE2	2.52	0.45
29:c:501:CLA:H191	29:c:507:CLA:HBB1	1.99	0.45
5:d:87:HIS:CD2	5:d:166:GLY:HA2	2.52	0.45
5:d:174:GLY:O	5:d:178:ILE:HG12	2.17	0.45
5:d:218:VAL:HG13	5:d:244:TYR:CD1	2.52	0.45
29:y:610:CLA:H41	29:y:612:CLA:H2	1.98	0.45
34:A1:414:SPH:H112	47:I1:102:4RF:H40	1.99	0.45
4:C1:333:PRO:HG3	14:O1:135:ARG:HH12	1.82	0.45
14:O1:211:LEU:HD13	14:O1:216:ARG:O	2.17	0.45
20:N1:59:TYR:OH	20:N1:71:ASP:OD2	2.25	0.45
22:R1:78:LEU:HD22	50:R1:621:XAT:H23	1.98	0.45
23:S1:109:ARG:NH1	48:S1:608:CHL:OBD	2.41	0.45
24:Y1:151:ILE:HG23	24:Y1:152:LEU:HD22	1.99	0.45
1:a1:33:PHE:CE2	1:a1:128:GLY:HA3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a1:94:TYR:H	1:a1:113:GLN:HE22	1.64	0.45
1:a1:96:ILE:HG22	1:a1:105:TRP:CZ2	2.52	0.45
1:a1:307:VAL:HG11	15:p1:90:LYS:NZ	2.32	0.45
2:b1:230:SER:OG	2:b1:236:SER:OG	2.33	0.45
5:d1:68:ILE:HG22	7:f1:39:MET:HE2	1.98	0.45
5:d1:181:PHE:HA	5:d1:184:PHE:CD2	2.51	0.45
29:n1:613:CLA:H101	40:n1:624:LHG:H142	1.99	0.45
21:g1:37:ARG:NH2	21:g1:53:LEU:O	2.50	0.45
29:g1:603:CLA:HMA3	29:g1:603:CLA:H51	2.00	0.45
31:B:618:BCR:H383	32:B:621:SQD:H252	1.99	0.44
4:C:394:SER:HA	4:C:408:VAL:HG23	1.99	0.44
37:C:519:DGD:HA21	39:J:101:DGA:HA72	1.98	0.44
14:O:235:ASP:OD1	14:O:235:ASP:N	2.50	0.44
29:N:602:CLA:H112	29:N:602:CLA:H152	1.67	0.44
29:N:613:CLA:H172	29:N:613:CLA:H13	1.74	0.44
22:R:214:PRO:HD2	29:R:610:CLA:OBD	2.17	0.44
38:S:626:3PH:H371	38:S:626:3PH:H342	1.70	0.44
4:c:323:THR:O	14:o:206:ARG:NH1	2.50	0.44
5:d:103:ARG:NH2	6:e:77:LYS:HA	2.32	0.44
29:n:613:CLA:HBA1	29:n:613:CLA:HBD	1.99	0.44
5:D1:8:TYR:HD2	5:D1:10:GLU:HG2	1.81	0.44
5:D1:117:HIS:O	5:D1:121:GLY:N	2.39	0.44
5:D1:171:PRO:HG3	5:D1:181:PHE:CD2	2.52	0.44
29:R1:612:CLA:H11	29:R1:612:CLA:H52	1.70	0.44
29:S1:613:CLA:H11	29:S1:613:CLA:H52	1.69	0.44
1:a1:222:SER:HB2	1:a1:247:ASN:HB2	1.99	0.44
29:b1:609:CLA:H51	39:b1:625:DGA:HAW1	1.99	0.44
4:c1:162:LEU:HD23	29:c1:502:CLA:H172	1.99	0.44
5:d1:103:ARG:NH2	6:e1:80:SER:OG	2.50	0.44
5:d1:160:TYR:O	5:d1:164:GLN:HG2	2.17	0.44
19:z1:33:TRP:HZ3	19:z1:40:VAL:HG11	1.83	0.44
20:n1:173:PRO:HG2	48:n1:608:CHL:HBB2	1.99	0.44
29:n1:604:CLA:H122	51:n1:623:NEX:H402	1.99	0.44
50:n1:622:XAT:C32	40:y1:624:LHG:H121	2.47	0.44
22:r1:207:ASP:HB3	22:r1:210:LYS:HD3	1.99	0.44
29:r1:609:CLA:H41	29:r1:609:CLA:H93	1.99	0.44
23:s1:110:TRP:CE2	48:s1:608:CHL:HED2	2.52	0.44
23:s1:141:ALA:N	48:s1:607:CHL:O1D	2.50	0.44
1:A:27:ARG:HG3	1:A:28:LEU:HD12	1.99	0.44
29:A:410:CLA:H62	29:A:410:CLA:H102	1.64	0.44
2:B:25:MET:HE3	31:B:618:BCR:H271	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:LEU:HD23	29:B:603:CLA:HAC2	1.99	0.44
2:B:238:LEU:HD22	29:B:613:CLA:HBC3	1.99	0.44
29:B:604:CLA:H112	29:B:604:CLA:H72	1.81	0.44
29:B:616:CLA:H61	29:B:617:CLA:HBB1	2.00	0.44
29:B:617:CLA:H51	29:B:617:CLA:H11	1.74	0.44
4:C:150:GLY:HA2	4:C:236:GLY:HA2	1.98	0.44
5:D:48:TRP:NE1	5:D:52:CYS:SG	2.91	0.44
5:D:221:THR:HG21	5:D:249:ALA:HB2	1.99	0.44
20:N:248:PHE:HZ	21:G:146:LEU:HD22	1.82	0.44
29:N:602:CLA:H92	29:N:603:CLA:HMA3	2.00	0.44
50:N:622:XAT:H15	50:N:622:XAT:H201	1.68	0.44
21:G:104:GLN:HG2	21:G:105:TYR:N	2.33	0.44
29:Y:611:CLA:H41	29:Y:611:CLA:H61	1.63	0.44
1:a:188:ALA:HB2	1:a:328:MET:HB3	1.98	0.44
2:b:41:GLU:O	2:b:45:PHE:HB2	2.17	0.44
2:b:330:MET:HG2	2:b:444:ARG:HB2	1.99	0.44
48:n:606:CHL:H192	38:s:626:3PH:H281	1.99	0.44
29:n:613:CLA:H2	29:n:613:CLA:H61	1.65	0.44
2:B1:22:VAL:HB	29:B1:613:CLA:HBB1	1.97	0.44
2:B1:399:VAL:HG12	2:B1:417:VAL:HG22	2.00	0.44
29:B1:614:CLA:H41	29:B1:614:CLA:H62	1.83	0.44
4:C1:406:ASN:HB2	37:C1:520:DGD:HE2	1.98	0.44
37:C1:519:DGD:HA21	39:J1:101:DGA:HA72	1.98	0.44
5:D1:43:PHE:HB3	5:D1:113:PHE:CE2	2.53	0.44
50:N1:622:XAT:H31	50:N1:622:XAT:H391	1.68	0.44
23:S1:267:HIS:HA	23:S1:274:TYR:HB3	2.00	0.44
24:Y1:129:ALA:N	48:Y1:607:CHL:O1D	2.50	0.44
1:a1:297:LEU:HD12	1:a1:297:LEU:HA	1.85	0.44
1:a1:333:GLU:O	1:a1:334:ARG:C	2.55	0.44
31:a1:411:BCR:H15C	31:a1:411:BCR:H351	1.75	0.44
2:b1:340:TRP:CD1	2:b1:342:GLY:H	2.35	0.44
4:c1:268:SER:O	4:c1:272:PHE:N	2.48	0.44
4:c1:328:TYR:O	4:c1:340:GLY:N	2.51	0.44
11:k1:36:ALA:O	11:k1:40:GLN:HG2	2.17	0.44
50:r1:621:XAT:H35	50:r1:621:XAT:H401	1.77	0.44
24:y1:76:LEU:HB3	24:y1:86:TYR:CE2	2.52	0.44
29:B:612:CLA:H193	29:B:612:CLA:H162	1.71	0.44
4:C:166:LYS:HA	4:C:170:PHE:HB2	2.00	0.44
29:C:504:CLA:H42	37:C:519:DGD:HB32	2.00	0.44
5:D:43:PHE:HD2	5:D:113:PHE:HZ	1.64	0.44
5:D:214:HIS:ND1	43:D:405:PL9:O2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:N:622:XAT:C34	29:Y:613:CLA:H111	2.48	0.44
50:G:622:XAT:H31	50:G:622:XAT:H391	1.72	0.44
38:S:626:3PH:H2C2	38:S:626:3PH:H2F2	1.74	0.44
29:Y:614:CLA:HAB	55:Y:626:PTY:H232	1.99	0.44
50:Y:622:XAT:H11	50:Y:622:XAT:H191	1.90	0.44
1:a:67:VAL:HG22	5:d:312:GLU:HG3	1.98	0.44
21:g:92:GLY:O	21:g:96:ILE:HG12	2.17	0.44
29:r:608:CLA:HBA2	29:r:608:CLA:H3A	1.49	0.44
24:y:228:VAL:HG23	24:y:229:THR:HG23	1.99	0.44
32:A1:412:SQD:O7	5:D1:233:ARG:NH2	2.38	0.44
2:B1:389:LYS:HD3	15:P1:98:GLU:HG3	1.99	0.44
2:B1:450:TRP:HD1	29:B1:608:CLA:HHB	1.83	0.44
47:I1:102:4RF:H60	47:I1:102:4RF:H54	1.81	0.44
47:I1:102:4RF:H73	22:r1:182:PHE:CE1	2.53	0.44
14:O1:274:GLN:HG2	14:O1:275:PRO:HD2	1.98	0.44
20:N1:80:GLU:HB3	20:N1:84:ARG:NH1	2.32	0.44
50:N1:622:XAT:H15	50:N1:622:XAT:H201	1.70	0.44
29:R1:603:CLA:H102	52:R1:625:LMT:H51	2.00	0.44
24:Y1:96:TRP:HA	24:Y1:99:LEU:HB2	1.99	0.44
29:Y1:611:CLA:H43	29:Y1:612:CLA:HMD2	1.99	0.44
29:b1:615:CLA:H91	29:b1:615:CLA:H112	1.75	0.44
4:c1:104:VAL:HG11	31:c1:514:BCR:HC32	1.99	0.44
4:c1:160:ALA:HB1	4:c1:228:ILE:HG23	1.99	0.44
4:c1:417:SER:HB3	37:c1:519:DGD:HBW2	1.99	0.44
5:d1:189:HIS:O	5:d1:294:ARG:HB2	2.16	0.44
24:y1:162:MET:HA	24:y1:165:ALA:HB3	1.99	0.44
2:B:226:TYR:HA	2:B:231:MET:HG3	2.00	0.44
2:B:382:PRO:HG3	2:B:391:SER:HB2	1.98	0.44
4:C:200:TYR:HB3	4:C:212:ILE:HG22	1.99	0.44
20:N:75:LEU:HD12	29:N:602:CLA:H11	2.00	0.44
29:N:612:CLA:HAB	49:N:620:LUT:C14	2.47	0.44
21:G:198:VAL:HA	21:G:201:ILE:HG22	1.98	0.44
49:R:620:LUT:H15	49:R:620:LUT:H201	1.85	0.44
24:Y:39:SER:O	24:Y:39:SER:OG	2.33	0.44
4:c:336:GLU:HG3	14:o:72:TYR:HE1	1.82	0.44
14:o:130:THR:HB	14:o:170:VAL:HB	1.98	0.44
20:n:201:GLU:O	20:n:205:LYS:HG3	2.16	0.44
55:y:626:PTY:H321	55:y:626:PTY:H112	1.99	0.44
1:A1:42:LEU:HB3	31:A1:411:BCR:H353	1.99	0.44
2:B1:120:LEU:HG	2:B1:122:LEU:H	1.83	0.44
4:C1:49:VAL:HG23	4:C1:106:HIS:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C1:251:ALA:HB2	9:I1:24:LEU:HD12	1.99	0.44
10:J1:32:TYR:HB2	39:J1:101:DGA:HA31	1.98	0.44
11:K1:12:PRO:HG2	11:K1:15:TYR:HB2	1.98	0.44
21:G1:178:GLY:O	21:G1:182:ASP:N	2.50	0.44
1:a1:304:GLN:HG2	1:a1:313:VAL:HG11	2.00	0.44
38:b1:624:3PH:H2D1	38:b1:624:3PH:H282	1.99	0.44
6:e1:15:THR:HG23	10:j1:10:ILE:O	2.18	0.44
48:n1:608:CHL:H11	29:n1:610:CLA:HMD2	2.00	0.44
40:n1:624:LHG:H201	40:n1:624:LHG:H172	1.83	0.44
49:r1:620:LUT:H15	49:r1:620:LUT:H201	1.80	0.44
29:s1:611:CLA:H3A	29:s1:611:CLA:HBA2	1.51	0.44
29:A:410:CLA:H142	29:A:410:CLA:H111	1.86	0.44
2:B:151:PHE:HB2	2:B:206:GLY:HA3	1.99	0.44
2:B:362:PHE:HB3	5:D:188:PHE:CD2	2.53	0.44
29:B:607:CLA:H111	29:B:607:CLA:H152	1.78	0.44
14:O:112:THR:HG23	14:O:292:GLY:HA2	2.00	0.44
20:N:89:GLU:OE1	20:N:207:ILE:HD11	2.18	0.44
21:G:150:VAL:HA	48:G:609:CHL:HBB2	1.99	0.44
29:Y:602:CLA:CAB	49:Y:621:LUT:H32	2.48	0.44
2:b:469:HIS:O	2:b:473:THR:HG23	2.17	0.44
29:b:603:CLA:H91	29:b:603:CLA:H112	1.79	0.44
4:c:15:ASP:HB3	11:k:46:ARG:HG2	1.99	0.44
4:c:331:ARG:HH21	14:o:82:ASN:HA	1.83	0.44
5:d:85:LEU:HD13	5:d:90:LEU:HD11	1.99	0.44
15:p:128:ILE:O	15:p:131:TYR:HB2	2.18	0.44
21:g:88:TRP:HZ2	21:g:153:MET:HE2	1.82	0.44
29:r:603:CLA:H51	52:r:625:LMT:H102	1.99	0.44
1:A1:230:ASN:ND2	22:R1:95:ASN:OD1	2.50	0.44
2:B1:68:ARG:HG3	2:B1:267:LEU:HD22	1.99	0.44
4:C1:30:LEU:HD13	4:C1:37:LEU:HA	1.99	0.44
4:C1:132:TYR:CE2	29:C1:513:CLA:HAA1	2.52	0.44
40:D1:409:LHG:H302	16:T1:21:ILE:HD13	2.00	0.44
18:X1:75:SER:O	18:X1:79:GLY:N	2.43	0.44
20:N1:125:LYS:HZ1	24:Y1:257:VAL:HA	1.83	0.44
20:N1:149:ASN:O	20:N1:153:THR:OG1	2.26	0.44
29:G1:611:CLA:H61	29:G1:611:CLA:H41	1.77	0.44
1:a1:104:GLU:OE2	17:w1:64:ARG:NH2	2.46	0.44
1:a1:196:PRO:HG3	37:c1:520:DGD:HA51	1.99	0.44
29:a1:405:CLA:NB	29:d1:402:CLA:HBB1	2.32	0.44
29:b1:603:CLA:H202	29:b1:603:CLA:H161	1.82	0.44
29:b1:605:CLA:H8	29:b1:605:CLA:H122	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c1:516:BCR:H351	31:c1:516:BCR:H15C	1.80	0.44
20:n1:217:CYS:HA	20:n1:220:PHE:CD2	2.52	0.44
48:g1:608:CHL:HBB1	48:g1:608:CHL:HHC	1.99	0.44
50:r1:621:XAT:H11	50:r1:621:XAT:H191	1.88	0.44
23:s1:75:LEU:HD21	23:s1:97:VAL:HG21	2.00	0.44
29:A:407:CLA:HBB1	30:A:409:PHO:H122	1.99	0.44
15:P:206:LYS:NZ	15:P:241:PHE:O	2.32	0.44
29:N:611:CLA:HAB	50:G:622:XAT:H221	1.99	0.44
49:S:621:LUT:H35	49:S:621:LUT:H401	1.82	0.44
1:a:309:SER:HA	7:f:44:ARG:HG2	1.99	0.44
2:b:57:ARG:NH2	2:b:334:ASP:OD1	2.45	0.44
5:d:123:ILE:HD11	33:h:102:LMG:H392	1.99	0.44
20:n:210:GLY:O	20:n:214:MET:HG3	2.18	0.44
29:n:603:CLA:HAC1	48:n:607:CHL:CBB	2.47	0.44
21:g:199:LYS:HD3	29:g:612:CLA:HBD	1.98	0.44
29:r:608:CLA:HMB1	51:r:622:NEX:H14	2.00	0.44
49:s:620:LUT:H15	49:s:620:LUT:H201	1.86	0.44
55:y:626:PTY:H181	55:y:626:PTY:H352	1.99	0.44
1:A1:133:LEU:HD23	5:D1:256:ILE:HG12	2.00	0.44
2:B1:181:VAL:HG13	2:B1:199:PRO:HG3	1.98	0.44
4:C1:75:ILE:HG13	4:C1:76:LEU:HD22	1.99	0.44
4:C1:277:PHE:HB3	4:C1:285:TYR:HE1	1.83	0.44
29:C1:513:CLA:H162	29:C1:513:CLA:H122	1.81	0.44
15:P1:187:PHE:N	15:P1:205:VAL:O	2.49	0.44
48:N1:607:CHL:C3C	48:Y1:601:CHL:H143	2.47	0.44
29:N1:612:CLA:H3A	29:N1:612:CLA:HBA1	1.77	0.44
23:S1:180:GLU:HG3	29:S1:609:CLA:NB	2.33	0.44
32:a1:412:SQD:H371	37:c1:519:DGD:HAW2	1.98	0.44
4:c1:29:ARG:HH22	11:k1:46:ARG:C	2.25	0.44
20:n1:167:TYR:CD1	20:n1:172:GLY:HA3	2.53	0.44
51:n1:623:NEX:H15	51:n1:623:NEX:H201	1.83	0.44
1:A:288:LEU:HD11	4:C:423:PHE:HD2	1.83	0.44
29:A:410:CLA:H92	17:W:89:LEU:HD11	2.00	0.44
2:B:394:GLN:NE2	15:P:149:ALA:HB2	2.32	0.44
29:C:513:CLA:H62	29:C:513:CLA:H41	1.73	0.44
37:C:519:DGD:HB81	37:C:519:DGD:HB52	1.83	0.44
5:D:126:MET:HE3	5:D:143:ALA:O	2.18	0.44
49:N:620:LUT:H35	49:N:620:LUT:H401	1.89	0.44
48:S:607:CHL:HHC	48:S:607:CHL:HBB1	2.00	0.44
1:a:225:ARG:HD2	22:r:97:ALA:HB1	1.99	0.44
19:z:9:LEU:O	19:z:13:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:n:622:XAT:H22	24:y:253:ALA:HA	2.00	0.44
23:s:234:LYS:HG3	29:s:611:CLA:HED2	2.00	0.44
29:s:604:CLA:H61	48:s:606:CHL:HBA2	2.00	0.44
24:y:76:LEU:HB3	24:y:86:TYR:HE2	1.82	0.44
1:A1:142:TRP:HE1	4:C1:431:TRP:HA	1.83	0.44
2:B1:40:PHE:CD1	38:B1:624:3PH:H282	2.53	0.44
2:B1:74:SER:OG	2:B1:94:GLU:OE2	2.35	0.44
2:B1:250:PHE:CE2	29:B1:603:CLA:H172	2.52	0.44
29:C1:508:CLA:H162	29:C1:508:CLA:H203	1.85	0.44
5:D1:54:PHE:HE1	7:F1:39:MET:HE1	1.83	0.44
50:Y1:622:XAT:H31	50:Y1:622:XAT:H391	1.80	0.44
2:b1:268:PHE:HB3	2:b1:448:ARG:HB2	1.99	0.44
29:b1:617:CLA:C3D	8:h1:26:LEU:HD23	2.47	0.44
4:c1:102:SER:C	4:c1:106:HIS:HD1	2.25	0.44
29:c1:504:CLA:H203	37:c1:519:DGD:HAF1	2.00	0.44
29:c1:512:CLA:H12	29:c1:512:CLA:HBA2	1.76	0.44
17:w1:72:LEU:HD23	17:w1:75:GLY:HA2	2.00	0.44
29:s1:610:CLA:H61	29:s1:610:CLA:H41	1.73	0.44
1:A:221:SER:OG	5:D:139:ARG:O	2.28	0.44
5:D:83:ASN:ND2	5:D:165:SER:OG	2.40	0.44
48:N:601:CHL:H161	40:N:624:LHG:H223	2.00	0.44
21:G:83:LEU:O	21:G:87:ARG:HG2	2.18	0.44
29:G:610:CLA:H13	29:G:610:CLA:H172	1.85	0.44
1:a:37:MET:HE1	1:a:129:ARG:NH1	2.33	0.44
1:a:126:TYR:HE2	40:d:409:LHG:H372	1.83	0.44
2:b:9:HIS:CG	29:b:613:CLA:HAB	2.53	0.44
2:b:236:SER:HA	2:b:473:THR:HG21	2.00	0.44
2:b:457:SER:HB2	33:b:622:LMG:H231	2.00	0.44
4:c:63:PHE:HZ	4:c:93:VAL:HG21	1.83	0.44
29:c:511:CLA:H143	19:z:20:VAL:HG13	1.99	0.44
5:d:172:SER:HB2	5:d:177:SER:HB2	2.00	0.44
7:f:39:MET:HA	7:f:42:ILE:HG13	1.99	0.44
20:n:150:ILE:HG22	55:y:626:PTY:HC32	1.99	0.44
21:g:202:LYS:NZ	40:g:624:LHG:O4	2.40	0.44
1:A1:76:ASN:O	1:A1:80:GLY:N	2.50	0.44
2:B1:16:PRO:HB3	2:B1:133:LEU:HD11	1.99	0.44
2:B1:377:VAL:HG21	5:D1:342:PRO:HD3	2.00	0.44
29:B1:603:CLA:H161	33:H1:102:LMG:H382	2.00	0.44
29:B1:612:CLA:HBC1	40:D1:408:LHG:H301	2.00	0.44
4:C1:277:PHE:HB3	4:C1:285:TYR:CE1	2.53	0.44
31:C1:516:BCR:H271	47:K1:101:4RF:H94	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D1:182:ILE:HG23	29:D1:402:CLA:HAC1	2.00	0.44
49:G1:621:LUT:H11	49:G1:621:LUT:H191	1.79	0.44
22:R1:213:TYR:HB3	29:R1:610:CLA:HED3	1.99	0.44
29:Y1:614:CLA:H62	34:Y1:625:SPH:H142	2.00	0.44
1:a1:97:TRP:CH2	9:i1:5:LYS:HE3	2.53	0.44
2:b1:64:PRO:HB2	2:b1:268:PHE:HE1	1.83	0.44
2:b1:130:LYS:HD2	22:r1:89:VAL:HG22	1.98	0.44
31:b1:619:BCR:H351	31:b1:619:BCR:H15C	1.79	0.44
4:c1:132:TYR:CZ	29:c1:513:CLA:HAA1	2.52	0.44
4:c1:174:TYR:HA	4:c1:184:VAL:HA	1.99	0.44
4:c1:274:ALA:HA	4:c1:277:PHE:CD2	2.52	0.44
31:c1:514:BCR:H281	40:c1:525:LHG:H101	2.00	0.44
5:d1:338:LYS:HD3	6:e1:65:LEU:HD22	2.00	0.44
29:r1:612:CLA:H11	29:r1:612:CLA:H52	1.75	0.44
23:s1:200:ASP:OD1	23:s1:201:SER:N	2.46	0.44
29:y1:612:CLA:H102	29:y1:612:CLA:H62	1.81	0.44
1:A:196:PRO:HG3	1:A:300:PHE:CE2	2.53	0.44
2:B:11:VAL:HG11	29:B:615:CLA:HED3	1.99	0.44
2:B:277:GLN:HB2	25:U:106:VAL:HB	2.00	0.44
38:B:624:3PH:H3G1	16:t:11:ILE:HD13	2.00	0.44
8:H:66:GLU:HG2	8:H:71:SER:HB2	2.00	0.44
47:I:102:4RF:H73	22:r:182:PHE:CE1	2.53	0.44
48:N:608:CHL:HMA2	51:N:623:NEX:H30	2.00	0.44
29:Y:604:CLA:H2	29:Y:604:CLA:H61	1.75	0.44
2:b:315:ILE:HG22	2:b:426:LEU:HB3	2.00	0.44
39:b:625:DGA:HA71	39:b:625:DGA:HB51	1.99	0.44
20:n:214:MET:HB2	29:n:602:CLA:HMC2	2.00	0.44
48:s:606:CHL:HBB2	48:s:607:CHL:CBB	2.48	0.44
2:B1:394:GLN:HG2	15:P1:147:ARG:HB3	1.99	0.44
4:C1:167:ALA:HA	4:C1:172:GLY:HA2	2.00	0.44
4:C1:238:TRP:HD1	34:Y1:625:SPH:H102	1.82	0.44
4:C1:331:ARG:HB2	14:O1:137:THR:HG22	2.00	0.44
29:C1:501:CLA:H51	29:C1:501:CLA:C3B	2.48	0.44
5:D1:19:ASP:OD1	5:D1:32:TRP:NE1	2.49	0.44
5:D1:213:ILE:O	5:D1:217:THR:N	2.42	0.44
6:E1:22:ILE:HG13	6:E1:23:HIS:ND1	2.33	0.44
29:S1:603:CLA:H11	29:S1:603:CLA:H51	1.82	0.44
24:Y1:99:LEU:HB3	29:Y1:604:CLA:HBB2	1.99	0.44
29:a1:405:CLA:H193	29:a1:406:CLA:H193	2.00	0.44
2:b1:149:LEU:HD22	29:b1:605:CLA:H172	1.99	0.44
2:b1:320:ALA:HB1	5:d1:292:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b1:611:CLA:H8	29:b1:611:CLA:H51	1.74	0.44
4:c1:213:VAL:HG13	37:c1:518:DGD:HD61	2.00	0.44
14:o1:260:ASP:HB3	14:o1:265:GLU:HG2	1.99	0.44
20:n1:135:GLY:HA2	20:n1:148:GLN:HG3	1.99	0.44
20:n1:161:MET:HE1	48:n1:609:CHL:C2C	2.48	0.44
21:g1:241:ALA:HB3	50:y1:622:XAT:H193	1.99	0.44
50:y1:622:XAT:H11	50:y1:622:XAT:H191	1.73	0.44
1:A:335:ASN:ND2	14:O:211:LEU:O	2.46	0.43
29:A:406:CLA:H202	29:A:406:CLA:H162	1.81	0.43
2:B:301:ALA:O	2:B:304:LYS:HB2	2.17	0.43
29:B:606:CLA:H61	29:B:606:CLA:H41	1.78	0.43
4:C:426:PHE:CE1	29:C:505:CLA:HAB	2.52	0.43
32:M:101:SQD:H132	13:m:23:LEU:HD21	2.00	0.43
48:N:601:CHL:H41	48:N:601:CHL:H61	1.72	0.43
49:N:621:LUT:H15	49:N:621:LUT:H201	1.80	0.43
1:a:325:ASN:HB3	4:c:400:THR:HG22	1.99	0.43
29:c:501:CLA:H171	29:c:507:CLA:H102	2.00	0.43
29:c:506:CLA:H71	39:c:524:DGA:HA71	2.00	0.43
48:s:608:CHL:HHC	48:s:608:CHL:HBB1	2.01	0.43
29:B1:602:CLA:H161	45:H1:101:RRX:H39	1.99	0.43
29:B1:607:CLA:H152	22:R1:189:TRP:CH2	2.53	0.43
29:C1:505:CLA:HBA1	9:I1:23:PHE:CE2	2.53	0.43
39:C1:524:DGA:HB71	17:W1:93:TRP:HZ3	1.83	0.43
5:D1:46:GLY:HA2	31:D1:404:BCR:H353	1.99	0.43
20:N1:46:ASN:OD1	20:N1:46:ASN:N	2.51	0.43
20:N1:93:ALA:HB1	20:N1:210:GLY:HA3	2.00	0.43
21:G1:199:LYS:HG3	29:G1:611:CLA:HED2	2.00	0.43
29:G1:602:CLA:H72	49:G1:621:LUT:H30	2.00	0.43
2:b1:55:MET:HE2	2:b1:64:PRO:HG3	2.00	0.43
2:b1:328:GLY:HA2	33:b1:622:LMG:O6	2.18	0.43
2:b1:348:ASP:HA	2:b1:397:VAL:HA	1.99	0.43
5:d1:159:ILE:HG21	5:d1:287:VAL:HG22	2.00	0.43
5:d1:263:ASN:HB3	5:d1:266:TRP:HB3	1.99	0.43
14:o1:224:ASN:HA	14:o1:240:LEU:HB2	2.00	0.43
21:g1:110:PHE:HE1	21:g1:131:LEU:HD23	1.83	0.43
29:g1:603:CLA:HBB1	29:g1:603:CLA:HHC	1.98	0.43
29:r1:603:CLA:NB	52:r1:625:LMT:H2'	2.33	0.43
23:s1:243:MET:O	23:s1:243:MET:HE3	2.18	0.43
24:y1:137:LEU:HB2	24:y1:148:ALA:HB3	2.00	0.43
1:A:27:ARG:NH2	5:D:258:GLY:O	2.39	0.43
1:A:32:TRP:O	1:A:35:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:405:CLA:H18	40:D:409:LHG:H332	2.01	0.43
3:V:33:LEU:HA	29:C:511:CLA:H42	2.00	0.43
4:C:135:PHE:HB3	29:C:512:CLA:HBC2	2.00	0.43
29:G:610:CLA:H51	29:G:612:CLA:HMA2	2.00	0.43
23:S:143:MET:HE2	48:S:606:CHL:HBC3	2.00	0.43
2:b:158:VAL:HG23	2:b:199:PRO:HB3	2.00	0.43
2:b:198:VAL:O	2:b:202:HIS:ND1	2.38	0.43
4:c:264:LEU:HD21	29:c:508:CLA:CAB	2.46	0.43
5:d:210:LEU:HD13	5:d:271:MET:HA	2.00	0.43
48:n:605:CHL:HBA2	38:s:626:3PH:H3C2	1.99	0.43
50:n:622:XAT:H11	50:n:622:XAT:H191	1.88	0.43
25:u:107:LYS:HA	25:u:110:ARG:HG2	2.01	0.43
2:B1:74:SER:HG	2:B1:94:GLU:CD	2.26	0.43
2:B1:390:TYR:OH	15:P1:96:GLU:OE2	2.29	0.43
29:B1:612:CLA:H112	29:B1:612:CLA:H72	1.71	0.43
32:B1:621:SQD:H262	32:M1:101:SQD:H111	2.00	0.43
29:C1:513:CLA:H112	40:C1:525:LHG:H141	2.00	0.43
14:O1:266:ILE:HD12	14:O1:266:ILE:HA	1.89	0.43
20:N1:111:ASP:OD1	20:N1:111:ASP:N	2.51	0.43
20:N1:173:PRO:HD2	20:N1:174:ALA:H	1.83	0.43
29:N1:613:CLA:H51	29:N1:613:CLA:NC	2.33	0.43
23:S1:192:PHE:HD1	23:S1:198:LYS:H	1.65	0.43
48:S1:606:CHL:HBA2	51:S1:623:NEX:H28	2.01	0.43
24:Y1:162:MET:HE3	48:Y1:606:CHL:HMB2	2.00	0.43
29:Y1:610:CLA:HBB2	49:Y1:620:LUT:H34	2.00	0.43
1:a1:297:LEU:HB2	4:c1:416:THR:HG21	1.99	0.43
30:a1:408:PHO:H192	30:a1:408:PHO:H162	1.84	0.43
2:b1:4:PRO:HD2	2:b1:7:ARG:HG3	1.99	0.43
2:b1:16:PRO:HA	2:b1:19:LEU:HB3	2.00	0.43
2:b1:259:GLY:HA3	8:h1:81:TRP:CZ2	2.52	0.43
29:b1:609:CLA:HBB2	5:d1:123:ILE:HG12	2.00	0.43
4:c1:73:GLY:HA2	4:c1:413:TRP:CZ3	2.53	0.43
5:d1:87:HIS:NE2	5:d1:164:GLN:O	2.35	0.43
14:o1:147:MET:HE1	14:o1:149:ILE:HD11	1.99	0.43
48:n1:606:CHL:HED1	48:n1:606:CHL:H2	1.99	0.43
29:n1:613:CLA:H2	29:n1:613:CLA:H61	1.70	0.43
22:r1:201:LEU:HA	22:r1:204:ASN:HB2	1.99	0.43
23:s1:85:TYR:CE1	48:s1:601:CHL:HAA2	2.54	0.43
24:y1:77:SER:HB3	24:y1:83:PHE:CG	2.53	0.43
24:y1:213:ARG:HA	24:y1:216:MET:HE2	2.00	0.43
1:A:59:ASP:HA	1:A:66:PRO:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C:507:CLA:H142	31:C:515:BCR:H362	1.99	0.43
31:C:514:BCR:H323	19:Z:55:GLY:HA2	2.00	0.43
6:E:32:ILE:HG23	6:E:35:TRP:HE3	1.84	0.43
20:N:205:LYS:HD3	29:N:612:CLA:HBD	1.99	0.43
29:Y:602:CLA:CBB	49:Y:621:LUT:H32	2.48	0.43
29:Y:610:CLA:H92	49:Y:620:LUT:H371	2.00	0.43
1:a:26:ASN:O	5:d:255:GLN:NE2	2.51	0.43
1:a:132:GLU:O	1:a:136:ARG:HG2	2.18	0.43
29:b:610:CLA:H92	29:b:610:CLA:H61	1.83	0.43
38:b:624:3PH:H2C2	38:b:624:3PH:H2F1	1.85	0.43
4:c:43:ALA:HB2	4:c:117:GLY:HA3	2.00	0.43
4:c:394:SER:HA	4:c:408:VAL:HG23	2.00	0.43
20:n:81:THR:OG1	24:y:75:GLY:O	2.22	0.43
29:g:602:CLA:H3A	29:g:602:CLA:HBA2	1.52	0.43
29:s:603:CLA:H51	29:s:603:CLA:H11	1.81	0.43
29:A1:405:CLA:H203	29:A1:405:CLA:H161	1.74	0.43
6:E1:64:PRO:HB3	6:E1:79:LEU:HG	2.00	0.43
29:R1:603:CLA:HBB2	50:R1:621:XAT:H191	2.00	0.43
24:Y1:110:LEU:HD23	24:Y1:115:VAL:HG21	2.00	0.43
1:a1:39:PRO:HB2	29:a1:410:CLA:HAB	1.99	0.43
1:a1:153:ALA:HB3	29:a1:405:CLA:H43	2.01	0.43
33:a1:413:LMG:H421	29:c1:505:CLA:H101	2.00	0.43
29:b1:605:CLA:HBB1	29:b1:614:CLA:C2C	2.47	0.43
4:c1:59:GLU:HG2	4:c1:77:LEU:HG	2.00	0.43
4:c1:73:GLY:HA2	4:c1:413:TRP:HZ3	1.83	0.43
4:c1:112:VAL:HB	31:c1:514:BCR:H362	1.99	0.43
5:d1:326:ARG:NH1	5:d1:326:ARG:HB3	2.33	0.43
20:n1:72:THR:OG1	49:n1:621:LUT:O23	2.25	0.43
22:r1:233:PHE:HA	22:r1:236:LYS:HE2	2.01	0.43
51:r1:622:NEX:H11	51:r1:622:NEX:H191	1.86	0.43
29:s1:610:CLA:H102	49:s1:620:LUT:H371	1.99	0.43
1:A:120:PHE:HE2	29:C:505:CLA:H13	1.84	0.43
2:B:474:ILE:HD11	29:B:609:CLA:HAA2	2.00	0.43
4:C:51:TRP:HB2	29:C:510:CLA:HAC2	2.00	0.43
29:C:504:CLA:H93	29:C:504:CLA:H61	1.80	0.43
22:R:140:HIS:HB3	22:R:247:MET:HE2	2.00	0.43
29:R:610:CLA:H52	49:R:620:LUT:H28	2.00	0.43
23:S:136:TRP:HZ2	23:S:250:ALA:HA	1.83	0.43
49:S:620:LUT:H15	49:S:620:LUT:H201	1.82	0.43
1:a:89:ILE:HD11	1:a:108:ASN:HB3	2.00	0.43
30:a:408:PHO:H43	40:d:409:LHG:H341	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:410:CLA:H102	29:a:410:CLA:H62	1.53	0.43
32:b:626:SQD:H142	32:b:626:SQD:H112	1.77	0.43
4:c:40:ALA:HB2	29:c:511:CLA:HMA2	2.00	0.43
5:d:43:PHE:HB3	5:d:113:PHE:CZ	2.54	0.43
12:l:13:LEU:HB2	13:m:25:LEU:HB3	1.99	0.43
29:n:603:CLA:H61	29:n:603:CLA:H102	1.50	0.43
21:g:85:HIS:CD2	21:g:208:MET:HE2	2.53	0.43
21:g:242:PHE:HB3	24:y:132:PHE:HZ	1.83	0.43
24:y:221:GLY:O	24:y:225:GLN:HG3	2.19	0.43
1:A1:300:PHE:HD1	4:C1:393:ASN:HD21	1.66	0.43
2:B1:60:MET:SD	2:B1:60:MET:N	2.91	0.43
29:B1:605:CLA:H93	29:B1:605:CLA:H61	1.80	0.43
3:V1:16:VAL:O	31:C1:516:BCR:H16C	2.18	0.43
4:C1:97:PHE:HA	4:C1:100:PHE:HB3	1.99	0.43
29:C1:507:CLA:H202	29:C1:507:CLA:H161	1.79	0.43
5:D1:253:TRP:CZ3	43:D1:405:PL9:HC72	2.53	0.43
14:O1:95:ARG:HH22	14:O1:153:GLY:HA2	1.83	0.43
29:N1:603:CLA:H61	29:N1:603:CLA:H102	1.75	0.43
29:N1:613:CLA:H51	29:N1:613:CLA:C4C	2.48	0.43
50:N1:622:XAT:H30	40:Y1:624:LHG:H342	2.01	0.43
24:Y1:60:TYR:CD1	24:Y1:61:LEU:HG	2.53	0.43
29:c1:511:CLA:H91	29:c1:511:CLA:H111	1.70	0.43
5:d1:53:THR:HG22	5:d1:67:TYR:CD2	2.54	0.43
8:h1:46:THR:OG1	8:h1:49:LEU:HB2	2.19	0.43
19:z1:1:MET:SD	19:z1:1:MET:N	2.90	0.43
29:n1:602:CLA:H52	49:n1:621:LUT:H28	2.00	0.43
21:g1:205:ARG:HA	21:g1:208:MET:HB3	2.00	0.43
22:r1:69:GLY:H	22:r1:237:THR:HG22	1.82	0.43
29:r1:604:CLA:H12	48:r1:606:CHL:CAD	2.49	0.43
23:s1:261:TYR:HA	23:s1:264:ILE:HG22	1.99	0.43
24:y1:120:ASP:HB2	24:y1:130:GLU:OE1	2.18	0.43
1:A:56:PRO:HD2	1:A:106:LEU:HD22	1.99	0.43
29:B:603:CLA:H93	29:B:610:CLA:H201	1.99	0.43
4:C:320:GLN:HB3	14:O:165:TYR:CE2	2.53	0.43
48:N:606:CHL:H41	48:N:606:CHL:H62	1.73	0.43
34:a:414:SPH:H183	34:a:414:SPH:H152	1.89	0.43
4:c:30:LEU:HD13	4:c:37:LEU:HA	2.00	0.43
4:c:71:GLU:HG2	4:c:386:HIS:CD2	2.53	0.43
40:c:525:LHG:H141	40:c:525:LHG:H111	1.79	0.43
5:d:69:GLU:OE1	6:e:55:TYR:OH	2.23	0.43
14:o:110:GLU:OE2	17:w:60:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:s:57:ARG:NH2	23:s:75:LEU:O	2.51	0.43
29:y:602:CLA:H102	29:y:602:CLA:H13	1.62	0.43
1:A1:337:HIS:HB2	5:D1:351:ALA:HB3	2.00	0.43
2:B1:333:GLY:HA2	2:B1:440:ASP:OD1	2.19	0.43
29:B1:604:CLA:H41	29:B1:604:CLA:H61	1.68	0.43
29:B1:611:CLA:HED2	29:B1:611:CLA:H2A	2.00	0.43
29:B1:612:CLA:H71	40:L1:101:LHG:H322	1.99	0.43
29:C1:504:CLA:C1D	37:C1:519:DGD:HB21	2.48	0.43
29:C1:509:CLA:H122	29:C1:509:CLA:H8	1.89	0.43
6:E1:8:ARG:NH1	6:E1:12:ASP:OD2	2.52	0.43
20:N1:214:MET:CE	29:N1:602:CLA:HAB	2.48	0.43
22:R1:194:LEU:HD22	51:R1:622:NEX:H15	2.00	0.43
29:R1:608:CLA:H92	29:R1:608:CLA:H62	1.84	0.43
24:Y1:71:TRP:CH2	49:Y1:621:LUT:H27	2.53	0.43
1:a1:94:TYR:N	1:a1:113:GLN:OE1	2.52	0.43
16:t1:17:ILE:HG22	38:t1:101:3PH:H2I2	2.01	0.43
29:g1:602:CLA:H2	49:g1:621:LUT:H28	1.99	0.43
1:A:335:ASN:OD1	5:D:350:ASN:ND2	2.52	0.43
2:B:198:VAL:HG13	2:B:202:HIS:CE1	2.53	0.43
29:C:501:CLA:H61	29:C:501:CLA:H41	1.65	0.43
5:D:107:LEU:HD23	6:E:66:ILE:HD13	2.00	0.43
20:N:126:ALA:HB1	29:N:604:CLA:HED1	2.01	0.43
20:N:192:LEU:HD23	20:N:192:LEU:HA	1.89	0.43
54:S:625:LPX:H9A	54:S:625:LPX:H12A	1.69	0.43
25:U:107:LYS:HA	25:U:110:ARG:HG2	2.01	0.43
29:b:606:CLA:HBB1	29:b:606:CLA:HMB3	2.01	0.43
32:b:621:SQD:H251	32:b:621:SQD:H132	2.00	0.43
40:d:409:LHG:H182	16:t:17:ILE:HD11	2.00	0.43
15:p:134:PRO:HB3	15:p:187:PHE:CE1	2.53	0.43
1:A1:201:GLY:HA3	1:A1:286:THR:HB	2.00	0.43
1:A1:317:TRP:CD1	5:D1:177:SER:HB3	2.53	0.43
2:B1:188:GLU:HA	8:H1:77:VAL:HG22	1.99	0.43
2:B1:251:VAL:HG22	29:B1:603:CLA:H72	2.01	0.43
2:B1:423:LYS:HD2	2:B1:429:ILE:HG23	2.00	0.43
2:B1:450:TRP:HD1	29:B1:608:CLA:CHB	2.31	0.43
29:B1:603:CLA:HAA1	8:H1:64:ILE:HD11	2.01	0.43
3:V1:28:VAL:HG23	3:V1:29:ARG:HG2	2.00	0.43
4:C1:280:PHE:HB3	37:C1:518:DGD:HD5	1.99	0.43
4:C1:329:LEU:HB3	4:C1:337:ILE:HD11	2.00	0.43
29:C1:506:CLA:H2	29:C1:507:CLA:H203	2.01	0.43
6:E1:44:TYR:CD2	6:E1:51:ARG:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L1:9:GLN:HE22	22:R1:95:ASN:HD21	1.66	0.43
29:N1:602:CLA:H93	29:N1:602:CLA:H111	1.73	0.43
23:S1:237:LYS:NZ	40:S1:624:LHG:O5	2.51	0.43
23:S1:264:ILE:HD12	49:S1:620:LUT:H22	2.01	0.43
51:Y1:623:NEX:H15	51:Y1:623:NEX:H201	1.85	0.43
1:a1:21:ILE:HG23	1:a1:22:THR:HG23	2.01	0.43
1:a1:43:THR:HG22	31:a1:411:BCR:H16C	2.01	0.43
1:a1:191:ASN:HB3	1:a1:194:MET:HE1	1.99	0.43
33:a1:413:LMG:H411	29:c1:505:CLA:H142	2.00	0.43
29:b1:608:CLA:HBB1	29:b1:608:CLA:HMB1	2.00	0.43
29:b1:612:CLA:H91	29:b1:614:CLA:H143	2.01	0.43
4:c1:262:TYR:HB3	29:c1:507:CLA:C4B	2.47	0.43
9:i1:22:GLY:O	9:i1:25:SER:OG	2.26	0.43
15:p1:177:LYS:HA	15:p1:183:THR:HA	2.00	0.43
48:r1:606:CHL:HBA1	51:r1:622:NEX:H31	2.00	0.43
20:N:138:TYR:OH	51:N:623:NEX:O23	2.23	0.43
50:N:622:XAT:H31	50:N:622:XAT:H391	1.71	0.43
29:G:602:CLA:HAB	49:G:621:LUT:H32	2.01	0.43
49:G:620:LUT:H11	49:G:620:LUT:H191	1.88	0.43
1:a:29:TYR:CG	1:a:133:LEU:HD13	2.54	0.43
29:b:615:CLA:H41	29:b:615:CLA:H62	1.63	0.43
29:b:616:CLA:H8	29:b:616:CLA:H52	1.80	0.43
4:c:378:ARG:O	4:c:382:GLU:HG2	2.19	0.43
20:n:157:GLN:OE1	48:n:607:CHL:HMC	2.19	0.43
20:n:231:PRO:O	49:n:620:LUT:O3	2.35	0.43
29:r:603:CLA:HAB	52:r:625:LMT:H22	2.00	0.43
2:B1:3:LEU:HA	2:B1:3:LEU:HD23	1.87	0.43
29:B1:609:CLA:HBA2	29:B1:609:CLA:H3A	1.73	0.43
4:C1:19:THR:HG21	4:C1:29:ARG:HG3	2.00	0.43
29:C1:513:CLA:NB	31:C1:514:BCR:H383	2.34	0.43
37:C1:519:DGD:HA92	37:C1:519:DGD:HA61	1.81	0.43
5:D1:111:TRP:O	5:D1:115:ALA:N	2.40	0.43
5:D1:123:ILE:HD11	33:H1:102:LMG:H392	2.01	0.43
31:D1:404:BCR:H351	31:D1:404:BCR:H15C	1.62	0.43
10:J1:13:TRP:O	10:J1:17:THR:HG23	2.19	0.43
48:N1:606:CHL:H62	48:N1:606:CHL:H41	1.72	0.43
22:R1:184:ILE:HD13	22:R1:184:ILE:HA	1.89	0.43
50:R1:621:XAT:H191	50:R1:621:XAT:H11	1.87	0.43
29:S1:602:CLA:H62	29:S1:602:CLA:H41	1.45	0.43
24:Y1:181:ASP:HB3	24:Y1:184:TYR:O	2.19	0.43
29:Y1:611:CLA:H142	29:Y1:611:CLA:H111	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:v1:26:LEU:HG	19:z1:25:VAL:HG22	2.01	0.43
5:d1:230:ASN:ND2	5:d1:232:PHE:HB2	2.33	0.43
5:d1:285:GLY:O	5:d1:289:LEU:N	2.50	0.43
29:d1:402:CLA:H62	29:d1:402:CLA:H41	1.58	0.43
6:e1:62:ASP:OD1	6:e1:62:ASP:N	2.49	0.43
20:n1:87:GLU:HA	20:n1:181:LEU:HD11	2.00	0.43
21:g1:136:LEU:HD23	21:g1:136:LEU:HA	1.90	0.43
22:r1:135:GLU:HG3	22:r1:212:ILE:HG12	2.01	0.43
29:s1:613:CLA:H61	29:s1:613:CLA:H41	1.74	0.43
24:y1:104:ILE:HD11	49:y1:621:LUT:H8	2.01	0.43
24:y1:219:CYS:HA	24:y1:222:PHE:CD2	2.53	0.43
2:B:4:PRO:HD2	2:B:7:ARG:HD2	2.00	0.43
29:B:607:CLA:H13	47:i:101:4RF:H63	2.01	0.43
29:S:603:CLA:H11	29:S:603:CLA:H51	1.78	0.43
29:Y:603:CLA:H161	29:Y:603:CLA:H192	1.79	0.43
2:b:281:GLN:O	2:b:285:GLN:HG3	2.19	0.43
29:c:506:CLA:H141	29:c:506:CLA:H161	1.86	0.43
7:f:19:TRP:HE3	7:f:20:LEU:HD22	1.83	0.43
20:n:96:ALA:HB3	20:n:214:MET:HG2	2.00	0.43
29:n:602:CLA:CBB	49:n:621:LUT:H32	2.49	0.43
48:n:607:CHL:H203	48:n:609:CHL:H51	1.99	0.43
21:g:39:LYS:HB3	21:g:45:SER:HB2	2.01	0.43
49:g:621:LUT:H15	49:g:621:LUT:H201	1.85	0.43
1:A1:277:VAL:O	1:A1:281:VAL:HG12	2.18	0.43
2:B1:142:HIS:ND1	29:B1:611:CLA:OBD	2.40	0.43
2:B1:239:SER:O	2:B1:466:HIS:ND1	2.52	0.43
29:C1:508:CLA:H91	40:D1:410:LHG:H352	2.00	0.43
5:D1:171:PRO:HG3	5:D1:181:PHE:CE2	2.54	0.43
5:D1:221:THR:HG22	5:D1:245:SER:H	1.84	0.43
11:K1:14:ALA:O	19:Z1:6:GLN:NE2	2.51	0.43
29:G1:614:CLA:H12	29:G1:614:CLA:HBA1	1.81	0.43
22:R1:216:GLY:HA2	22:R1:219:ASP:HB3	2.01	0.43
29:R1:602:CLA:HED2	29:R1:602:CLA:H2A	2.00	0.43
1:a1:149:ALA:HB2	1:a1:280:VAL:HG13	2.01	0.43
29:b1:609:CLA:C4C	29:b1:610:CLA:H102	2.48	0.43
4:c1:249:ARG:HA	4:c1:254:TRP:HE1	1.82	0.43
4:c1:367:LYS:HB2	4:c1:367:LYS:HE3	1.83	0.43
5:d1:328:TRP:CZ2	5:d1:346:LEU:HB3	2.54	0.43
14:o1:208:SER:HA	14:o1:245:TYR:CZ	2.53	0.43
15:p1:173:VAL:HG12	15:p1:187:PHE:HD1	1.84	0.43
19:z1:1:MET:HA	19:z1:4:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:n1:74:GLY:HA3	21:g1:77:ARG:HD2	2.00	0.43
29:g1:613:CLA:HBB1	49:g1:620:LUT:H7	2.00	0.43
29:r1:609:CLA:H61	29:r1:609:CLA:H102	1.74	0.43
23:s1:236:ILE:HG23	23:s1:240:ARG:HH21	1.83	0.43
24:y1:120:ASP:HB3	24:y1:126:LYS:HG3	2.00	0.43
2:B:144:PHE:HZ	52:R:625:LMT:H3'	1.83	0.43
2:B:282:GLN:HG3	25:U:107:LYS:HG2	2.00	0.43
2:B:288:VAL:O	2:B:292:THR:OG1	2.32	0.43
29:C:513:CLA:CAB	31:C:514:BCR:H24C	2.47	0.43
20:N:154:LEU:HD21	50:N:622:XAT:H202	2.01	0.43
50:G:622:XAT:H15	50:G:622:XAT:H201	1.85	0.43
29:Y:614:CLA:H62	34:Y:625:SPH:H141	1.99	0.43
1:a:274:PHE:HA	1:a:277:VAL:HG12	2.00	0.43
2:b:119:ASP:OD1	2:b:124:ARG:NH2	2.52	0.43
32:b:621:SQD:H271	32:m:101:SQD:H131	2.01	0.43
4:c:48:ILE:HG22	29:c:503:CLA:HHD	2.00	0.43
4:c:154:ILE:HA	4:c:233:ILE:HD13	2.01	0.43
29:c:506:CLA:H152	29:c:506:CLA:H111	1.71	0.43
37:c:518:DGD:HB61	37:c:518:DGD:HB92	1.62	0.43
33:c:523:LMG:HC1	29:y:611:CLA:H3A	2.00	0.43
20:n:77:ALA:HB1	21:g:73:GLN:HE21	1.83	0.43
21:g:91:LEU:HD11	29:g:610:CLA:HAC1	2.01	0.43
50:y:622:XAT:H11	50:y:622:XAT:H191	1.91	0.43
1:A1:42:LEU:HD23	1:A1:42:LEU:HA	1.88	0.43
33:A1:413:LMG:H401	4:C1:272:PHE:CD2	2.54	0.43
2:B1:144:PHE:CE1	2:B1:210:VAL:HG13	2.54	0.43
2:B1:315:ILE:HG23	2:B1:443:PHE:CE2	2.53	0.43
2:B1:323:GLY:HA2	5:D1:294:ARG:N	2.33	0.43
4:C1:19:THR:OG1	4:C1:29:ARG:NE	2.37	0.43
29:C1:513:CLA:H62	40:C1:525:LHG:H292	2.00	0.43
20:N1:41:TYR:CE2	20:N1:200:ALA:HB1	2.54	0.43
24:Y1:168:PHE:HD2	29:Y1:608:CLA:HAB	1.81	0.43
55:Y1:626:PTY:H112	55:Y1:626:PTY:H332	1.99	0.43
29:b1:604:CLA:H192	29:b1:610:CLA:H91	2.00	0.43
31:b1:619:BCR:H333	33:b1:622:LMG:H352	1.99	0.43
4:c1:330:MET:HG3	4:c1:331:ARG:H	1.83	0.43
5:d1:153:PHE:HE1	5:d1:173:PHE:HZ	1.66	0.43
15:p1:113:VAL:HG22	15:p1:201:ARG:HH21	1.84	0.43
33:w1:201:LMG:H352	33:w1:201:LMG:H382	1.83	0.43
20:n1:94:ARG:NH2	48:n1:608:CHL:O1D	2.37	0.43
20:n1:238:HIS:CG	29:n1:613:CLA:HAA1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r1:69:GLY:N	22:r1:237:THR:HG22	2.34	0.43
24:y1:159:VAL:HA	48:y1:609:CHL:HBB2	2.01	0.43
1:A:67:VAL:HG22	5:D:312:GLU:HG2	1.99	0.43
1:A:308:ASP:HB2	6:E:52:PRO:O	2.18	0.43
2:B:468:TRP:NE1	29:B:612:CLA:O1D	2.48	0.43
29:B:602:CLA:H3A	29:B:602:CLA:HBA2	1.50	0.43
4:C:55:MET:HE1	29:C:504:CLA:ND	2.33	0.43
4:C:321:GLY:HA2	4:C:327:LYS:HG3	2.01	0.43
29:C:503:CLA:H61	29:C:503:CLA:H41	1.78	0.43
15:P:168:ALA:HB1	15:P:189:ILE:HD11	2.01	0.43
22:R:162:TRP:HZ2	22:R:253:PHE:HB3	1.83	0.43
24:Y:86:TYR:O	24:Y:89:ILE:HG22	2.19	0.43
29:c:504:CLA:H43	37:c:520:DGD:HB32	2.01	0.43
29:c:506:CLA:H8	29:c:506:CLA:H122	1.68	0.43
33:c:523:LMG:H402	34:y:625:SPH:H142	2.00	0.43
6:e:51:ARG:NH1	6:e:54:GLU:OE2	2.52	0.43
8:h:50:MET:O	8:h:54:ILE:HG12	2.18	0.43
20:n:70:TRP:HZ2	48:g:609:CHL:H11	1.84	0.43
21:g:85:HIS:HE2	49:g:621:LUT:H15	1.83	0.43
48:g:601:CHL:HBA1	48:g:601:CHL:H3A	1.85	0.43
30:A1:409:PHO:H3A	30:A1:409:PHO:HBA1	1.78	0.43
2:B1:389:LYS:H	5:D1:344:GLU:CD	2.26	0.43
43:D1:405:PL9:H201	40:L1:101:LHG:H171	2.01	0.43
8:H1:69:ASN:HD22	33:H1:102:LMG:HC92	1.84	0.43
14:O1:119:GLU:HG2	14:O1:125:GLU:HG2	2.01	0.43
14:O1:140:LEU:HD12	14:O1:140:LEU:HA	1.81	0.43
18:X1:83:LEU:HA	18:X1:86:ILE:HG12	2.01	0.43
24:Y1:152:LEU:HA	24:Y1:155:LEU:HG	2.01	0.43
2:b1:227:PHE:CE1	22:r1:101:LYS:HG3	2.54	0.43
2:b1:470:GLY:HA2	29:b1:609:CLA:HED1	2.01	0.43
29:b1:604:CLA:H141	29:b1:604:CLA:H161	1.71	0.43
29:b1:607:CLA:H161	29:b1:607:CLA:H193	1.83	0.43
31:b1:619:BCR:HC32	33:b1:622:LMG:H131	2.00	0.43
3:v1:8:GLN:O	3:v1:12:LEU:N	2.37	0.43
29:c1:513:CLA:C3B	31:c1:514:BCR:H24C	2.48	0.43
31:c1:515:BCR:H351	31:c1:515:BCR:H15C	1.52	0.43
5:d1:214:HIS:CD2	5:d1:271:MET:HE1	2.54	0.43
7:f1:37:THR:HG23	10:j1:29:ILE:HG21	2.01	0.43
17:w1:92:ILE:HA	17:w1:95:ILE:HD12	2.00	0.43
20:n1:73:ALA:HA	21:g1:81:ILE:HD11	2.01	0.43
21:g1:94:LEU:HB3	29:g1:604:CLA:HMC1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:s1:623:NEX:H15	51:s1:623:NEX:H201	1.85	0.43
54:s1:625:LPX:H10	38:s1:626:3PH:H2C1	2.01	0.43
29:y1:613:CLA:H2	29:y1:613:CLA:H61	1.82	0.43
29:B:604:CLA:CAB	29:B:606:CLA:H161	2.49	0.42
32:B:621:SQD:H161	32:B:621:SQD:H281	2.01	0.42
5:D:51:GLY:HA3	5:D:78:VAL:HG22	2.01	0.42
4:c:120:HIS:HA	4:c:124:GLY:HA3	2.00	0.42
4:c:374:PRO:O	4:c:378:ARG:HG3	2.19	0.42
4:c:378:ARG:HE	4:c:378:ARG:HB2	1.59	0.42
5:d:312:GLU:OE1	5:d:316:THR:OG1	2.37	0.42
19:z:33:TRP:O	19:z:37:LYS:HG2	2.18	0.42
29:s:611:CLA:H161	29:s:611:CLA:H143	1.84	0.42
1:A1:267:ASN:HB3	1:A1:270:SER:HB2	2.01	0.42
29:A1:410:CLA:H141	33:A1:413:LMG:H292	1.99	0.42
32:A1:412:SQD:H111	47:K1:101:4RF:H22	2.00	0.42
33:A1:413:LMG:HC61	17:W1:75:GLY:HA2	2.00	0.42
2:B1:75:TRP:CE3	32:B1:626:SQD:H45	2.54	0.42
29:B1:615:CLA:H111	32:M1:101:SQD:H301	2.01	0.42
4:C1:27:ASN:HB3	29:C1:509:CLA:HAB	2.01	0.42
17:W1:86:ALA:O	33:W1:201:LMG:H371	2.19	0.42
20:N1:205:LYS:O	20:N1:209:ASN:ND2	2.32	0.42
23:S1:237:LYS:HZ2	40:S1:624:LHG:HC62	1.84	0.42
3:v1:33:LEU:OXT	11:k1:46:ARG:NH2	2.52	0.42
4:c1:280:PHE:CE2	37:c1:518:DGD:HD3	2.54	0.42
4:c1:351:GLY:H	4:c1:354:VAL:HG22	1.84	0.42
5:d1:110:LEU:HA	5:d1:113:PHE:HB3	2.01	0.42
14:o1:217:GLY:HA2	14:o1:243:LYS:HG3	2.01	0.42
29:n1:613:CLA:HBB1	49:n1:620:LUT:H181	2.00	0.42
29:g1:602:CLA:H93	29:g1:602:CLA:H111	1.84	0.42
49:g1:620:LUT:H11	49:g1:620:LUT:H191	1.89	0.42
24:y1:151:ILE:HD12	24:y1:154:THR:HB	2.01	0.42
1:A:281:VAL:HG11	32:A:412:SQD:H161	2.00	0.42
39:B:625:DGA:HAE2	39:B:625:DGA:HAF2	1.77	0.42
29:C:503:CLA:H61	29:C:503:CLA:H101	1.76	0.42
5:D:289:LEU:HD22	5:D:294:ARG:HG2	2.02	0.42
15:P:81:ASP:OD1	15:P:81:ASP:N	2.53	0.42
20:N:207:ILE:O	20:N:211:ARG:HG3	2.20	0.42
50:N:622:XAT:H34	29:Y:613:CLA:H111	2.00	0.42
48:G:607:CHL:H143	48:G:609:CHL:H92	2.01	0.42
50:R:621:XAT:H391	50:R:621:XAT:H31	1.64	0.42
54:S:625:LPX:H8	38:S:626:3PH:H292	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:170:ASP:CG	2:b:174:LEU:H	2.25	0.42
2:b:424:ALA:HB2	2:b:429:ILE:HD11	2.00	0.42
2:b:462:PHE:CE2	29:b:612:CLA:HAB	2.53	0.42
4:c:49:VAL:HG12	4:c:106:HIS:O	2.19	0.42
12:l:24:LEU:O	12:l:28:LEU:HD23	2.18	0.42
14:o:279:GLU:HB2	14:o:282:ALA:HB3	2.00	0.42
20:n:229:LYS:HB2	20:n:234:ASN:HD21	1.84	0.42
21:g:90:LEU:HD13	29:g:610:CLA:HHC	2.01	0.42
23:s:276:LEU:O	23:s:280:LEU:HG	2.18	0.42
49:s:621:LUT:H15	49:s:621:LUT:H201	1.91	0.42
1:A1:213:ALA:O	1:A1:217:SER:OG	2.30	0.42
29:B1:609:CLA:H61	29:B1:610:CLA:H121	1.99	0.42
33:B1:622:LMG:H152	33:B1:622:LMG:H121	1.90	0.42
4:C1:390:GLY:HA3	4:C1:408:VAL:HG22	2.00	0.42
33:D1:411:LMG:H202	33:D1:411:LMG:H172	1.83	0.42
47:K1:101:4RF:H47	47:K1:101:4RF:H43	1.70	0.42
48:N1:607:CHL:H162	48:N1:609:CHL:H101	2.01	0.42
21:G1:135:SER:O	21:G1:135:SER:OG	2.37	0.42
49:R1:620:LUT:H11	49:R1:620:LUT:H191	1.81	0.42
52:R1:625:LMT:H61	52:R1:625:LMT:H91	1.64	0.42
53:R1:626:ERG:H212	53:R1:626:ERG:H162	1.75	0.42
24:Y1:214:LEU:HB2	40:Y1:624:LHG:H242	2.00	0.42
29:Y1:602:CLA:HBB2	49:Y1:621:LUT:H34	2.01	0.42
1:a1:38:ILE:HG12	38:t1:101:3PH:H251	2.01	0.42
2:b1:233:SER:HB2	2:b1:235:GLU:HG2	2.00	0.42
29:b1:606:CLA:HMB2	29:b1:607:CLA:H12	2.01	0.42
29:b1:617:CLA:H11	29:b1:617:CLA:H51	1.84	0.42
4:c1:168:LEU:HD23	4:c1:169:TYR:CD1	2.54	0.42
4:c1:425:PHE:HE1	29:c1:508:CLA:CAB	2.32	0.42
5:d1:188:PHE:HA	5:d1:326:ARG:NE	2.29	0.42
8:h1:60:PHE:HA	8:h1:63:ILE:HG12	2.00	0.42
14:o1:276:SER:HB3	14:o1:288:ILE:HD11	2.00	0.42
24:y1:104:ILE:HG13	49:y1:621:LUT:H182	2.01	0.42
24:y1:214:LEU:HD23	40:y1:624:LHG:H242	2.00	0.42
29:y1:602:CLA:H142	49:y1:621:LUT:H361	2.01	0.42
4:C:205:PRO:HG3	37:C:518:DGD:HA81	2.02	0.42
37:C:518:DGD:HA72	37:C:518:DGD:HA42	1.90	0.42
40:D:409:LHG:H322	16:T:21:ILE:HD11	2.00	0.42
8:H:31:ARG:HD2	8:H:31:ARG:HA	1.82	0.42
13:M:26:TYR:HE2	32:m:101:SQD:H92	1.84	0.42
20:N:231:PRO:HB2	49:N:620:LUT:H21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:103:GLU:CD	25:U:103:GLU:H	2.27	0.42
3:v:16:VAL:HG13	31:c:516:BCR:H362	2.01	0.42
12:l:29:ALA:O	12:l:33:SER:OG	2.36	0.42
17:w:79:GLY:HA2	33:w:201:LMG:HC72	2.00	0.42
48:n:601:CHL:HBA1	48:n:601:CHL:H3A	1.79	0.42
49:n:620:LUT:H15	49:n:620:LUT:H201	1.79	0.42
21:g:229:LEU:HB2	49:g:620:LUT:H22	2.00	0.42
24:y:108:GLU:HB2	24:y:122:ALA:O	2.19	0.42
24:y:151:ILE:HA	24:y:154:THR:HG22	2.00	0.42
1:A1:194:MET:HG2	1:A1:300:PHE:HB2	2.01	0.42
2:B1:141:ILE:CD1	29:B1:616:CLA:HBB1	2.46	0.42
3:V1:11:ALA:HB1	11:K1:21:ILE:HD13	2.01	0.42
3:V1:33:LEU:HB2	29:C1:511:CLA:H42	2.01	0.42
4:C1:68:PRO:HG2	4:C1:71:GLU:HG3	2.02	0.42
4:C1:142:LYS:HD3	4:C1:254:TRP:CE3	2.54	0.42
29:C1:512:CLA:HBB1	29:C1:512:CLA:H18	2.01	0.42
12:L1:26:PHE:O	12:L1:30:VAL:HG23	2.18	0.42
20:N1:212:LEU:HA	20:N1:215:PHE:CD2	2.52	0.42
21:G1:89:ALA:O	21:G1:93:ALA:N	2.46	0.42
24:Y1:98:LEU:HD21	49:Y1:620:LUT:C33	2.50	0.42
29:b1:613:CLA:H43	29:b1:616:CLA:CGA	2.50	0.42
4:c1:281:ASN:O	4:c1:411:ARG:NH1	2.44	0.42
29:c1:506:CLA:H161	29:c1:506:CLA:H141	1.83	0.42
14:o1:138:TYR:CE2	17:w1:61:VAL:HG22	2.47	0.42
29:n1:613:CLA:H91	40:n1:624:LHG:H311	2.01	0.42
21:g1:112:GLU:H	21:g1:121:GLN:NE2	2.17	0.42
29:s1:609:CLA:H143	29:s1:609:CLA:H112	1.81	0.42
24:y1:50:LEU:HB2	24:y1:54:SER:HA	2.01	0.42
49:y1:620:LUT:H191	49:y1:620:LUT:H11	1.80	0.42
29:B:608:CLA:H2	33:B:622:LMG:H151	2.01	0.42
4:C:15:ASP:O	4:C:19:THR:OG1	2.35	0.42
17:W:95:ILE:HA	17:W:98:VAL:HG22	2.02	0.42
48:G:607:CHL:H161	48:G:607:CHL:H141	1.84	0.42
22:R:79:SER:OG	29:R:602:CLA:O1A	2.28	0.42
29:R:608:CLA:H91	29:R:608:CLA:H111	1.67	0.42
24:Y:145:LEU:HD22	29:Y:604:CLA:H91	2.00	0.42
29:Y:612:CLA:HED2	29:Y:612:CLA:H12	2.01	0.42
4:c:41:HIS:CE1	29:c:509:CLA:H193	2.55	0.42
29:c:509:CLA:HBB1	29:c:509:CLA:HMB3	2.01	0.42
5:d:49:LEU:HD23	5:d:49:LEU:HA	1.77	0.42
5:d:103:ARG:NH1	6:e:77:LYS:HG2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:l:101:LHG:H111	40:l:101:LHG:HC61	2.00	0.42
20:n:45:ARG:NE	20:n:67:ASP:O	2.50	0.42
29:n:613:CLA:C12	50:g:622:XAT:H34	2.48	0.42
23:s:152:PHE:HD1	23:s:158:VAL:H	1.67	0.42
1:A1:14:TRP:HB3	17:W1:99:SER:HB2	2.02	0.42
1:A1:97:TRP:CZ3	9:I1:8:VAL:HG11	2.55	0.42
29:A1:407:CLA:C1B	30:A1:409:PHO:H202	2.49	0.42
30:A1:409:PHO:H142	30:A1:409:PHO:H112	1.77	0.42
33:A1:413:LMG:H371	37:C1:518:DGD:HB41	2.01	0.42
2:B1:141:ILE:O	2:B1:145:LEU:N	2.42	0.42
29:B1:617:CLA:H51	29:B1:617:CLA:H11	1.77	0.42
14:O1:120:ASP:HB2	14:O1:124:ARG:HB3	2.01	0.42
14:O1:158:ARG:HH22	14:O1:188:ASP:HB3	1.85	0.42
23:S1:237:LYS:HB3	29:S1:611:CLA:HMD1	2.01	0.42
2:b1:170:ASP:CG	2:b1:174:LEU:H	2.28	0.42
2:b1:226:TYR:HA	2:b1:231:MET:CG	2.49	0.42
29:c1:509:CLA:HMB1	29:c1:511:CLA:HBB1	2.02	0.42
5:d1:85:LEU:HD13	5:d1:90:LEU:HD21	1.99	0.42
5:d1:210:LEU:HD11	5:d1:270:PHE:CE2	2.55	0.42
20:n1:103:MET:HE1	20:n1:123:TRP:CD1	2.55	0.42
20:n1:145:ILE:HD11	29:n1:604:CLA:H12	2.00	0.42
29:n1:603:CLA:HMA3	29:n1:603:CLA:H2	2.01	0.42
21:g1:121:GLN:HB2	21:g1:128:LEU:HD12	2.02	0.42
40:g1:624:LHG:H121	50:y1:622:XAT:H403	2.00	0.42
29:C:513:CLA:H91	29:C:513:CLA:H112	1.79	0.42
6:E:22:ILE:HG13	6:E:23:HIS:ND1	2.34	0.42
17:W:80:ILE:HG12	53:r:626:ERG:H162	2.01	0.42
40:Y:624:LHG:H361	40:Y:624:LHG:H332	1.77	0.42
29:c:502:CLA:H61	29:c:512:CLA:H42	2.00	0.42
14:o:187:PHE:HD1	14:o:200:PHE:HB3	1.84	0.42
20:n:182:TYR:HB3	29:n:610:CLA:HED3	2.02	0.42
21:g:134:GLU:OE2	21:g:138:HIS:NE2	2.52	0.42
23:s:136:TRP:HZ2	23:s:250:ALA:HA	1.83	0.42
34:y:625:SPH:H162	34:y:625:SPH:H131	1.82	0.42
2:B1:340:TRP:HA	2:B1:430:PHE:HD1	1.84	0.42
2:B1:370:LEU:HD23	2:B1:370:LEU:HA	1.82	0.42
29:B1:616:CLA:H93	29:B1:616:CLA:H111	1.88	0.42
4:C1:323:THR:OG1	4:C1:325:LEU:HD22	2.20	0.42
6:E1:65:LEU:HA	6:E1:65:LEU:HD12	1.79	0.42
14:O1:104:LEU:HD23	14:O1:147:MET:HB2	2.01	0.42
38:T1:101:3PH:H2C1	38:T1:101:3PH:H2H1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a1:147:TYR:O	1:a1:150:PRO:HG2	2.20	0.42
29:a1:406:CLA:H111	40:d1:409:LHG:H181	2.00	0.42
2:b1:30:VAL:HG12	29:b1:614:CLA:C3C	2.49	0.42
2:b1:422:ARG:HH22	14:o1:229:PRO:HA	1.84	0.42
29:b1:611:CLA:H192	29:b1:613:CLA:HMD2	2.01	0.42
8:h1:57:PHE:HB2	45:h1:101:RRX:C22	2.50	0.42
11:k1:25:LEU:HD23	11:k1:25:LEU:HA	1.86	0.42
29:n1:603:CLA:H152	48:n1:609:CHL:H112	2.01	0.42
29:g1:611:CLA:H112	29:g1:611:CLA:H142	1.75	0.42
29:g1:613:CLA:H52	29:g1:613:CLA:NC	2.34	0.42
29:s1:603:CLA:HHB	29:s1:609:CLA:H12	2.01	0.42
24:y1:123:ILE:HB	24:y1:126:LYS:HG2	2.00	0.42
48:y1:607:CHL:H62	48:y1:607:CHL:H2	1.81	0.42
29:y1:610:CLA:CBB	49:y1:620:LUT:H32	2.49	0.42
50:y1:622:XAT:H15	50:y1:622:XAT:H201	1.73	0.42
1:A:201:GLY:HA3	1:A:286:THR:HB	1.99	0.42
1:A:310:ASN:O	15:P:89:SER:OG	2.30	0.42
1:A:330:VAL:HA	5:D:352:LEU:HD23	2.01	0.42
2:B:155:ALA:O	2:B:159:THR:OG1	2.36	0.42
2:B:391:SER:O	2:B:395:VAL:HG22	2.20	0.42
29:B:607:CLA:H62	29:B:607:CLA:H41	1.79	0.42
31:C:515:BCR:H351	31:C:515:BCR:H15C	1.75	0.42
19:Z:60:PHE:CZ	23:S:280:LEU:HD23	2.55	0.42
29:N:603:CLA:H61	29:N:603:CLA:H102	1.75	0.42
21:G:84:ILE:HD13	21:G:84:ILE:HA	1.90	0.42
22:R:133:PHE:HA	22:R:136:THR:HG1	1.84	0.42
22:R:174:GLN:HA	22:R:180:LEU:HG	2.00	0.42
22:R:220:PRO:HD2	49:R:620:LUT:H23	2.01	0.42
29:S:602:CLA:H62	29:S:602:CLA:H41	1.63	0.42
29:a:406:CLA:H202	29:a:406:CLA:H161	1.85	0.42
29:a:410:CLA:H61	29:a:410:CLA:H41	1.80	0.42
2:b:366:PHE:HB3	2:b:425:GLN:NE2	2.31	0.42
40:g:624:LHG:H151	40:g:624:LHG:H181	1.83	0.42
23:s:118:ILE:HG23	23:s:136:TRP:HB3	2.01	0.42
34:A1:414:SPH:H183	34:A1:414:SPH:H152	1.77	0.42
2:B1:400:THR:OG1	2:B1:401:PHE:N	2.53	0.42
29:B1:606:CLA:HAB	29:B1:607:CLA:H51	2.01	0.42
29:B1:611:CLA:HBD	29:B1:611:CLA:H152	2.01	0.42
4:C1:261:SER:HA	4:C1:264:LEU:HD12	2.01	0.42
29:C1:505:CLA:H172	37:C1:518:DGD:HA71	2.02	0.42
29:R1:609:CLA:H121	52:R1:625:LMT:H111	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:S1:614:CLA:HBC1	40:S1:624:LHG:H371	2.02	0.42
24:Y1:58:PRO:HG2	24:Y1:61:LEU:HD12	2.00	0.42
2:b1:49:ASP:OD2	2:b1:52:LEU:HB2	2.20	0.42
29:b1:610:CLA:H143	29:b1:610:CLA:H161	1.85	0.42
39:b1:625:DGA:HA21	5:d1:131:GLU:HA	2.02	0.42
4:c1:187:ILE:HD13	4:c1:218:LEU:HG	2.00	0.42
39:c1:524:DGA:HB22	39:c1:524:DGA:HB52	1.70	0.42
20:n1:226:VAL:HG21	50:g1:622:XAT:H21	1.99	0.42
29:g1:602:CLA:H101	49:g1:621:LUT:H361	2.00	0.42
23:s1:234:LYS:HG2	29:s1:611:CLA:OBD	2.20	0.42
29:s1:611:CLA:H112	29:s1:611:CLA:H91	1.86	0.42
40:s1:624:LHG:H122	40:s1:624:LHG:HC92	1.71	0.42
24:y1:82:THR:HA	24:y1:85:ARG:HB2	2.01	0.42
2:B:324:LEU:N	5:D:294:ARG:O	2.40	0.42
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.22	0.42
21:G:245:ALA:HA	50:Y:622:XAT:H22	2.00	0.42
29:G:610:CLA:H72	49:G:620:LUT:H30	2.01	0.42
24:Y:42:TYR:CE1	24:Y:202:ALA:HB1	2.54	0.42
5:d:87:HIS:CD2	5:d:162:LEU:HA	2.55	0.42
14:o:207:GLY:HA3	15:p:157:GLU:OE1	2.20	0.42
15:p:88:PRO:HG2	15:p:91:TRP:CD2	2.55	0.42
23:s:105:LEU:O	23:s:109:ARG:HG3	2.19	0.42
49:y:621:LUT:H11	49:y:621:LUT:H191	1.92	0.42
1:A1:265:PHE:HB3	1:A1:271:LEU:HB2	2.01	0.42
2:B1:58:GLN:HB2	2:B1:60:MET:HE1	2.00	0.42
2:B1:281:GLN:HE21	2:B1:358:ARG:CZ	2.32	0.42
2:B1:282:GLN:NE2	25:U1:107:LYS:HB2	2.35	0.42
29:B1:605:CLA:H51	29:B1:606:CLA:C1C	2.50	0.42
4:C1:33:LEU:HB3	4:C1:36:LYS:HB3	2.02	0.42
4:C1:62:HIS:ND1	33:C1:521:LMG:O4	2.32	0.42
4:C1:118:VAL:HG23	29:C1:511:CLA:H91	2.02	0.42
4:C1:333:PRO:O	14:O1:136:LEU:HB2	2.20	0.42
5:D1:89:LEU:HD21	33:H1:102:LMG:H301	2.01	0.42
15:P1:97:LYS:NZ	15:P1:100:ASP:HA	2.34	0.42
20:N1:192:LEU:HB3	29:N1:610:CLA:HBA1	2.01	0.42
21:G1:42:GLY:HA3	21:G1:43:PRO:HD3	1.91	0.42
29:S1:604:CLA:H12	51:S1:623:NEX:H241	2.00	0.42
24:Y1:111:ALA:HB2	24:Y1:117:PHE:HD2	1.84	0.42
48:Y1:606:CHL:HHC	48:Y1:606:CHL:HBB1	2.01	0.42
30:a1:409:PHO:H142	30:a1:409:PHO:H112	1.84	0.42
2:b1:447:PRO:HA	2:b1:450:TRP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b1:617:CLA:H162	29:b1:617:CLA:H141	1.70	0.42
38:b1:624:3PH:H3G2	38:b1:624:3PH:H3D2	1.78	0.42
4:c1:275:CYS:SG	4:c1:418:HIS:HB2	2.59	0.42
4:c1:429:HIS:HE1	29:c1:505:CLA:ND	2.17	0.42
29:c1:501:CLA:H203	29:c1:507:CLA:H13	2.02	0.42
8:h1:60:PHE:HB2	45:h1:101:RRX:H33	2.01	0.42
15:p1:116:VAL:HG23	15:p1:219:VAL:HG22	2.01	0.42
20:n1:95:TRP:O	20:n1:99:GLY:N	2.51	0.42
20:n1:218:LEU:HD13	29:n1:603:CLA:HAB	2.02	0.42
48:n1:601:CHL:H61	48:n1:601:CHL:H41	1.88	0.42
23:s1:255:VAL:HG13	23:s1:256:THR:HG23	2.00	0.42
29:s1:603:CLA:H18	29:s1:609:CLA:HBB1	2.01	0.42
29:y1:602:CLA:H2A	29:y1:602:CLA:HED2	2.01	0.42
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.90	0.42
1:A:326:LEU:HD11	15:P:110:PHE:HE1	1.84	0.42
2:B:269:GLY:O	2:B:448:ARG:NH2	2.38	0.42
29:B:611:CLA:H141	29:B:613:CLA:HBD	2.01	0.42
4:C:270:MET:HE1	29:C:507:CLA:H11	2.02	0.42
5:D:40:CYS:SG	29:D:403:CLA:HBB1	2.59	0.42
5:D:66:SER:OG	5:D:68:ILE:HG22	2.19	0.42
6:E:37:PHE:CD1	6:E:42:LEU:HB3	2.55	0.42
23:S:176:LEU:HD13	29:S:609:CLA:HMC2	2.01	0.42
1:a:121:LEU:HD21	29:c:505:CLA:H162	2.01	0.42
29:c:513:CLA:H122	31:c:514:BCR:H23C	2.01	0.42
51:n:623:NEX:H171	29:s:612:CLA:HED3	2.02	0.42
29:y:612:CLA:H61	29:y:612:CLA:H41	1.86	0.42
51:y:623:NEX:H201	51:y:623:NEX:H15	1.76	0.42
1:A1:323:ARG:C	5:D1:329:MET:HE1	2.45	0.42
2:B1:245:VAL:HG11	29:B1:614:CLA:HMB1	2.02	0.42
2:B1:332:SER:OG	2:B1:444:ARG:NH1	2.53	0.42
2:B1:348:ASP:OD1	2:B1:352:ARG:N	2.52	0.42
3:V1:33:LEU:OXT	11:K1:46:ARG:NH2	2.48	0.42
29:C1:512:CLA:O2D	29:C1:513:CLA:HBB2	2.20	0.42
40:C1:525:LHG:H161	40:C1:525:LHG:H192	1.95	0.42
8:H1:19:GLU:HA	8:H1:20:PRO:HD3	1.85	0.42
21:G1:130:TYR:HB2	21:G1:137:ILE:HG12	2.01	0.42
29:G1:603:CLA:H141	29:G1:603:CLA:H162	1.76	0.42
22:R1:78:LEU:HB3	29:R1:602:CLA:O2A	2.20	0.42
29:Y1:611:CLA:H172	29:Y1:612:CLA:CBB	2.49	0.42
4:c1:274:ALA:HB2	29:c1:501:CLA:H43	2.01	0.42
29:g1:610:CLA:H172	49:g1:620:LUT:H393	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:s1:178:ALA:HA	23:s1:181:LYS:HE3	2.01	0.42
30:A:408:PHO:HAB	5:D:205:LEU:HD13	2.02	0.42
29:B:616:CLA:H111	29:B:616:CLA:H91	1.73	0.42
13:M:31:ALA:HB2	13:m:28:LYS:HG3	2.02	0.42
22:R:221:LEU:HA	24:y:188:PRO:HB3	2.02	0.42
29:R:612:CLA:H111	29:R:612:CLA:H142	1.83	0.42
23:S:181:LYS:HB2	23:S:181:LYS:HE2	1.83	0.42
29:Y:613:CLA:H112	29:Y:613:CLA:H71	1.75	0.42
1:a:217:SER:O	1:a:221:SER:OG	2.36	0.42
1:a:330:VAL:HA	5:d:352:LEU:HD23	2.00	0.42
1:a:340:PRO:HB3	15:p:198:GLU:C	2.44	0.42
31:a:411:BCR:H351	31:a:411:BCR:H15C	1.72	0.42
29:g:602:CLA:H62	29:g:602:CLA:H41	1.83	0.42
23:s:134:GLY:HA2	29:s:604:CLA:HED1	2.02	0.42
29:s:602:CLA:H62	29:s:602:CLA:H41	1.72	0.42
29:y:614:CLA:H161	29:y:614:CLA:H143	1.80	0.42
29:B1:616:CLA:HAB	29:R1:609:CLA:H43	2.02	0.42
4:C1:72:GLN:HB2	4:C1:74:LEU:HG	2.02	0.42
4:C1:128:LEU:HD13	4:C1:135:PHE:HB3	2.01	0.42
4:C1:322:PRO:HB2	14:O1:206:ARG:NH2	2.35	0.42
4:C1:323:THR:HA	14:O1:206:ARG:CD	2.49	0.42
29:C1:501:CLA:HBB1	29:C1:507:CLA:H41	2.01	0.42
5:D1:53:THR:HG23	5:D1:67:TYR:HD2	1.84	0.42
29:N1:613:CLA:H112	29:N1:613:CLA:H91	1.85	0.42
2:b1:223:ILE:HD12	22:r1:85:LEU:HD11	2.01	0.42
2:b1:277:GLN:O	25:u1:105:THR:HA	2.20	0.42
38:b1:624:3PH:H11	13:m1:6:LEU:HD13	2.01	0.42
48:s1:607:CHL:HHC	48:s1:607:CHL:HBB1	2.01	0.42
38:s1:626:3PH:H351	38:s1:626:3PH:H321	1.84	0.42
40:y1:624:LHG:H272	40:y1:624:LHG:H242	1.83	0.42
1:A:267:ASN:HB3	1:A:270:SER:HB2	2.02	0.42
1:A:323:ARG:HE	1:A:323:ARG:HB3	1.67	0.42
29:A:406:CLA:H92	29:A:406:CLA:H62	1.87	0.42
29:A:410:CLA:H12	33:A:413:LMG:H121	2.01	0.42
29:B:603:CLA:H202	29:B:603:CLA:H161	1.72	0.42
5:D:263:ASN:HB3	5:D:266:TRP:HB3	2.02	0.42
48:N:605:CHL:HHC	48:N:605:CHL:HBB1	2.02	0.42
29:b:606:CLA:H202	29:b:606:CLA:H161	1.77	0.42
5:d:202:ALA:HB2	43:d:405:PL9:H353	2.02	0.42
55:y:626:PTY:H131	55:y:626:PTY:H162	1.79	0.42
29:A1:405:CLA:H203	29:A1:406:CLA:H8	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:4:PRO:HD2	2:B1:7:ARG:HB2	2.02	0.42
2:B1:46:ASP:HB3	2:B1:58:GLN:HE22	1.85	0.42
29:B1:611:CLA:H141	29:B1:613:CLA:HBD	2.02	0.42
5:D1:188:PHE:CD1	5:D1:326:ARG:HG2	2.54	0.42
43:D1:405:PL9:H122	43:D1:405:PL9:H101	1.79	0.42
9:I1:21:PHE:HD1	9:I1:24:LEU:HD23	1.85	0.42
14:O1:252:ALA:HA	14:O1:272:SER:HA	2.02	0.42
15:P1:187:PHE:HB2	15:P1:205:VAL:HB	2.02	0.42
20:N1:48:TRP:HD1	20:N1:68:TYR:O	2.03	0.42
20:N1:168:ARG:HH12	48:N1:609:CHL:HED2	1.85	0.42
21:G1:214:PHE:HZ	49:G1:620:LUT:H8	1.84	0.42
22:R1:244:ARG:HA	22:R1:247:MET:HE2	2.01	0.42
23:S1:120:ILE:HD13	23:S1:120:ILE:HA	1.89	0.42
24:Y1:40:ALA:O	24:Y1:46:ARG:HA	2.19	0.42
29:a1:410:CLA:HBA1	29:a1:410:CLA:H12	1.80	0.42
4:c1:107:LEU:HD21	31:c1:517:BCR:HC41	2.02	0.42
4:c1:227:TRP:HZ3	55:y1:626:PTY:H191	1.85	0.42
29:c1:508:CLA:CAB	29:c1:510:CLA:HMA3	2.50	0.42
31:d1:404:BCR:H373	7:f1:33:LEU:HD21	2.02	0.42
29:g1:611:CLA:H61	29:g1:611:CLA:H41	1.85	0.42
22:r1:63:LEU:HB3	22:r1:70:ASP:OD2	2.20	0.42
23:s1:191:GLY:HA2	23:s1:199:PHE:CZ	2.55	0.42
23:s1:225:PRO:HA	23:s1:228:PHE:HB3	2.02	0.42
1:A:186:PHE:CE2	1:A:192:ILE:HD12	2.55	0.41
1:A:297:LEU:HD12	1:A:297:LEU:HA	1.82	0.41
2:B:75:TRP:CE3	32:B:626:SQD:H45	2.54	0.41
2:B:318:ASN:HB3	2:B:321:LYS:HG2	2.00	0.41
3:V:11:ALA:HB2	11:K:21:ILE:HG22	2.02	0.41
4:C:309:ASP:OD2	4:C:328:TYR:OH	2.27	0.41
4:C:358:ARG:HG2	4:C:363:LEU:HD23	2.01	0.41
48:G:606:CHL:HBB1	48:G:606:CHL:HHC	2.02	0.41
23:S:172:GLU:HG3	23:S:176:LEU:HD12	2.02	0.41
29:S:613:CLA:H52	29:S:613:CLA:H11	1.73	0.41
30:a:408:PHO:H8	30:a:408:PHO:H121	1.75	0.41
32:a:412:SQD:H261	32:a:412:SQD:H292	1.82	0.41
2:b:193:TYR:HB3	8:h:84:LEU:HD12	2.01	0.41
2:b:413:ASP:HB3	2:b:416:THR:HG22	2.02	0.41
2:b:467:ILE:O	2:b:471:SER:OG	2.34	0.41
29:b:610:CLA:H193	29:b:610:CLA:H162	1.86	0.41
31:b:618:BCR:H15C	31:b:618:BCR:H351	1.83	0.41
5:d:259:VAL:HG21	40:d:409:LHG:H271	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:n:221:PHE:CD2	29:n:603:CLA:HBB2	2.55	0.41
48:n:607:CHL:H93	48:n:607:CHL:H61	1.93	0.41
51:n:623:NEX:H15	51:n:623:NEX:H201	1.93	0.41
21:g:188:ASP:OD1	21:g:188:ASP:N	2.51	0.41
1:A1:309:SER:HA	7:F1:44:ARG:HG2	2.02	0.41
32:A1:412:SQD:H383	37:C1:519:DGD:HAT2	2.01	0.41
32:A1:412:SQD:H332	29:C1:504:CLA:H201	2.02	0.41
2:B1:454:GLY:HA2	33:B1:622:LMG:H191	2.02	0.41
4:C1:30:LEU:HD22	4:C1:36:LYS:HG2	2.02	0.41
14:O1:192:THR:HG23	14:O1:195:SER:H	1.85	0.41
14:O1:228:LEU:HA	14:O1:229:PRO:HD3	1.85	0.41
17:W1:83:TRP:CD2	33:W1:201:LMG:H292	2.55	0.41
20:N1:158:VAL:HG13	50:N1:622:XAT:H402	2.01	0.41
21:G1:192:THR:O	21:G1:196:LEU:N	2.43	0.41
29:G1:603:CLA:H161	29:G1:603:CLA:H193	1.81	0.41
50:G1:622:XAT:H15	50:G1:622:XAT:H201	1.88	0.41
24:Y1:124:TRP:HB2	49:Y1:621:LUT:H41	2.02	0.41
24:Y1:248:ASN:ND2	24:Y1:250:PHE:HB2	2.35	0.41
1:a1:56:PRO:HD2	1:a1:106:LEU:HD12	2.02	0.41
1:a1:269:ARG:HD3	5:d1:222:LEU:HD13	2.01	0.41
1:a1:340:PRO:HB3	15:p1:198:GLU:HA	2.01	0.41
2:b1:130:LYS:HE2	22:r1:89:VAL:HG13	2.02	0.41
29:b1:612:CLA:H122	29:b1:612:CLA:H161	1.87	0.41
14:o1:133:LEU:HD11	14:o1:171:LYS:HB2	2.01	0.41
14:o1:181:LEU:C	14:o1:274:GLN:HE22	2.26	0.41
20:n1:94:ARG:NE	48:n1:608:CHL:OBD	2.53	0.41
48:g1:609:CHL:H161	48:g1:609:CHL:H141	1.78	0.41
51:s1:623:NEX:H35	51:s1:623:NEX:H401	1.83	0.41
24:y1:137:LEU:HD23	24:y1:137:LEU:HA	1.91	0.41
29:y1:613:CLA:H42	29:y1:613:CLA:C1D	2.50	0.41
1:A:270:SER:OG	32:A:412:SQD:O2	2.33	0.41
2:B:10:THR:HG21	29:B:612:CLA:HED1	2.02	0.41
2:B:121:GLU:HG2	8:H:23:VAL:HG22	2.02	0.41
29:B:609:CLA:H8	29:B:610:CLA:H121	2.01	0.41
4:C:135:PHE:CZ	31:C:514:BCR:H282	2.55	0.41
47:K:101:4RF:H50	47:K:101:4RF:H55	1.91	0.41
22:R:145:MET:HA	22:R:148:THR:HG22	2.02	0.41
29:R:608:CLA:HBA2	29:R:608:CLA:H3A	1.57	0.41
49:Y:621:LUT:H15	49:Y:621:LUT:H201	1.79	0.41
1:a:42:LEU:HB3	31:a:411:BCR:H353	2.02	0.41
1:a:131:TRP:HE1	4:c:434:GLY:HA2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:410:CLA:H13	29:a:410:CLA:H101	1.74	0.41
4:c:118:VAL:HG22	29:c:511:CLA:H91	2.02	0.41
15:p:128:ILE:HG23	15:p:209:VAL:HG13	2.02	0.41
23:s:53:TYR:HE2	23:s:229:ALA:HB1	1.85	0.41
4:C1:421:LEU:HD23	29:C1:502:CLA:HMC2	2.02	0.41
29:C1:511:CLA:H143	19:Z1:20:VAL:HG23	2.01	0.41
43:D1:405:PL9:H13	43:D1:405:PL9:H172	1.73	0.41
19:Z1:17:PHE:HA	19:Z1:20:VAL:HG12	2.03	0.41
29:R1:603:CLA:H111	52:R1:625:LMT:H32	2.02	0.41
23:S1:61:LEU:HD22	23:S1:65:LEU:HD23	2.02	0.41
29:Y1:613:CLA:H41	40:Y1:624:LHG:H191	2.02	0.41
40:Y1:624:LHG:H361	40:Y1:624:LHG:H332	1.77	0.41
2:b1:30:VAL:HG23	29:b1:606:CLA:HAC2	2.02	0.41
2:b1:209:GLY:HA3	29:b1:606:CLA:H201	2.01	0.41
29:b1:612:CLA:H193	29:b1:612:CLA:H162	1.87	0.41
4:c1:75:ILE:C	4:c1:78:PRO:HD2	2.45	0.41
4:c1:282:ASN:OD1	37:c1:518:DGD:O5E	2.32	0.41
5:d1:186:GLN:HB2	29:d1:402:CLA:HBC1	2.01	0.41
5:d1:318:ASN:O	5:d1:322:ASN:N	2.48	0.41
29:y1:604:CLA:H122	29:y1:604:CLA:H161	1.88	0.41
2:B:208:LEU:HD12	2:B:208:LEU:HA	1.88	0.41
4:C:282:ASN:OD1	37:C:518:DGD:O5E	2.34	0.41
29:C:509:CLA:HBB1	29:C:509:CLA:HMB3	2.01	0.41
5:D:72:ASN:HA	33:D:411:LMG:HC1	2.02	0.41
24:Y:185:PRO:HG3	29:Y:608:CLA:HBC2	2.02	0.41
29:Y:613:CLA:H121	40:Y:624:LHG:H332	2.02	0.41
40:d:409:LHG:H292	16:t:17:ILE:HG23	2.01	0.41
7:f:33:LEU:HD23	7:f:33:LEU:HA	1.77	0.41
20:n:116:MET:HE3	20:n:116:MET:HB2	1.88	0.41
49:n:620:LUT:H11	49:n:620:LUT:H191	1.88	0.41
23:s:143:MET:HG3	23:s:165:LEU:HB2	2.02	0.41
24:y:155:LEU:O	24:y:159:VAL:HG23	2.20	0.41
1:A1:142:TRP:CZ2	4:C1:435:ARG:HB2	2.56	0.41
2:B1:124:ARG:HG2	2:B1:131:THR:HA	2.02	0.41
29:B1:616:CLA:HBA1	29:B1:616:CLA:H3A	1.73	0.41
4:C1:147:ASN:HB3	4:C1:151:TYR:CZ	2.55	0.41
5:D1:261:PHE:HE1	5:D1:266:TRP:CD1	2.38	0.41
5:D1:330:ALA:HB3	5:D1:339:LEU:HD22	2.02	0.41
9:I1:3:THR:HG23	22:r1:181:PRO:HB2	2.02	0.41
20:N1:98:LEU:HD21	29:N1:610:CLA:HBC3	2.02	0.41
48:N1:606:CHL:H71	38:S1:626:3PH:H3I3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:G1:602:CLA:H93	29:G1:602:CLA:H111	1.85	0.41
29:Y1:612:CLA:H41	29:Y1:612:CLA:H61	1.65	0.41
2:b1:57:ARG:HH12	2:b1:334:ASP:CG	2.28	0.41
2:b1:259:GLY:HA3	8:h1:81:TRP:HZ2	1.84	0.41
29:b1:604:CLA:H152	29:b1:604:CLA:H111	1.97	0.41
4:c1:20:GLY:O	5:d1:230:ASN:N	2.53	0.41
29:c1:502:CLA:H172	29:c1:502:CLA:H13	1.83	0.41
40:c1:525:LHG:H191	32:c1:526:SQD:H383	2.02	0.41
6:e1:10:PHE:CZ	7:f1:18:ARG:HD2	2.55	0.41
15:p1:93:PRO:HB3	15:p1:106:TYR:CE1	2.54	0.41
23:s1:177:GLY:HA2	29:s1:609:CLA:HAB	2.03	0.41
29:B:605:CLA:H92	29:B:605:CLA:H61	1.85	0.41
6:E:32:ILE:O	6:E:36:LEU:HG	2.20	0.41
40:L:101:LHG:HC61	40:L:101:LHG:H111	2.02	0.41
20:N:99:GLY:O	20:N:103:MET:HG3	2.21	0.41
49:R:620:LUT:H31	49:R:620:LUT:H391	1.97	0.41
38:S:626:3PH:H2E2	38:S:626:3PH:H2H1	1.91	0.41
24:Y:61:LEU:HB3	24:Y:68:ASP:OD1	2.20	0.41
25:U:98:ASP:HB2	25:U:107:LYS:NZ	2.34	0.41
2:b:157:HIS:HA	2:b:163:GLY:HA3	2.02	0.41
2:b:352:ARG:HD2	2:b:378:ARG:HE	1.85	0.41
31:b:618:BCR:H331	38:b:624:3PH:H252	2.02	0.41
5:d:270:PHE:HZ	43:d:405:PL9:H203	1.85	0.41
6:e:10:PHE:HA	6:e:13:ILE:HG22	2.02	0.41
14:o:252:ALA:HA	14:o:272:SER:HA	2.03	0.41
15:p:177:LYS:HB2	15:p:177:LYS:HE2	1.81	0.41
20:n:67:ASP:HA	29:n:602:CLA:CGD	2.49	0.41
20:n:94:ARG:HA	20:n:97:LEU:HD12	2.02	0.41
50:g:622:XAT:H11	50:g:622:XAT:H191	1.96	0.41
24:y:102:LEU:HG	29:y:604:CLA:HAC1	2.02	0.41
1:A1:223:LEU:O	2:B1:482:ILE:HG12	2.21	0.41
2:B1:314:TYR:HE1	2:B1:426:LEU:HB3	1.84	0.41
2:B1:341:LEU:HB2	2:B1:429:ILE:HG22	2.03	0.41
29:B1:604:CLA:H201	8:H1:58:ALA:HB2	2.03	0.41
47:K1:101:4RF:H55	47:K1:101:4RF:H50	1.73	0.41
12:L1:19:TYR:HE1	16:T1:19:PHE:HB3	1.86	0.41
16:T1:1:MET:HE3	16:T1:1:MET:HB3	1.87	0.41
20:N1:125:LYS:HZ1	24:Y1:257:VAL:HG13	1.85	0.41
49:G1:620:LUT:H15	49:G1:620:LUT:H201	1.83	0.41
34:Y1:625:SPH:H131	34:Y1:625:SPH:H161	1.74	0.41
2:b1:99:SER:OG	29:b1:607:CLA:H61	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:338:VAL:HB	2:b1:431:GLU:HB3	2.03	0.41
2:b1:376:VAL:HG13	15:p1:97:LYS:H	1.85	0.41
2:b1:458:PHE:HB3	29:b1:605:CLA:HMC1	2.02	0.41
29:b1:605:CLA:H93	29:b1:605:CLA:H61	1.91	0.41
4:c1:197:ILE:HG21	4:c1:227:TRP:CD1	2.56	0.41
4:c1:261:SER:HA	4:c1:264:LEU:HD12	2.02	0.41
29:c1:501:CLA:H162	29:c1:507:CLA:HMB3	2.01	0.41
40:n1:624:LHG:HC91	50:g1:622:XAT:H393	2.03	0.41
48:g1:601:CHL:HMD1	40:g1:624:LHG:H241	2.00	0.41
22:r1:252:GLY:HA2	22:r1:255:ILE:HG12	2.02	0.41
23:s1:209:LYS:HA	23:s1:209:LYS:HD3	1.90	0.41
23:s1:212:PRO:HG3	48:s1:608:CHL:HBC2	2.02	0.41
29:s1:613:CLA:HAB	40:s1:624:LHG:H302	2.02	0.41
25:u1:91:VAL:HA	25:u1:94:VAL:HG12	2.02	0.41
1:A:127:MET:HG2	1:A:144:ALA:HB1	2.03	0.41
1:A:230:ASN:HB3	22:R:94:GLN:HG3	2.02	0.41
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.02	0.41
4:C:246:PRO:HA	4:C:249:ARG:HD2	2.03	0.41
14:O:107:PHE:HE1	14:O:294:TRP:CE3	2.37	0.41
15:P:105:ARG:HG3	15:P:117:TYR:HB3	2.02	0.41
29:N:610:CLA:H91	29:N:610:CLA:H111	1.81	0.41
21:G:119:GLY:HA2	48:G:606:CHL:HAC2	2.03	0.41
29:Y:614:CLA:H143	29:Y:614:CLA:H161	1.85	0.41
2:b:282:GLN:O	2:b:286:LYS:HB2	2.20	0.41
29:c:509:CLA:H112	29:c:509:CLA:H142	1.70	0.41
21:g:128:LEU:HG	21:g:137:ILE:HD11	2.01	0.41
21:g:193:PHE:CZ	21:g:197:LYS:HD2	2.55	0.41
29:g:603:CLA:H122	48:g:609:CHL:H101	2.03	0.41
29:r:612:CLA:H11	29:r:612:CLA:H52	1.79	0.41
50:r:621:XAT:H31	50:r:621:XAT:H391	1.81	0.41
29:s:611:CLA:H192	29:s:611:CLA:H162	1.83	0.41
29:B1:606:CLA:H202	29:B1:606:CLA:H161	1.79	0.41
4:C1:104:VAL:HG11	31:C1:514:BCR:HC32	2.02	0.41
4:C1:295:PRO:HA	4:C1:346:PHE:CG	2.56	0.41
33:C1:523:LMG:H132	29:Y1:611:CLA:C1C	2.50	0.41
5:D1:299:VAL:O	5:D1:303:ILE:HG12	2.20	0.41
6:E1:45:ASP:OD2	15:P1:60:GLY:HA2	2.20	0.41
48:N1:607:CHL:C1B	48:Y1:601:CHL:H172	2.51	0.41
51:S1:623:NEX:H192	51:S1:623:NEX:H171	2.03	0.41
2:b1:191:ASP:HB3	2:b1:194:ASN:HB3	2.03	0.41
29:b1:603:CLA:HBA2	29:b1:603:CLA:H12	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c1:112:VAL:HA	4:c1:115:PHE:CD2	2.55	0.41
37:c1:519:DGD:HB81	37:c1:519:DGD:HB52	1.75	0.41
6:e1:22:ILE:HD13	44:f1:101:HEM:HMA2	2.01	0.41
8:h1:63:ILE:HA	8:h1:66:GLU:OE2	2.21	0.41
29:g1:602:CLA:HAB	49:g1:621:LUT:C32	2.51	0.41
22:r1:247:MET:HE3	22:r1:251:LEU:HD13	2.02	0.41
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.02	0.41
2:B:391:SER:OG	2:B:393:GLU:OE1	2.37	0.41
29:B:617:CLA:H91	29:B:617:CLA:H112	1.81	0.41
4:C:381:ALA:HA	4:C:384:MET:HE2	2.02	0.41
15:P:116:VAL:HG23	15:P:219:VAL:HG22	2.01	0.41
20:N:205:LYS:HG2	29:N:611:CLA:OBD	2.20	0.41
21:G:188:ASP:OD1	21:G:188:ASP:N	2.53	0.41
48:G:601:CHL:ND	40:G:624:LHG:HC82	2.35	0.41
50:R:621:XAT:H201	50:R:621:XAT:H15	1.71	0.41
4:c:431:TRP:CZ3	40:d:410:LHG:H281	2.56	0.41
39:c:524:DGA:HAN1	17:w:74:PHE:HE2	1.84	0.41
8:h:39:LYS:NZ	22:r:84:SEP:O1P	2.51	0.41
1:A1:195:HIS:HA	1:A1:196:PRO:HD3	1.91	0.41
1:A1:332:HIS:HA	28:A1:403:CL:CL	2.57	0.41
2:B1:303:ALA:HB2	2:B1:403:GLY:HA2	2.02	0.41
29:B1:607:CLA:H111	29:B1:607:CLA:H151	1.78	0.41
29:B1:610:CLA:C3D	8:H1:50:MET:HE1	2.51	0.41
29:B1:615:CLA:H141	29:B1:615:CLA:H162	1.80	0.41
5:D1:55:VAL:HG21	5:D1:110:LEU:HD13	2.02	0.41
49:N1:620:LUT:H11	49:N1:620:LUT:H191	1.87	0.41
29:Y1:611:CLA:H122	29:Y1:611:CLA:H161	1.89	0.41
1:a1:157:VAL:HG11	1:a1:172:MET:SD	2.61	0.41
30:a1:408:PHO:H162	30:a1:408:PHO:H141	1.71	0.41
2:b1:440:ASP:OD1	2:b1:441:GLY:N	2.53	0.41
29:b1:602:CLA:H143	29:b1:602:CLA:H111	1.78	0.41
38:b1:624:3PH:H2H1	38:b1:624:3PH:H2E1	1.82	0.41
4:c1:72:GLN:O	4:c1:72:GLN:NE2	2.52	0.41
29:c1:506:CLA:H112	29:c1:507:CLA:H141	2.02	0.41
5:d1:21:TRP:CE3	18:x1:90:VAL:HG23	2.56	0.41
5:d1:156:VAL:HG22	5:d1:286:VAL:HG11	2.03	0.41
5:d1:249:ALA:O	5:d1:253:TRP:N	2.44	0.41
8:h1:54:ILE:HA	45:h1:101:RRX:H21	2.01	0.41
21:g1:235:ASP:HB3	21:g1:238:VAL:HG12	2.01	0.41
23:s1:193:SER:OG	23:s1:215:PRO:O	2.24	0.41
29:s1:613:CLA:H42	29:s1:613:CLA:C4C	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:y1:626:PTY:H362	55:y1:626:PTY:H331	1.79	0.41
2:B:260:SER:N	2:B:263:THR:OG1	2.51	0.41
29:B:614:CLA:H62	29:B:614:CLA:H41	1.85	0.41
31:D:404:BCR:H351	31:D:404:BCR:H15C	1.79	0.41
7:F:35:ALA:O	7:F:39:MET:HG2	2.20	0.41
15:P:205:VAL:HG22	15:P:218:LYS:HG3	2.02	0.41
21:G:146:LEU:HD21	50:G:622:XAT:H202	2.03	0.41
22:R:135:GLU:HG3	22:R:212:ILE:CG1	2.50	0.41
23:S:268:LEU:HD23	54:S:625:LPX:H8A	2.01	0.41
24:Y:76:LEU:HD21	29:Y:602:CLA:H42	1.97	0.41
1:a:63:ILE:HG21	1:a:336:ALA:HA	2.03	0.41
2:b:191:ASP:HB3	2:b:194:ASN:HB2	2.02	0.41
29:b:610:CLA:HMA3	29:b:611:CLA:C1C	2.51	0.41
6:e:55:TYR:O	6:e:60:ARG:NH2	2.46	0.41
7:f:32:PHE:O	7:f:36:ILE:HD12	2.21	0.41
14:o:218:GLY:N	14:o:245:TYR:OH	2.49	0.41
29:r:602:CLA:H2A	29:r:602:CLA:HED2	2.03	0.41
23:s:283:ASP:OD1	23:s:283:ASP:N	2.53	0.41
51:s:623:NEX:H11	51:s:623:NEX:H191	1.89	0.41
2:B1:256:MET:HG2	2:B1:451:PHE:HD2	1.86	0.41
29:C1:506:CLA:H62	39:C1:524:DGA:HA62	2.01	0.41
33:C1:523:LMG:H332	33:C1:523:LMG:H131	2.02	0.41
5:D1:67:TYR:HA	5:D1:71:CYS:O	2.21	0.41
5:D1:111:TRP:NE1	5:D1:115:ALA:HB2	2.35	0.41
5:D1:111:TRP:CD1	5:D1:115:ALA:HB2	2.55	0.41
29:N1:603:CLA:ND	48:N1:609:CHL:H72	2.36	0.41
48:N1:607:CHL:H141	48:Y1:601:CHL:H201	2.03	0.41
29:N1:611:CLA:H12	29:N1:611:CLA:H3A	2.02	0.41
29:G1:611:CLA:HAB	50:Y1:622:XAT:H221	2.02	0.41
24:Y1:50:LEU:HD21	48:Y1:601:CHL:HAA1	2.03	0.41
1:a1:9:GLU:OE1	1:a1:9:GLU:N	2.53	0.41
2:b1:271:THR:O	2:b1:274:GLN:NE2	2.28	0.41
29:b1:604:CLA:NC	29:b1:606:CLA:H71	2.36	0.41
4:c1:423:PHE:HE1	37:c1:518:DGD:HBF2	1.84	0.41
29:c1:501:CLA:H203	29:c1:507:CLA:H162	2.01	0.41
5:d1:80:THR:HG22	5:d1:111:TRP:CE2	2.55	0.41
5:d1:196:PHE:HA	5:d1:199:MET:HE3	2.02	0.41
20:n1:229:LYS:HB3	20:n1:233:GLU:HG3	2.03	0.41
48:n1:606:CHL:HBB2	48:n1:607:CHL:HAB	2.03	0.41
29:n1:612:CLA:H3A	29:n1:612:CLA:HBA1	1.83	0.41
51:n1:623:NEX:H373	51:n1:623:NEX:H23	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:g1:603:CLA:H52	29:y1:603:CLA:H52	2.02	0.41
24:y1:233:PRO:HG2	24:y1:234:ILE:HD12	2.03	0.41
1:A:41:LEU:HD23	1:A:41:LEU:HA	1.85	0.41
1:A:329:GLU:HG3	1:A:332:HIS:HE1	1.86	0.41
4:C:225:HIS:HA	4:C:228:ILE:HG22	2.02	0.41
6:E:8:ARG:HB3	6:E:13:ILE:HD11	2.02	0.41
13:M:24:ILE:HG21	32:M:101:SQD:H251	2.02	0.41
15:P:204:LEU:HB3	15:P:238:LEU:HD13	2.01	0.41
51:R:622:NEX:H35	51:R:622:NEX:H401	1.89	0.41
24:Y:185:PRO:HB2	24:Y:189:PHE:HD2	1.86	0.41
30:a:408:PHO:H61	30:a:408:PHO:H2	1.84	0.41
29:b:609:CLA:H93	39:b:625:DGA:HBS1	2.02	0.41
32:b:621:SQD:H82	32:b:621:SQD:H111	1.82	0.41
39:c:524:DGA:HBG2	39:c:524:DGA:HBN2	1.72	0.41
5:d:199:MET:HG2	43:d:405:PL9:H321	2.03	0.41
5:d:257:PHE:CE1	40:d:409:LHG:H321	2.56	0.41
6:e:10:PHE:HE2	7:f:18:ARG:HD2	1.85	0.41
22:r:231:LYS:HB2	22:r:231:LYS:HE2	1.85	0.41
55:y:626:PTY:H391	55:y:626:PTY:H422	1.92	0.41
1:A1:222:SER:HA	5:D1:138:LEU:HD22	2.02	0.41
1:A1:300:PHE:HA	4:C1:393:ASN:OD1	2.20	0.41
2:B1:69:LEU:HD11	29:B1:604:CLA:HMD1	2.02	0.41
2:B1:321:LYS:NZ	2:B1:363:PHE:O	2.54	0.41
2:B1:382:PRO:HB3	5:D1:344:GLU:HG3	2.03	0.41
4:C1:137:TYR:CE1	29:C1:512:CLA:HBC1	2.56	0.41
5:D1:82:ALA:HB1	5:D1:336:HIS:NE2	2.35	0.41
29:D1:402:CLA:H62	29:D1:402:CLA:H41	1.81	0.41
8:H1:54:ILE:HA	45:H1:101:RRX:H21	2.03	0.41
16:T1:14:LEU:HD22	38:T1:101:3PH:H2G1	2.02	0.41
29:N1:610:CLA:H52	29:N1:610:CLA:H8	1.72	0.41
29:N1:611:CLA:HAB	50:G1:622:XAT:H222	2.03	0.41
21:G1:90:LEU:HA	21:G1:93:ALA:HB3	2.02	0.41
40:G1:624:LHG:H221	29:Y1:603:CLA:H201	2.02	0.41
1:a1:36:ILE:HA	29:a1:410:CLA:CBB	2.50	0.41
1:a1:289:GLY:O	1:a1:293:MET:HG2	2.21	0.41
1:a1:308:ASP:OD1	1:a1:312:ARG:N	2.54	0.41
2:b1:144:PHE:CE1	2:b1:210:VAL:HG13	2.55	0.41
2:b1:462:PHE:HA	29:b1:612:CLA:HMC2	2.01	0.41
4:c1:347:TRP:CZ3	14:o1:76:LYS:HE2	2.56	0.41
4:c1:425:PHE:HA	29:c1:508:CLA:HMC2	2.02	0.41
29:c1:508:CLA:H192	29:c1:508:CLA:H162	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d1:313:THR:OG1	5:d1:316:THR:HG23	2.20	0.41
29:n1:613:CLA:H122	29:n1:613:CLA:H8	1.76	0.41
2:B:39:LEU:HD12	38:B:624:3PH:H3D2	2.02	0.41
29:B:604:CLA:H2	29:B:606:CLA:H91	2.03	0.41
4:C:14:ARG:O	4:C:29:ARG:NH1	2.54	0.41
4:C:454:VAL:HG21	5:D:248:THR:HG23	2.02	0.41
29:D:402:CLA:H41	29:D:402:CLA:H62	1.62	0.41
43:D:405:PL9:H403	12:L:27:VAL:HG13	2.03	0.41
14:O:243:LYS:HD2	14:O:280:MET:SD	2.61	0.41
20:N:229:LYS:HD3	20:N:233:GLU:CD	2.46	0.41
23:S:99:LYS:HE2	23:S:99:LYS:HB2	1.83	0.41
24:Y:102:LEU:O	24:Y:106:THR:OG1	2.33	0.41
24:Y:145:LEU:HD21	22:r:176:LEU:HD22	2.02	0.41
29:Y:611:CLA:H111	29:Y:611:CLA:H72	1.90	0.41
29:Y:613:CLA:H12	29:Y:614:CLA:HED2	2.03	0.41
1:a:42:LEU:HD23	1:a:42:LEU:HA	1.83	0.41
2:b:25:MET:HE3	2:b:25:MET:O	2.20	0.41
2:b:120:LEU:HD13	29:b:617:CLA:HMD2	2.02	0.41
2:b:172:TYR:CE1	2:b:283:GLU:HB2	2.56	0.41
2:b:235:GLU:HB3	2:b:473:THR:HG22	2.02	0.41
2:b:302:TRP:O	2:b:305:ILE:HB	2.21	0.41
2:b:382:PRO:HB3	5:d:344:GLU:HG2	2.03	0.41
29:c:508:CLA:H192	29:c:508:CLA:H162	1.77	0.41
37:c:519:DGD:HBF2	37:c:519:DGD:HBE2	1.83	0.41
8:h:53:ALA:O	45:h:101:RRX:H21	2.20	0.41
33:h:102:LMG:H111	33:h:102:LMG:H141	1.87	0.41
23:s:96:GLN:N	23:s:96:GLN:OE1	2.54	0.41
51:s:623:NEX:H15	51:s:623:NEX:H201	1.88	0.41
24:y:85:ARG:O	24:y:88:THR:OG1	2.28	0.41
24:y:168:PHE:CD2	29:y:608:CLA:HAB	2.46	0.41
1:A1:280:VAL:HA	30:A1:408:PHO:HBC1	2.02	0.41
2:B1:75:TRP:HD1	2:B1:88:PRO:HG2	1.86	0.41
2:B1:293:SER:OG	2:B1:294:GLU:OE1	2.33	0.41
29:B1:605:CLA:H61	29:B1:605:CLA:H41	1.89	0.41
29:B1:605:CLA:HMC2	29:B1:612:CLA:H201	2.03	0.41
29:B1:609:CLA:H62	29:B1:610:CLA:H93	2.01	0.41
29:B1:617:CLA:H193	29:B1:617:CLA:H161	1.78	0.41
4:C1:69:MET:SD	4:C1:289:PHE:HA	2.60	0.41
4:C1:330:MET:O	4:C1:337:ILE:HD12	2.20	0.41
37:C1:519:DGD:HBE2	37:C1:519:DGD:HBF2	1.80	0.41
40:D1:409:LHG:O9	12:L1:20:TRP:NE1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H1:55:LEU:O	8:H1:59:VAL:HG23	2.21	0.41
15:P1:94:SER:HB2	15:P1:105:ARG:NH1	2.36	0.41
15:P1:134:PRO:HA	15:P1:137:PHE:HD2	1.86	0.41
20:N1:70:TRP:CZ3	48:N1:601:CHL:HAA2	2.52	0.41
20:N1:125:LYS:HZ2	24:Y1:257:VAL:HG22	1.86	0.41
20:N1:125:LYS:HD2	48:N1:607:CHL:HED3	2.03	0.41
20:N1:165:GLU:OE1	20:N1:168:ARG:NH2	2.44	0.41
20:N1:231:PRO:HA	20:N1:234:ASN:HB2	2.02	0.41
48:N1:601:CHL:H202	48:G1:607:CHL:H13	2.02	0.41
21:G1:65:THR:HA	24:Y1:85:ARG:NH2	2.36	0.41
53:R1:626:ERG:H192	53:R1:626:ERG:H111	1.83	0.41
23:S1:285:ARG:HH12	23:S1:287:PRO:HA	1.86	0.41
29:S1:611:CLA:H143	29:S1:611:CLA:H161	1.93	0.41
24:Y1:152:LEU:HD13	24:Y1:155:LEU:HD21	2.01	0.41
49:Y1:620:LUT:H31	49:Y1:620:LUT:H391	1.89	0.41
1:a1:153:ALA:HA	1:a1:156:ALA:HB3	2.02	0.41
1:a1:220:THR:HA	1:a1:223:LEU:HG	2.03	0.41
29:a1:407:CLA:HAB	5:d1:157:PHE:CE1	2.56	0.41
2:b1:26:HIS:CE1	29:b1:613:CLA:HMA3	2.56	0.41
2:b1:157:HIS:HA	2:b1:163:GLY:HA3	2.03	0.41
2:b1:379:ALA:HA	2:b1:390:TYR:HB3	2.02	0.41
2:b1:476:ARG:NH2	22:r1:99:ASN:HB3	2.36	0.41
4:c1:48:ILE:HG21	29:c1:503:CLA:H191	2.02	0.41
4:c1:168:LEU:HA	4:c1:187:ILE:HG22	2.03	0.41
4:c1:351:GLY:O	4:c1:355:GLU:HG2	2.21	0.41
29:c1:501:CLA:H171	29:c1:507:CLA:H111	2.02	0.41
29:c1:502:CLA:H41	29:c1:502:CLA:H62	1.87	0.41
29:c1:510:CLA:H143	29:c1:510:CLA:H111	1.83	0.41
29:c1:513:CLA:H121	31:c1:514:BCR:H392	2.03	0.41
40:c1:525:LHG:H331	40:c1:525:LHG:H361	1.79	0.41
5:d1:297:ASP:OD1	5:d1:297:ASP:N	2.49	0.41
5:d1:334:GLN:HB3	5:d1:336:HIS:CD2	2.56	0.41
5:d1:343:GLU:HB2	15:p1:112:ALA:HB3	2.03	0.41
40:d1:410:LHG:O3	40:d1:410:LHG:O1	2.30	0.41
6:e1:75:GLN:HG3	6:e1:78:LYS:HE2	2.03	0.41
10:j1:28:ALA:HB1	39:j1:101:DGA:HB92	2.02	0.41
14:o1:253:VAL:N	14:o1:271:GLU:O	2.41	0.41
14:o1:259:VAL:HG13	14:o1:266:ILE:HG22	2.02	0.41
20:n1:63:GLU:HG3	20:n1:64:PHE:CD2	2.56	0.41
48:n1:601:CHL:HHD	40:n1:624:LHG:HC41	2.03	0.41
21:g1:171:ASP:OD1	21:g1:171:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:g1:604:CLA:C3B	49:g1:621:LUT:H183	2.50	0.41
40:g1:624:LHG:H182	40:g1:624:LHG:H212	1.77	0.41
22:r1:202:ARG:NH2	29:r1:609:CLA:O1D	2.54	0.41
23:s1:258:GLU:HB2	23:s1:262:ALA:HB3	2.01	0.41
29:s1:614:CLA:HBA2	29:s1:614:CLA:H3A	1.53	0.41
24:y1:90:GLU:OE2	24:y1:213:ARG:NH2	2.54	0.41
29:y1:602:CLA:H92	29:y1:603:CLA:HMA1	2.01	0.41
25:u1:111:LYS:HD2	25:u1:111:LYS:HA	1.91	0.41
1:A:39:PRO:HB3	31:A:411:BCR:H10C	2.03	0.41
2:B:25:MET:HG2	31:B:618:BCR:H23C	2.02	0.41
2:B:359:MET:HB2	2:B:425:GLN:HG2	2.03	0.41
29:C:506:CLA:HMD3	33:C:523:LMG:H301	2.02	0.41
32:M:101:SQD:H92	13:m:26:TYR:HE2	1.84	0.41
14:O:228:LEU:HD11	14:O:231:LYS:HB3	2.02	0.41
29:N:613:CLA:H62	29:N:613:CLA:H2	1.82	0.41
2:b:30:VAL:HG22	29:b:614:CLA:C3C	2.51	0.41
29:b:610:CLA:OBD	8:h:46:THR:OG1	2.29	0.41
37:b:623:DGD:O5D	37:b:623:DGD:O4D	2.29	0.41
5:d:336:HIS:ND1	25:u:104:GLU:OE2	2.34	0.41
21:g:83:LEU:HD12	21:g:83:LEU:HA	1.88	0.41
1:A1:293:MET:HE2	1:A1:297:LEU:HB3	2.03	0.41
2:B1:114:HIS:HE1	29:B1:617:CLA:NA	2.19	0.41
2:B1:321:LYS:NZ	2:B1:359:MET:SD	2.82	0.41
4:C1:74:LEU:HD13	4:C1:77:LEU:HD12	2.02	0.41
4:C1:94:LEU:HA	23:S1:289:LEU:HD13	2.03	0.41
4:C1:142:LYS:HD3	4:C1:254:TRP:CD2	2.56	0.41
4:C1:316:VAL:HB	4:C1:328:TYR:HB2	2.03	0.41
29:C1:512:CLA:HMB2	40:C1:525:LHG:H122	2.03	0.41
21:G1:92:GLY:HA2	49:G1:621:LUT:H181	2.02	0.41
21:G1:207:ALA:O	21:G1:210:SER:HB3	2.21	0.41
29:R1:602:CLA:CBB	50:R1:621:XAT:H32	2.50	0.41
48:R1:606:CHL:HHC	48:R1:606:CHL:HBB1	2.02	0.41
23:S1:143:MET:HE2	48:S1:606:CHL:HAC1	2.03	0.41
23:S1:268:LEU:HD13	54:S1:625:LPX:H8A	2.03	0.41
24:Y1:105:ILE:HG23	24:Y1:234:ILE:HG13	2.03	0.41
24:Y1:137:LEU:HD21	29:Y1:604:CLA:HAA2	2.03	0.41
25:U1:106:VAL:HG23	25:U1:110:ARG:HH12	1.86	0.41
1:a1:19:GLU:HA	9:i1:30:ARG:HH12	1.86	0.41
30:a1:408:PHO:H121	30:a1:408:PHO:H8	1.65	0.41
29:a1:410:CLA:HBB1	29:a1:410:CLA:HMB3	2.03	0.41
2:b1:51:VAL:HG12	2:b1:308:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c1:249:ARG:HA	4:c1:254:TRP:NE1	2.36	0.41
31:c1:517:BCR:H351	31:c1:517:BCR:H15C	1.47	0.41
8:h1:78:THR:HB	8:h1:83:SER:OG	2.21	0.41
51:n1:623:NEX:H35	51:n1:623:NEX:H401	1.78	0.41
22:r1:180:LEU:HA	22:r1:181:PRO:HD3	1.98	0.41
22:r1:221:LEU:HB3	22:r1:223:LEU:HG	2.04	0.41
29:r1:610:CLA:H2	49:r1:620:LUT:H28	2.03	0.41
29:s1:611:CLA:H193	29:s1:611:CLA:H162	1.81	0.41
3:V:15:VAL:O	31:C:516:BCR:H14C	2.21	0.40
29:G:602:CLA:H111	29:G:602:CLA:H93	1.85	0.40
29:R:602:CLA:H71	29:R:602:CLA:H111	1.76	0.40
24:Y:85:ARG:HD2	24:Y:85:ARG:HA	1.82	0.40
29:Y:610:CLA:H111	29:Y:610:CLA:H91	1.85	0.40
29:Y:614:CLA:H61	29:Y:614:CLA:H41	1.67	0.40
1:a:308:ASP:O	7:f:44:ARG:HD2	2.22	0.40
29:b:617:CLA:H41	51:r:622:NEX:H22	2.02	0.40
4:c:119:TYR:OH	29:c:513:CLA:O1D	2.30	0.40
4:c:265:ALA:HB2	4:c:429:HIS:CG	2.56	0.40
15:p:93:PRO:HB3	15:p:106:TYR:CE1	2.56	0.40
17:w:62:ASP:OD1	17:w:62:ASP:N	2.54	0.40
50:n:622:XAT:H15	50:n:622:XAT:H201	1.73	0.40
23:s:171:ILE:O	23:s:175:LEU:HB2	2.21	0.40
49:y:620:LUT:H11	49:y:620:LUT:H191	1.95	0.40
1:A1:84:PRO:HA	1:A1:112:TYR:CG	2.56	0.40
4:C1:37:LEU:O	4:C1:41:HIS:ND1	2.51	0.40
4:C1:40:ALA:HB1	29:C1:509:CLA:HBB1	2.02	0.40
4:C1:120:HIS:HA	4:C1:124:GLY:HA3	2.03	0.40
37:C1:520:DGD:HBT1	37:C1:520:DGD:HA61	2.02	0.40
5:D1:151:ALA:HB2	5:D1:280:TRP:CE2	2.56	0.40
5:D1:270:PHE:HZ	43:D1:405:PL9:H203	1.85	0.40
5:D1:336:HIS:HD1	6:E1:65:LEU:HD21	1.85	0.40
14:O1:97:LEU:HD13	14:O1:149:ILE:HD13	2.03	0.40
15:P1:75:PHE:HB3	15:P1:86:LEU:HB3	2.02	0.40
38:T1:101:3PH:H2H1	38:T1:101:3PH:H2E1	1.73	0.40
21:G1:220:VAL:HA	21:G1:248:PHE:HE2	1.85	0.40
23:S1:252:GLN:HB3	23:S1:263:ASN:ND2	2.36	0.40
3:v1:3:LEU:O	3:v1:7:LEU:HD23	2.21	0.40
5:d1:25:ASP:HA	5:d1:29:PHE:CE2	2.55	0.40
14:o1:277:ASP:CG	14:o1:279:GLU:H	2.28	0.40
48:n1:601:CHL:H111	40:n1:624:LHG:H202	2.04	0.40
21:g1:76:ALA:HA	21:g1:79:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:g1:601:CHL:HHD	40:g1:624:LHG:HC41	2.03	0.40
49:g1:621:LUT:H391	49:g1:621:LUT:H31	1.76	0.40
23:s1:125:GLN:HG3	23:s1:131:ILE:HB	2.04	0.40
23:s1:228:PHE:HE1	29:s1:610:CLA:H2A	1.86	0.40
4:C:252:PHE:HE2	29:C:506:CLA:HAA2	1.87	0.40
4:C:277:PHE:CD2	29:C:501:CLA:H12	2.55	0.40
4:C:344:MET:O	4:C:347:TRP:HB3	2.22	0.40
5:D:155:SER:HA	5:D:159:ILE:HB	2.02	0.40
31:D:404:BCR:H381	10:J:23:ALA:HB1	2.03	0.40
14:O:233:ASP:N	14:O:233:ASP:OD1	2.53	0.40
53:R:626:ERG:H162	17:w:80:ILE:HG12	2.03	0.40
23:S:109:ARG:O	23:S:113:LEU:HD12	2.22	0.40
48:S:608:CHL:H92	48:S:608:CHL:H62	1.90	0.40
29:Y:614:CLA:H142	29:Y:614:CLA:H112	1.85	0.40
1:a:224:ILE:HD12	2:b:484:GLU:OE1	2.22	0.40
2:b:304:LYS:HE3	2:b:304:LYS:HB3	1.78	0.40
5:d:104:TRP:NE1	5:d:109:GLY:HA3	2.36	0.40
5:d:200:GLY:HA3	5:d:282:SER:OG	2.21	0.40
29:d:403:CLA:H141	29:d:403:CLA:H161	1.91	0.40
31:d:404:BCR:H363	7:f:32:PHE:HB3	2.01	0.40
7:f:44:ARG:NH2	10:j:42:LEU:O	2.54	0.40
29:n:602:CLA:H151	29:n:602:CLA:H18	1.50	0.40
1:A1:180:PHE:HA	1:A1:183:MET:HG3	2.02	0.40
33:A1:413:LMG:H391	37:C1:518:DGD:HB61	2.02	0.40
2:B1:55:MET:HB2	2:B1:63:LEU:HD23	2.03	0.40
2:B1:106:LEU:HD23	2:B1:106:LEU:HA	1.96	0.40
3:V1:20:PRO:HA	3:V1:23:VAL:HG12	2.03	0.40
29:C1:504:CLA:H61	29:C1:504:CLA:H93	1.75	0.40
29:C1:513:CLA:H112	29:C1:513:CLA:H91	1.74	0.40
5:D1:53:THR:C	5:D1:66:SER:HB2	2.47	0.40
15:P1:231:ASP:OD1	15:P1:232:LYS:N	2.54	0.40
20:N1:113:ASP:OD1	20:N1:113:ASP:N	2.54	0.40
29:N1:610:CLA:H3A	29:N1:610:CLA:HBA2	1.65	0.40
29:G1:604:CLA:C2B	49:G1:621:LUT:H183	2.51	0.40
24:Y1:105:ILE:HG12	24:Y1:234:ILE:HD11	2.04	0.40
24:Y1:231:LYS:HB3	24:Y1:235:GLN:CD	2.46	0.40
1:a1:105:TRP:HZ2	1:a1:114:LEU:HD23	1.85	0.40
1:a1:287:ALA:O	1:a1:291:SER:OG	2.28	0.40
29:b1:608:CLA:H152	29:b1:608:CLA:H112	1.81	0.40
29:b1:610:CLA:H112	29:b1:610:CLA:H151	1.71	0.40
29:c1:513:CLA:H62	40:c1:525:LHG:H292	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:t1:14:LEU:HD23	16:t1:17:ILE:HD12	2.02	0.40
29:r1:608:CLA:H93	29:r1:608:CLA:H111	1.75	0.40
29:s1:604:CLA:C2B	51:s1:623:NEX:H383	2.51	0.40
29:y1:611:CLA:H72	29:y1:612:CLA:ND	2.35	0.40
29:B:615:CLA:H43	32:M:101:SQD:H241	2.02	0.40
4:C:57:LEU:HA	4:C:60:VAL:HG22	2.02	0.40
29:C:509:CLA:H93	29:C:509:CLA:H62	1.99	0.40
20:N:170:ASN:C	20:N:170:ASN:HD22	2.30	0.40
29:N:602:CLA:H141	29:N:602:CLA:H162	1.93	0.40
21:G:115:TRP:HE3	49:G:621:LUT:H21	1.87	0.40
49:S:621:LUT:H3	49:S:621:LUT:H162	1.91	0.40
1:a:47:VAL:HG21	1:a:114:LEU:HD22	2.03	0.40
5:d:25:ASP:OD1	5:d:25:ASP:N	2.52	0.40
20:n:47:LYS:HE2	20:n:56:THR:HG21	2.03	0.40
20:n:247:ALA:HB2	29:n:613:CLA:CAD	2.51	0.40
53:r:626:ERG:C3	53:r:626:ERG:HO1	2.13	0.40
38:s:626:3PH:H3F1	38:s:626:3PH:H3C1	1.89	0.40
29:B1:608:CLA:H143	29:B1:614:CLA:H172	2.02	0.40
4:C1:228:ILE:HD13	4:C1:228:ILE:HA	1.94	0.40
33:C1:523:LMG:H171	33:C1:523:LMG:H202	1.86	0.40
5:D1:104:TRP:NE1	5:D1:109:GLY:HA3	2.36	0.40
6:E1:68:ASP:HA	25:U1:109:LEU:O	2.21	0.40
12:L1:34:SER:HA	16:T1:6:TYR:OH	2.22	0.40
13:M1:15:ILE:HD13	13:M1:15:ILE:HA	1.98	0.40
14:O1:111:PRO:HA	14:O1:292:GLY:HA3	2.03	0.40
14:O1:270:PHE:HB3	14:O1:294:TRP:CD1	2.57	0.40
29:N1:602:CLA:H41	29:N1:602:CLA:H61	1.65	0.40
29:N1:604:CLA:H142	29:N1:604:CLA:H112	1.86	0.40
29:N1:604:CLA:HBA1	48:N1:606:CHL:CHD	2.51	0.40
29:G1:611:CLA:C4C	40:G1:624:LHG:HC62	2.51	0.40
50:R1:621:XAT:H31	50:R1:621:XAT:H391	1.75	0.40
23:S1:116:ALA:HB3	29:S1:604:CLA:HMC2	2.02	0.40
23:S1:244:ILE:HD12	23:S1:244:ILE:H	1.86	0.40
23:S1:270:ASP:OD1	23:S1:270:ASP:N	2.54	0.40
24:Y1:49:PHE:CD2	24:Y1:50:LEU:HG	2.56	0.40
1:a1:180:PHE:HE2	5:d1:186:GLN:HE21	1.70	0.40
1:a1:229:GLU:HB3	22:r1:94:GLN:HB3	2.03	0.40
2:b1:475:PHE:O	5:d1:139:ARG:NH1	2.49	0.40
2:b1:476:ARG:HH21	22:r1:99:ASN:HB3	1.86	0.40
29:b1:607:CLA:H161	29:b1:607:CLA:H141	1.88	0.40
5:d1:73:PHE:HB3	33:d1:411:LMG:H121	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d1:181:PHE:HA	5:d1:184:PHE:HD2	1.86	0.40
14:o1:107:PHE:HD2	14:o1:143:MET:HE2	1.85	0.40
15:p1:202:HIS:HB2	15:p1:221:ALA:HB3	2.03	0.40
20:n1:167:TYR:HB3	48:n1:608:CHL:CMC	2.51	0.40
29:g1:602:CLA:H92	29:g1:603:CLA:HMA1	2.03	0.40
29:r1:602:CLA:H72	50:r1:621:XAT:C28	2.48	0.40
23:s1:149:LEU:HD21	29:s1:604:CLA:HED2	2.02	0.40
29:s1:602:CLA:H61	29:s1:602:CLA:H92	1.83	0.40
1:A:21:ILE:HD13	1:A:21:ILE:HA	1.92	0.40
20:N:158:VAL:HG13	48:N:609:CHL:HBB2	2.03	0.40
29:R:608:CLA:H62	29:R:608:CLA:H92	1.77	0.40
23:S:171:ILE:HA	23:S:174:VAL:HG22	2.03	0.40
4:c:333:PRO:HB3	14:o:135:ARG:HD3	2.03	0.40
19:z:3:SER:O	19:z:7:ILE:HG12	2.22	0.40
20:n:184:GLY:HA3	29:n:610:CLA:HED2	2.04	0.40
48:n:605:CHL:H143	29:s:612:CLA:HBB1	2.03	0.40
29:g:603:CLA:H91	29:g:603:CLA:H111	1.83	0.40
24:y:49:PHE:HB3	24:y:69:TYR:HB3	2.02	0.40
24:y:197:ASP:OD1	24:y:197:ASP:N	2.50	0.40
1:A1:24:THR:O	5:D1:255:GLN:NE2	2.48	0.40
2:B1:74:SER:HB2	2:B1:93:TYR:CD2	2.56	0.40
29:B1:616:CLA:H151	8:H1:26:LEU:HD21	2.03	0.40
4:C1:177:TRP:HE1	4:C1:283:THR:HG23	1.86	0.40
29:C1:507:CLA:H142	31:C1:515:BCR:H362	2.04	0.40
31:C1:517:BCR:H351	31:C1:517:BCR:H15C	1.80	0.40
12:L1:18:LEU:HD11	13:M1:26:TYR:CD2	2.57	0.40
14:O1:97:LEU:HD21	14:O1:193:LEU:HD11	2.03	0.40
14:O1:149:ILE:HA	14:O1:155:VAL:HG12	2.02	0.40
20:N1:37:ILE:O	20:N1:41:TYR:N	2.54	0.40
20:N1:75:LEU:HD13	29:N1:602:CLA:H42	2.04	0.40
29:N1:613:CLA:C13	50:G1:622:XAT:H34	2.49	0.40
21:G1:94:LEU:HB2	49:G1:620:LUT:H35	2.03	0.40
29:G1:603:CLA:HAC1	48:G1:607:CHL:HBB2	2.04	0.40
29:R1:603:CLA:H71	52:R1:625:LMT:H51	2.03	0.40
24:Y1:209:ILE:HD12	24:Y1:209:ILE:HA	1.90	0.40
1:a1:94:TYR:CD1	1:a1:98:GLU:HB3	2.56	0.40
29:a1:407:CLA:C1B	30:a1:409:PHO:H202	2.52	0.40
4:c1:83:LEU:HD13	4:c1:166:LYS:HZ1	1.86	0.40
29:c1:512:CLA:H112	32:c1:526:SQD:H341	2.03	0.40
33:c1:523:LMG:H291	29:y1:611:CLA:H42	2.02	0.40
40:c1:525:LHG:H251	29:s1:611:CLA:HAB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d1:129:GLN:NE2	5:d1:143:ALA:HA	2.36	0.40
16:t1:16:ILE:O	16:t1:20:SER:N	2.54	0.40
20:n1:156:VAL:HG11	48:n1:606:CHL:HED3	2.04	0.40
49:g1:620:LUT:H15	49:g1:620:LUT:H201	1.85	0.40
22:r1:225:ASP:CG	22:r1:226:GLU:H	2.30	0.40
23:s1:124:LEU:HD23	23:s1:124:LEU:HA	1.89	0.40
29:s1:610:CLA:HBA2	29:s1:610:CLA:H3A	1.59	0.40
29:s1:614:CLA:H41	29:s1:614:CLA:H61	1.46	0.40
24:y1:108:GLU:HG3	24:y1:122:ALA:HB1	2.03	0.40
29:y1:603:CLA:HHD	48:y1:607:CHL:H202	2.04	0.40
50:y1:622:XAT:H31	50:y1:622:XAT:H391	1.94	0.40
51:y1:623:NEX:H191	51:y1:623:NEX:H11	1.84	0.40
2:B:247:TRP:HB2	29:B:609:CLA:HBC1	2.03	0.40
29:B:608:CLA:H62	29:B:608:CLA:H41	1.65	0.40
29:B:614:CLA:H71	29:B:614:CLA:H112	1.87	0.40
4:C:64:VAL:O	4:C:72:GLN:NE2	2.49	0.40
4:C:389:LEU:HD22	4:C:398:VAL:HG12	2.03	0.40
29:C:506:CLA:H111	29:C:506:CLA:H152	1.75	0.40
40:D:408:LHG:H152	12:L:24:LEU:HD11	2.04	0.40
14:O:160:ASP:OD1	14:O:161:GLU:N	2.55	0.40
14:O:179:PRO:O	14:O:276:SER:OG	2.39	0.40
33:a:413:LMG:H332	37:c:518:DGD:HA81	2.03	0.40
2:b:201:HIS:HB2	29:b:603:CLA:C1B	2.51	0.40
37:b:623:DGD:HD61	22:r:170:LEU:HD11	2.02	0.40
4:c:68:PRO:HG2	4:c:71:GLU:HG3	2.01	0.40
15:p:134:PRO:HB3	15:p:187:PHE:HE1	1.87	0.40
18:x:77:VAL:O	18:x:81:VAL:HG23	2.21	0.40
51:n:623:NEX:H35	51:n:623:NEX:H401	1.83	0.40
40:g:624:LHG:HC81	50:y:622:XAT:H371	2.03	0.40
29:r:604:CLA:HBA2	29:r:604:CLA:H3A	1.68	0.40
29:r:610:CLA:H61	29:r:610:CLA:H92	1.81	0.40
3:V1:26:LEU:HD23	3:V1:26:LEU:HA	1.91	0.40
4:C1:57:LEU:HD11	4:C1:104:VAL:HG22	2.04	0.40
4:C1:177:TRP:HZ3	4:C1:355:GLU:HG3	1.85	0.40
29:C1:507:CLA:H92	29:C1:507:CLA:H62	1.84	0.40
43:D1:405:PL9:H201	43:D1:405:PL9:H221	1.82	0.40
44:F1:101:HEM:HMC2	44:F1:101:HEM:HBC2	2.04	0.40
14:O1:269:VAL:HG12	14:O1:293:LEU:HG	2.04	0.40
17:W1:81:LEU:HA	17:W1:84:VAL:HG12	2.03	0.40
17:W1:83:TRP:CE2	33:W1:201:LMG:H292	2.57	0.40
20:N1:202:LEU:HB3	29:N1:610:CLA:HMA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N1:609:CHL:HAB	48:N1:609:CHL:HHC	1.92	0.40
21:G1:202:LYS:HE3	40:G1:624:LHG:HC61	2.03	0.40
23:S1:108:ALA:O	23:S1:112:MET:HG3	2.21	0.40
49:S1:621:LUT:H35	49:S1:621:LUT:H401	1.77	0.40
29:Y1:604:CLA:H91	29:Y1:604:CLA:H112	1.84	0.40
1:a1:120:PHE:CZ	37:c1:518:DGD:HBT1	2.51	0.40
1:a1:187:GLN:OE1	1:a1:193:LEU:HG	2.22	0.40
29:b1:613:CLA:H122	29:b1:613:CLA:H62	2.03	0.40
29:b1:616:CLA:H92	29:b1:616:CLA:H61	1.90	0.40
5:d1:338:LYS:HB2	25:u1:103:GLU:OE1	2.21	0.40
6:e1:68:ASP:OD1	25:u1:110:ARG:NH1	2.54	0.40
17:w1:83:TRP:HE1	24:y1:113:ASN:CG	2.29	0.40
20:n1:163:LEU:HB3	20:n1:167:TYR:CE2	2.57	0.40
21:g1:241:ALA:HB1	50:y1:622:XAT:H161	2.04	0.40
29:g1:613:CLA:H51	29:g1:613:CLA:H8	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/336 (100%)	321 (96%)	14 (4%)	0	100	100
1	A1	335/336 (100%)	313 (93%)	22 (7%)	0	100	100
1	a	335/336 (100%)	318 (95%)	17 (5%)	0	100	100
1	a1	335/336 (100%)	314 (94%)	21 (6%)	0	100	100
2	B	482/484 (100%)	464 (96%)	18 (4%)	0	100	100
2	B1	482/484 (100%)	447 (93%)	35 (7%)	0	100	100
2	b	482/484 (100%)	464 (96%)	18 (4%)	0	100	100
2	b1	482/484 (100%)	454 (94%)	28 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	V	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	V1	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v	30/32 (94%)	30 (100%)	0	0	100	100
3	v1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	430 (96%)	17 (4%)	0	100	100
4	C1	447/449 (100%)	421 (94%)	26 (6%)	0	100	100
4	c	447/449 (100%)	431 (96%)	16 (4%)	0	100	100
4	c1	447/449 (100%)	421 (94%)	25 (6%)	1 (0%)	43	72
5	D	346/348 (99%)	330 (95%)	16 (5%)	0	100	100
5	D1	346/348 (99%)	324 (94%)	22 (6%)	0	100	100
5	d	346/348 (99%)	331 (96%)	15 (4%)	0	100	100
5	d1	346/348 (99%)	324 (94%)	22 (6%)	0	100	100
6	E	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	E1	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	e	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
6	e1	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	F1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
7	f1	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
8	H1	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
8	h	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
8	h1	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	I1	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
9	i	33/35 (94%)	29 (88%)	4 (12%)	0	100	100
9	i1	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
10	J1	34/36 (94%)	34 (100%)	0	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	j1	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
11	K	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	K1	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k1	35/37 (95%)	35 (100%)	0	0	100	100
12	L	36/38 (95%)	36 (100%)	0	0	100	100
12	L1	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	29/31 (94%)	29 (100%)	0	0	100	100
13	M1	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
13	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	m1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
14	O	236/238 (99%)	215 (91%)	19 (8%)	2 (1%)	16	49
14	O1	236/238 (99%)	212 (90%)	23 (10%)	1 (0%)	30	61
14	o	236/238 (99%)	218 (92%)	17 (7%)	1 (0%)	30	61
14	o1	236/238 (99%)	210 (89%)	25 (11%)	1 (0%)	30	61
15	P	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
15	P1	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
15	p	185/187 (99%)	170 (92%)	15 (8%)	0	100	100
15	p1	185/187 (99%)	169 (91%)	16 (9%)	0	100	100
16	T	28/30 (93%)	27 (96%)	0	1 (4%)	2	22
16	T1	28/30 (93%)	25 (89%)	2 (7%)	1 (4%)	2	22
16	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	t1	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
17	W	42/44 (96%)	38 (90%)	4 (10%)	0	100	100
17	W1	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w1	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
18	X	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
18	X1	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	x1	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
19	Z1	59/61 (97%)	55 (93%)	4 (7%)	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
19	z1	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
20	N	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	14	46
20	N1	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	14	46
20	n	218/222 (98%)	199 (91%)	17 (8%)	2 (1%)	14	46
20	n1	218/222 (98%)	202 (93%)	14 (6%)	2 (1%)	14	46
21	G	219/221 (99%)	196 (90%)	23 (10%)	0	100	100
21	G1	219/221 (99%)	195 (89%)	24 (11%)	0	100	100
21	g	219/221 (99%)	197 (90%)	22 (10%)	0	100	100
21	g1	219/221 (99%)	195 (89%)	24 (11%)	0	100	100
22	R	191/196 (97%)	177 (93%)	14 (7%)	0	100	100
22	R1	191/196 (97%)	176 (92%)	15 (8%)	0	100	100
22	r	191/196 (97%)	177 (93%)	14 (7%)	0	100	100
22	r1	191/196 (97%)	176 (92%)	15 (8%)	0	100	100
23	S	241/243 (99%)	219 (91%)	21 (9%)	1 (0%)	30	61
23	S1	241/243 (99%)	208 (86%)	32 (13%)	1 (0%)	30	61
23	s	241/243 (99%)	219 (91%)	20 (8%)	2 (1%)	16	49
23	s1	241/243 (99%)	214 (89%)	26 (11%)	1 (0%)	30	61
24	Y	220/222 (99%)	212 (96%)	7 (3%)	1 (0%)	24	57
24	Y1	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	24	57
24	y	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	24	57
24	y1	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	24	57
25	U	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
25	U1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
25	u	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
25	u1	25/27 (93%)	25 (100%)	0	0	100	100
All	All	14636/14846 (99%)	13696 (94%)	915 (6%)	25 (0%)	44	72

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	O	205	TYR
20	N	192	LEU
14	o	205	TYR
20	n	192	LEU
23	s	284	ASP
14	O1	205	TYR
20	N1	192	LEU
23	s1	284	ASP
20	N	145	ILE
24	Y	146	ILE
24	y	146	ILE
14	o1	205	TYR
20	n1	192	LEU
20	n	145	ILE
23	s	92	LYS
24	Y1	146	ILE
23	S	284	ASP
24	y1	146	ILE
14	O	216	ARG
23	S1	92	LYS
4	c1	211	TRP
20	N1	145	ILE
20	n1	145	ILE
16	T	29	ILE
16	T1	29	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/275 (100%)	276 (100%)	0	100	100
1	A1	276/275 (100%)	276 (100%)	0	100	100
1	a	276/275 (100%)	276 (100%)	0	100	100
1	a1	276/275 (100%)	276 (100%)	0	100	100
2	B	388/388 (100%)	388 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B1	388/388 (100%)	388 (100%)	0	100	100
2	b	388/388 (100%)	388 (100%)	0	100	100
2	b1	388/388 (100%)	387 (100%)	1 (0%)	86	83
3	V	25/25 (100%)	25 (100%)	0	100	100
3	V1	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100
3	v1	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	350 (100%)	0	100	100
4	C1	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	350 (100%)	0	100	100
4	c1	350/350 (100%)	350 (100%)	0	100	100
5	D	279/279 (100%)	279 (100%)	0	100	100
5	D1	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	279 (100%)	0	100	100
5	d1	279/279 (100%)	279 (100%)	0	100	100
6	E	68/68 (100%)	68 (100%)	0	100	100
6	E1	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
6	e1	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	F1	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
7	f1	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	H1	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
8	h1	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	I1	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
9	i1	31/31 (100%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	27/27 (100%)	27 (100%)	0	100	100
10	J1	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
10	j1	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	K1	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100
11	k1	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	L1	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
13	M1	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100
13	m1	26/26 (100%)	26 (100%)	0	100	100
14	O	195/195 (100%)	195 (100%)	0	100	100
14	O1	195/195 (100%)	194 (100%)	1 (0%)	81	80
14	o	195/195 (100%)	195 (100%)	0	100	100
14	o1	195/195 (100%)	194 (100%)	1 (0%)	81	80
15	P	151/151 (100%)	151 (100%)	0	100	100
15	P1	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	151 (100%)	0	100	100
15	p1	151/151 (100%)	151 (100%)	0	100	100
16	T	26/26 (100%)	26 (100%)	0	100	100
16	T1	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
16	t1	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	W1	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
17	w1	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	X	21/21 (100%)	21 (100%)	0	100	100
18	X1	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
18	x1	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	Z1	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100
19	z1	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100
20	N1	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	170 (99%)	1 (1%)	78	79
20	n1	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	168 (100%)	0	100	100
21	G1	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
21	g1	168/168 (100%)	168 (100%)	0	100	100
22	R	151/151 (100%)	151 (100%)	0	100	100
22	R1	151/151 (100%)	151 (100%)	0	100	100
22	r	151/151 (100%)	151 (100%)	0	100	100
22	r1	151/151 (100%)	151 (100%)	0	100	100
23	S	190/190 (100%)	190 (100%)	0	100	100
23	S1	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	190 (100%)	0	100	100
23	s1	190/190 (100%)	190 (100%)	0	100	100
24	Y	167/167 (100%)	167 (100%)	0	100	100
24	Y1	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
24	y1	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	26 (100%)	0	100	100
25	U1	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	u1	26/26 (100%)	26 (100%)	0	100	100
All	All	11841/11837 (100%)	11837 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	n	46	ASN
14	O1	138	TYR
2	b1	425	GLN
14	o1	138	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
1	A	247	ASN
2	B	9	HIS
2	B	26	HIS
2	B	343	HIS
2	B	407	ASN
4	C	16	GLN
4	C	147	ASN
4	C	315	ASN
4	C	370	ASN
5	D	255	GLN
5	D	263	ASN
5	D	350	ASN
12	L	9	GLN
13	M	4	ASN
15	P	121	GLN
17	W	100	GLN
21	G	129	ASN
21	G	133	ASN
21	G	239	ASN
24	Y	149	GLN
24	Y	211	ASN
24	Y	235	GLN
24	Y	238	GLN
1	a	195	HIS
1	a	234	ASN
1	a	247	ASN

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Mol	Chain	Res	Type
1	a	267	ASN
1	a	301	ASN
1	a	335	ASN
2	b	58	GLN
2	b	438	GLN
4	c	56	ASN
4	c	320	GLN
4	c	373	GLN
5	d	106	GLN
5	d	186	GLN
5	d	194	ASN
5	d	301	GLN
5	d	322	ASN
7	f	23	HIS
7	f	40	GLN
7	f	43	GLN
13	m	4	ASN
14	o	150	ASN
14	o	242	ASN
14	o	274	GLN
15	p	140	GLN
17	w	100	GLN
20	n	149	ASN
21	g	85	HIS
21	g	129	ASN
23	s	238	ASN
24	y	138	ASN
1	A1	108	ASN
1	A1	191	ASN
1	A1	230	ASN
1	A1	304	GLN
1	A1	325	ASN
1	A1	335	ASN
2	B1	58	GLN
2	B1	100	HIS
2	B1	281	GLN
2	B1	282	GLN
2	B1	455	HIS
4	C1	44	HIS
4	C1	56	ASN
4	C1	299	GLN
4	C1	301	GLN

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Mol	Chain	Res	Type
4	C1	320	GLN
5	D1	117	HIS
5	D1	164	GLN
5	D1	230	ASN
5	D1	350	ASN
6	E1	61	GLN
6	E1	82	GLN
7	F1	43	GLN
12	L1	9	GLN
14	O1	82	ASN
14	O1	274	GLN
14	O1	283	HIS
15	P1	140	GLN
19	Z1	58	ASN
20	N1	148	GLN
20	N1	157	GLN
21	G1	109	GLN
21	G1	129	ASN
21	G1	133	ASN
21	G1	162	ASN
21	G1	227	GLN
22	R1	99	ASN
22	R1	174	GLN
24	Y1	142	ASN
24	Y1	144	ASN
24	Y1	149	GLN
24	Y1	247	ASN
1	a1	26	ASN
1	a1	108	ASN
1	a1	187	GLN
1	a1	310	ASN
1	a1	325	ASN
2	b1	26	HIS
2	b1	114	HIS
2	b1	317	ASN
2	b1	425	GLN
2	b1	438	GLN
4	c1	44	HIS
4	c1	143	ASN
4	c1	299	GLN
4	c1	403	ASN
4	c1	429	HIS

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Mol	Chain	Res	Type
5	d1	129	GLN
5	d1	186	GLN
5	d1	334	GLN
8	h1	69	ASN
8	h1	79	ASN
14	o1	82	ASN
14	o1	224	ASN
14	o1	297	GLN
18	x1	71	ASN
20	n1	46	ASN
20	n1	245	ASN
21	g1	121	GLN
21	g1	129	ASN
22	r1	99	ASN
22	r1	140	HIS
22	r1	203	ASN
23	s1	161	ASN
23	s1	232	GLN
24	y1	149	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	SEP	R	84	22	8,9,10	1.58	1 (12%)	8,12,14	1.40	2 (25%)
22	SEP	R1	84	22	8,9,10	1.52	1 (12%)	8,12,14	1.71	2 (25%)
22	SEP	r	84	22	8,9,10	1.51	1 (12%)	8,12,14	1.39	2 (25%)
22	SEP	r1	84	22	8,9,10	1.53	1 (12%)	8,12,14	1.69	2 (25%)

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
22	SEP	R	84	22	-	2/5/8/10	-
22	SEP	R1	84	22	-	4/5/8/10	-
22	SEP	r	84	22	-	2/5/8/10	-
22	SEP	r1	84	22	-	5/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	84	SEP	P-O1P	3.37	1.61	1.50
22	r1	84	SEP	P-O1P	3.30	1.61	1.50
22	R1	84	SEP	P-O1P	3.29	1.61	1.50
22	r	84	SEP	P-O1P	3.22	1.60	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r1	84	SEP	P-OG-CB	-3.36	109.03	118.30
22	R1	84	SEP	OG-CB-CA	3.23	111.29	108.14
22	R1	84	SEP	P-OG-CB	-3.07	109.85	118.30
22	r1	84	SEP	OG-CB-CA	2.79	110.86	108.14
22	r	84	SEP	P-OG-CB	-2.56	111.25	118.30
22	R	84	SEP	OG-CB-CA	2.49	110.57	108.14
22	r	84	SEP	OG-CB-CA	2.30	110.39	108.14
22	R	84	SEP	P-OG-CB	-2.07	112.59	118.30

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	R	84	SEP	N-CA-CB-OG
22	R1	84	SEP	N-CA-CB-OG
22	R1	84	SEP	CB-OG-P-O2P
22	R1	84	SEP	CB-OG-P-O3P
22	r1	84	SEP	N-CA-CB-OG
22	r1	84	SEP	CB-OG-P-O2P
22	R1	84	SEP	CB-OG-P-O1P
22	r1	84	SEP	CB-OG-P-O1P

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Mol	Chain	Res	Type	Atoms
22	r	84	SEP	CB-OG-P-O2P
22	r1	84	SEP	CB-OG-P-O3P
22	R	84	SEP	CA-CB-OG-P
22	r	84	SEP	N-CA-CB-OG
22	r1	84	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	R	84	SEP	1	0
22	r	84	SEP	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 721 ligands modelled in this entry, 16 are monoatomic - leaving 705 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	$\#\|Z\| > 2$
29	CLA	y	612	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	19 (22%)
40	LHG	L1	101	-	48,48,48	0.37	0	51,54,54	1.11	3 (5%)
29	CLA	C1	505	4	69,73,73	1.37	7 (10%)	83,113,113	1.91	18 (21%)
29	CLA	S1	602	23	64,68,73	1.40	8 (12%)	77,107,113	2.06	18 (23%)
46	GOL	I1	101	-	5,5,5	0.56	0	5,5,5	0.31	0
49	LUT	y	621	-	42,43,43	2.36	1 (2%)	51,60,60	1.98	14 (27%)
39	DGA	J1	101	-	28,28,43	1.27	2 (7%)	30,30,45	1.34	2 (6%)
49	LUT	y1	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.97	10 (19%)
29	CLA	B	617	2	69,73,73	1.37	7 (10%)	83,113,113	1.98	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
29	CLA	s	617	-	54,58,73	1.55	7 (12%)	65,95,113	2.25	18 (27%)
29	CLA	c	507	-	69,73,73	1.39	7 (10%)	83,113,113	1.98	18 (21%)
32	SQD	c	526	-	53,54,54	0.79	0	62,65,65	0.92	2 (3%)
48	CHL	n1	608	-	54,58,74	0.92	2 (3%)	59,94,114	1.31	9 (15%)
29	CLA	c	501	4	69,73,73	1.35	7 (10%)	83,113,113	2.01	18 (21%)
29	CLA	y	610	24	69,73,73	1.35	7 (10%)	83,113,113	1.97	18 (21%)
34	SPH	y	625	-	19,20,20	0.61	0	18,21,21	1.21	2 (11%)
50	XAT	g1	622	-	39,47,47	0.75	1 (2%)	54,74,74	1.88	16 (29%)
55	PTY	y1	627	-	18,18,49	1.27	2 (11%)	21,23,54	1.45	2 (9%)
40	LHG	D	408	-	43,43,48	0.41	0	46,49,54	1.10	2 (4%)
55	PTY	y1	626	-	49,49,49	0.87	4 (8%)	52,54,54	1.08	2 (3%)
29	CLA	B	603	2	69,73,73	1.37	8 (11%)	83,113,113	1.91	19 (22%)
29	CLA	b	602	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	20 (24%)
29	CLA	g	614	-	53,57,73	1.57	8 (15%)	62,93,113	2.15	17 (27%)
29	CLA	a	406	-	69,73,73	1.36	7 (10%)	83,113,113	2.15	19 (22%)
29	CLA	d1	402	-	69,73,73	1.40	8 (11%)	83,113,113	1.91	19 (22%)
29	CLA	C1	508	4	69,73,73	1.40	8 (11%)	83,113,113	1.81	15 (18%)
26	OEX	A1	401	1,4	0,14,14	-	-	-		
33	LMG	d	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.19	4 (7%)
29	CLA	B1	609	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	16 (19%)
31	BCR	C	515	-	41,41,41	1.83	6 (14%)	56,56,56	4.20	16 (28%)
48	CHL	s	606	-	48,52,74	1.06	2 (4%)	53,87,114	1.39	7 (13%)
29	CLA	b1	613	-	69,73,73	1.38	7 (10%)	83,113,113	2.01	17 (20%)
49	LUT	R	620	-	42,43,43	2.33	1 (2%)	51,60,60	2.03	17 (33%)
29	CLA	N	610	-	69,73,73	1.36	6 (8%)	83,113,113	2.03	20 (24%)
29	CLA	c	504	-	69,73,73	1.33	7 (10%)	83,113,113	1.99	18 (21%)
29	CLA	A1	406	-	69,73,73	1.40	7 (10%)	83,113,113	1.96	19 (22%)
29	CLA	Y1	611	-	69,73,73	1.35	7 (10%)	83,113,113	1.91	18 (21%)
29	CLA	r	603	-	64,68,73	1.45	7 (10%)	77,107,113	1.89	17 (22%)
38	3PH	s	626	-	47,47,47	0.87	3 (6%)	51,52,52	4.40	4 (7%)
50	XAT	G	622	-	39,47,47	0.71	1 (2%)	54,74,74	2.11	15 (27%)
31	BCR	B1	619	-	41,41,41	1.82	4 (9%)	56,56,56	4.44	18 (32%)
32	SQD	b1	626	-	53,54,54	0.80	0	62,65,65	0.93	2 (3%)
51	NEX	S	623	-	38,46,46	3.42	10 (26%)	50,70,70	1.71	12 (24%)
53	ERG	r	626	-	31,32,32	7.80	18 (58%)	47,50,50	3.01	16 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
48	CHL	G1	601	21	70,74,74	0.84	2 (2%)	80,114,114	1.33	14 (17%)
40	LHG	g1	624	-	48,48,48	0.41	0	51,54,54	1.11	3 (5%)
48	CHL	g1	609	-	70,74,74	0.85	2 (2%)	80,114,114	1.25	10 (12%)
29	CLA	r	608	-	64,68,73	1.42	9 (14%)	77,107,113	1.90	17 (22%)
29	CLA	B1	610	-	69,73,73	1.38	7 (10%)	83,113,113	1.84	14 (16%)
52	LMT	r	625	-	36,36,36	1.22	5 (13%)	47,47,47	1.16	3 (6%)
29	CLA	g1	610	-	69,73,73	1.32	6 (8%)	83,113,113	2.19	20 (24%)
32	SQD	m	101	-	41,42,54	0.91	0	50,53,65	0.99	3 (6%)
29	CLA	C1	512	-	69,73,73	1.38	7 (10%)	83,113,113	1.97	22 (26%)
48	CHL	G1	605	21	52,56,74	0.91	2 (3%)	58,92,114	1.41	11 (18%)
33	LMG	b1	622	-	44,44,55	0.86	2 (4%)	52,52,63	1.17	3 (5%)
44	HEM	f1	101	7	50,50,50	1.59	7 (14%)	66,82,82	1.14	7 (10%)
48	CHL	Y1	609	-	70,74,74	0.79	2 (2%)	80,114,114	1.27	11 (13%)
29	CLA	y1	604	-	69,73,73	1.34	6 (8%)	83,113,113	2.03	17 (20%)
29	CLA	s	604	-	59,63,73	1.48	6 (10%)	71,101,113	2.01	15 (21%)
47	4RF	K	101	-	56,56,56	1.08	3 (5%)	59,59,59	0.91	3 (5%)
40	LHG	d1	408	-	43,43,48	0.40	0	46,49,54	1.05	2 (4%)
29	CLA	b	616	2	69,73,73	1.35	7 (10%)	83,113,113	1.84	17 (20%)
31	BCR	d1	404	-	41,41,41	1.88	4 (9%)	56,56,56	4.27	22 (39%)
29	CLA	b1	614	-	69,73,73	1.38	9 (13%)	83,113,113	1.88	18 (21%)
29	CLA	C1	501	4	69,73,73	1.36	7 (10%)	83,113,113	2.08	21 (25%)
29	CLA	G	602	-	69,73,73	1.37	7 (10%)	83,113,113	2.01	20 (24%)
29	CLA	y	608	-	54,58,73	1.58	8 (14%)	65,95,113	2.16	17 (26%)
47	4RF	I1	102	-	56,56,56	1.06	4 (7%)	59,59,59	0.98	3 (5%)
29	CLA	a	410	1	64,68,73	1.41	8 (12%)	77,107,113	2.08	20 (25%)
29	CLA	g1	612	21	47,51,73	1.65	8 (17%)	56,86,113	2.21	15 (26%)
29	CLA	N	611	-	53,57,73	1.57	6 (11%)	62,93,113	2.15	17 (27%)
48	CHL	y1	607	-	70,74,74	0.78	2 (2%)	80,114,114	1.28	11 (13%)
29	CLA	n1	611	-	53,57,73	1.57	6 (11%)	62,93,113	2.20	17 (27%)
49	LUT	G1	620	-	42,43,43	2.26	1 (2%)	51,60,60	1.86	13 (25%)
37	DGD	C1	518	-	56,56,67	0.98	4 (7%)	70,70,81	1.07	6 (8%)
51	NEX	S1	623	-	38,46,46	3.20	9 (23%)	50,70,70	1.79	10 (20%)
34	SPH	a1	414	-	19,20,20	0.73	1 (5%)	18,21,21	0.98	1 (5%)
29	CLA	N1	603	-	69,73,73	1.36	6 (8%)	83,113,113	2.06	23 (27%)
31	BCR	C	517	-	41,41,41	1.87	5 (12%)	56,56,56	4.32	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
29	CLA	g1	602	-	69,73,73	1.38	8 (11%)	83,113,113	1.91	21 (25%)
50	XAT	Y1	622	-	39,47,47	0.69	1 (2%)	54,74,74	3.83	20 (37%)
29	CLA	A	407	-	54,58,73	1.55	8 (14%)	65,95,113	2.21	18 (27%)
31	BCR	c1	515	-	41,41,41	1.91	4 (9%)	56,56,56	4.38	13 (23%)
37	DGD	c	520	-	60,60,67	1.05	4 (6%)	74,74,81	1.03	3 (4%)
39	DGA	j	101	-	28,28,43	1.28	3 (10%)	30,30,45	1.28	2 (6%)
47	4RF	i1	101	-	56,56,56	1.06	3 (5%)	59,59,59	0.92	3 (5%)
49	LUT	S	621	-	42,43,43	2.25	1 (2%)	51,60,60	2.10	19 (37%)
48	CHL	y	606	-	70,74,74	0.86	3 (4%)	80,114,114	1.24	11 (13%)
29	CLA	R	604	-	53,57,73	1.55	7 (13%)	62,93,113	2.22	16 (25%)
29	CLA	s	603	-	69,73,73	1.39	7 (10%)	83,113,113	1.98	19 (22%)
29	CLA	S	605	23	54,58,73	1.59	8 (14%)	65,95,113	2.32	17 (26%)
48	CHL	g	606	-	54,58,74	0.94	2 (3%)	59,94,114	1.53	10 (16%)
50	XAT	n1	622	-	39,47,47	0.71	1 (2%)	54,74,74	2.04	14 (25%)
44	HEM	F	101	6,7	50,50,50	1.34	7 (14%)	66,82,82	1.16	5 (7%)
48	CHL	G1	609	-	70,74,74	0.90	2 (2%)	80,114,114	1.22	11 (13%)
29	CLA	A1	410	-	64,68,73	1.40	7 (10%)	77,107,113	2.06	21 (27%)
50	XAT	r1	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.16	18 (33%)
37	DGD	C	520	-	60,60,67	1.06	6 (10%)	74,74,81	1.07	3 (4%)
41	LMK	c1	527	-	38,39,53	1.51	3 (7%)	41,46,60	1.24	2 (4%)
36	C7Z	b	620	-	43,43,43	5.32	27 (62%)	58,60,60	2.48	19 (32%)
55	PTY	y	627	-	18,18,49	1.29	3 (16%)	21,23,54	1.50	2 (9%)
29	CLA	s1	605	-	54,58,73	1.58	9 (16%)	65,95,113	2.20	20 (30%)
51	NEX	s	623	-	38,46,46	3.52	11 (28%)	50,70,70	2.12	14 (28%)
52	LMT	R1	625	-	36,36,36	1.27	8 (22%)	47,47,47	1.15	4 (8%)
49	LUT	S1	621	-	42,43,43	2.39	2 (4%)	51,60,60	1.99	19 (37%)
47	4RF	i	101	-	56,56,56	1.07	3 (5%)	59,59,59	0.93	3 (5%)
48	CHL	N	608	-	54,58,74	0.99	3 (5%)	59,94,114	1.30	9 (15%)
31	BCR	b	619	-	41,41,41	1.83	5 (12%)	56,56,56	4.15	16 (28%)
29	CLA	c	513	-	69,73,73	1.41	8 (11%)	83,113,113	2.03	18 (21%)
29	CLA	B	604	-	69,73,73	1.39	6 (8%)	83,113,113	1.89	16 (19%)
29	CLA	R1	609	-	64,68,73	1.39	7 (10%)	77,107,113	4.35	21 (27%)
29	CLA	y1	614	-	69,73,73	1.38	8 (11%)	83,113,113	1.87	21 (25%)
33	LMG	B	622	-	44,44,55	0.86	3 (6%)	52,52,63	1.24	2 (3%)
29	CLA	Y1	610	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
38	3PH	t	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.19	2 (3%)
54	LPX	s1	625	-	29,29,29	1.01	2 (6%)	31,33,33	1.05	2 (6%)
41	LMK	C	527	-	38,39,53	1.47	2 (5%)	41,46,60	1.56	4 (9%)
48	CHL	N	601	20	70,74,74	0.81	2 (2%)	80,114,114	1.36	11 (13%)
29	CLA	S1	609	-	64,68,73	1.40	7 (10%)	77,107,113	2.04	18 (23%)
29	CLA	C	506	-	69,73,73	1.41	7 (10%)	83,113,113	1.99	19 (22%)
29	CLA	C	512	-	69,73,73	1.38	6 (8%)	83,113,113	1.92	17 (20%)
40	LHG	N1	624	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
29	CLA	y1	603	-	69,73,73	1.38	7 (10%)	83,113,113	1.90	18 (21%)
29	CLA	G1	602	-	69,73,73	1.42	6 (8%)	83,113,113	2.04	22 (26%)
30	PHO	a	408	-	58,69,69	2.01	12 (20%)	56,99,99	1.62	7 (12%)
37	DGD	c1	519	-	63,63,67	1.14	6 (9%)	77,77,81	1.04	3 (3%)
51	NEX	G	623	-	38,46,46	3.37	11 (28%)	50,70,70	1.92	12 (24%)
48	CHL	N	605	20	70,74,74	0.87	3 (4%)	80,114,114	1.27	12 (15%)
48	CHL	g1	608	-	48,52,74	0.97	2 (4%)	53,87,114	1.39	8 (15%)
33	LMG	C1	523	-	55,55,55	1.12	6 (10%)	63,63,63	1.15	6 (9%)
43	PL9	d	405	-	55,55,55	1.75	10 (18%)	68,69,69	1.54	11 (16%)
29	CLA	s1	602	-	64,68,73	1.41	7 (10%)	77,107,113	2.19	21 (27%)
48	CHL	N	607	-	70,74,74	0.85	2 (2%)	80,114,114	1.18	12 (15%)
29	CLA	r	602	22	64,68,73	1.45	7 (10%)	77,107,113	1.92	19 (24%)
48	CHL	N1	601	-	70,74,74	0.88	2 (2%)	80,114,114	1.40	12 (15%)
29	CLA	R	608	-	64,68,73	1.47	9 (14%)	77,107,113	2.02	17 (22%)
30	PHO	a1	409	-	58,69,69	2.09	10 (17%)	56,99,99	1.82	9 (16%)
29	CLA	g1	604	-	53,57,73	1.54	7 (13%)	62,93,113	2.18	17 (27%)
51	NEX	N1	623	-	38,46,46	3.26	10 (26%)	50,70,70	1.68	10 (20%)
36	C7Z	B	620	-	43,43,43	5.27	26 (60%)	58,60,60	2.44	22 (37%)
49	LUT	Y	621	-	42,43,43	2.32	1 (2%)	51,60,60	2.00	15 (29%)
37	DGD	C	519	-	63,63,67	1.13	7 (11%)	77,77,81	1.01	2 (2%)
29	CLA	y	603	-	69,73,73	1.36	8 (11%)	83,113,113	2.09	19 (22%)
47	4RF	k1	101	-	56,56,56	1.04	3 (5%)	59,59,59	0.88	3 (5%)
49	LUT	G	621	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	12 (23%)
39	DGA	c	524	-	43,43,43	1.10	3 (6%)	45,45,45	1.55	3 (6%)
29	CLA	c1	505	-	69,73,73	1.34	8 (11%)	83,113,113	2.02	18 (21%)
29	CLA	y	602	24	69,73,73	1.40	6 (8%)	83,113,113	1.86	16 (19%)
33	LMG	B1	622	-	44,44,55	0.88	3 (6%)	52,52,63	1.08	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
48	CHL	r1	607	-	54,58,74	0.95	2 (3%)	59,94,114	1.59	12 (20%)
29	CLA	c	506	4	69,73,73	1.39	8 (11%)	83,113,113	1.96	17 (20%)
30	PHO	A	408	-	58,69,69	1.96	9 (15%)	56,99,99	1.56	7 (12%)
29	CLA	c1	506	-	69,73,73	1.34	6 (8%)	83,113,113	1.98	19 (22%)
49	LUT	n	620	-	42,43,43	2.35	1 (2%)	51,60,60	2.09	17 (33%)
33	LMG	b	622	-	44,44,55	0.87	3 (6%)	52,52,63	1.15	2 (3%)
37	DGD	C1	520	-	60,60,67	1.08	5 (8%)	74,74,81	0.95	2 (2%)
40	LHG	D	410	-	38,38,48	0.42	0	41,44,54	1.16	4 (9%)
29	CLA	B	612	2	69,73,73	1.39	6 (8%)	83,113,113	1.88	15 (18%)
51	NEX	r1	622	-	38,46,46	3.37	9 (23%)	50,70,70	1.83	12 (24%)
29	CLA	N	612	-	49,53,73	1.64	8 (16%)	59,89,113	2.00	14 (23%)
38	3PH	B1	624	-	47,47,47	0.86	3 (6%)	51,52,52	1.11	2 (3%)
29	CLA	C1	503	4	69,73,73	1.40	8 (11%)	83,113,113	1.94	21 (25%)
29	CLA	B1	613	-	69,73,73	1.38	7 (10%)	83,113,113	1.92	16 (19%)
29	CLA	S1	614	-	59,63,73	1.49	6 (10%)	71,101,113	2.08	19 (26%)
48	CHL	Y	607	-	70,74,74	0.81	2 (2%)	80,114,114	1.22	9 (11%)
53	ERG	R	626	-	31,32,32	7.79	18 (58%)	47,50,50	3.10	19 (40%)
31	BCR	a1	411	-	41,41,41	1.92	5 (12%)	56,56,56	4.06	15 (26%)
29	CLA	b1	605	2	69,73,73	1.34	6 (8%)	83,113,113	2.05	21 (25%)
48	CHL	S	606	-	48,52,74	0.95	2 (4%)	53,87,114	1.46	11 (20%)
29	CLA	B	615	-	69,73,73	1.38	8 (11%)	83,113,113	1.94	18 (21%)
32	SQD	B	621	-	41,42,54	0.88	0	50,53,65	1.01	3 (6%)
31	BCR	c1	517	-	41,41,41	1.91	5 (12%)	56,56,56	4.37	19 (33%)
29	CLA	B	610	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	19 (22%)
31	BCR	C1	515	-	41,41,41	1.93	4 (9%)	56,56,56	3.77	16 (28%)
29	CLA	S1	605	-	54,58,73	1.58	8 (14%)	65,95,113	2.13	19 (29%)
29	CLA	Y1	614	-	69,73,73	1.36	6 (8%)	83,113,113	1.98	19 (22%)
33	LMG	c	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.16	4 (6%)
39	DGA	C1	524	-	43,43,43	1.17	3 (6%)	45,45,45	1.54	4 (8%)
37	DGD	c1	518	-	56,56,67	1.02	5 (8%)	70,70,81	1.11	4 (5%)
29	CLA	y1	611	40	69,73,73	1.36	7 (10%)	83,113,113	1.99	18 (21%)
29	CLA	c1	513	-	69,73,73	1.40	8 (11%)	83,113,113	2.01	20 (24%)
29	CLA	n	611	-	53,57,73	1.56	6 (11%)	62,93,113	2.21	19 (30%)
29	CLA	C	502	-	69,73,73	1.38	7 (10%)	83,113,113	1.95	17 (20%)
40	LHG	c1	525	-	46,46,48	0.39	0	49,52,54	1.01	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
48	CHL	g	607	-	70,74,74	0.85	2 (2%)	80,114,114	1.22	11 (13%)
48	CHL	y1	606	-	70,74,74	0.82	2 (2%)	80,114,114	1.20	12 (15%)
29	CLA	R	610	-	64,68,73	1.49	9 (14%)	77,107,113	2.14	23 (29%)
40	LHG	d1	409	-	48,48,48	0.40	0	51,54,54	1.03	2 (3%)
32	SQD	B	626	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
49	LUT	N	620	-	42,43,43	2.34	1 (2%)	51,60,60	1.92	15 (29%)
40	LHG	s	624	29	44,44,48	0.43	0	47,50,54	1.13	3 (6%)
49	LUT	n1	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.77	10 (19%)
48	CHL	g1	605	-	52,56,74	0.89	1 (1%)	58,92,114	1.49	11 (18%)
42	BCT	D	401	27	2,3,3	1.26	0	2,3,3	2.71	2 (100%)
29	CLA	c	509	4	69,73,73	1.37	6 (8%)	83,113,113	1.84	15 (18%)
29	CLA	g	612	-	47,51,73	1.69	6 (12%)	56,86,113	2.10	15 (26%)
40	LHG	y	624	29	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
29	CLA	c1	509	4	69,73,73	1.38	8 (11%)	83,113,113	1.76	16 (19%)
40	LHG	C	525	-	46,46,48	0.42	0	49,52,54	1.04	2 (4%)
29	CLA	Y	602	-	69,73,73	1.41	7 (10%)	83,113,113	1.98	19 (22%)
29	CLA	s1	614	-	59,63,73	1.48	8 (13%)	71,101,113	2.11	18 (25%)
26	OEX	a1	401	1	0,14,14	-	-	-		
29	CLA	B1	607	-	69,73,73	1.35	7 (10%)	83,113,113	2.05	21 (25%)
29	CLA	b	617	2	69,73,73	1.36	7 (10%)	83,113,113	1.95	17 (20%)
48	CHL	n1	601	-	70,74,74	0.79	2 (2%)	80,114,114	1.29	10 (12%)
29	CLA	b	614	-	69,73,73	1.36	7 (10%)	83,113,113	2.06	16 (19%)
29	CLA	G	614	-	53,57,73	1.58	7 (13%)	62,93,113	2.20	19 (30%)
54	LPX	S	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.94	1 (3%)
29	CLA	b1	608	-	69,73,73	1.40	7 (10%)	83,113,113	1.93	20 (24%)
50	XAT	r	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	13 (24%)
31	BCR	b1	618	-	41,41,41	2.03	4 (9%)	56,56,56	4.25	19 (33%)
29	CLA	N	614	-	53,57,73	1.57	6 (11%)	62,93,113	2.27	17 (27%)
48	CHL	r	607	-	54,58,74	0.95	2 (3%)	59,94,114	1.44	10 (16%)
29	CLA	C	508	4	69,73,73	1.45	6 (8%)	83,113,113	1.93	22 (26%)
29	CLA	n1	614	-	53,57,73	1.54	7 (13%)	62,93,113	2.30	17 (27%)
48	CHL	s	607	-	47,51,74	0.98	2 (4%)	52,86,114	1.51	11 (21%)
29	CLA	A1	405	-	69,73,73	1.36	7 (10%)	83,113,113	1.92	17 (20%)
29	CLA	c1	503	4	69,73,73	1.36	8 (11%)	83,113,113	2.02	21 (25%)
48	CHL	r1	606	-	48,52,74	1.07	3 (6%)	53,87,114	1.21	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	CLA	C	509	4	69,73,73	1.38	7 (10%)	83,113,113	1.99	19 (22%)
29	CLA	b	615	-	69,73,73	1.36	7 (10%)	83,113,113	1.99	18 (21%)
29	CLA	C1	510	-	69,73,73	1.36	8 (11%)	83,113,113	1.89	17 (20%)
29	CLA	N1	612	-	49,53,73	1.62	7 (14%)	59,89,113	2.09	14 (23%)
40	LHG	d	409	-	48,48,48	0.41	0	51,54,54	1.06	3 (5%)
33	LMG	A	413	-	48,48,55	1.01	5 (10%)	56,56,63	1.20	4 (7%)
48	CHL	n	605	20	70,74,74	0.89	3 (4%)	80,114,114	1.27	10 (12%)
54	LPX	S1	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.93	1 (3%)
29	CLA	R1	610	-	64,68,73	1.45	8 (12%)	77,107,113	2.21	19 (24%)
48	CHL	Y	606	-	70,74,74	0.85	2 (2%)	80,114,114	1.20	9 (11%)
49	LUT	s1	620	-	42,43,43	2.39	1 (2%)	51,60,60	2.02	16 (31%)
39	DGA	B1	625	-	43,43,43	1.14	3 (6%)	45,45,45	1.46	3 (6%)
29	CLA	g	611	-	69,73,73	1.35	6 (8%)	83,113,113	2.04	19 (22%)
30	PHO	a	409	-	58,69,69	1.98	9 (15%)	56,99,99	1.63	11 (19%)
49	LUT	G1	621	-	42,43,43	2.23	1 (2%)	51,60,60	2.08	10 (19%)
48	CHL	S	607	-	47,51,74	1.01	2 (4%)	52,86,114	1.45	9 (17%)
29	CLA	S1	613	-	59,63,73	1.43	6 (10%)	71,101,113	2.10	18 (25%)
49	LUT	y1	621	-	42,43,43	2.37	1 (2%)	51,60,60	2.41	16 (31%)
29	CLA	N1	610	-	69,73,73	1.34	6 (8%)	83,113,113	1.92	19 (22%)
33	LMG	c1	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.13	3 (4%)
29	CLA	a1	407	-	53,57,73	1.57	7 (13%)	62,93,113	2.31	17 (27%)
43	PL9	d1	405	-	55,55,55	1.13	3 (5%)	68,69,69	1.57	14 (20%)
50	XAT	n	622	-	39,47,47	0.78	1 (2%)	54,74,74	2.09	13 (24%)
29	CLA	G1	603	-	69,73,73	1.35	6 (8%)	83,113,113	2.00	19 (22%)
52	LMT	R	625	-	36,36,36	1.22	6 (16%)	47,47,47	1.14	3 (6%)
31	BCR	c	517	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	17 (30%)
52	LMT	r1	625	-	36,36,36	1.18	4 (11%)	47,47,47	1.08	4 (8%)
29	CLA	C1	504	-	69,73,73	1.38	6 (8%)	83,113,113	1.97	19 (22%)
29	CLA	a1	405	-	69,73,73	1.35	6 (8%)	83,113,113	2.02	17 (20%)
44	HEM	f	101	6,7	50,50,50	1.43	5 (10%)	66,82,82	1.15	7 (10%)
48	CHL	N1	606	-	70,74,74	0.88	2 (2%)	80,114,114	1.19	10 (12%)
29	CLA	B1	616	-	69,73,73	1.34	7 (10%)	83,113,113	1.97	18 (21%)
29	CLA	C1	507	-	69,73,73	1.39	7 (10%)	83,113,113	1.89	19 (22%)
48	CHL	g1	601	-	70,74,74	0.77	1 (1%)	80,114,114	1.30	11 (13%)
53	ERG	R1	626	-	31,32,32	7.67	19 (61%)	47,50,50	2.83	19 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	CLA	Y1	608	-	54,58,73	1.58	7 (12%)	65,95,113	2.19	18 (27%)
29	CLA	s	602	-	64,68,73	1.41	7 (10%)	77,107,113	2.04	22 (28%)
29	CLA	R1	612	-	64,68,73	1.44	6 (9%)	77,107,113	2.02	19 (24%)
29	CLA	g1	611	-	69,73,73	1.39	8 (11%)	83,113,113	1.84	17 (20%)
29	CLA	s1	611	40	69,73,73	1.38	6 (8%)	83,113,113	1.97	20 (24%)
26	OEX	A	401	1,4	0,14,14	-	-	-		
32	SQD	M	101	-	41,42,54	0.90	0	50,53,65	0.98	3 (6%)
29	CLA	N	602	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	21 (25%)
33	LMG	w	201	-	39,39,55	0.89	2 (5%)	47,47,63	1.29	4 (8%)
48	CHL	g	609	-	70,74,74	0.87	2 (2%)	80,114,114	1.29	10 (12%)
29	CLA	n1	602	20	69,73,73	1.33	7 (10%)	83,113,113	1.98	20 (24%)
54	LPX	s	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.94	1 (3%)
29	CLA	C	501	4	69,73,73	1.36	7 (10%)	83,113,113	1.98	20 (24%)
29	CLA	G1	610	-	69,73,73	1.38	8 (11%)	83,113,113	2.00	20 (24%)
31	BCR	c1	514	-	41,41,41	1.85	4 (9%)	56,56,56	4.49	17 (30%)
48	CHL	n1	607	-	70,74,74	0.78	2 (2%)	80,114,114	1.24	9 (11%)
29	CLA	s	613	-	59,63,73	1.44	6 (10%)	71,101,113	2.18	19 (26%)
49	LUT	r1	620	-	42,43,43	2.36	2 (4%)	51,60,60	2.32	15 (29%)
50	XAT	R1	621	-	39,47,47	0.68	1 (2%)	54,74,74	1.91	18 (33%)
29	CLA	Y	604	-	69,73,73	1.34	5 (7%)	83,113,113	1.93	17 (20%)
48	CHL	y1	609	-	70,74,74	0.85	2 (2%)	80,114,114	1.35	11 (13%)
48	CHL	R1	607	-	54,58,74	0.89	2 (3%)	59,94,114	1.43	11 (18%)
31	BCR	C1	517	-	41,41,41	1.87	4 (9%)	56,56,56	4.45	16 (28%)
41	LMK	C1	527	-	38,39,53	1.50	2 (5%)	41,46,60	1.47	2 (4%)
47	4RF	I	102	-	56,56,56	1.05	4 (7%)	59,59,59	0.97	3 (5%)
45	RRX	h	101	-	42,42,42	4.74	24 (57%)	57,58,58	3.10	25 (43%)
29	CLA	y1	610	24	69,73,73	1.41	8 (11%)	83,113,113	1.96	22 (26%)
48	CHL	y	607	-	70,74,74	0.83	2 (2%)	80,114,114	1.26	12 (15%)
32	SQD	b	621	-	41,42,54	0.87	0	50,53,65	1.02	3 (6%)
29	CLA	b1	606	-	69,73,73	1.38	7 (10%)	83,113,113	1.98	18 (21%)
29	CLA	S	617	23	54,58,73	1.52	7 (12%)	65,95,113	2.21	19 (29%)
40	LHG	C1	525	-	46,46,48	0.39	0	49,52,54	1.04	3 (6%)
51	NEX	g1	623	-	38,46,46	3.26	10 (26%)	50,70,70	1.91	15 (30%)
34	SPH	A1	414	-	19,20,20	0.67	1 (5%)	18,21,21	1.17	1 (5%)
29	CLA	C	511	-	69,73,73	1.36	7 (10%)	83,113,113	1.90	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	CLA	S1	611	40	69,73,73	1.41	8 (11%)	83,113,113	1.93	17 (20%)
48	CHL	R	607	-	54,58,74	0.93	2 (3%)	59,94,114	1.45	11 (18%)
29	CLA	b	611	-	69,73,73	1.38	6 (8%)	83,113,113	1.94	20 (24%)
40	LHG	D1	408	-	43,43,48	0.41	0	46,49,54	1.03	2 (4%)
48	CHL	g	605	21	52,56,74	0.91	2 (3%)	58,92,114	1.59	13 (22%)
29	CLA	B	613	2	69,73,73	1.41	7 (10%)	83,113,113	1.94	15 (18%)
40	LHG	S	624	29	44,44,48	0.43	0	47,50,54	1.05	3 (6%)
29	CLA	N	613	-	69,73,73	1.38	6 (8%)	83,113,113	1.96	15 (18%)
36	C7Z	B1	620	-	43,43,43	5.38	26 (60%)	58,60,60	2.39	22 (37%)
51	NEX	G1	623	-	38,46,46	3.38	10 (26%)	50,70,70	1.77	11 (22%)
29	CLA	n1	612	-	49,53,73	1.64	8 (16%)	59,89,113	1.98	15 (25%)
29	CLA	b	605	-	69,73,73	1.39	7 (10%)	83,113,113	2.14	23 (27%)
32	SQD	a1	412	-	50,51,54	0.82	0	59,62,65	0.95	2 (3%)
55	PTY	y	626	-	49,49,49	0.88	3 (6%)	52,54,54	1.12	3 (5%)
49	LUT	Y	620	-	42,43,43	2.31	1 (2%)	51,60,60	1.81	13 (25%)
49	LUT	G	620	-	42,43,43	2.25	1 (2%)	51,60,60	1.99	17 (33%)
29	CLA	Y	603	-	69,73,73	1.37	7 (10%)	83,113,113	2.00	21 (25%)
29	CLA	c1	501	-	69,73,73	1.40	7 (10%)	83,113,113	2.00	20 (24%)
29	CLA	y1	612	-	69,73,73	1.35	7 (10%)	83,113,113	1.97	21 (25%)
40	LHG	l	101	-	48,48,48	0.38	0	51,54,54	4.45	4 (7%)
49	LUT	n1	621	-	42,43,43	2.34	1 (2%)	51,60,60	2.13	18 (35%)
49	LUT	g	620	-	42,43,43	2.32	1 (2%)	51,60,60	2.16	16 (31%)
34	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.00	0
29	CLA	G1	611	-	69,73,73	1.36	6 (8%)	83,113,113	1.96	17 (20%)
40	LHG	S1	624	29	44,44,48	0.44	0	47,50,54	1.12	4 (8%)
48	CHL	y1	601	24	70,74,74	0.79	2 (2%)	80,114,114	1.22	9 (11%)
45	RRX	H	101	-	42,42,42	4.84	24 (57%)	57,58,58	2.85	22 (38%)
29	CLA	c	508	4	69,73,73	1.39	7 (10%)	83,113,113	1.88	16 (19%)
48	CHL	S1	601	23	50,54,74	0.95	3 (6%)	56,90,114	1.42	10 (17%)
29	CLA	c	503	4	69,73,73	1.38	7 (10%)	83,113,113	1.90	20 (24%)
29	CLA	b1	615	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	14 (16%)
48	CHL	G	601	21	70,74,74	0.82	2 (2%)	80,114,114	1.27	12 (15%)
48	CHL	y	605	24	50,54,74	0.96	2 (4%)	56,90,114	1.49	11 (19%)
49	LUT	g1	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.33	14 (27%)
29	CLA	C	505	4	69,73,73	1.39	7 (10%)	83,113,113	1.97	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
31	BCR	C	514	-	41,41,41	1.87	5 (12%)	56,56,56	4.28	14 (25%)
39	DGA	c1	524	-	43,43,43	1.14	3 (6%)	45,45,45	1.51	3 (6%)
31	BCR	b	618	-	41,41,41	1.89	5 (12%)	56,56,56	4.48	20 (35%)
29	CLA	b	604	-	69,73,73	1.40	7 (10%)	83,113,113	1.82	16 (19%)
29	CLA	B	602	-	69,73,73	1.35	6 (8%)	83,113,113	1.92	17 (20%)
48	CHL	Y1	601	-	70,74,74	0.91	3 (4%)	80,114,114	1.15	9 (11%)
29	CLA	C1	509	-	69,73,73	1.36	7 (10%)	83,113,113	1.99	17 (20%)
29	CLA	b1	609	-	69,73,73	1.36	7 (10%)	83,113,113	2.01	17 (20%)
32	SQD	B1	626	-	53,54,54	0.80	0	62,65,65	0.92	2 (3%)
49	LUT	g1	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.93	11 (21%)
29	CLA	N	604	-	69,73,73	1.38	6 (8%)	83,113,113	2.01	20 (24%)
29	CLA	R	612	-	64,68,73	1.43	8 (12%)	77,107,113	2.10	20 (25%)
29	CLA	n1	604	-	69,73,73	1.37	7 (10%)	83,113,113	1.92	16 (19%)
29	CLA	B1	606	-	69,73,73	1.37	8 (11%)	83,113,113	1.97	19 (22%)
29	CLA	s	612	-	49,53,73	1.63	8 (16%)	59,89,113	2.05	15 (25%)
29	CLA	B	608	-	69,73,73	1.36	6 (8%)	83,113,113	1.95	16 (19%)
29	CLA	A	410	1	64,68,73	1.45	8 (12%)	77,107,113	2.06	20 (25%)
29	CLA	Y	613	24	69,73,73	1.38	7 (10%)	83,113,113	2.10	23 (27%)
29	CLA	G	613	-	69,73,73	1.35	7 (10%)	83,113,113	2.00	22 (26%)
29	CLA	n	610	-	69,73,73	1.40	8 (11%)	83,113,113	2.06	20 (24%)
29	CLA	C1	502	-	69,73,73	1.39	6 (8%)	83,113,113	1.94	19 (22%)
31	BCR	D1	404	-	41,41,41	1.85	4 (9%)	56,56,56	4.33	16 (28%)
29	CLA	N1	611	-	53,57,73	1.56	7 (13%)	62,93,113	2.22	18 (29%)
29	CLA	N1	602	-	69,73,73	1.38	7 (10%)	83,113,113	1.92	18 (21%)
29	CLA	B1	614	-	69,73,73	1.38	8 (11%)	83,113,113	1.94	14 (16%)
48	CHL	G1	608	-	48,52,74	1.03	2 (4%)	53,87,114	1.46	9 (16%)
55	PTY	Y	626	-	49,49,49	0.88	3 (6%)	52,54,54	1.02	2 (3%)
33	LMG	w1	201	-	39,39,55	0.85	2 (5%)	47,47,63	1.17	3 (6%)
29	CLA	N1	613	-	69,73,73	1.37	7 (10%)	83,113,113	1.94	17 (20%)
48	CHL	Y	609	-	70,74,74	0.87	3 (4%)	80,114,114	1.43	15 (18%)
40	LHG	G	624	29	48,48,48	0.37	0	51,54,54	1.06	3 (5%)
30	PHO	A1	409	-	58,69,69	2.04	9 (15%)	56,99,99	1.75	8 (14%)
43	PL9	D	405	-	55,55,55	1.56	5 (9%)	68,69,69	1.47	12 (17%)
48	CHL	Y	601	24	70,74,74	0.94	3 (4%)	80,114,114	1.17	9 (11%)
47	4RF	k	101	-	56,56,56	1.06	5 (8%)	59,59,59	0.83	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	CLA	S1	612	-	49,53,73	1.61	6 (12%)	59,89,113	2.03	14 (23%)
29	CLA	g	603	-	69,73,73	1.38	8 (11%)	83,113,113	1.98	19 (22%)
42	BCT	d	401	-	2,3,3	1.27	0	2,3,3	2.80	2 (100%)
29	CLA	g	604	-	53,57,73	1.56	8 (15%)	62,93,113	2.13	18 (29%)
29	CLA	Y1	612	-	69,73,73	1.39	7 (10%)	83,113,113	1.93	20 (24%)
48	CHL	Y	605	24	50,54,74	0.98	2 (4%)	56,90,114	1.50	11 (19%)
48	CHL	G	605	21	52,56,74	0.93	2 (3%)	58,92,114	1.31	9 (15%)
29	CLA	d	402	-	69,73,73	1.37	7 (10%)	83,113,113	1.91	18 (21%)
31	BCR	D	404	-	41,41,41	1.86	4 (9%)	56,56,56	4.18	16 (28%)
50	XAT	G1	622	-	39,47,47	0.76	1 (2%)	54,74,74	1.88	17 (31%)
29	CLA	R1	608	-	64,68,73	1.43	7 (10%)	77,107,113	2.03	18 (23%)
51	NEX	Y	623	-	38,46,46	3.34	9 (23%)	50,70,70	1.85	12 (24%)
29	CLA	G1	613	-	69,73,73	1.35	7 (10%)	83,113,113	2.10	20 (24%)
34	SPH	a	414	-	19,20,20	0.70	1 (5%)	18,21,21	1.10	1 (5%)
40	LHG	c	525	-	46,46,48	0.40	0	49,52,54	1.12	3 (6%)
29	CLA	b	612	-	69,73,73	1.37	7 (10%)	83,113,113	2.00	16 (19%)
29	CLA	S1	617	23	54,58,73	1.54	8 (14%)	65,95,113	2.21	18 (27%)
48	CHL	G1	607	-	70,74,74	0.86	2 (2%)	80,114,114	1.12	8 (10%)
33	LMG	W1	201	-	39,39,55	0.87	2 (5%)	47,47,63	1.37	6 (12%)
48	CHL	n	607	-	70,74,74	0.83	2 (2%)	80,114,114	1.21	11 (13%)
29	CLA	b	606	-	69,73,73	1.37	7 (10%)	83,113,113	2.02	16 (19%)
29	CLA	S	609	-	64,68,73	1.42	7 (10%)	77,107,113	1.93	18 (23%)
33	LMG	h	102	-	48,48,55	1.01	5 (10%)	56,56,63	1.22	4 (7%)
34	SPH	A	414	-	19,20,20	0.66	0	18,21,21	1.13	2 (11%)
38	3PH	b1	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.15	2 (3%)
29	CLA	c1	511	-	69,73,73	1.36	6 (8%)	83,113,113	2.03	19 (22%)
29	CLA	s1	603	-	69,73,73	1.36	7 (10%)	83,113,113	2.02	19 (22%)
29	CLA	S	614	-	59,63,73	1.49	6 (10%)	71,101,113	2.05	17 (23%)
48	CHL	n1	606	-	70,74,74	0.81	2 (2%)	80,114,114	1.24	11 (13%)
29	CLA	B1	602	-	69,73,73	1.40	7 (10%)	83,113,113	1.98	18 (21%)
43	PL9	D1	405	-	55,55,55	1.18	5 (9%)	68,69,69	1.72	15 (22%)
48	CHL	n	609	-	70,74,74	0.79	2 (2%)	80,114,114	1.40	13 (16%)
48	CHL	R1	606	-	48,52,74	1.00	2 (4%)	53,87,114	1.35	11 (20%)
29	CLA	S	604	-	59,63,73	1.45	7 (11%)	71,101,113	2.13	19 (26%)
29	CLA	b1	617	2	69,73,73	1.38	5 (7%)	83,113,113	1.92	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	CLA	y1	602	-	69,73,73	1.36	9 (13%)	83,113,113	1.97	21 (25%)
38	3PH	T1	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.09	2 (3%)
48	CHL	g1	607	-	70,74,74	0.82	2 (2%)	80,114,114	1.19	9 (11%)
29	CLA	n1	603	-	69,73,73	1.35	6 (8%)	83,113,113	1.98	18 (21%)
29	CLA	Y	612	-	69,73,73	1.37	7 (10%)	83,113,113	1.95	19 (22%)
29	CLA	G	612	-	47,51,73	1.65	5 (10%)	56,86,113	2.12	16 (28%)
29	CLA	B1	617	-	69,73,73	1.39	7 (10%)	83,113,113	1.93	18 (21%)
32	SQD	b	626	-	53,54,54	0.82	0	62,65,65	0.91	3 (4%)
40	LHG	d1	410	-	38,38,48	0.44	0	41,44,54	1.04	2 (4%)
29	CLA	S	613	-	59,63,73	1.49	7 (11%)	71,101,113	2.08	16 (22%)
29	CLA	D1	402	-	69,73,73	1.38	7 (10%)	83,113,113	1.99	20 (24%)
40	LHG	Y	624	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
55	PTY	Y1	626	-	49,49,49	0.89	4 (8%)	52,54,54	1.04	2 (3%)
34	SPH	y1	625	-	19,20,20	0.62	0	18,21,21	1.27	2 (11%)
49	LUT	N	621	-	42,43,43	2.39	1 (2%)	51,60,60	1.97	12 (23%)
48	CHL	Y1	605	-	50,54,74	0.96	2 (4%)	56,90,114	1.39	9 (16%)
49	LUT	n	621	-	42,43,43	2.39	1 (2%)	51,60,60	1.78	12 (23%)
29	CLA	R1	602	-	64,68,73	1.45	8 (12%)	77,107,113	2.00	19 (24%)
31	BCR	A1	411	-	41,41,41	1.88	4 (9%)	56,56,56	4.17	15 (26%)
51	NEX	Y1	623	-	38,46,46	3.15	10 (26%)	50,70,70	1.99	13 (26%)
29	CLA	c	510	4	69,73,73	1.37	6 (8%)	83,113,113	2.01	19 (22%)
29	CLA	R	603	-	64,68,73	1.47	8 (12%)	77,107,113	1.94	17 (22%)
29	CLA	y1	608	-	54,58,73	1.55	8 (14%)	65,95,113	2.13	19 (29%)
48	CHL	G1	606	-	54,58,74	1.02	2 (3%)	59,94,114	1.36	11 (18%)
32	SQD	B1	621	-	41,42,54	0.89	0	50,53,65	0.96	2 (4%)
29	CLA	B	605	2	69,73,73	1.40	7 (10%)	83,113,113	2.03	20 (24%)
29	CLA	b	608	-	69,73,73	1.34	6 (8%)	83,113,113	1.93	15 (18%)
29	CLA	b1	611	-	69,73,73	1.44	6 (8%)	83,113,113	1.98	20 (24%)
40	LHG	y1	624	29	48,48,48	0.41	0	51,54,54	0.98	2 (3%)
48	CHL	G	609	21	70,74,74	0.84	2 (2%)	80,114,114	1.20	13 (16%)
29	CLA	s1	610	-	69,73,73	1.37	6 (8%)	83,113,113	1.94	19 (22%)
29	CLA	C	504	-	69,73,73	1.34	7 (10%)	83,113,113	1.89	14 (16%)
33	LMG	D1	411	-	46,46,55	0.91	4 (8%)	54,54,63	1.12	3 (5%)
29	CLA	S	603	-	69,73,73	1.37	8 (11%)	83,113,113	1.83	19 (22%)
32	SQD	A	412	-	50,51,54	0.81	0	59,62,65	0.94	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
29	CLA	R	602	-	64,68,73	1.46	8 (12%)	77,107,113	1.94	20 (25%)
48	CHL	Y1	607	-	70,74,74	0.87	3 (4%)	80,114,114	1.15	9 (11%)
29	CLA	y1	613	-	69,73,73	1.34	6 (8%)	83,113,113	2.01	19 (22%)
29	CLA	b1	607	-	69,73,73	1.37	7 (10%)	83,113,113	1.95	20 (24%)
29	CLA	C	507	-	69,73,73	1.39	7 (10%)	83,113,113	1.99	17 (20%)
29	CLA	b	610	-	69,73,73	1.35	7 (10%)	83,113,113	1.95	17 (20%)
29	CLA	r1	602	-	64,68,73	1.42	6 (9%)	77,107,113	2.03	20 (25%)
32	SQD	C	526	-	53,54,54	0.81	1 (1%)	62,65,65	0.94	3 (4%)
33	LMG	c	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.12	3 (4%)
40	LHG	L	101	-	48,48,48	0.38	0	51,54,54	4.46	5 (9%)
42	BCT	d1	401	-	2,3,3	1.18	0	2,3,3	4.36	2 (100%)
32	SQD	b1	621	-	41,42,54	0.89	0	50,53,65	0.98	3 (6%)
33	LMG	A1	413	-	48,48,55	1.00	5 (10%)	56,56,63	1.20	5 (8%)
40	LHG	d	410	-	38,38,48	0.43	0	41,44,54	1.11	3 (7%)
29	CLA	C	513	-	69,73,73	1.38	6 (8%)	83,113,113	1.94	19 (22%)
37	DGD	B	623	-	44,44,67	0.89	1 (2%)	58,58,81	1.36	6 (10%)
29	CLA	C1	511	-	69,73,73	1.36	7 (10%)	83,113,113	2.09	21 (25%)
29	CLA	s1	617	-	54,58,73	1.53	8 (14%)	65,95,113	2.14	19 (29%)
37	DGD	b	623	-	44,44,67	0.89	2 (4%)	58,58,81	1.26	6 (10%)
49	LUT	g	621	-	42,43,43	2.37	2 (4%)	51,60,60	1.91	12 (23%)
29	CLA	c1	502	-	69,73,73	1.41	7 (10%)	83,113,113	1.82	15 (18%)
29	CLA	B	611	-	69,73,73	1.39	7 (10%)	83,113,113	1.95	19 (22%)
29	CLA	g1	613	-	69,73,73	1.37	7 (10%)	83,113,113	2.00	18 (21%)
31	BCR	C1	516	-	41,41,41	1.89	4 (9%)	56,56,56	4.66	17 (30%)
48	CHL	s1	601	23	50,54,74	1.01	3 (6%)	56,90,114	1.44	12 (21%)
29	CLA	Y	614	-	69,73,73	1.36	8 (11%)	83,113,113	1.99	21 (25%)
48	CHL	s1	607	-	47,51,74	0.94	2 (4%)	52,86,114	1.47	11 (21%)
51	NEX	s1	623	-	38,46,46	3.40	12 (31%)	50,70,70	2.71	15 (30%)
31	BCR	B1	618	-	41,41,41	1.88	4 (9%)	56,56,56	4.43	19 (33%)
29	CLA	B1	604	-	69,73,73	1.39	6 (8%)	83,113,113	1.78	16 (19%)
39	DGA	B	625	-	43,43,43	1.09	2 (4%)	45,45,45	1.52	3 (6%)
29	CLA	A	405	-	69,73,73	1.38	6 (8%)	83,113,113	1.98	16 (19%)
29	CLA	R1	603	-	64,68,73	1.46	7 (10%)	77,107,113	1.84	16 (20%)
51	NEX	y1	623	-	38,46,46	3.26	10 (26%)	50,70,70	2.03	18 (36%)
29	CLA	c1	507	-	69,73,73	1.38	7 (10%)	83,113,113	1.98	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
29	CLA	Y1	602	-	69,73,73	1.39	8 (11%)	83,113,113	2.03	19 (22%)
29	CLA	b1	602	-	69,73,73	1.38	9 (13%)	83,113,113	1.90	20 (24%)
40	LHG	n1	624	-	48,48,48	0.41	0	51,54,54	1.07	3 (5%)
48	CHL	y	609	-	70,74,74	0.84	3 (4%)	80,114,114	1.24	10 (12%)
29	CLA	B1	608	-	69,73,73	1.38	7 (10%)	83,113,113	1.93	18 (21%)
33	LMG	a	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.19	4 (7%)
49	LUT	N1	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.99	14 (27%)
32	SQD	C1	526	-	53,54,54	0.81	0	62,65,65	0.88	2 (3%)
51	NEX	n1	623	-	38,46,46	3.26	9 (23%)	50,70,70	1.71	11 (22%)
48	CHL	g	601	21	70,74,74	0.83	3 (4%)	80,114,114	1.28	11 (13%)
29	CLA	B1	605	-	69,73,73	1.35	7 (10%)	83,113,113	2.00	18 (21%)
49	LUT	s1	621	-	42,43,43	2.25	1 (2%)	51,60,60	2.37	13 (25%)
31	BCR	C1	514	-	41,41,41	1.84	5 (12%)	56,56,56	4.05	13 (23%)
50	XAT	y1	622	-	39,47,47	0.74	1 (2%)	54,74,74	3.88	20 (37%)
29	CLA	n	604	-	69,73,73	1.35	7 (10%)	83,113,113	1.95	18 (21%)
29	CLA	S1	610	-	69,73,73	1.37	6 (8%)	83,113,113	1.97	18 (21%)
29	CLA	A	406	-	69,73,73	1.36	7 (10%)	83,113,113	2.01	16 (19%)
29	CLA	b1	616	2	69,73,73	1.40	6 (8%)	83,113,113	1.90	15 (18%)
29	CLA	a1	406	-	69,73,73	1.39	8 (11%)	83,113,113	1.99	20 (24%)
29	CLA	r1	609	-	64,68,73	1.40	7 (10%)	77,107,113	2.02	20 (25%)
32	SQD	M1	101	-	41,42,54	0.90	0	50,53,65	0.97	2 (4%)
29	CLA	d1	403	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	19 (22%)
33	LMG	W	201	-	39,39,55	0.85	2 (5%)	47,47,63	1.21	4 (8%)
29	CLA	G	604	-	53,57,73	1.58	7 (13%)	62,93,113	2.15	17 (27%)
29	CLA	a	405	-	69,73,73	1.38	6 (8%)	83,113,113	1.97	19 (22%)
29	CLA	N1	614	-	53,57,73	1.55	7 (13%)	62,93,113	2.21	17 (27%)
29	CLA	G1	612	-	47,51,73	1.69	7 (14%)	56,86,113	2.10	14 (25%)
29	CLA	Y1	613	-	69,73,73	1.35	7 (10%)	83,113,113	2.05	18 (21%)
37	DGD	C1	519	-	63,63,67	1.10	7 (11%)	77,77,81	1.05	3 (3%)
29	CLA	G	611	40	69,73,73	1.37	6 (8%)	83,113,113	1.96	18 (21%)
40	LHG	G1	624	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
47	4RF	K1	101	-	56,56,56	1.07	3 (5%)	59,59,59	0.84	3 (5%)
29	CLA	r1	604	-	53,57,73	1.57	7 (13%)	62,93,113	2.14	16 (25%)
29	CLA	s1	612	-	49,53,73	1.67	9 (18%)	59,89,113	1.93	13 (22%)
48	CHL	N	606	-	70,74,74	0.86	2 (2%)	80,114,114	1.25	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
46	GOL	I	101	-	5,5,5	0.54	0	5,5,5	0.39	0
38	3PH	T	101	-	47,47,47	0.85	3 (6%)	51,52,52	1.19	2 (3%)
33	LMG	d1	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.11	3 (5%)
29	CLA	s	614	-	59,63,73	1.48	6 (10%)	71,101,113	2.03	16 (22%)
29	CLA	S	610	-	69,73,73	1.39	8 (11%)	83,113,113	1.87	21 (25%)
29	CLA	b	603	2	69,73,73	1.39	7 (10%)	83,113,113	1.98	18 (21%)
31	BCR	a	411	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	14 (25%)
29	CLA	S	611	40	69,73,73	1.36	6 (8%)	83,113,113	1.91	18 (21%)
34	SPH	Y1	625	-	19,20,20	0.64	0	18,21,21	1.03	1 (5%)
29	CLA	s	605	-	54,58,73	1.55	7 (12%)	65,95,113	2.21	18 (27%)
29	CLA	S1	603	-	69,73,73	1.39	7 (10%)	83,113,113	1.96	18 (21%)
29	CLA	n	602	-	69,73,73	1.42	7 (10%)	83,113,113	1.90	21 (25%)
48	CHL	g	608	-	48,52,74	0.97	2 (4%)	53,87,114	1.46	13 (24%)
29	CLA	c	502	4	69,73,73	1.37	6 (8%)	83,113,113	1.99	16 (19%)
29	CLA	C1	506	-	69,73,73	1.36	6 (8%)	83,113,113	1.97	19 (22%)
48	CHL	g1	606	-	54,58,74	1.01	4 (7%)	59,94,114	1.37	10 (16%)
29	CLA	b1	610	-	69,73,73	1.37	8 (11%)	83,113,113	1.87	18 (21%)
29	CLA	S1	604	-	59,63,73	1.49	7 (11%)	71,101,113	2.14	20 (28%)
29	CLA	d	403	-	69,73,73	1.38	7 (10%)	83,113,113	1.94	17 (20%)
51	NEX	y	623	-	38,46,46	3.41	9 (23%)	50,70,70	1.96	15 (30%)
33	LMG	H1	102	-	48,48,55	1.02	5 (10%)	56,56,63	1.16	3 (5%)
29	CLA	B	607	2	69,73,73	1.38	8 (11%)	83,113,113	1.89	16 (19%)
37	DGD	c	518	-	56,56,67	0.98	4 (7%)	70,70,81	1.14	4 (5%)
53	ERG	r1	626	-	31,32,32	7.77	19 (61%)	47,50,50	2.72	18 (38%)
45	RRX	h1	101	-	42,42,42	4.84	24 (57%)	57,58,58	2.65	25 (43%)
29	CLA	Y1	604	-	69,73,73	1.38	5 (7%)	83,113,113	1.92	17 (20%)
48	CHL	S	601	23	50,54,74	1.04	3 (6%)	56,90,114	1.43	9 (16%)
48	CHL	N1	605	20	70,74,74	0.89	2 (2%)	80,114,114	1.31	13 (16%)
33	LMG	a1	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.31	4 (7%)
50	XAT	g	622	-	39,47,47	0.80	1 (2%)	54,74,74	2.22	16 (29%)
48	CHL	N1	607	-	70,74,74	0.83	2 (2%)	80,114,114	1.22	11 (13%)
29	CLA	g	613	-	69,73,73	1.34	6 (8%)	83,113,113	1.99	20 (24%)
49	LUT	y	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.92	15 (29%)
29	CLA	B	609	2	69,73,73	1.38	7 (10%)	83,113,113	2.13	17 (20%)
29	CLA	C1	513	4	69,73,73	1.37	7 (10%)	83,113,113	1.89	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
48	CHL	S	608	-	65,69,74	0.84	2 (3%)	74,108,114	1.29	12 (16%)
33	LMG	c1	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.10	3 (5%)
29	CLA	n	613	-	69,73,73	1.38	6 (8%)	83,113,113	2.04	18 (21%)
40	LHG	d	408	-	43,43,48	0.40	0	46,49,54	1.04	3 (6%)
29	CLA	s	609	-	64,68,73	1.43	8 (12%)	77,107,113	1.97	16 (20%)
41	LMK	c	527	-	38,39,53	1.50	2 (5%)	41,46,60	1.25	2 (4%)
26	OEX	a	401	1,4	0,14,14	-	-	-		
40	LHG	D1	410	-	38,38,48	0.43	0	41,44,54	1.09	3 (7%)
30	PHO	A	409	-	58,69,69	1.98	9 (15%)	56,99,99	1.70	8 (14%)
29	CLA	B	606	2	69,73,73	1.36	7 (10%)	83,113,113	2.04	16 (19%)
29	CLA	s1	604	-	59,63,73	1.48	5 (8%)	71,101,113	2.10	17 (23%)
29	CLA	G	603	21	69,73,73	1.35	7 (10%)	83,113,113	1.99	22 (26%)
30	PHO	a1	408	-	58,69,69	2.04	10 (17%)	56,99,99	1.48	9 (16%)
29	CLA	c	512	-	69,73,73	1.43	9 (13%)	83,113,113	1.89	20 (24%)
48	CHL	s1	608	-	65,69,74	0.95	4 (6%)	74,108,114	1.39	12 (16%)
31	BCR	A	411	-	41,41,41	1.86	4 (9%)	56,56,56	4.22	14 (25%)
48	CHL	s1	606	-	48,52,74	0.96	2 (4%)	53,87,114	1.31	8 (15%)
29	CLA	s1	609	-	64,68,73	1.39	7 (10%)	77,107,113	2.12	17 (22%)
31	BCR	b1	619	-	41,41,41	1.91	4 (9%)	56,56,56	4.36	15 (26%)
29	CLA	N	603	-	69,73,73	1.33	7 (10%)	83,113,113	2.02	20 (24%)
55	PTY	Y	627	-	18,18,49	1.31	3 (16%)	21,23,54	1.40	2 (9%)
29	CLA	n	603	-	69,73,73	1.36	7 (10%)	83,113,113	2.01	22 (26%)
33	LMG	C	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.19	3 (5%)
38	3PH	t1	101	-	47,47,47	0.87	3 (6%)	51,52,52	1.05	2 (3%)
29	CLA	y	614	-	69,73,73	1.34	6 (8%)	83,113,113	1.97	20 (24%)
51	NEX	R	622	-	38,46,46	3.42	11 (28%)	50,70,70	1.98	12 (24%)
48	CHL	S1	608	-	65,69,74	0.83	2 (3%)	74,108,114	1.33	12 (16%)
39	DGA	b	625	-	43,43,43	1.11	2 (4%)	45,45,45	1.45	3 (6%)
29	CLA	s1	613	-	59,63,73	1.51	8 (13%)	71,101,113	2.05	19 (26%)
29	CLA	Y	611	-	69,73,73	1.35	8 (11%)	83,113,113	1.84	13 (15%)
29	CLA	c1	510	-	69,73,73	1.40	7 (10%)	83,113,113	1.89	17 (20%)
29	CLA	B1	611	-	69,73,73	1.40	6 (8%)	83,113,113	2.03	17 (20%)
29	CLA	r1	612	-	64,68,73	1.43	7 (10%)	77,107,113	1.96	19 (24%)
29	CLA	a	407	-	53,57,73	1.55	6 (11%)	62,93,113	2.39	18 (29%)
48	CHL	n	601	20	70,74,74	0.87	3 (4%)	80,114,114	1.28	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
29	CLA	b	607	-	69,73,73	1.37	7 (10%)	83,113,113	1.94	20 (24%)
32	SQD	c1	526	-	53,54,54	0.80	0	62,65,65	0.93	2 (3%)
48	CHL	y1	605	24	50,54,74	0.97	2 (4%)	56,90,114	1.35	10 (17%)
29	CLA	S	612	-	49,53,73	1.64	7 (14%)	59,89,113	2.09	13 (22%)
49	LUT	S	620	-	42,43,43	2.29	1 (2%)	51,60,60	2.12	18 (35%)
29	CLA	Y	610	-	69,73,73	1.38	7 (10%)	83,113,113	2.06	18 (21%)
29	CLA	G	610	21	69,73,73	1.38	7 (10%)	83,113,113	1.96	18 (21%)
51	NEX	n	623	-	38,46,46	3.48	11 (28%)	50,70,70	1.66	11 (22%)
37	DGD	b1	623	-	44,44,67	0.92	2 (4%)	58,58,81	1.32	5 (8%)
49	LUT	Y1	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.87	14 (27%)
29	CLA	g1	603	-	69,73,73	1.40	8 (11%)	83,113,113	1.84	17 (20%)
29	CLA	B	616	-	69,73,73	1.36	9 (13%)	83,113,113	1.93	21 (25%)
29	CLA	C	510	4	69,73,73	1.39	6 (8%)	83,113,113	1.90	18 (21%)
48	CHL	Y1	606	-	70,74,74	0.85	3 (4%)	80,114,114	1.29	11 (13%)
29	CLA	b	609	2	69,73,73	1.42	9 (13%)	83,113,113	1.93	20 (24%)
29	CLA	R	609	-	64,68,73	1.43	7 (10%)	77,107,113	4.30	20 (25%)
29	CLA	B1	612	-	69,73,73	1.37	6 (8%)	83,113,113	2.02	20 (24%)
48	CHL	S1	607	-	47,51,74	0.97	2 (4%)	52,86,114	1.49	10 (19%)
33	LMG	h1	102	-	48,48,55	1.00	4 (8%)	56,56,63	1.23	4 (7%)
29	CLA	A1	407	-	54,58,73	1.57	7 (12%)	65,95,113	2.10	17 (26%)
31	BCR	c	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	14 (25%)
29	CLA	Y1	603	-	69,73,73	1.38	8 (11%)	83,113,113	1.91	18 (21%)
50	XAT	R	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	18 (33%)
37	DGD	c1	520	-	60,60,67	1.09	6 (10%)	74,74,81	1.00	3 (4%)
29	CLA	B1	615	-	69,73,73	1.38	7 (10%)	83,113,113	1.91	18 (21%)
29	CLA	N1	604	-	69,73,73	1.36	7 (10%)	83,113,113	2.11	18 (21%)
32	SQD	A1	412	-	50,51,54	0.81	0	59,62,65	0.98	4 (6%)
33	LMG	H	102	-	48,48,55	1.01	5 (10%)	56,56,63	1.10	2 (3%)
50	XAT	N1	622	-	39,47,47	0.72	1 (2%)	54,74,74	2.10	15 (27%)
55	PTY	Y1	627	-	18,18,49	1.28	2 (11%)	21,23,54	1.41	2 (9%)
29	CLA	r1	610	-	64,68,73	1.45	7 (10%)	77,107,113	1.92	17 (22%)
40	LHG	g	624	-	48,48,48	0.39	0	51,54,54	0.97	2 (3%)
49	LUT	S1	620	-	42,43,43	2.32	1 (2%)	51,60,60	1.76	9 (17%)
49	LUT	Y1	621	-	42,43,43	2.32	1 (2%)	51,60,60	2.33	13 (25%)
29	CLA	g	602	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	22 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
29	CLA	D	403	-	69,73,73	1.35	7 (10%)	83,113,113	2.02	20 (24%)
33	LMG	D	411	-	46,46,55	0.91	4 (8%)	54,54,63	0.99	2 (3%)
40	LHG	N	624	-	48,48,48	0.40	0	51,54,54	1.08	3 (5%)
40	LHG	n	624	-	48,48,48	0.38	0	51,54,54	1.08	2 (3%)
48	CHL	N	609	-	70,74,74	0.82	3 (4%)	80,114,114	1.17	10 (12%)
48	CHL	n1	609	-	70,74,74	0.80	2 (2%)	80,114,114	1.30	12 (15%)
48	CHL	r	606	-	48,52,74	0.96	2 (4%)	53,87,114	1.38	9 (16%)
48	CHL	R	606	-	48,52,74	1.08	2 (4%)	53,87,114	1.34	8 (15%)
29	CLA	c1	512	-	69,73,73	1.40	7 (10%)	83,113,113	1.93	18 (21%)
37	DGD	B1	623	-	44,44,67	0.86	1 (2%)	58,58,81	1.21	6 (10%)
38	3PH	B	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.12	2 (3%)
32	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.92	2 (3%)
32	SQD	m1	101	-	41,42,54	0.88	0	50,53,65	0.99	3 (6%)
50	XAT	Y	622	-	39,47,47	0.70	1 (2%)	54,74,74	3.77	16 (29%)
31	BCR	c	516	-	41,41,41	1.87	4 (9%)	56,56,56	4.24	12 (21%)
31	BCR	B	618	-	41,41,41	1.88	5 (12%)	56,56,56	4.32	18 (32%)
51	NEX	N	623	-	38,46,46	3.40	9 (23%)	50,70,70	1.64	11 (22%)
29	CLA	n1	613	-	69,73,73	1.36	7 (10%)	83,113,113	2.10	19 (22%)
37	DGD	c	519	-	63,63,67	1.12	5 (7%)	77,77,81	1.01	2 (2%)
50	XAT	N	622	-	39,47,47	0.70	1 (2%)	54,74,74	2.21	13 (24%)
29	CLA	D1	403	-	69,73,73	1.37	9 (13%)	83,113,113	1.96	22 (26%)
36	C7Z	b1	620	-	43,43,43	5.40	26 (60%)	58,60,60	2.51	22 (37%)
40	LHG	s1	624	29	44,44,48	0.43	0	47,50,54	1.08	4 (8%)
29	CLA	g1	614	-	53,57,73	1.60	9 (16%)	62,93,113	2.21	18 (29%)
38	3PH	s1	626	-	47,47,47	0.86	3 (6%)	51,52,52	4.37	4 (7%)
49	LUT	r	620	-	42,43,43	2.34	1 (2%)	51,60,60	2.12	14 (27%)
49	LUT	s	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.91	15 (29%)
33	LMG	C1	521	-	51,51,55	1.07	5 (9%)	59,59,63	1.14	2 (3%)
48	CHL	s	601	-	50,54,74	0.99	2 (4%)	56,90,114	1.52	12 (21%)
31	BCR	d	404	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	16 (28%)
51	NEX	r	622	-	38,46,46	3.31	9 (23%)	50,70,70	1.78	11 (22%)
29	CLA	c	505	4	69,73,73	1.40	7 (10%)	83,113,113	1.94	17 (20%)
31	BCR	C	516	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	16 (28%)
29	CLA	G1	604	-	53,57,73	1.57	6 (11%)	62,93,113	2.26	20 (32%)
29	CLA	G1	614	-	53,57,73	1.54	6 (11%)	62,93,113	2.24	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
29	CLA	b1	612	-	69,73,73	1.38	7 (10%)	83,113,113	2.06	18 (21%)
31	BCR	B	619	-	41,41,41	1.85	4 (9%)	56,56,56	3.81	21 (37%)
48	CHL	G	608	-	48,52,74	1.00	2 (4%)	53,87,114	1.46	9 (16%)
40	LHG	Y1	624	-	48,48,48	0.40	0	51,54,54	1.11	4 (7%)
29	CLA	r	610	-	64,68,73	1.42	8 (12%)	77,107,113	2.13	21 (27%)
29	CLA	s	610	-	69,73,73	1.38	8 (11%)	83,113,113	1.94	19 (22%)
29	CLA	R1	604	-	53,57,73	1.57	7 (13%)	62,93,113	2.22	14 (22%)
44	HEM	F1	101	7	50,50,50	1.40	5 (10%)	66,82,82	1.32	9 (13%)
29	CLA	s	611	40	69,73,73	1.36	7 (10%)	83,113,113	1.89	15 (18%)
30	PHO	A1	408	-	58,69,69	2.07	10 (17%)	56,99,99	1.65	8 (14%)
29	CLA	y	604	-	69,73,73	1.36	7 (10%)	83,113,113	1.99	18 (21%)
39	DGA	j1	101	-	28,28,43	1.32	3 (10%)	30,30,45	1.26	2 (6%)
37	DGD	C	518	-	56,56,67	0.98	4 (7%)	70,70,81	0.95	2 (2%)
29	CLA	n1	610	-	69,73,73	1.35	5 (7%)	83,113,113	1.95	18 (21%)
48	CHL	N1	608	-	54,58,74	1.01	2 (3%)	59,94,114	1.43	9 (15%)
38	3PH	S	626	-	47,47,47	0.87	2 (4%)	51,52,52	4.41	4 (7%)
45	RRX	H1	101	-	42,42,42	4.95	24 (57%)	57,58,58	2.34	19 (33%)
29	CLA	y	611	40	69,73,73	1.37	7 (10%)	83,113,113	1.80	15 (18%)
29	CLA	c	511	4	69,73,73	1.38	7 (10%)	83,113,113	1.92	19 (22%)
49	LUT	N1	621	-	42,43,43	2.33	2 (4%)	51,60,60	2.10	13 (25%)
40	LHG	D1	409	-	48,48,48	0.41	0	51,54,54	1.07	3 (5%)
29	CLA	a1	410	1	64,68,73	1.45	8 (12%)	77,107,113	2.08	20 (25%)
31	BCR	c1	516	-	41,41,41	1.91	4 (9%)	56,56,56	4.43	13 (23%)
39	DGA	C	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.50	3 (6%)
29	CLA	y	613	-	69,73,73	1.39	7 (10%)	83,113,113	1.95	17 (20%)
48	CHL	G	607	-	70,74,74	0.90	2 (2%)	80,114,114	1.19	10 (12%)
48	CHL	S1	606	-	48,52,74	1.01	2 (4%)	53,87,114	1.49	9 (16%)
29	CLA	r	612	-	64,68,73	1.43	7 (10%)	77,107,113	1.98	18 (23%)
51	NEX	g	623	-	38,46,46	3.48	11 (28%)	50,70,70	1.86	15 (30%)
29	CLA	B1	603	2	69,73,73	1.40	8 (11%)	83,113,113	2.06	20 (24%)
49	LUT	s	621	-	42,43,43	2.30	1 (2%)	51,60,60	1.98	16 (31%)
48	CHL	N1	609	-	70,74,74	0.82	2 (2%)	80,114,114	1.46	13 (16%)
49	LUT	R1	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	10 (19%)
29	CLA	D	402	-	69,73,73	1.39	8 (11%)	83,113,113	1.88	15 (18%)
38	3PH	S1	626	-	47,47,47	0.87	4 (8%)	51,52,52	4.40	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
51	NEX	R1	622	-	38,46,46	3.31	9 (23%)	50,70,70	1.93	14 (28%)
39	DGA	b1	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.50	3 (6%)
48	CHL	y	601	24	70,74,74	0.90	3 (4%)	80,114,114	1.31	12 (15%)
40	LHG	D	409	-	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
39	DGA	J	101	-	28,28,43	1.31	3 (10%)	30,30,45	1.27	2 (6%)
29	CLA	g	610	-	69,73,73	1.35	7 (10%)	83,113,113	2.04	20 (24%)
48	CHL	s	608	-	65,69,74	0.85	2 (3%)	74,108,114	1.34	13 (17%)
29	CLA	r	609	-	64,68,73	1.43	6 (9%)	77,107,113	1.98	18 (23%)
29	CLA	n	612	-	49,53,73	1.62	6 (12%)	59,89,113	2.01	15 (25%)
29	CLA	Y	608	-	54,58,73	1.55	8 (14%)	65,95,113	2.20	18 (27%)
29	CLA	n	614	-	53,57,73	1.55	7 (13%)	62,93,113	2.27	22 (35%)
29	CLA	C	503	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	19 (22%)
42	BCT	D1	401	27	2,3,3	1.29	0	2,3,3	3.02	2 (100%)
29	CLA	b1	604	-	69,73,73	1.38	7 (10%)	83,113,113	1.99	19 (22%)
29	CLA	c1	508	4	69,73,73	1.38	8 (11%)	83,113,113	1.89	19 (22%)
31	BCR	c	515	-	41,41,41	1.88	5 (12%)	56,56,56	4.18	16 (28%)
29	CLA	c1	504	-	69,73,73	1.38	7 (10%)	83,113,113	2.04	15 (18%)
29	CLA	r	604	-	53,57,73	1.54	7 (13%)	62,93,113	2.28	15 (24%)
50	XAT	y	622	-	39,47,47	0.73	1 (2%)	54,74,74	3.68	19 (35%)
29	CLA	r1	603	22	64,68,73	1.40	7 (10%)	77,107,113	2.04	19 (24%)
48	CHL	n1	605	-	70,74,74	0.88	3 (4%)	80,114,114	1.28	11 (13%)
48	CHL	G	606	-	54,58,74	0.94	2 (3%)	59,94,114	1.48	12 (20%)
38	3PH	b	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.18	3 (5%)
29	CLA	B	614	-	69,73,73	1.36	7 (10%)	83,113,113	1.97	18 (21%)
29	CLA	S	602	-	64,68,73	1.47	7 (10%)	77,107,113	2.07	17 (22%)
33	LMG	C	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.13	2 (3%)
29	CLA	b	613	-	69,73,73	1.37	7 (10%)	83,113,113	1.92	13 (15%)
48	CHL	n	608	-	54,58,74	1.02	3 (5%)	59,94,114	1.21	10 (16%)
48	CHL	n	606	-	70,74,74	0.88	3 (4%)	80,114,114	1.27	13 (16%)
29	CLA	r1	608	-	64,68,73	1.44	7 (10%)	77,107,113	1.99	18 (23%)
29	CLA	b1	603	-	69,73,73	1.37	6 (8%)	83,113,113	1.97	21 (25%)

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
29	CLA	y	612	-	-	19/39/115/115	-
40	LHG	L1	101	-	-	36/53/53/53	-
29	CLA	C1	505	4	-	19/39/115/115	-
29	CLA	S1	602	23	-	19/33/109/115	-
46	GOL	I1	101	-	-	2/4/4/4	-
49	LUT	y	621	-	-	2/29/67/67	0/2/2/2
39	DGA	J1	101	-	-	15/30/30/45	-
49	LUT	y1	620	-	-	3/29/67/67	0/2/2/2
29	CLA	B	617	2	-	19/39/115/115	-
29	CLA	s	617	-	-	8/21/97/115	-
29	CLA	c	507	-	-	17/39/115/115	-
32	SQD	c	526	-	-	20/49/69/69	0/1/1/1
48	CHL	n1	608	-	-	8/22/98/117	-
29	CLA	c	501	4	-	21/39/115/115	-
29	CLA	y	610	24	-	15/39/115/115	-
34	SPH	y	625	-	-	8/21/21/21	-
50	XAT	g1	622	-	1/1/12/26	7/31/93/93	0/4/4/4
55	PTY	y1	627	-	-	11/20/20/53	-
40	LHG	D	408	-	-	23/48/48/53	-
55	PTY	y1	626	-	-	33/53/53/53	-
29	CLA	B	603	2	-	23/39/115/115	-
29	CLA	b	602	-	-	23/39/115/115	-
29	CLA	g	614	-	-	13/20/96/115	-
29	CLA	a	406	-	-	17/39/115/115	-
29	CLA	d1	402	-	-	12/39/115/115	-
29	CLA	C1	508	4	-	13/39/115/115	-
33	LMG	d	411	-	-	19/41/61/70	0/1/1/1
29	CLA	B1	609	-	-	17/39/115/115	-
31	BCR	C	515	-	-	9/29/63/63	0/2/2/2
48	CHL	s	606	-	-	3/15/91/117	-
29	CLA	b1	613	-	-	17/39/115/115	-
49	LUT	R	620	-	1/1/12/27	2/29/67/67	0/2/2/2
29	CLA	N	610	-	-	21/39/115/115	-
29	CLA	c	504	-	-	20/39/115/115	-
29	CLA	A1	406	-	-	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	Y1	611	-	-	18/39/115/115	-
29	CLA	r	603	-	-	19/33/109/115	-
50	XAT	G	622	-	1/1/12/26	2/31/93/93	0/4/4/4
38	3PH	s	626	-	-	22/49/49/49	-
31	BCR	B1	619	-	-	6/29/63/63	0/2/2/2
32	SQD	b1	626	-	-	26/49/69/69	0/1/1/1
51	NEX	S	623	-	-	8/27/83/83	0/3/3/3
53	ERG	r	626	-	5/5/11/15	8/13/71/71	0/4/4/4
48	CHL	G1	601	21	1/1/15/21	13/41/117/117	-
48	CHL	g1	609	-	1/1/15/21	7/41/117/117	-
40	LHG	g1	624	-	-	35/53/53/53	-
29	CLA	r	608	-	-	17/33/109/115	-
29	CLA	B1	610	-	-	23/39/115/115	-
52	LMT	r	625	-	-	13/21/61/61	0/2/2/2
29	CLA	g1	610	-	-	18/39/115/115	-
32	SQD	m	101	-	-	20/37/57/69	0/1/1/1
29	CLA	C1	512	-	-	16/39/115/115	-
48	CHL	G1	605	21	1/1/11/21	5/20/96/117	-
33	LMG	b1	622	-	-	19/39/59/70	0/1/1/1
48	CHL	Y1	609	-	1/1/15/21	8/41/117/117	-
44	HEM	f1	101	7	-	2/14/54/54	-
29	CLA	y1	604	-	-	15/39/115/115	-
29	CLA	s	604	-	-	11/27/103/115	-
47	4RF	K	101	-	-	32/59/59/59	-
40	LHG	d1	408	-	-	30/48/48/53	-
29	CLA	b	616	2	-	17/39/115/115	-
31	BCR	d1	404	-	-	12/29/63/63	0/2/2/2
29	CLA	b1	614	-	-	12/39/115/115	-
29	CLA	C1	501	4	-	15/39/115/115	-
29	CLA	G	602	-	-	17/39/115/115	-
29	CLA	y	608	-	-	10/21/97/115	-
47	4RF	I1	102	-	-	24/59/59/59	-
29	CLA	a	410	1	-	15/33/109/115	-
29	CLA	g1	612	21	-	5/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	N	611	-	-	9/20/96/115	-
48	CHL	y1	607	-	1/1/15/21	4/41/117/117	-
29	CLA	n1	611	-	-	11/20/96/115	-
49	LUT	G1	620	-	-	5/29/67/67	0/2/2/2
37	DGD	C1	518	-	-	12/44/84/95	0/2/2/2
51	NEX	S1	623	-	-	4/27/83/83	0/3/3/3
34	SPH	a1	414	-	-	10/21/21/21	-
29	CLA	N1	603	-	-	17/39/115/115	-
31	BCR	C	517	-	-	13/29/63/63	0/2/2/2
50	XAT	Y1	622	-	1/1/12/26	4/31/93/93	0/4/4/4
29	CLA	g1	602	-	-	19/39/115/115	-
29	CLA	A	407	-	-	9/21/97/115	-
31	BCR	c1	515	-	-	11/29/63/63	0/2/2/2
37	DGD	c	520	-	-	9/48/88/95	0/2/2/2
39	DGA	j	101	-	-	20/30/30/45	-
47	4RF	i1	101	-	-	30/59/59/59	-
49	LUT	S	621	-	-	4/29/67/67	0/2/2/2
48	CHL	y	606	-	1/1/15/21	12/41/117/117	-
29	CLA	R	604	-	-	10/20/96/115	-
29	CLA	s	603	-	-	17/39/115/115	-
29	CLA	S	605	23	-	11/21/97/115	-
48	CHL	g	606	-	-	4/22/98/117	-
50	XAT	n1	622	-	-	4/31/93/93	0/4/4/4
44	HEM	F	101	6,7	-	1/14/54/54	-
48	CHL	G1	609	-	1/1/15/21	10/41/117/117	-
29	CLA	A1	410	-	-	12/33/109/115	-
50	XAT	r1	621	-	1/1/12/26	2/31/93/93	0/4/4/4
37	DGD	C	520	-	-	14/48/88/95	0/2/2/2
41	LMK	c1	527	-	2/2/6/6	14/46/46/60	-
36	C7Z	b	620	-	1/1/12/26	13/29/67/67	0/2/2/2
55	PTY	y	627	-	-	15/20/20/53	-
29	CLA	s1	605	-	-	11/21/97/115	-
51	NEX	s	623	-	-	4/27/83/83	0/3/3/3
52	LMT	R1	625	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	LUT	S1	621	-	-	7/29/67/67	0/2/2/2
47	4RF	i	101	-	-	31/59/59/59	-
48	CHL	N	608	-	-	3/22/98/117	-
31	BCR	b	619	-	-	6/29/63/63	0/2/2/2
29	CLA	c	513	-	-	23/39/115/115	-
29	CLA	B	604	-	-	18/39/115/115	-
29	CLA	R1	609	-	-	16/33/109/115	-
29	CLA	y1	614	-	-	18/39/115/115	-
33	LMG	B	622	-	-	20/39/59/70	0/1/1/1
29	CLA	Y1	610	-	-	12/39/115/115	-
38	3PH	t	101	-	-	27/49/49/49	-
54	LPX	s1	625	-	-	18/31/31/31	-
41	LMK	C	527	-	2/2/6/6	21/46/46/60	-
48	CHL	N	601	20	1/1/15/21	5/41/117/117	-
29	CLA	S1	609	-	-	12/33/109/115	-
29	CLA	C	506	-	-	15/39/115/115	-
29	CLA	C	512	-	-	15/39/115/115	-
40	LHG	N1	624	-	-	34/53/53/53	-
29	CLA	y1	603	-	-	20/39/115/115	-
29	CLA	G1	602	-	-	23/39/115/115	-
30	PHO	a	408	-	-	11/37/103/103	0/5/6/6
37	DGD	c1	519	-	-	24/51/91/95	0/2/2/2
51	NEX	G	623	-	-	5/27/83/83	0/3/3/3
48	CHL	N	605	20	1/1/15/21	10/41/117/117	-
48	CHL	g1	608	-	-	1/15/91/117	-
33	LMG	C1	523	-	-	19/50/70/70	0/1/1/1
43	PL9	d	405	-	-	9/53/73/73	0/1/1/1
29	CLA	s1	602	-	-	13/33/109/115	-
48	CHL	N	607	-	1/1/15/21	8/41/117/117	-
29	CLA	r	602	22	-	14/33/109/115	-
48	CHL	N1	601	-	1/1/15/21	10/41/117/117	-
29	CLA	R	608	-	-	21/33/109/115	-
30	PHO	a1	409	-	-	12/37/103/103	0/5/6/6
29	CLA	g1	604	-	-	9/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	NEX	N1	623	-	-	6/27/83/83	0/3/3/3
36	C7Z	B	620	-	1/1/12/26	9/29/67/67	0/2/2/2
49	LUT	Y	621	-	-	4/29/67/67	0/2/2/2
49	LUT	G	621	-	1/1/12/27	4/29/67/67	0/2/2/2
29	CLA	y	603	-	-	20/39/115/115	-
37	DGD	C	519	-	-	26/51/91/95	0/2/2/2
47	4RF	k1	101	-	-	37/59/59/59	-
39	DGA	c	524	-	-	31/45/45/45	-
29	CLA	c1	505	-	-	18/39/115/115	-
29	CLA	y	602	24	-	17/39/115/115	-
33	LMG	B1	622	-	-	19/39/59/70	0/1/1/1
48	CHL	r1	607	-	-	5/22/98/117	-
29	CLA	c	506	4	-	17/39/115/115	-
30	PHO	A	408	-	-	8/37/103/103	0/5/6/6
29	CLA	c1	506	-	-	16/39/115/115	-
49	LUT	n	620	-	-	3/29/67/67	0/2/2/2
33	LMG	b	622	-	-	17/39/59/70	0/1/1/1
37	DGD	C1	520	-	-	16/48/88/95	0/2/2/2
40	LHG	D	410	-	-	26/43/43/53	-
29	CLA	B	612	2	-	16/39/115/115	-
51	NEX	r1	622	-	-	8/27/83/83	0/3/3/3
29	CLA	N	612	-	-	6/15/91/115	-
38	3PH	B1	624	-	-	27/49/49/49	-
29	CLA	C1	503	4	-	19/39/115/115	-
29	CLA	B1	613	-	-	21/39/115/115	-
48	CHL	Y	607	-	1/1/15/21	7/41/117/117	-
53	ERG	R	626	-	5/5/11/15	6/13/71/71	0/4/4/4
29	CLA	S1	614	-	-	10/27/103/115	-
31	BCR	a1	411	-	-	6/29/63/63	0/2/2/2
29	CLA	b1	605	2	-	20/39/115/115	-
48	CHL	S	606	-	-	2/15/91/117	-
29	CLA	B	615	-	-	15/39/115/115	-
32	SQD	B	621	-	-	20/37/57/69	0/1/1/1
31	BCR	c1	517	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	610	-	-	23/39/115/115	-
31	BCR	C1	515	-	-	12/29/63/63	0/2/2/2
29	CLA	S1	605	-	-	10/21/97/115	-
29	CLA	Y1	614	-	-	14/39/115/115	-
33	LMG	c	521	-	-	14/46/66/70	0/1/1/1
39	DGA	C1	524	-	-	23/45/45/45	-
37	DGD	c1	518	-	-	14/44/84/95	0/2/2/2
29	CLA	y1	611	40	-	20/39/115/115	-
29	CLA	c1	513	-	-	25/39/115/115	-
29	CLA	n	611	-	-	10/20/96/115	-
29	CLA	C	502	-	-	15/39/115/115	-
40	LHG	c1	525	-	-	33/51/51/53	-
48	CHL	g	607	-	1/1/15/21	11/41/117/117	-
48	CHL	y1	606	-	1/1/15/21	6/41/117/117	-
29	CLA	R	610	-	-	16/33/109/115	-
40	LHG	d1	409	-	-	30/53/53/53	-
32	SQD	B	626	-	-	23/49/69/69	0/1/1/1
49	LUT	N	620	-	-	2/29/67/67	0/2/2/2
40	LHG	s	624	29	-	26/49/49/53	-
49	LUT	n1	620	-	-	5/29/67/67	0/2/2/2
48	CHL	g1	605	-	1/1/11/21	7/20/96/117	-
29	CLA	c	509	4	-	16/39/115/115	-
29	CLA	g	612	-	-	8/13/89/115	-
40	LHG	y	624	29	-	30/53/53/53	-
29	CLA	c1	509	4	-	20/39/115/115	-
40	LHG	C	525	-	-	32/51/51/53	-
29	CLA	Y	602	-	-	18/39/115/115	-
29	CLA	s1	614	-	-	17/27/103/115	-
29	CLA	B1	607	-	-	16/39/115/115	-
48	CHL	n1	601	-	1/1/15/21	11/41/117/117	-
29	CLA	b	617	2	-	15/39/115/115	-
29	CLA	b	614	-	-	13/39/115/115	-
29	CLA	G	614	-	-	10/20/96/115	-
54	LPX	S	625	-	-	14/31/31/31	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b1	608	-	-	25/39/115/115	-
50	XAT	r	621	-	2/2/12/26	2/31/93/93	0/4/4/4
31	BCR	b1	618	-	-	11/29/63/63	0/2/2/2
29	CLA	N	614	-	-	7/20/96/115	-
48	CHL	r	607	-	-	4/22/98/117	-
29	CLA	C	508	4	-	12/39/115/115	-
29	CLA	n1	614	-	-	11/20/96/115	-
48	CHL	s	607	-	-	1/14/90/117	-
29	CLA	A1	405	-	-	12/39/115/115	-
29	CLA	c1	503	4	-	20/39/115/115	-
48	CHL	r1	606	-	-	4/15/91/117	-
29	CLA	C	509	4	-	20/39/115/115	-
29	CLA	b	615	-	-	19/39/115/115	-
29	CLA	C1	510	-	-	19/39/115/115	-
29	CLA	N1	612	-	-	6/15/91/115	-
40	LHG	d	409	-	-	26/53/53/53	-
33	LMG	A	413	-	-	15/43/63/70	0/1/1/1
48	CHL	n	605	20	1/1/15/21	8/41/117/117	-
54	LPX	S1	625	-	-	15/31/31/31	-
29	CLA	R1	610	-	-	19/33/109/115	-
48	CHL	Y	606	-	1/1/15/21	7/41/117/117	-
49	LUT	s1	620	-	-	6/29/67/67	0/2/2/2
39	DGA	B1	625	-	-	26/45/45/45	-
29	CLA	g	611	-	-	17/39/115/115	-
30	PHO	a	409	-	-	11/37/103/103	0/5/6/6
49	LUT	G1	621	-	-	3/29/67/67	0/2/2/2
48	CHL	S	607	-	-	1/14/90/117	-
29	CLA	S1	613	-	-	11/27/103/115	-
49	LUT	y1	621	-	-	4/29/67/67	0/2/2/2
29	CLA	N1	610	-	-	21/39/115/115	-
33	LMG	c1	523	-	-	18/50/70/70	0/1/1/1
29	CLA	a1	407	-	-	7/20/96/115	-
43	PL9	d1	405	-	-	20/53/73/73	0/1/1/1
50	XAT	n	622	-	1/1/12/26	4/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G1	603	-	-	25/39/115/115	-
52	LMT	R	625	-	-	9/21/61/61	0/2/2/2
31	BCR	c	517	-	-	10/29/63/63	0/2/2/2
52	LMT	r1	625	-	-	10/21/61/61	0/2/2/2
29	CLA	C1	504	-	-	20/39/115/115	-
29	CLA	a1	405	-	-	17/39/115/115	-
44	HEM	f	101	6,7	-	1/14/54/54	-
48	CHL	N1	606	-	1/1/15/21	12/41/117/117	-
48	CHL	g1	601	-	1/1/15/21	12/41/117/117	-
53	ERG	R1	626	-	5/5/11/15	9/13/71/71	0/4/4/4
29	CLA	B1	616	-	-	18/39/115/115	-
29	CLA	C1	507	-	-	16/39/115/115	-
29	CLA	Y1	608	-	-	9/21/97/115	-
29	CLA	s	602	-	-	18/33/109/115	-
29	CLA	R1	612	-	-	21/33/109/115	-
29	CLA	g1	611	-	-	20/39/115/115	-
29	CLA	s1	611	40	-	22/39/115/115	-
32	SQD	M	101	-	-	24/37/57/69	0/1/1/1
48	CHL	g	609	-	1/1/15/21	10/41/117/117	-
29	CLA	N	602	-	-	15/39/115/115	-
33	LMG	w	201	-	-	17/34/54/70	0/1/1/1
29	CLA	n1	602	20	-	19/39/115/115	-
54	LPX	s	625	-	-	15/31/31/31	-
29	CLA	C	501	4	-	20/39/115/115	-
29	CLA	G1	610	-	-	17/39/115/115	-
31	BCR	c1	514	-	-	12/29/63/63	0/2/2/2
48	CHL	n1	607	-	1/1/15/21	7/41/117/117	-
29	CLA	s	613	-	-	11/27/103/115	-
49	LUT	r1	620	-	-	4/29/67/67	0/2/2/2
50	XAT	R1	621	-	-	4/31/93/93	0/4/4/4
29	CLA	Y	604	-	-	17/39/115/115	-
48	CHL	y1	609	-	1/1/15/21	8/41/117/117	-
48	CHL	R1	607	-	-	4/22/98/117	-
31	BCR	C1	517	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LMK	C1	527	-	2/2/6/6	19/46/46/60	-
47	4RF	I	102	-	-	30/59/59/59	-
45	RRX	h	101	-	1/1/11/25	4/29/65/65	0/2/2/2
48	CHL	y	607	-	1/1/15/21	9/41/117/117	-
29	CLA	y1	610	24	-	13/39/115/115	-
32	SQD	b	621	-	-	19/37/57/69	0/1/1/1
29	CLA	b1	606	-	-	13/39/115/115	-
29	CLA	S	617	23	-	9/21/97/115	-
51	NEX	g1	623	-	1/1/12/25	7/27/83/83	0/3/3/3
40	LHG	C1	525	-	-	30/51/51/53	-
34	SPH	A1	414	-	-	16/21/21/21	-
29	CLA	C	511	-	-	14/39/115/115	-
29	CLA	S1	611	40	-	18/39/115/115	-
48	CHL	R	607	-	-	7/22/98/117	-
48	CHL	g	605	21	1/1/11/21	5/20/96/117	-
29	CLA	b	611	-	-	7/39/115/115	-
40	LHG	D1	408	-	-	26/48/48/53	-
29	CLA	B	613	2	-	18/39/115/115	-
40	LHG	S	624	29	-	27/49/49/53	-
29	CLA	N	613	-	-	19/39/115/115	-
36	C7Z	B1	620	-	1/1/12/26	7/29/67/67	0/2/2/2
51	NEX	G1	623	-	-	12/27/83/83	0/3/3/3
29	CLA	n1	612	-	-	7/15/91/115	-
29	CLA	b	605	-	-	21/39/115/115	-
32	SQD	a1	412	-	-	19/46/66/69	0/1/1/1
55	PTY	y	626	-	-	27/53/53/53	-
49	LUT	Y	620	-	-	5/29/67/67	0/2/2/2
49	LUT	G	620	-	-	3/29/67/67	0/2/2/2
29	CLA	Y	603	-	-	19/39/115/115	-
29	CLA	c1	501	-	-	19/39/115/115	-
49	LUT	n1	621	-	1/1/12/27	5/29/67/67	0/2/2/2
29	CLA	y1	612	-	-	18/39/115/115	-
40	LHG	l	101	-	-	38/53/53/53	-
49	LUT	g	620	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SPH	Y	625	-	-	10/21/21/21	-
29	CLA	G1	611	-	-	21/39/115/115	-
40	LHG	S1	624	29	-	32/49/49/53	-
48	CHL	y1	601	24	1/1/15/21	5/41/117/117	-
45	RRX	H	101	-	1/1/11/25	7/29/65/65	0/2/2/2
29	CLA	c	508	4	-	12/39/115/115	-
48	CHL	S1	601	23	-	3/17/93/117	-
29	CLA	c	503	4	-	20/39/115/115	-
29	CLA	b1	615	-	-	17/39/115/115	-
48	CHL	G	601	21	1/1/15/21	11/41/117/117	-
48	CHL	y	605	24	-	3/17/93/117	-
49	LUT	g1	621	-	-	6/29/67/67	0/2/2/2
29	CLA	C	505	4	-	18/39/115/115	-
31	BCR	C	514	-	-	17/29/63/63	0/2/2/2
48	CHL	Y1	601	-	1/1/15/21	7/41/117/117	-
31	BCR	b	618	-	-	9/29/63/63	0/2/2/2
29	CLA	b	604	-	-	16/39/115/115	-
29	CLA	B	602	-	-	20/39/115/115	-
39	DGA	c1	524	-	-	28/45/45/45	-
29	CLA	C1	509	-	-	10/39/115/115	-
29	CLA	b1	609	-	-	18/39/115/115	-
32	SQD	B1	626	-	-	17/49/69/69	0/1/1/1
49	LUT	g1	620	-	-	6/29/67/67	0/2/2/2
29	CLA	N	604	-	-	21/39/115/115	-
29	CLA	R	612	-	-	12/33/109/115	-
29	CLA	n1	604	-	-	15/39/115/115	-
29	CLA	B1	606	-	-	20/39/115/115	-
29	CLA	s	612	-	-	5/15/91/115	-
29	CLA	B	608	-	-	27/39/115/115	-
29	CLA	A	410	1	-	14/33/109/115	-
29	CLA	Y	613	24	-	24/39/115/115	-
29	CLA	G	613	-	-	21/39/115/115	-
29	CLA	n	610	-	-	20/39/115/115	-
29	CLA	C1	502	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	D1	404	-	-	14/29/63/63	0/2/2/2
29	CLA	N1	611	-	-	12/20/96/115	-
29	CLA	N1	602	-	-	17/39/115/115	-
29	CLA	B1	614	-	-	16/39/115/115	-
48	CHL	G1	608	-	-	1/15/91/117	-
55	PTY	Y	626	-	-	31/53/53/53	-
33	LMG	w1	201	-	-	17/34/54/70	0/1/1/1
29	CLA	N1	613	-	-	14/39/115/115	-
48	CHL	Y	609	-	1/1/15/21	6/41/117/117	-
40	LHG	G	624	29	-	33/53/53/53	-
30	PHO	A1	409	-	-	11/37/103/103	0/5/6/6
43	PL9	D	405	-	-	9/53/73/73	0/1/1/1
48	CHL	Y	601	24	1/1/15/21	7/41/117/117	-
47	4RF	k	101	-	-	31/59/59/59	-
29	CLA	S1	612	-	-	6/15/91/115	-
29	CLA	g	603	-	-	23/39/115/115	-
29	CLA	g	604	-	-	9/20/96/115	-
29	CLA	Y1	612	-	-	20/39/115/115	-
48	CHL	Y	605	24	-	3/17/93/117	-
48	CHL	G	605	21	1/1/11/21	6/20/96/117	-
50	XAT	G1	622	-	1/1/12/26	2/31/93/93	0/4/4/4
29	CLA	d	402	-	-	13/39/115/115	-
31	BCR	D	404	-	-	13/29/63/63	0/2/2/2
29	CLA	R1	608	-	-	11/33/109/115	-
51	NEX	Y	623	-	-	7/27/83/83	0/3/3/3
29	CLA	G1	613	-	-	15/39/115/115	-
34	SPH	a	414	-	-	11/21/21/21	-
40	LHG	c	525	-	-	30/51/51/53	-
29	CLA	b	612	-	-	16/39/115/115	-
29	CLA	S1	617	23	-	7/21/97/115	-
48	CHL	G1	607	-	1/1/15/21	11/41/117/117	-
48	CHL	n	607	-	1/1/15/21	8/41/117/117	-
33	LMG	W1	201	-	-	16/34/54/70	0/1/1/1
29	CLA	b	606	-	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	S	609	-	-	12/33/109/115	-
33	LMG	h	102	-	-	11/43/63/70	0/1/1/1
34	SPH	A	414	-	-	12/21/21/21	-
38	3PH	b1	624	-	-	24/49/49/49	-
29	CLA	c1	511	-	-	20/39/115/115	-
29	CLA	s1	603	-	-	17/39/115/115	-
29	CLA	S	614	-	-	8/27/103/115	-
48	CHL	n1	606	-	1/1/15/21	8/41/117/117	-
29	CLA	B1	602	-	-	25/39/115/115	-
48	CHL	n	609	-	1/1/15/21	5/41/117/117	-
43	PL9	D1	405	-	-	18/53/73/73	0/1/1/1
48	CHL	R1	606	-	-	4/15/91/117	-
29	CLA	S	604	-	-	11/27/103/115	-
29	CLA	b1	617	2	-	16/39/115/115	-
29	CLA	y1	602	-	-	17/39/115/115	-
38	3PH	T1	101	-	-	29/49/49/49	-
48	CHL	g1	607	-	1/1/15/21	8/41/117/117	-
29	CLA	n1	603	-	-	14/39/115/115	-
29	CLA	Y	612	-	-	15/39/115/115	-
29	CLA	G	612	-	-	7/13/89/115	-
29	CLA	B1	617	-	-	18/39/115/115	-
32	SQD	b	626	-	-	17/49/69/69	0/1/1/1
40	LHG	d1	410	-	-	33/43/43/53	-
29	CLA	S	613	-	-	12/27/103/115	-
29	CLA	D1	402	-	-	13/39/115/115	-
40	LHG	Y	624	-	-	29/53/53/53	-
55	PTY	Y1	626	-	-	26/53/53/53	-
34	SPH	y1	625	-	-	12/21/21/21	-
49	LUT	N	621	-	-	4/29/67/67	0/2/2/2
48	CHL	Y1	605	-	-	3/17/93/117	-
49	LUT	n	621	-	-	2/29/67/67	0/2/2/2
29	CLA	R1	602	-	-	14/33/109/115	-
31	BCR	A1	411	-	-	9/29/63/63	0/2/2/2
51	NEX	Y1	623	-	-	8/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	c	510	4	-	16/39/115/115	-
29	CLA	R	603	-	-	18/33/109/115	-
29	CLA	y1	608	-	-	11/21/97/115	-
48	CHL	G1	606	-	-	4/22/98/117	-
32	SQD	B1	621	-	-	11/37/57/69	0/1/1/1
29	CLA	B	605	2	-	21/39/115/115	-
29	CLA	b	608	-	-	28/39/115/115	-
29	CLA	b1	611	-	-	10/39/115/115	-
48	CHL	G	609	21	1/1/15/21	10/41/117/117	-
40	LHG	y1	624	29	-	25/53/53/53	-
29	CLA	s1	610	-	-	20/39/115/115	-
29	CLA	C	504	-	-	18/39/115/115	-
33	LMG	D1	411	-	-	10/41/61/70	0/1/1/1
29	CLA	S	603	-	-	19/39/115/115	-
32	SQD	A	412	-	-	24/46/66/69	0/1/1/1
29	CLA	R	602	-	-	12/33/109/115	-
48	CHL	Y1	607	-	1/1/15/21	12/41/117/117	-
29	CLA	y1	613	-	-	20/39/115/115	-
29	CLA	b1	607	-	-	14/39/115/115	-
29	CLA	C	507	-	-	14/39/115/115	-
29	CLA	b	610	-	-	15/39/115/115	-
29	CLA	r1	602	-	-	13/33/109/115	-
32	SQD	C	526	-	-	23/49/69/69	0/1/1/1
33	LMG	c	523	-	-	21/50/70/70	0/1/1/1
40	LHG	L	101	-	-	38/53/53/53	-
32	SQD	b1	621	-	-	17/37/57/69	0/1/1/1
33	LMG	A1	413	-	-	18/43/63/70	0/1/1/1
40	LHG	d	410	-	-	20/43/43/53	-
29	CLA	C	513	-	-	22/39/115/115	-
37	DGD	B	623	-	-	15/32/72/95	0/2/2/2
29	CLA	C1	511	-	-	12/39/115/115	-
29	CLA	s1	617	-	-	11/21/97/115	-
37	DGD	b	623	-	-	13/32/72/95	0/2/2/2
49	LUT	g	621	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	c1	502	-	-	16/39/115/115	-
29	CLA	B	611	-	-	13/39/115/115	-
29	CLA	g1	613	-	-	24/39/115/115	-
31	BCR	C1	516	-	-	15/29/63/63	0/2/2/2
48	CHL	s1	601	23	-	4/17/93/117	-
29	CLA	Y	614	-	-	19/39/115/115	-
48	CHL	s1	607	-	-	0/14/90/117	-
51	NEX	s1	623	-	-	3/27/83/83	0/3/3/3
31	BCR	B1	618	-	-	15/29/63/63	0/2/2/2
29	CLA	B1	604	-	-	14/39/115/115	-
39	DGA	B	625	-	-	23/45/45/45	-
29	CLA	A	405	-	-	14/39/115/115	-
29	CLA	R1	603	-	-	19/33/109/115	-
51	NEX	y1	623	-	-	10/27/83/83	0/3/3/3
29	CLA	c1	507	-	-	16/39/115/115	-
29	CLA	Y1	602	-	-	20/39/115/115	-
29	CLA	b1	602	-	-	22/39/115/115	-
40	LHG	n1	624	-	-	29/53/53/53	-
48	CHL	y	609	-	1/1/15/21	6/41/117/117	-
29	CLA	B1	608	-	-	28/39/115/115	-
33	LMG	a	413	-	-	20/43/63/70	0/1/1/1
49	LUT	N1	620	-	-	8/29/67/67	0/2/2/2
32	SQD	C1	526	-	-	25/49/69/69	0/1/1/1
51	NEX	n1	623	-	-	5/27/83/83	0/3/3/3
48	CHL	g	601	21	1/1/15/21	16/41/117/117	-
29	CLA	B1	605	-	-	17/39/115/115	-
49	LUT	s1	621	-	-	5/29/67/67	0/2/2/2
31	BCR	C1	514	-	-	12/29/63/63	0/2/2/2
50	XAT	y1	622	-	-	7/31/93/93	0/4/4/4
29	CLA	n	604	-	-	15/39/115/115	-
29	CLA	S1	610	-	-	22/39/115/115	-
29	CLA	A	406	-	-	14/39/115/115	-
29	CLA	b1	616	2	-	9/39/115/115	-
29	CLA	a1	406	-	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	r1	609	-	-	19/33/109/115	-
32	SQD	M1	101	-	-	17/37/57/69	0/1/1/1
29	CLA	d1	403	-	-	12/39/115/115	-
33	LMG	W	201	-	-	14/34/54/70	0/1/1/1
29	CLA	G	604	-	-	8/20/96/115	-
29	CLA	a	405	-	-	15/39/115/115	-
29	CLA	N1	614	-	-	7/20/96/115	-
29	CLA	G1	612	-	-	8/13/89/115	-
29	CLA	Y1	613	-	-	21/39/115/115	-
37	DGD	C1	519	-	-	22/51/91/95	0/2/2/2
29	CLA	G	611	40	-	19/39/115/115	-
40	LHG	G1	624	-	-	29/53/53/53	-
47	4RF	K1	101	-	-	32/59/59/59	-
29	CLA	r1	604	-	-	10/20/96/115	-
29	CLA	s1	612	-	-	8/15/91/115	-
48	CHL	N	606	-	1/1/15/21	10/41/117/117	-
46	GOL	I	101	-	-	2/4/4/4	-
38	3PH	T	101	-	-	26/49/49/49	-
33	LMG	d1	411	-	-	19/41/61/70	0/1/1/1
29	CLA	s	614	-	-	4/27/103/115	-
29	CLA	S	610	-	-	22/39/115/115	-
29	CLA	b	603	2	-	22/39/115/115	-
31	BCR	a	411	-	-	11/29/63/63	0/2/2/2
29	CLA	S	611	40	-	18/39/115/115	-
34	SPH	Y1	625	-	-	9/21/21/21	-
29	CLA	s	605	-	-	13/21/97/115	-
29	CLA	S1	603	-	-	14/39/115/115	-
29	CLA	n	602	-	-	16/39/115/115	-
48	CHL	g	608	-	-	3/15/91/117	-
29	CLA	c	502	4	-	14/39/115/115	-
29	CLA	C1	506	-	-	21/39/115/115	-
48	CHL	g1	606	-	-	3/22/98/117	-
29	CLA	b1	610	-	-	19/39/115/115	-
29	CLA	S1	604	-	-	12/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	d	403	-	-	16/39/115/115	-
51	NEX	y	623	-	-	6/27/83/83	0/3/3/3
33	LMG	H1	102	-	-	17/43/63/70	0/1/1/1
29	CLA	B	607	2	-	18/39/115/115	-
37	DGD	c	518	-	-	9/44/84/95	0/2/2/2
53	ERG	r1	626	-	5/5/11/15	8/13/71/71	0/4/4/4
45	RRX	h1	101	-	1/1/11/25	10/29/65/65	0/2/2/2
29	CLA	Y1	604	-	-	15/39/115/115	-
48	CHL	S	601	23	-	3/17/93/117	-
48	CHL	N1	605	20	1/1/15/21	9/41/117/117	-
50	XAT	g	622	-	2/2/12/26	3/31/93/93	0/4/4/4
33	LMG	a1	413	-	-	20/43/63/70	0/1/1/1
48	CHL	N1	607	-	1/1/15/21	11/41/117/117	-
29	CLA	g	613	-	-	21/39/115/115	-
49	LUT	y	620	-	-	4/29/67/67	0/2/2/2
29	CLA	B	609	2	-	12/39/115/115	-
29	CLA	C1	513	4	-	16/39/115/115	-
48	CHL	S	608	-	1/1/14/21	7/35/111/117	-
33	LMG	c1	521	-	-	14/46/66/70	0/1/1/1
29	CLA	n	613	-	-	18/39/115/115	-
40	LHG	d	408	-	-	26/48/48/53	-
29	CLA	s	609	-	-	18/33/109/115	-
41	LMK	c	527	-	2/2/6/6	13/46/46/60	-
40	LHG	D1	410	-	-	25/43/43/53	-
30	PHO	A	409	-	-	14/37/103/103	0/5/6/6
29	CLA	B	606	2	-	20/39/115/115	-
29	CLA	s1	604	-	-	8/27/103/115	-
29	CLA	G	603	21	-	16/39/115/115	-
30	PHO	a1	408	-	-	17/37/103/103	0/5/6/6
29	CLA	c	512	-	-	18/39/115/115	-
48	CHL	s1	608	-	1/1/14/21	5/35/111/117	-
31	BCR	A	411	-	-	12/29/63/63	0/2/2/2
48	CHL	s1	606	-	-	0/15/91/117	-
29	CLA	s1	609	-	-	19/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	b1	619	-	-	9/29/63/63	0/2/2/2
29	CLA	N	603	-	-	19/39/115/115	-
55	PTY	Y	627	-	-	15/20/20/53	-
29	CLA	n	603	-	-	25/39/115/115	-
33	LMG	C	521	-	-	16/46/66/70	0/1/1/1
38	3PH	t1	101	-	-	30/49/49/49	-
29	CLA	y	614	-	-	17/39/115/115	-
51	NEX	R	622	-	-	8/27/83/83	0/3/3/3
48	CHL	S1	608	-	1/1/14/21	10/35/111/117	-
39	DGA	b	625	-	-	26/45/45/45	-
29	CLA	s1	613	-	-	13/27/103/115	-
29	CLA	Y	611	-	-	12/39/115/115	-
29	CLA	c1	510	-	-	14/39/115/115	-
29	CLA	B1	611	-	-	13/39/115/115	-
29	CLA	r1	612	-	-	16/33/109/115	-
29	CLA	a	407	-	-	9/20/96/115	-
48	CHL	n	601	20	1/1/15/21	4/41/117/117	-
29	CLA	b	607	-	-	18/39/115/115	-
32	SQD	c1	526	-	-	22/49/69/69	0/1/1/1
48	CHL	y1	605	24	-	4/17/93/117	-
29	CLA	S	612	-	-	6/15/91/115	-
49	LUT	S	620	-	-	3/29/67/67	0/2/2/2
29	CLA	Y	610	-	-	12/39/115/115	-
29	CLA	G	610	21	-	16/39/115/115	-
51	NEX	n	623	-	-	5/27/83/83	1/3/3/3
37	DGD	b1	623	-	-	14/32/72/95	0/2/2/2
49	LUT	Y1	620	-	-	8/29/67/67	0/2/2/2
29	CLA	g1	603	-	-	18/39/115/115	-
29	CLA	B	616	-	-	7/39/115/115	-
29	CLA	C	510	4	-	13/39/115/115	-
48	CHL	Y1	606	-	1/1/15/21	7/41/117/117	-
29	CLA	b	609	2	-	13/39/115/115	-
29	CLA	R	609	-	-	15/33/109/115	-
29	CLA	B1	612	-	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	CHL	S1	607	-	-	2/14/90/117	-
33	LMG	h1	102	-	-	22/43/63/70	0/1/1/1
29	CLA	A1	407	-	-	9/21/97/115	-
31	BCR	c	514	-	-	14/29/63/63	0/2/2/2
29	CLA	Y1	603	-	-	16/39/115/115	-
50	XAT	R	621	-	-	2/31/93/93	0/4/4/4
37	DGD	c1	520	-	-	11/48/88/95	0/2/2/2
29	CLA	B1	615	-	-	14/39/115/115	-
29	CLA	N1	604	-	-	20/39/115/115	-
32	SQD	A1	412	-	-	15/46/66/69	0/1/1/1
50	XAT	N1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
33	LMG	H	102	-	-	14/43/63/70	0/1/1/1
55	PTY	Y1	627	-	-	12/20/20/53	-
29	CLA	r1	610	-	-	15/33/109/115	-
40	LHG	g	624	-	-	27/53/53/53	-
49	LUT	S1	620	-	-	4/29/67/67	0/2/2/2
49	LUT	Y1	621	-	-	6/29/67/67	0/2/2/2
48	CHL	N	609	-	1/1/15/21	11/41/117/117	-
29	CLA	D	403	-	-	18/39/115/115	-
29	CLA	g	602	-	-	22/39/115/115	-
33	LMG	D	411	-	-	11/41/61/70	0/1/1/1
40	LHG	N	624	-	-	31/53/53/53	-
48	CHL	n1	609	-	1/1/15/21	5/41/117/117	-
40	LHG	n	624	-	-	35/53/53/53	-
48	CHL	r	606	-	-	3/15/91/117	-
48	CHL	R	606	-	-	1/15/91/117	-
29	CLA	c1	512	-	-	17/39/115/115	-
37	DGD	B1	623	-	-	11/32/72/95	0/2/2/2
38	3PH	B	624	-	-	34/49/49/49	-
32	SQD	a	412	-	-	14/46/66/69	0/1/1/1
32	SQD	m1	101	-	-	22/37/57/69	0/1/1/1
50	XAT	Y	622	-	-	7/31/93/93	0/4/4/4
31	BCR	c	516	-	-	15/29/63/63	0/2/2/2
31	BCR	B	618	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	NEX	N	623	-	-	4/27/83/83	1/3/3/3
29	CLA	n1	613	-	-	22/39/115/115	-
37	DGD	c	519	-	-	23/51/91/95	0/2/2/2
50	XAT	N	622	-	1/1/12/26	2/31/93/93	0/4/4/4
36	C7Z	b1	620	-	1/1/12/26	11/29/67/67	0/2/2/2
29	CLA	D1	403	-	-	17/39/115/115	-
40	LHG	s1	624	29	-	27/49/49/53	-
29	CLA	g1	614	-	-	13/20/96/115	-
38	3PH	s1	626	-	-	27/49/49/49	-
49	LUT	r	620	-	-	6/29/67/67	0/2/2/2
49	LUT	s	620	-	-	1/29/67/67	0/2/2/2
33	LMG	C1	521	-	-	12/46/66/70	0/1/1/1
48	CHL	s	601	-	-	4/17/93/117	-
31	BCR	d	404	-	-	13/29/63/63	0/2/2/2
51	NEX	r	622	-	-	9/27/83/83	0/3/3/3
29	CLA	c	505	4	-	21/39/115/115	-
31	BCR	C	516	-	-	13/29/63/63	0/2/2/2
29	CLA	G1	604	-	-	10/20/96/115	-
29	CLA	G1	614	-	-	8/20/96/115	-
29	CLA	b1	612	-	-	18/39/115/115	-
31	BCR	B	619	-	-	8/29/63/63	0/2/2/2
48	CHL	G	608	-	-	1/15/91/117	-
40	LHG	Y1	624	-	-	18/53/53/53	-
29	CLA	r	610	-	-	13/33/109/115	-
29	CLA	s	610	-	-	20/39/115/115	-
29	CLA	R1	604	-	-	12/20/96/115	-
44	HEM	F1	101	7	-	1/14/54/54	-
29	CLA	s	611	40	-	17/39/115/115	-
30	PHO	A1	408	-	-	6/37/103/103	0/5/6/6
29	CLA	y	604	-	-	15/39/115/115	-
39	DGA	j1	101	-	-	20/30/30/45	-
37	DGD	C	518	-	-	18/44/84/95	0/2/2/2
29	CLA	n1	610	-	-	22/39/115/115	-
48	CHL	N1	608	-	-	6/22/98/117	-
45	RRX	H1	101	-	1/1/11/25	9/29/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	3PH	S	626	-	-	24/49/49/49	-
29	CLA	y	611	40	-	16/39/115/115	-
29	CLA	c	511	4	-	9/39/115/115	-
49	LUT	N1	621	-	-	4/29/67/67	0/2/2/2
40	LHG	D1	409	-	-	31/53/53/53	-
29	CLA	a1	410	1	-	13/33/109/115	-
31	BCR	c1	516	-	-	12/29/63/63	0/2/2/2
39	DGA	C	524	-	-	18/45/45/45	-
29	CLA	y	613	-	-	24/39/115/115	-
48	CHL	G	607	-	1/1/15/21	11/41/117/117	-
48	CHL	S1	606	-	-	2/15/91/117	-
29	CLA	r	612	-	-	16/33/109/115	-
51	NEX	g	623	-	1/1/12/25	9/27/83/83	0/3/3/3
29	CLA	B1	603	2	-	21/39/115/115	-
49	LUT	s	621	-	-	3/29/67/67	0/2/2/2
48	CHL	N1	609	-	1/1/15/21	10/41/117/117	-
49	LUT	R1	620	-	-	9/29/67/67	0/2/2/2
29	CLA	D	402	-	-	19/39/115/115	-
38	3PH	S1	626	-	-	30/49/49/49	-
51	NEX	R1	622	-	-	14/27/83/83	0/3/3/3
39	DGA	b1	625	-	-	22/45/45/45	-
48	CHL	y	601	24	1/1/15/21	9/41/117/117	-
40	LHG	D	409	-	-	25/53/53/53	-
39	DGA	J	101	-	-	12/30/30/45	-
48	CHL	s	608	-	1/1/14/21	5/35/111/117	-
29	CLA	g	610	-	-	21/39/115/115	-
29	CLA	r	609	-	-	12/33/109/115	-
29	CLA	n	612	-	-	7/15/91/115	-
29	CLA	Y	608	-	-	9/21/97/115	-
29	CLA	n	614	-	-	6/20/96/115	-
29	CLA	C	503	-	-	20/39/115/115	-
29	CLA	b1	604	-	-	20/39/115/115	-
29	CLA	c1	508	4	-	12/39/115/115	-
31	BCR	c	515	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	c1	504	-	-	21/39/115/115	-
29	CLA	r	604	-	-	11/20/96/115	-
50	XAT	y	622	-	-	8/31/93/93	0/4/4/4
48	CHL	n1	605	-	1/1/15/21	7/41/117/117	-
29	CLA	r1	603	22	-	20/33/109/115	-
48	CHL	G	606	-	-	5/22/98/117	-
38	3PH	b	624	-	-	23/49/49/49	-
29	CLA	B	614	-	-	14/39/115/115	-
29	CLA	S	602	-	-	16/33/109/115	-
33	LMG	C	523	-	-	21/50/70/70	0/1/1/1
29	CLA	b	613	-	-	21/39/115/115	-
48	CHL	n	608	-	-	6/22/98/117	-
48	CHL	n	606	-	1/1/15/21	7/41/117/117	-
29	CLA	r1	608	-	-	16/33/109/115	-
29	CLA	b1	603	-	-	21/39/115/115	-

All (3547) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	R	626	ERG	C1-C10	-23.16	1.10	1.54
53	r	626	ERG	C1-C10	-22.96	1.10	1.54
53	R1	626	ERG	C1-C10	-22.89	1.10	1.54
53	r1	626	ERG	C1-C10	-22.73	1.11	1.54
53	r	626	ERG	C10-C9	-20.15	1.28	1.55
53	r1	626	ERG	C10-C9	-20.12	1.28	1.55
53	R	626	ERG	C10-C9	-19.91	1.29	1.55
53	R1	626	ERG	C10-C9	-19.17	1.30	1.55
36	b1	620	C7Z	C25-C26	16.02	1.62	1.34
36	B1	620	C7Z	C25-C26	15.63	1.61	1.34
45	H1	101	RRX	C26-C25	15.53	1.61	1.34
45	H	101	RRX	C26-C25	15.52	1.61	1.34
45	h	101	RRX	C26-C25	15.42	1.61	1.34
45	h1	101	RRX	C26-C25	15.41	1.61	1.34
36	B	620	C7Z	C25-C26	15.22	1.60	1.34
36	b	620	C7Z	C5-C6	15.22	1.60	1.34
36	b	620	C7Z	C25-C26	15.11	1.60	1.34
45	H1	101	RRX	C5-C6	14.93	1.60	1.34
36	B1	620	C7Z	C5-C6	14.92	1.60	1.34
36	b1	620	C7Z	C5-C6	14.80	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	h1	101	RRX	C5-C6	14.61	1.59	1.34
49	s1	620	LUT	C24-C25	14.59	1.51	1.33
36	B	620	C7Z	C5-C6	14.59	1.59	1.34
49	N	621	LUT	C24-C25	14.58	1.51	1.33
49	n1	620	LUT	C24-C25	14.58	1.51	1.33
49	Y1	620	LUT	C24-C25	14.57	1.51	1.33
49	y1	621	LUT	C24-C25	14.55	1.51	1.33
49	N1	620	LUT	C24-C25	14.53	1.51	1.33
45	H	101	RRX	C5-C6	14.51	1.59	1.34
49	g1	621	LUT	C24-C25	14.50	1.51	1.33
49	g	621	LUT	C24-C25	14.44	1.51	1.33
49	n	621	LUT	C24-C25	14.43	1.51	1.33
49	s	620	LUT	C24-C25	14.43	1.51	1.33
49	S1	621	LUT	C24-C25	14.39	1.51	1.33
49	y1	620	LUT	C24-C25	14.36	1.51	1.33
49	r	620	LUT	C24-C25	14.36	1.51	1.33
49	G	621	LUT	C24-C25	14.35	1.51	1.33
49	R1	620	LUT	C24-C25	14.34	1.51	1.33
49	n1	621	LUT	C24-C25	14.29	1.50	1.33
49	N	620	LUT	C24-C25	14.26	1.50	1.33
49	y	621	LUT	C24-C25	14.24	1.50	1.33
49	r1	620	LUT	C24-C25	14.24	1.50	1.33
49	n	620	LUT	C24-C25	14.24	1.50	1.33
49	g1	620	LUT	C24-C25	14.22	1.50	1.33
49	S1	620	LUT	C24-C25	14.19	1.50	1.33
49	R	620	LUT	C24-C25	14.19	1.50	1.33
49	Y1	621	LUT	C24-C25	14.19	1.50	1.33
49	g	620	LUT	C24-C25	14.13	1.50	1.33
49	N1	621	LUT	C24-C25	14.10	1.50	1.33
49	y	620	LUT	C24-C25	14.09	1.50	1.33
49	Y	621	LUT	C24-C25	14.09	1.50	1.33
49	Y	620	LUT	C24-C25	14.00	1.50	1.33
45	h	101	RRX	C5-C6	13.99	1.58	1.34
53	R	626	ERG	C10-C5	-13.96	1.25	1.52
53	R1	626	ERG	C10-C5	-13.92	1.25	1.52
53	r	626	ERG	C4-C3	-13.88	1.27	1.52
49	G1	620	LUT	C24-C25	13.85	1.50	1.33
49	s	621	LUT	C24-C25	13.84	1.50	1.33
53	r1	626	ERG	C4-C3	-13.82	1.28	1.52
49	s1	621	LUT	C24-C25	13.78	1.50	1.33
53	r1	626	ERG	C10-C5	-13.77	1.25	1.52
49	S	620	LUT	C24-C25	13.73	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	G	620	LUT	C24-C25	13.69	1.50	1.33
53	r	626	ERG	C10-C5	-13.64	1.25	1.52
53	R	626	ERG	C4-C3	-13.62	1.28	1.52
49	G1	621	LUT	C24-C25	13.62	1.50	1.33
49	S	621	LUT	C24-C25	13.59	1.50	1.33
53	R1	626	ERG	C4-C3	-13.30	1.28	1.52
36	B1	620	C7Z	C24-C23	12.05	1.73	1.52
36	b1	620	C7Z	C24-C23	12.04	1.73	1.52
53	r	626	ERG	C2-C3	-11.64	1.23	1.51
36	B	620	C7Z	C24-C23	11.64	1.72	1.52
53	r1	626	ERG	C2-C3	-11.30	1.24	1.51
36	b	620	C7Z	C24-C23	11.27	1.71	1.52
36	b	620	C7Z	C2-C3	-11.04	1.36	1.52
53	R	626	ERG	C2-C3	-10.99	1.25	1.51
53	R1	626	ERG	C2-C3	-10.68	1.26	1.51
36	b	620	C7Z	C22-C23	-10.65	1.37	1.52
45	H	101	RRX	C29-C28	-10.54	1.37	1.52
36	B1	620	C7Z	C2-C3	-10.44	1.37	1.52
45	h	101	RRX	C29-C28	-10.44	1.37	1.52
45	H1	101	RRX	C29-C28	-10.35	1.37	1.52
36	b1	620	C7Z	C22-C23	-10.28	1.37	1.52
45	h1	101	RRX	C29-C28	-10.21	1.37	1.52
36	B	620	C7Z	C2-C3	-10.10	1.37	1.52
36	B1	620	C7Z	C22-C23	-10.08	1.37	1.52
36	B	620	C7Z	C22-C23	-10.05	1.37	1.52
36	b1	620	C7Z	C2-C3	-10.00	1.37	1.52
30	a1	409	PHO	C1B-C2B	9.95	1.50	1.39
30	A1	409	PHO	C1B-C2B	9.72	1.50	1.39
30	A1	408	PHO	C1B-C2B	9.54	1.50	1.39
53	R	626	ERG	C12-C13	9.14	1.70	1.54
30	a1	408	PHO	C1B-C2B	9.14	1.49	1.39
30	a	409	PHO	C1B-C2B	9.12	1.49	1.39
53	R	626	ERG	O1-C3	9.12	1.70	1.43
53	r1	626	ERG	O1-C3	9.11	1.70	1.43
53	R1	626	ERG	O1-C3	9.08	1.70	1.43
53	r	626	ERG	O1-C3	9.03	1.70	1.43
53	R1	626	ERG	C6-C5	8.97	1.54	1.33
30	A	409	PHO	C1B-C2B	8.96	1.49	1.39
53	r	626	ERG	C6-C5	8.94	1.54	1.33
36	b1	620	C7Z	C4-C3	8.92	1.67	1.52
53	R	626	ERG	C6-C5	8.89	1.54	1.33
53	r1	626	ERG	C6-C5	8.81	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	r	626	ERG	C12-C13	8.79	1.69	1.54
30	A	408	PHO	C1B-C2B	8.71	1.49	1.39
53	R1	626	ERG	C12-C13	8.67	1.69	1.54
53	r1	626	ERG	C12-C13	8.63	1.69	1.54
30	a	408	PHO	C1B-C2B	8.61	1.49	1.39
31	C1	515	BCR	C10-C9	8.52	1.47	1.35
31	b1	618	BCR	C10-C9	8.45	1.47	1.35
36	B1	620	C7Z	C4-C3	8.41	1.66	1.52
36	B	620	C7Z	C4-C3	8.29	1.66	1.52
36	b	620	C7Z	C4-C3	8.29	1.66	1.52
51	n	623	NEX	C14-C13	-8.18	1.24	1.35
51	s	623	NEX	C14-C13	-8.10	1.25	1.35
31	c1	517	BCR	C10-C9	8.03	1.46	1.35
51	y	623	NEX	C34-C33	-8.01	1.25	1.35
45	H1	101	RRX	C27-C28	7.97	1.66	1.52
45	h1	101	RRX	C27-C28	7.93	1.66	1.52
51	g	623	NEX	C10-C9	-7.92	1.25	1.35
51	y	623	NEX	C14-C13	-7.90	1.25	1.35
51	s	623	NEX	C34-C33	-7.89	1.25	1.35
51	n	623	NEX	C10-C9	-7.88	1.25	1.35
51	s	623	NEX	C10-C9	-7.88	1.25	1.35
51	N	623	NEX	C10-C9	-7.86	1.25	1.35
51	g	623	NEX	C14-C13	-7.86	1.25	1.35
51	N	623	NEX	C30-C29	-7.86	1.25	1.35
51	R	622	NEX	C34-C33	-7.85	1.25	1.35
51	G1	623	NEX	C34-C33	-7.82	1.25	1.35
51	g	623	NEX	C34-C33	-7.80	1.25	1.35
51	n	623	NEX	C34-C33	-7.78	1.25	1.35
51	G1	623	NEX	C10-C9	-7.78	1.25	1.35
45	H	101	RRX	C27-C28	7.77	1.65	1.52
51	R	622	NEX	C14-C13	-7.77	1.25	1.35
51	R1	622	NEX	C10-C9	-7.75	1.25	1.35
51	n	623	NEX	C30-C29	-7.75	1.25	1.35
30	a	408	PHO	C3B-C4B	7.75	1.50	1.41
51	G	623	NEX	C14-C13	-7.72	1.25	1.35
31	C1	516	BCR	C10-C9	7.71	1.46	1.35
51	r1	622	NEX	C14-C13	-7.69	1.25	1.35
51	s	623	NEX	C30-C29	-7.67	1.25	1.35
51	G	623	NEX	C34-C33	-7.62	1.25	1.35
31	d1	404	BCR	C10-C9	7.62	1.45	1.35
31	B1	618	BCR	C10-C9	7.61	1.45	1.35
51	s1	623	NEX	C14-C13	-7.60	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c1	516	BCR	C10-C9	7.59	1.45	1.35
31	b1	619	BCR	C10-C9	7.57	1.45	1.35
51	Y	623	NEX	C34-C33	-7.56	1.25	1.35
51	Y	623	NEX	C30-C29	-7.55	1.25	1.35
30	A1	409	PHO	C3B-C4B	7.54	1.50	1.41
51	r1	622	NEX	C10-C9	-7.54	1.25	1.35
51	s1	623	NEX	C10-C9	-7.54	1.25	1.35
51	y	623	NEX	C30-C29	-7.52	1.25	1.35
51	S	623	NEX	C14-C13	-7.52	1.25	1.35
51	N	623	NEX	C14-C13	-7.52	1.25	1.35
51	y	623	NEX	C10-C9	-7.50	1.25	1.35
51	G1	623	NEX	C14-C13	-7.49	1.25	1.35
51	n1	623	NEX	C14-C13	-7.49	1.25	1.35
51	R	622	NEX	C30-C29	-7.49	1.25	1.35
51	G	623	NEX	C30-C29	-7.47	1.25	1.35
51	N1	623	NEX	C14-C13	-7.47	1.25	1.35
51	g	623	NEX	C30-C29	-7.47	1.25	1.35
51	S	623	NEX	C30-C29	-7.46	1.25	1.35
31	a1	411	BCR	C10-C9	7.46	1.45	1.35
51	G1	623	NEX	C30-C29	-7.46	1.25	1.35
51	r	622	NEX	C14-C13	-7.45	1.25	1.35
30	A	408	PHO	C3B-C4B	7.44	1.50	1.41
30	a	409	PHO	C3B-C4B	7.44	1.50	1.41
30	a1	408	PHO	C3B-C4B	7.42	1.50	1.41
51	r1	622	NEX	C30-C29	-7.41	1.26	1.35
51	y1	623	NEX	C10-C9	-7.40	1.26	1.35
51	G	623	NEX	C10-C9	-7.38	1.26	1.35
51	g1	623	NEX	C10-C9	-7.38	1.26	1.35
51	N	623	NEX	C34-C33	-7.37	1.26	1.35
31	C	517	BCR	C10-C9	7.37	1.45	1.35
51	S	623	NEX	C34-C33	-7.36	1.26	1.35
51	R1	622	NEX	C14-C13	-7.34	1.26	1.35
51	Y	623	NEX	C14-C13	-7.34	1.26	1.35
45	h	101	RRX	C27-C28	7.33	1.65	1.52
31	D	404	BCR	C10-C9	7.32	1.45	1.35
51	y1	623	NEX	C14-C13	-7.32	1.26	1.35
51	N1	623	NEX	C10-C9	-7.32	1.26	1.35
31	c1	515	BCR	C10-C9	7.30	1.45	1.35
30	A1	408	PHO	C3B-C4B	7.29	1.49	1.41
51	n1	623	NEX	C10-C9	-7.29	1.26	1.35
51	r	622	NEX	C30-C29	-7.28	1.26	1.35
30	A	409	PHO	C3B-C4B	7.26	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	618	BCR	C10-C9	7.24	1.45	1.35
51	r	622	NEX	C34-C33	-7.23	1.26	1.35
51	S1	623	NEX	C30-C29	-7.21	1.26	1.35
31	B	618	BCR	C10-C9	7.21	1.45	1.35
51	Y	623	NEX	C10-C9	-7.21	1.26	1.35
31	d	404	BCR	C10-C9	7.21	1.45	1.35
51	g1	623	NEX	C14-C13	-7.20	1.26	1.35
31	c1	514	BCR	C10-C9	7.19	1.45	1.35
51	g1	623	NEX	C30-C29	-7.19	1.26	1.35
51	N1	623	NEX	C34-C33	-7.18	1.26	1.35
51	r	622	NEX	C10-C9	-7.17	1.26	1.35
51	R1	622	NEX	C34-C33	-7.16	1.26	1.35
30	a1	409	PHO	C3B-C4B	7.15	1.49	1.41
41	c	527	LMK	O3-C4	7.15	1.44	1.22
31	C1	517	BCR	C10-C9	7.15	1.45	1.35
31	B1	619	BCR	C10-C9	7.14	1.45	1.35
51	S1	623	NEX	C14-C13	-7.13	1.26	1.35
41	C1	527	LMK	O3-C4	7.13	1.43	1.22
51	S1	623	NEX	C34-C33	-7.12	1.26	1.35
51	r1	622	NEX	C34-C33	-7.11	1.26	1.35
51	N1	623	NEX	C30-C29	-7.10	1.26	1.35
51	S	623	NEX	C10-C9	-7.10	1.26	1.35
31	A1	411	BCR	C10-C9	7.10	1.45	1.35
41	c1	527	LMK	O3-C4	7.07	1.43	1.22
41	C	527	LMK	O3-C4	7.03	1.43	1.22
43	d	405	PL9	C7-C3	-7.00	1.44	1.51
51	g1	623	NEX	C34-C33	-7.00	1.26	1.35
51	R	622	NEX	C10-C9	-7.00	1.26	1.35
51	Y1	623	NEX	C14-C13	-6.99	1.26	1.35
51	n1	623	NEX	C34-C33	-6.99	1.26	1.35
51	R1	622	NEX	C30-C29	-6.98	1.26	1.35
31	C	516	BCR	C10-C9	6.98	1.45	1.35
51	s1	623	NEX	C34-C33	-6.96	1.26	1.35
51	S1	623	NEX	C10-C9	-6.96	1.26	1.35
31	c	516	BCR	C10-C9	6.94	1.45	1.35
51	R	622	NEX	C35-C15	-6.92	1.18	1.36
31	c	517	BCR	C10-C9	6.91	1.44	1.35
51	n	623	NEX	C35-C15	-6.89	1.18	1.36
51	G	623	NEX	C35-C15	-6.86	1.18	1.36
51	y1	623	NEX	C30-C29	-6.85	1.26	1.35
51	y	623	NEX	C35-C15	-6.84	1.18	1.36
51	G1	623	NEX	C35-C15	-6.81	1.18	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	n1	623	NEX	C35-C15	-6.80	1.18	1.36
51	y1	623	NEX	C34-C33	-6.80	1.26	1.35
51	s	623	NEX	C35-C15	-6.80	1.18	1.36
51	Y1	623	NEX	C34-C33	-6.78	1.26	1.35
51	N	623	NEX	C35-C15	-6.76	1.18	1.36
51	S	623	NEX	C35-C15	-6.74	1.18	1.36
51	Y1	623	NEX	C10-C9	-6.73	1.26	1.35
51	Y	623	NEX	C35-C15	-6.72	1.18	1.36
51	r	622	NEX	C35-C15	-6.72	1.18	1.36
51	g	623	NEX	C35-C15	-6.71	1.18	1.36
51	r1	622	NEX	C35-C15	-6.71	1.18	1.36
29	B1	603	CLA	MG-NA	6.70	2.22	2.06
31	a	411	BCR	C10-C9	6.66	1.44	1.35
51	R	622	NEX	C11-C12	-6.65	1.17	1.34
31	c	514	BCR	C10-C9	6.65	1.44	1.35
51	n1	623	NEX	C30-C29	-6.63	1.27	1.35
29	r1	612	CLA	MG-NA	6.60	2.22	2.06
45	H	101	RRX	C2-C3	-6.60	1.36	1.52
31	D1	404	BCR	C10-C9	6.60	1.44	1.35
51	g1	623	NEX	C35-C15	-6.59	1.18	1.36
29	b1	602	CLA	MG-NA	6.58	2.21	2.06
45	H	101	RRX	C1-C6	-6.57	1.44	1.53
51	N1	623	NEX	C35-C15	-6.56	1.18	1.36
31	A	411	BCR	C10-C9	6.56	1.44	1.35
51	s	623	NEX	C11-C12	-6.55	1.17	1.34
51	R1	622	NEX	C35-C15	-6.55	1.18	1.36
51	S	623	NEX	C7-C8	6.55	1.42	1.32
29	R1	612	CLA	MG-NA	6.55	2.21	2.06
51	g	623	NEX	C11-C12	-6.54	1.17	1.34
29	R	612	CLA	MG-NA	6.54	2.21	2.06
51	S1	623	NEX	C35-C15	-6.54	1.19	1.36
51	s	623	NEX	C31-C32	-6.52	1.17	1.34
29	S1	611	CLA	MG-NA	6.52	2.21	2.06
45	h1	101	RRX	C2-C3	-6.51	1.36	1.52
51	Y1	623	NEX	C35-C15	-6.51	1.19	1.36
29	g1	614	CLA	MG-NA	6.51	2.21	2.06
51	n	623	NEX	C11-C12	-6.50	1.17	1.34
29	B1	602	CLA	MG-NA	6.49	2.21	2.06
29	s1	613	CLA	MG-NA	6.48	2.21	2.06
29	s	603	CLA	MG-NA	6.47	2.21	2.06
45	h	101	RRX	C2-C3	-6.47	1.36	1.52
29	G1	602	CLA	MG-NA	6.47	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	n	623	NEX	C31-C32	-6.47	1.17	1.34
29	s1	612	CLA	MG-NA	6.47	2.21	2.06
29	N	612	CLA	MG-NA	6.46	2.21	2.06
29	n	602	CLA	MG-NA	6.46	2.21	2.06
29	R	603	CLA	MG-NA	6.46	2.21	2.06
29	s1	614	CLA	MG-NA	6.46	2.21	2.06
51	s1	623	NEX	C35-C15	-6.46	1.19	1.36
31	C	514	BCR	C10-C9	6.46	1.44	1.35
51	Y1	623	NEX	C30-C29	-6.45	1.27	1.35
29	S	603	CLA	MG-NA	6.45	2.21	2.06
29	b1	616	CLA	MG-NA	6.45	2.21	2.06
29	s1	611	CLA	MG-NA	6.44	2.21	2.06
29	s	617	CLA	MG-NA	6.44	2.21	2.06
51	S	623	NEX	C11-C12	-6.43	1.18	1.34
29	g	614	CLA	MG-NA	6.43	2.21	2.06
45	H1	101	RRX	C2-C3	-6.43	1.36	1.52
29	r	612	CLA	MG-NA	6.43	2.21	2.06
29	C1	503	CLA	MG-NA	6.42	2.21	2.06
29	b1	614	CLA	MG-NA	6.42	2.21	2.06
29	r1	603	CLA	MG-NA	6.42	2.21	2.06
29	g1	612	CLA	MG-NA	6.42	2.21	2.06
29	s1	605	CLA	MG-NA	6.42	2.21	2.06
51	s1	623	NEX	C30-C29	-6.42	1.27	1.35
29	y	602	CLA	MG-NA	6.41	2.21	2.06
29	G	612	CLA	MG-NA	6.41	2.21	2.06
29	N1	614	CLA	MG-NA	6.41	2.21	2.06
29	B	616	CLA	MG-NA	6.41	2.21	2.06
29	g	612	CLA	MG-NA	6.41	2.21	2.06
29	g1	611	CLA	MG-NA	6.40	2.21	2.06
29	S	605	CLA	MG-NA	6.40	2.21	2.06
45	H1	101	RRX	C1-C6	-6.40	1.45	1.53
29	c	512	CLA	MG-NA	6.39	2.21	2.06
29	R1	608	CLA	MG-NA	6.39	2.21	2.06
31	B	619	BCR	C10-C9	6.39	1.44	1.35
51	N	623	NEX	C11-C12	-6.39	1.18	1.34
29	N	611	CLA	MG-NA	6.39	2.21	2.06
51	r1	622	NEX	C31-C32	-6.39	1.18	1.34
31	C1	514	BCR	C10-C9	6.39	1.44	1.35
51	N	623	NEX	C31-C32	-6.38	1.18	1.34
29	n	612	CLA	MG-NA	6.38	2.21	2.06
29	r	602	CLA	MG-NA	6.38	2.21	2.06
51	Y	623	NEX	C31-C32	-6.37	1.18	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	603	CLA	MG-NA	6.37	2.21	2.06
29	b	602	CLA	MG-NA	6.37	2.21	2.06
29	Y1	603	CLA	MG-NA	6.37	2.21	2.06
29	y	608	CLA	MG-NA	6.36	2.21	2.06
29	Y1	612	CLA	MG-NA	6.36	2.21	2.06
29	n1	612	CLA	MG-NA	6.36	2.21	2.06
29	S1	605	CLA	MG-NA	6.35	2.21	2.06
29	R	608	CLA	MG-NA	6.35	2.21	2.06
29	c1	512	CLA	MG-NA	6.35	2.21	2.06
29	r1	602	CLA	MG-NA	6.34	2.21	2.06
29	G	614	CLA	MG-NA	6.34	2.21	2.06
29	B1	616	CLA	MG-NA	6.34	2.21	2.06
29	n	611	CLA	MG-NA	6.34	2.21	2.06
45	h	101	RRX	C1-C6	-6.33	1.45	1.53
29	R1	602	CLA	MG-NA	6.33	2.21	2.06
29	g1	603	CLA	MG-NA	6.33	2.21	2.06
51	r1	622	NEX	C7-C8	6.33	1.42	1.32
29	r1	604	CLA	MG-NA	6.32	2.21	2.06
51	g1	623	NEX	C11-C12	-6.32	1.18	1.34
51	N1	623	NEX	C11-C12	-6.32	1.18	1.34
29	R1	603	CLA	MG-NA	6.32	2.21	2.06
29	y1	611	CLA	MG-NA	6.32	2.21	2.06
31	b	619	BCR	C10-C9	6.32	1.44	1.35
29	s	605	CLA	MG-NA	6.31	2.21	2.06
51	y	623	NEX	C31-C32	-6.31	1.18	1.34
29	s1	609	CLA	MG-NA	6.31	2.21	2.06
29	c1	513	CLA	MG-NA	6.31	2.21	2.06
29	b	605	CLA	MG-NA	6.31	2.21	2.06
29	r1	608	CLA	MG-NA	6.30	2.21	2.06
29	G	604	CLA	MG-NA	6.30	2.21	2.06
29	s	612	CLA	MG-NA	6.30	2.21	2.06
29	r	603	CLA	MG-NA	6.30	2.21	2.06
29	G	611	CLA	MG-NA	6.30	2.21	2.06
29	d1	403	CLA	MG-NA	6.30	2.21	2.06
29	y	613	CLA	MG-NA	6.30	2.21	2.06
29	S1	603	CLA	MG-NA	6.29	2.21	2.06
29	S1	617	CLA	MG-NA	6.29	2.21	2.06
29	a1	406	CLA	MG-NA	6.29	2.21	2.06
29	R1	604	CLA	MG-NA	6.29	2.21	2.06
29	S	611	CLA	MG-NA	6.29	2.21	2.06
53	R	626	ERG	C16-C17	-6.28	1.41	1.54
29	B1	608	CLA	MG-NA	6.28	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s1	603	CLA	MG-NA	6.28	2.21	2.06
51	G	623	NEX	C31-C32	-6.28	1.18	1.34
29	Y1	608	CLA	MG-NA	6.28	2.21	2.06
29	d1	402	CLA	MG-NA	6.28	2.21	2.06
29	n	614	CLA	MG-NA	6.28	2.21	2.06
51	g	623	NEX	C31-C32	-6.28	1.18	1.34
29	c1	503	CLA	MG-NA	6.27	2.21	2.06
29	a	407	CLA	MG-NA	6.27	2.21	2.06
29	c1	511	CLA	MG-NA	6.27	2.21	2.06
29	s	610	CLA	MG-NA	6.27	2.21	2.06
29	y	603	CLA	MG-NA	6.27	2.21	2.06
29	C	502	CLA	MG-NA	6.27	2.21	2.06
29	G1	604	CLA	MG-NA	6.27	2.21	2.06
51	G1	623	NEX	C31-C32	-6.27	1.18	1.34
29	B	605	CLA	MG-NA	6.26	2.21	2.06
29	C	503	CLA	MG-NA	6.26	2.21	2.06
29	N	614	CLA	MG-NA	6.26	2.21	2.06
29	c1	510	CLA	MG-NA	6.26	2.21	2.06
29	N1	612	CLA	MG-NA	6.26	2.21	2.06
51	Y	623	NEX	C11-C12	-6.26	1.18	1.34
29	C	513	CLA	MG-NA	6.26	2.21	2.06
29	c1	501	CLA	MG-NA	6.26	2.21	2.06
29	r	608	CLA	MG-NA	6.26	2.21	2.06
29	s1	604	CLA	MG-NA	6.25	2.21	2.06
29	b1	604	CLA	MG-NA	6.25	2.21	2.06
29	S	602	CLA	MG-NA	6.25	2.21	2.06
51	y	623	NEX	C11-C12	-6.25	1.18	1.34
29	B1	615	CLA	MG-NA	6.25	2.21	2.06
29	Y	613	CLA	MG-NA	6.24	2.21	2.06
29	C	510	CLA	MG-NA	6.24	2.21	2.06
29	y1	608	CLA	MG-NA	6.24	2.21	2.06
29	s1	602	CLA	MG-NA	6.24	2.21	2.06
51	R1	622	NEX	C7-C8	6.24	1.42	1.32
29	c1	509	CLA	MG-NA	6.24	2.21	2.06
29	r1	610	CLA	MG-NA	6.24	2.21	2.06
29	S	609	CLA	MG-NA	6.23	2.21	2.06
29	G1	612	CLA	MG-NA	6.23	2.21	2.06
29	B1	605	CLA	MG-NA	6.23	2.21	2.06
29	n	613	CLA	MG-NA	6.23	2.21	2.06
51	R	622	NEX	C31-C32	-6.23	1.18	1.34
29	b1	608	CLA	MG-NA	6.23	2.21	2.06
29	N	613	CLA	MG-NA	6.23	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	y1	610	CLA	MG-NA	6.23	2.21	2.06
29	y	611	CLA	MG-NA	6.23	2.21	2.06
29	Y1	602	CLA	MG-NA	6.23	2.21	2.06
29	g1	613	CLA	MG-NA	6.23	2.21	2.06
51	y1	623	NEX	C35-C15	-6.22	1.19	1.36
29	n1	603	CLA	MG-NA	6.22	2.21	2.06
51	s1	623	NEX	C11-C12	-6.22	1.18	1.34
29	s	609	CLA	MG-NA	6.22	2.21	2.06
29	b1	606	CLA	MG-NA	6.22	2.21	2.06
29	Y	614	CLA	MG-NA	6.22	2.21	2.06
29	Y	612	CLA	MG-NA	6.22	2.21	2.06
29	s	604	CLA	MG-NA	6.22	2.21	2.06
29	n1	614	CLA	MG-NA	6.22	2.21	2.06
29	y1	614	CLA	MG-NA	6.22	2.21	2.06
51	G1	623	NEX	C11-C12	-6.22	1.18	1.34
29	Y1	604	CLA	MG-NA	6.22	2.21	2.06
29	N1	603	CLA	MG-NA	6.21	2.21	2.06
29	B	607	CLA	MG-NA	6.21	2.21	2.06
51	r	622	NEX	C31-C32	-6.21	1.18	1.34
29	C	507	CLA	MG-NA	6.21	2.21	2.06
29	b1	612	CLA	MG-NA	6.21	2.21	2.06
29	d	403	CLA	MG-NA	6.21	2.21	2.06
29	n1	611	CLA	MG-NA	6.21	2.21	2.06
29	s1	617	CLA	MG-NA	6.21	2.21	2.06
29	c	507	CLA	MG-NA	6.21	2.21	2.06
29	D1	403	CLA	MG-NA	6.21	2.21	2.06
51	R1	622	NEX	C11-C12	-6.21	1.18	1.34
29	G	602	CLA	MG-NA	6.21	2.21	2.06
29	c	511	CLA	MG-NA	6.20	2.21	2.06
51	r	622	NEX	C11-C12	-6.20	1.18	1.34
29	C	511	CLA	MG-NA	6.20	2.21	2.06
29	C1	501	CLA	MG-NA	6.20	2.21	2.06
29	s1	610	CLA	MG-NA	6.20	2.21	2.06
29	g	603	CLA	MG-NA	6.20	2.21	2.06
29	a1	407	CLA	MG-NA	6.20	2.21	2.06
29	n	610	CLA	MG-NA	6.19	2.21	2.06
29	g	604	CLA	MG-NA	6.19	2.21	2.06
29	G1	614	CLA	MG-NA	6.19	2.21	2.06
29	c	510	CLA	MG-NA	6.19	2.21	2.06
29	b1	611	CLA	MG-NA	6.19	2.21	2.06
29	b1	617	CLA	MG-NA	6.19	2.21	2.06
29	n1	604	CLA	MG-NA	6.19	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c1	502	CLA	MG-NA	6.18	2.21	2.06
29	y1	612	CLA	MG-NA	6.18	2.21	2.06
29	S	612	CLA	MG-NA	6.18	2.21	2.06
29	B	602	CLA	MG-NA	6.18	2.20	2.06
29	B	610	CLA	MG-NA	6.18	2.20	2.06
29	s	611	CLA	MG-NA	6.18	2.20	2.06
29	r	610	CLA	MG-NA	6.18	2.20	2.06
29	c	502	CLA	MG-NA	6.18	2.20	2.06
51	n1	623	NEX	C11-C12	-6.18	1.18	1.34
29	N	604	CLA	MG-NA	6.17	2.20	2.06
29	y	604	CLA	MG-NA	6.17	2.20	2.06
29	Y	608	CLA	MG-NA	6.17	2.20	2.06
29	b1	609	CLA	MG-NA	6.17	2.20	2.06
29	G	613	CLA	MG-NA	6.17	2.20	2.06
29	C1	502	CLA	MG-NA	6.17	2.20	2.06
29	R1	609	CLA	MG-NA	6.17	2.20	2.06
29	b1	607	CLA	MG-NA	6.17	2.20	2.06
29	g	613	CLA	MG-NA	6.16	2.20	2.06
29	Y	603	CLA	MG-NA	6.16	2.20	2.06
29	b	611	CLA	MG-NA	6.16	2.20	2.06
29	G	603	CLA	MG-NA	6.16	2.20	2.06
29	c1	507	CLA	MG-NA	6.16	2.20	2.06
51	S	623	NEX	C31-C32	-6.16	1.18	1.34
29	R	602	CLA	MG-NA	6.16	2.20	2.06
29	b1	605	CLA	MG-NA	6.15	2.20	2.06
29	C1	513	CLA	MG-NA	6.15	2.20	2.06
29	C1	512	CLA	MG-NA	6.15	2.20	2.06
29	R	604	CLA	MG-NA	6.15	2.20	2.06
29	Y1	610	CLA	MG-NA	6.15	2.20	2.06
29	B1	604	CLA	MG-NA	6.15	2.20	2.06
29	D1	402	CLA	MG-NA	6.15	2.20	2.06
29	c	506	CLA	MG-NA	6.15	2.20	2.06
29	b	608	CLA	MG-NA	6.15	2.20	2.06
29	b1	603	CLA	MG-NA	6.15	2.20	2.06
29	G1	610	CLA	MG-NA	6.14	2.20	2.06
29	B1	617	CLA	MG-NA	6.14	2.20	2.06
29	n	603	CLA	MG-NA	6.14	2.20	2.06
29	b1	615	CLA	MG-NA	6.14	2.20	2.06
29	G1	603	CLA	MG-NA	6.14	2.20	2.06
29	C	501	CLA	MG-NA	6.14	2.20	2.06
29	B1	612	CLA	MG-NA	6.14	2.20	2.06
29	S1	604	CLA	MG-NA	6.14	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b1	610	CLA	MG-NA	6.13	2.20	2.06
29	c	503	CLA	MG-NA	6.13	2.20	2.06
29	G1	613	CLA	MG-NA	6.13	2.20	2.06
29	y1	603	CLA	MG-NA	6.13	2.20	2.06
29	a1	410	CLA	MG-NA	6.13	2.20	2.06
29	b	609	CLA	MG-NA	6.13	2.20	2.06
29	y	612	CLA	MG-NA	6.13	2.20	2.06
51	S1	623	NEX	C31-C32	-6.13	1.18	1.34
29	C	512	CLA	MG-NA	6.12	2.20	2.06
29	c1	508	CLA	MG-NA	6.12	2.20	2.06
29	y1	613	CLA	MG-NA	6.12	2.20	2.06
29	g	602	CLA	MG-NA	6.12	2.20	2.06
29	N1	611	CLA	MG-NA	6.12	2.20	2.06
29	c1	506	CLA	MG-NA	6.12	2.20	2.06
29	N1	613	CLA	MG-NA	6.12	2.20	2.06
29	A1	407	CLA	MG-NA	6.12	2.20	2.06
29	A1	406	CLA	MG-NA	6.11	2.20	2.06
29	S1	612	CLA	MG-NA	6.11	2.20	2.06
31	b1	618	BCR	C24-C23	6.11	1.51	1.33
29	S	613	CLA	MG-NA	6.11	2.20	2.06
29	A	407	CLA	MG-NA	6.11	2.20	2.06
29	g1	602	CLA	MG-NA	6.11	2.20	2.06
29	B	608	CLA	MG-NA	6.11	2.20	2.06
51	G	623	NEX	C11-C12	-6.10	1.18	1.34
29	G1	611	CLA	MG-NA	6.10	2.20	2.06
29	n1	613	CLA	MG-NA	6.10	2.20	2.06
29	c	505	CLA	MG-NA	6.10	2.20	2.06
29	r	604	CLA	MG-NA	6.10	2.20	2.06
29	Y	602	CLA	MG-NA	6.10	2.20	2.06
29	B1	613	CLA	MG-NA	6.10	2.20	2.06
29	B1	610	CLA	MG-NA	6.09	2.20	2.06
29	B1	614	CLA	MG-NA	6.09	2.20	2.06
29	N1	602	CLA	MG-NA	6.09	2.20	2.06
29	D	403	CLA	MG-NA	6.09	2.20	2.06
29	C1	511	CLA	MG-NA	6.09	2.20	2.06
29	s	602	CLA	MG-NA	6.09	2.20	2.06
29	B1	609	CLA	MG-NA	6.08	2.20	2.06
29	Y	611	CLA	MG-NA	6.08	2.20	2.06
29	S	614	CLA	MG-NA	6.07	2.20	2.06
29	C	505	CLA	MG-NA	6.07	2.20	2.06
29	B	609	CLA	MG-NA	6.07	2.20	2.06
29	b	603	CLA	MG-NA	6.07	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R1	610	CLA	MG-NA	6.07	2.20	2.06
29	N	610	CLA	MG-NA	6.07	2.20	2.06
29	c	513	CLA	MG-NA	6.06	2.20	2.06
31	c1	516	BCR	C24-C23	6.06	1.51	1.33
29	N	602	CLA	MG-NA	6.06	2.20	2.06
29	C1	506	CLA	MG-NA	6.06	2.20	2.06
29	B	612	CLA	MG-NA	6.06	2.20	2.06
31	C	515	BCR	C10-C9	6.06	1.43	1.35
29	n1	610	CLA	MG-NA	6.05	2.20	2.06
53	r	626	ERG	C16-C17	-6.05	1.41	1.54
29	g1	604	CLA	MG-NA	6.05	2.20	2.06
29	C1	504	CLA	MG-NA	6.05	2.20	2.06
29	c	501	CLA	MG-NA	6.05	2.20	2.06
29	N1	604	CLA	MG-NA	6.05	2.20	2.06
29	Y1	614	CLA	MG-NA	6.05	2.20	2.06
29	b	607	CLA	MG-NA	6.05	2.20	2.06
29	S	617	CLA	MG-NA	6.05	2.20	2.06
29	a	410	CLA	MG-NA	6.05	2.20	2.06
29	b	604	CLA	MG-NA	6.04	2.20	2.06
29	C1	508	CLA	MG-NA	6.04	2.20	2.06
51	S1	623	NEX	C11-C12	-6.04	1.19	1.34
29	B	615	CLA	MG-NA	6.04	2.20	2.06
29	B	606	CLA	MG-NA	6.03	2.20	2.06
29	c1	505	CLA	MG-NA	6.03	2.20	2.06
29	S1	609	CLA	MG-NA	6.03	2.20	2.06
29	c	509	CLA	MG-NA	6.03	2.20	2.06
29	g	611	CLA	MG-NA	6.03	2.20	2.06
29	r1	609	CLA	MG-NA	6.03	2.20	2.06
29	C1	507	CLA	MG-NA	6.02	2.20	2.06
29	r	609	CLA	MG-NA	6.02	2.20	2.06
29	B	614	CLA	MG-NA	6.02	2.20	2.06
29	s	613	CLA	MG-NA	6.02	2.20	2.06
51	n1	623	NEX	C7-C8	6.02	1.42	1.32
29	C	508	CLA	MG-NA	6.02	2.20	2.06
29	Y	604	CLA	MG-NA	6.01	2.20	2.06
29	b	614	CLA	MG-NA	6.01	2.20	2.06
29	B	604	CLA	MG-NA	6.01	2.20	2.06
29	n	604	CLA	MG-NA	6.01	2.20	2.06
29	B1	611	CLA	MG-NA	6.00	2.20	2.06
29	a	406	CLA	MG-NA	6.00	2.20	2.06
29	y1	602	CLA	MG-NA	6.00	2.20	2.06
29	b	616	CLA	MG-NA	6.00	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	508	CLA	MG-NA	5.99	2.20	2.06
51	r1	622	NEX	C11-C12	-5.99	1.19	1.34
29	b	617	CLA	MG-NA	5.99	2.20	2.06
29	b	612	CLA	MG-NA	5.99	2.20	2.06
31	B1	618	BCR	C24-C23	5.99	1.51	1.33
51	N1	623	NEX	C31-C32	-5.99	1.19	1.34
29	b	615	CLA	MG-NA	5.98	2.20	2.06
51	n1	623	NEX	C31-C32	-5.98	1.19	1.34
53	R1	626	ERG	C16-C17	-5.98	1.42	1.54
29	C	506	CLA	MG-NA	5.98	2.20	2.06
29	B	617	CLA	MG-NA	5.97	2.20	2.06
29	R	610	CLA	MG-NA	5.97	2.20	2.06
29	S1	614	CLA	MG-NA	5.97	2.20	2.06
29	S1	613	CLA	MG-NA	5.97	2.20	2.06
29	C	509	CLA	MG-NA	5.97	2.20	2.06
29	y1	604	CLA	MG-NA	5.97	2.20	2.06
29	b	610	CLA	MG-NA	5.97	2.20	2.06
31	b1	619	BCR	C24-C23	5.96	1.51	1.33
53	r1	626	ERG	C13-C14	-5.96	1.46	1.56
29	B	611	CLA	MG-NA	5.96	2.20	2.06
29	C	504	CLA	MG-NA	5.96	2.20	2.06
51	s1	623	NEX	C7-C8	5.96	1.41	1.32
29	y	614	CLA	MG-NA	5.96	2.20	2.06
51	s1	623	NEX	C31-C32	-5.96	1.19	1.34
29	C1	509	CLA	MG-NA	5.95	2.20	2.06
29	A1	410	CLA	MG-NA	5.95	2.20	2.06
31	C1	517	BCR	C24-C23	5.95	1.51	1.33
29	G	610	CLA	MG-NA	5.95	2.20	2.06
51	R1	622	NEX	C31-C32	-5.95	1.19	1.34
29	c1	504	CLA	MG-NA	5.94	2.20	2.06
51	Y1	623	NEX	C31-C32	-5.94	1.19	1.34
29	C1	510	CLA	MG-NA	5.94	2.20	2.06
29	d	402	CLA	MG-NA	5.94	2.20	2.06
29	R	609	CLA	MG-NA	5.94	2.20	2.06
29	N	603	CLA	MG-NA	5.94	2.20	2.06
29	B1	606	CLA	MG-NA	5.93	2.20	2.06
29	y	610	CLA	MG-NA	5.93	2.20	2.06
29	S1	602	CLA	MG-NA	5.93	2.20	2.06
29	A1	405	CLA	MG-NA	5.93	2.20	2.06
31	c	515	BCR	C11-C12	-5.93	1.19	1.34
29	n1	602	CLA	MG-NA	5.92	2.20	2.06
29	A	406	CLA	MG-NA	5.92	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	g1	623	NEX	C31-C32	-5.92	1.19	1.34
29	S	610	CLA	MG-NA	5.92	2.20	2.06
29	g1	610	CLA	MG-NA	5.91	2.20	2.06
29	s	614	CLA	MG-NA	5.91	2.20	2.06
29	N1	610	CLA	MG-NA	5.90	2.20	2.06
36	B	620	C7Z	C1-C6	-5.90	1.45	1.53
29	b1	613	CLA	MG-NA	5.90	2.20	2.06
29	Y1	611	CLA	MG-NA	5.90	2.20	2.06
29	Y1	613	CLA	MG-NA	5.89	2.20	2.06
29	c	504	CLA	MG-NA	5.89	2.20	2.06
29	a1	405	CLA	MG-NA	5.88	2.20	2.06
29	C1	505	CLA	MG-NA	5.88	2.20	2.06
53	r1	626	ERG	C16-C17	-5.88	1.42	1.54
29	S	604	CLA	MG-NA	5.87	2.20	2.06
36	B1	620	C7Z	C12-C13	5.87	1.58	1.45
51	y1	623	NEX	C11-C12	-5.86	1.19	1.34
51	y1	623	NEX	C31-C32	-5.86	1.19	1.34
29	A	410	CLA	MG-NA	5.85	2.20	2.06
29	B	613	CLA	MG-NA	5.85	2.20	2.06
51	y1	623	NEX	C7-C8	5.85	1.41	1.32
51	s	623	NEX	C7-C8	5.83	1.41	1.32
29	D	402	CLA	MG-NA	5.83	2.20	2.06
29	b	606	CLA	MG-NA	5.81	2.20	2.06
29	a	405	CLA	MG-NA	5.80	2.20	2.06
29	b	613	CLA	MG-NA	5.80	2.20	2.06
29	B1	607	CLA	MG-NA	5.77	2.20	2.06
29	A	405	CLA	MG-NA	5.77	2.20	2.06
36	b1	620	C7Z	C1-C6	-5.76	1.45	1.53
31	b	619	BCR	C24-C23	5.76	1.50	1.33
43	D	405	PL9	C7-C3	-5.75	1.45	1.51
31	A1	411	BCR	C24-C23	5.74	1.50	1.33
31	D1	404	BCR	C24-C23	5.74	1.50	1.33
31	d1	404	BCR	C24-C23	5.73	1.50	1.33
36	b1	620	C7Z	C12-C13	5.72	1.58	1.45
51	r	622	NEX	C7-C8	5.72	1.41	1.32
31	D	404	BCR	C24-C23	5.71	1.50	1.33
31	c1	515	BCR	C24-C23	5.68	1.50	1.33
31	C1	514	BCR	C24-C23	5.68	1.50	1.33
29	S1	610	CLA	MG-NA	5.67	2.19	2.06
51	Y1	623	NEX	C7-C8	5.66	1.41	1.32
31	c	516	BCR	C24-C23	5.66	1.50	1.33
53	R1	626	ERG	C1-C2	5.65	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	g	623	NEX	C7-C8	5.64	1.41	1.32
31	b	618	BCR	C24-C23	5.64	1.50	1.33
31	c	515	BCR	C10-C9	5.63	1.43	1.35
31	d	404	BCR	C24-C23	5.63	1.50	1.33
31	C	514	BCR	C11-C12	-5.63	1.20	1.34
51	Y1	623	NEX	C11-C12	-5.63	1.20	1.34
29	g	610	CLA	MG-NA	5.62	2.19	2.06
31	c1	514	BCR	C24-C23	5.62	1.50	1.33
31	B	619	BCR	C24-C23	5.61	1.50	1.33
31	B1	619	BCR	C24-C23	5.60	1.50	1.33
29	Y	610	CLA	MG-NA	5.60	2.19	2.06
31	C1	516	BCR	C24-C23	5.57	1.49	1.33
31	C	516	BCR	C24-C23	5.56	1.49	1.33
36	B	620	C7Z	C12-C13	5.55	1.57	1.45
31	a1	411	BCR	C24-C23	5.54	1.49	1.33
31	a1	411	BCR	C11-C12	-5.54	1.20	1.34
36	b	620	C7Z	C1-C6	-5.53	1.46	1.53
31	c1	515	BCR	C11-C12	-5.51	1.20	1.34
31	c	514	BCR	C24-C23	5.50	1.49	1.33
31	c1	517	BCR	C24-C23	5.49	1.49	1.33
36	B	620	C7Z	C24-C25	-5.49	1.42	1.51
45	H1	101	RRX	C19-C18	5.49	1.57	1.45
31	A	411	BCR	C24-C23	5.48	1.49	1.33
31	C1	514	BCR	C11-C12	-5.48	1.20	1.34
31	a	411	BCR	C24-C23	5.48	1.49	1.33
51	Y	623	NEX	C28-C29	-5.48	1.34	1.45
31	C	514	BCR	C24-C23	5.47	1.49	1.33
31	C	515	BCR	C24-C23	5.46	1.49	1.33
31	A	411	BCR	C11-C12	-5.46	1.20	1.34
31	b	619	BCR	C11-C12	-5.45	1.20	1.34
31	B	619	BCR	C11-C12	-5.45	1.20	1.34
51	g	623	NEX	C28-C29	-5.44	1.34	1.45
31	C	517	BCR	C24-C23	5.42	1.49	1.33
53	R1	626	ERG	C13-C14	-5.41	1.47	1.56
31	B	618	BCR	C24-C23	5.41	1.49	1.33
51	n	623	NEX	C28-C29	-5.41	1.34	1.45
31	c	517	BCR	C24-C23	5.40	1.49	1.33
51	R	622	NEX	C28-C29	-5.39	1.34	1.45
31	c	514	BCR	C11-C12	-5.39	1.20	1.34
51	Y	623	NEX	C7-C8	5.38	1.40	1.32
36	B1	620	C7Z	C28-C29	5.38	1.57	1.45
31	D1	404	BCR	C11-C12	-5.37	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	620	C7Z	C12-C13	5.37	1.57	1.45
36	B1	620	C7Z	C1-C6	-5.36	1.46	1.53
51	s	623	NEX	C28-C29	-5.36	1.34	1.45
31	C1	515	BCR	C24-C23	5.35	1.49	1.33
51	y1	623	NEX	C28-C29	-5.35	1.34	1.45
53	R	626	ERG	C1-C2	5.34	1.64	1.53
51	G1	623	NEX	C7-C8	5.33	1.40	1.32
51	N	623	NEX	C28-C29	-5.33	1.34	1.45
31	a	411	BCR	C11-C12	-5.33	1.20	1.34
51	R	622	NEX	C7-C8	5.32	1.40	1.32
36	b1	620	C7Z	C28-C29	5.31	1.57	1.45
31	C	515	BCR	C11-C12	-5.29	1.20	1.34
36	b	620	C7Z	C24-C25	-5.29	1.42	1.51
31	c	516	BCR	C11-C12	-5.28	1.21	1.34
31	c	515	BCR	C24-C23	5.27	1.49	1.33
31	C	517	BCR	C11-C12	-5.27	1.21	1.34
51	g1	623	NEX	C28-C29	-5.26	1.34	1.45
51	g1	623	NEX	C7-C8	5.26	1.40	1.32
51	S1	623	NEX	C28-C29	-5.26	1.34	1.45
31	B	618	BCR	C11-C12	-5.20	1.21	1.34
31	C1	517	BCR	C11-C12	-5.20	1.21	1.34
31	A1	411	BCR	C11-C12	-5.19	1.21	1.34
51	y	623	NEX	C28-C29	-5.18	1.34	1.45
31	c	517	BCR	C11-C12	-5.18	1.21	1.34
53	r	626	ERG	C13-C14	-5.17	1.47	1.56
51	r	622	NEX	C28-C29	-5.17	1.34	1.45
31	C	516	BCR	C11-C12	-5.16	1.21	1.34
31	b1	619	BCR	C11-C12	-5.16	1.21	1.34
45	h1	101	RRX	C2-C1	5.16	1.66	1.54
53	r1	626	ERG	C1-C2	5.15	1.64	1.53
45	h1	101	RRX	C1-C6	-5.14	1.46	1.53
51	N	623	NEX	C7-C8	5.13	1.40	1.32
31	c1	514	BCR	C11-C12	-5.13	1.21	1.34
51	R1	622	NEX	C28-C29	-5.13	1.34	1.45
51	y	623	NEX	C7-C8	5.12	1.40	1.32
51	G	623	NEX	C28-C29	-5.10	1.35	1.45
45	h1	101	RRX	C30-C25	-5.10	1.46	1.53
51	r1	622	NEX	C28-C29	-5.10	1.35	1.45
31	c1	517	BCR	C11-C12	-5.09	1.21	1.34
51	S	623	NEX	C28-C29	-5.08	1.35	1.45
53	R	626	ERG	C13-C14	-5.07	1.47	1.56
53	r	626	ERG	C12-C11	-5.06	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	618	BCR	C11-C12	-5.06	1.21	1.34
45	H	101	RRX	C2-C1	5.06	1.65	1.54
51	N1	623	NEX	C7-C8	5.04	1.40	1.32
51	N1	623	NEX	C28-C29	-5.04	1.35	1.45
45	h1	101	RRX	C19-C18	5.02	1.56	1.45
45	H1	101	RRX	C30-C25	-5.01	1.46	1.53
31	c1	516	BCR	C11-C12	-5.01	1.21	1.34
31	B1	619	BCR	C11-C12	-5.00	1.21	1.34
51	Y1	623	NEX	C28-C29	-5.00	1.35	1.45
45	H1	101	RRX	C2-C1	4.99	1.65	1.54
31	D	404	BCR	C11-C12	-4.98	1.21	1.34
31	C1	516	BCR	C11-C12	-4.98	1.21	1.34
31	d	404	BCR	C11-C12	-4.97	1.21	1.34
45	h1	101	RRX	C8-C9	4.97	1.56	1.45
51	n	623	NEX	C7-C8	4.97	1.40	1.32
36	B1	620	C7Z	C32-C33	4.96	1.56	1.45
51	G1	623	NEX	C28-C29	-4.96	1.35	1.45
36	b1	620	C7Z	C32-C33	4.96	1.56	1.45
51	s1	623	NEX	C1-C6	-4.92	1.46	1.54
53	r1	626	ERG	C12-C11	-4.91	1.42	1.53
53	r1	626	ERG	C7-C6	-4.89	1.27	1.41
53	R	626	ERG	C7-C6	-4.88	1.27	1.41
53	R1	626	ERG	C7-C6	-4.87	1.27	1.41
45	h	101	RRX	C2-C1	4.86	1.65	1.54
31	c	515	BCR	C16-C17	-4.86	1.28	1.43
31	b1	618	BCR	C11-C12	-4.86	1.22	1.34
31	d1	404	BCR	C11-C12	-4.85	1.22	1.34
45	h	101	RRX	C27-C26	-4.85	1.43	1.51
53	R	626	ERG	C12-C11	-4.84	1.43	1.53
36	B	620	C7Z	C28-C29	4.83	1.56	1.45
45	H1	101	RRX	C8-C9	4.82	1.56	1.45
45	H	101	RRX	C19-C18	4.78	1.56	1.45
45	h	101	RRX	C8-C9	4.75	1.56	1.45
53	r	626	ERG	C7-C6	-4.75	1.27	1.41
36	B	620	C7Z	C4-C5	-4.75	1.43	1.51
51	n1	623	NEX	C28-C29	-4.74	1.35	1.45
43	d	405	PL9	C3-C4	-4.73	1.41	1.49
53	R1	626	ERG	C12-C11	-4.73	1.43	1.53
51	s1	623	NEX	C28-C29	-4.72	1.35	1.45
45	H	101	RRX	C30-C25	-4.71	1.47	1.53
53	r	626	ERG	C1-C2	4.71	1.63	1.53
31	A	411	BCR	C16-C17	-4.70	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f1	101	HEM	FE-ND	4.70	2.09	1.94
31	B	619	BCR	C16-C17	-4.67	1.29	1.43
45	h	101	RRX	C19-C18	4.66	1.56	1.45
31	B1	618	BCR	C11-C12	-4.66	1.22	1.34
36	B1	620	C7Z	C31-C30	4.66	1.57	1.43
36	B	620	C7Z	C32-C33	4.64	1.55	1.45
31	C	515	BCR	C16-C17	-4.62	1.29	1.43
36	B1	620	C7Z	C24-C25	-4.61	1.43	1.51
29	C1	508	CLA	MG-ND	-4.61	1.96	2.05
36	B1	620	C7Z	C4-C5	-4.59	1.43	1.51
31	C1	515	BCR	C11-C12	-4.59	1.22	1.34
29	b	609	CLA	MG-ND	-4.57	1.96	2.05
36	b	620	C7Z	C28-C29	4.56	1.55	1.45
45	H	101	RRX	C8-C9	4.55	1.55	1.45
36	b	620	C7Z	C32-C33	4.53	1.55	1.45
51	S1	623	NEX	C7-C8	4.52	1.39	1.32
29	R	603	CLA	MG-ND	-4.52	1.96	2.05
31	a	411	BCR	C16-C17	-4.51	1.29	1.43
29	S1	611	CLA	MG-ND	-4.51	1.96	2.05
31	C	514	BCR	C16-C17	-4.51	1.29	1.43
31	c1	515	BCR	C16-C17	-4.50	1.29	1.43
43	D	405	PL9	C3-C4	-4.50	1.42	1.49
36	B1	620	C7Z	C8-C9	4.49	1.55	1.45
36	b1	620	C7Z	C4-C5	-4.49	1.44	1.51
45	H1	101	RRX	C23-C22	4.48	1.55	1.45
29	Y	610	CLA	C1C-NC	-4.48	1.31	1.37
48	N1	608	CHL	CBB-CAB	4.48	1.52	1.30
29	c	505	CLA	MG-ND	-4.47	1.96	2.05
29	r	603	CLA	MG-ND	-4.47	1.96	2.05
53	r	626	ERG	C13-C17	4.47	1.63	1.55
31	A1	411	BCR	C16-C17	-4.47	1.29	1.43
29	b1	611	CLA	MG-ND	-4.46	1.96	2.05
48	Y1	601	CHL	CBB-CAB	4.46	1.52	1.30
48	y1	609	CHL	CBB-CAB	4.44	1.52	1.30
29	C	508	CLA	MG-ND	-4.44	1.97	2.05
31	b	619	BCR	C16-C17	-4.43	1.29	1.43
45	h	101	RRX	C30-C25	-4.43	1.47	1.53
44	f1	101	HEM	FE-NB	4.42	2.08	1.94
37	c1	518	DGD	O1G-C1A	4.41	1.46	1.33
48	N1	601	CHL	CBB-CAB	4.41	1.52	1.30
29	s1	613	CLA	CBB-CAB	4.41	1.52	1.30
37	B	623	DGD	O1G-C1A	4.41	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y1	608	CLA	MG-ND	-4.41	1.97	2.05
48	S1	608	CHL	CBB-CAB	4.41	1.52	1.30
31	a1	411	BCR	C16-C17	-4.40	1.29	1.43
29	B1	609	CLA	MG-ND	-4.40	1.97	2.05
29	B1	611	CLA	C1C-NC	-4.40	1.31	1.37
29	N1	602	CLA	CBB-CAB	4.40	1.52	1.30
31	c	514	BCR	C16-C17	-4.40	1.29	1.43
44	f	101	HEM	FE-NB	4.40	2.08	1.94
43	D	405	PL9	C6-C1	-4.40	1.40	1.48
53	R1	626	ERG	C13-C17	4.39	1.63	1.55
37	b	623	DGD	O1G-C1A	4.39	1.46	1.33
29	s1	602	CLA	CBB-CAB	4.39	1.52	1.30
48	G1	606	CHL	CBB-CAB	4.39	1.52	1.30
36	b1	620	C7Z	C24-C25	-4.39	1.44	1.51
48	Y1	607	CHL	CBB-CAB	4.39	1.52	1.30
48	n1	609	CHL	CBB-CAB	4.38	1.52	1.30
48	y1	606	CHL	CBB-CAB	4.38	1.52	1.30
36	b1	620	C7Z	C31-C30	4.38	1.57	1.43
29	C1	505	CLA	MG-ND	-4.38	1.97	2.05
29	y1	602	CLA	CBB-CAB	4.37	1.52	1.30
29	B1	604	CLA	CBB-CAB	4.37	1.52	1.30
53	R	626	ERG	C13-C17	4.37	1.63	1.55
37	b1	623	DGD	O1G-C1A	4.37	1.46	1.33
31	c	517	BCR	C16-C17	-4.37	1.29	1.43
29	n1	602	CLA	CBB-CAB	4.37	1.51	1.30
48	G	605	CHL	CBB-CAB	4.37	1.51	1.30
31	C1	516	BCR	C16-C17	-4.36	1.29	1.43
29	B	614	CLA	CBB-CAB	4.36	1.51	1.30
29	b1	608	CLA	CBB-CAB	4.36	1.51	1.30
48	g1	609	CHL	CBB-CAB	4.36	1.51	1.30
29	R1	608	CLA	CBB-CAB	4.36	1.51	1.30
29	C	505	CLA	MG-ND	-4.36	1.97	2.05
37	c1	519	DGD	O1G-C1A	4.36	1.46	1.33
45	h1	101	RRX	C23-C22	4.36	1.55	1.45
29	B1	611	CLA	CBB-CAB	4.36	1.51	1.30
48	g	609	CHL	CBB-CAB	4.35	1.51	1.30
29	B	606	CLA	CBB-CAB	4.35	1.51	1.30
48	G1	609	CHL	CBB-CAB	4.35	1.51	1.30
29	n	610	CLA	CBB-CAB	4.35	1.51	1.30
29	b1	611	CLA	C1C-NC	-4.35	1.31	1.37
29	b	611	CLA	CBB-CAB	4.35	1.51	1.30
48	y	607	CHL	CBB-CAB	4.35	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c1	508	CLA	CBB-CAB	4.35	1.51	1.30
48	N1	605	CHL	CBB-CAB	4.35	1.51	1.30
29	c1	501	CLA	CBB-CAB	4.35	1.51	1.30
29	N1	614	CLA	CBB-CAB	4.35	1.51	1.30
29	s1	610	CLA	CBB-CAB	4.35	1.51	1.30
48	S1	606	CHL	CBB-CAB	4.35	1.51	1.30
29	b1	617	CLA	CBB-CAB	4.35	1.51	1.30
29	b1	616	CLA	CBB-CAB	4.35	1.51	1.30
37	c	519	DGD	O1G-C1A	4.35	1.46	1.33
29	g	611	CLA	CBB-CAB	4.35	1.51	1.30
29	R1	612	CLA	CBB-CAB	4.35	1.51	1.30
31	c	516	BCR	C16-C17	-4.35	1.30	1.43
29	S1	610	CLA	CBB-CAB	4.34	1.51	1.30
29	c1	502	CLA	MG-ND	-4.34	1.97	2.05
48	N1	607	CHL	CBB-CAB	4.34	1.51	1.30
48	g1	601	CHL	CBB-CAB	4.34	1.51	1.30
29	R	608	CLA	CBB-CAB	4.34	1.51	1.30
29	b	606	CLA	CBB-CAB	4.34	1.51	1.30
29	g1	611	CLA	CBB-CAB	4.34	1.51	1.30
29	c1	503	CLA	CBB-CAB	4.34	1.51	1.30
29	s1	612	CLA	CBB-CAB	4.34	1.51	1.30
48	g1	607	CHL	CBB-CAB	4.34	1.51	1.30
29	C	506	CLA	MG-ND	-4.34	1.97	2.05
48	n	608	CHL	CBB-CAB	4.34	1.51	1.30
29	g	602	CLA	CBB-CAB	4.34	1.51	1.30
48	N	609	CHL	CBB-CAB	4.34	1.51	1.30
36	b1	620	C7Z	C8-C9	4.34	1.55	1.45
29	G1	614	CLA	CBB-CAB	4.34	1.51	1.30
29	G	614	CLA	CBB-CAB	4.33	1.51	1.30
29	G1	603	CLA	CBB-CAB	4.33	1.51	1.30
29	c1	507	CLA	CBB-CAB	4.33	1.51	1.30
48	Y1	609	CHL	CBB-CAB	4.33	1.51	1.30
29	G1	612	CLA	MG-ND	-4.33	1.97	2.05
29	G1	612	CLA	CBB-CAB	4.33	1.51	1.30
29	d1	403	CLA	CBB-CAB	4.33	1.51	1.30
29	c	513	CLA	MG-ND	-4.33	1.97	2.05
29	C1	512	CLA	CBB-CAB	4.33	1.51	1.30
29	b1	604	CLA	CBB-CAB	4.33	1.51	1.30
29	N1	610	CLA	CBB-CAB	4.33	1.51	1.30
48	N	608	CHL	CBB-CAB	4.33	1.51	1.30
29	C1	507	CLA	MG-ND	-4.33	1.97	2.05
45	H1	101	RRX	C12-C13	4.33	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	s1	606	CHL	CBB-CAB	4.33	1.51	1.30
48	r1	607	CHL	CBB-CAB	4.33	1.51	1.30
29	y1	613	CLA	CBB-CAB	4.33	1.51	1.30
29	B	604	CLA	MG-ND	-4.33	1.97	2.05
48	Y1	605	CHL	CBB-CAB	4.33	1.51	1.30
29	r1	609	CLA	CBB-CAB	4.32	1.51	1.30
29	B1	602	CLA	CBB-CAB	4.32	1.51	1.30
31	C	516	BCR	C16-C17	-4.32	1.30	1.43
29	c1	506	CLA	CBB-CAB	4.32	1.51	1.30
29	n1	612	CLA	CBB-CAB	4.32	1.51	1.30
29	g1	610	CLA	CBB-CAB	4.32	1.51	1.30
29	r	608	CLA	CBB-CAB	4.32	1.51	1.30
29	b1	611	CLA	CBB-CAB	4.32	1.51	1.30
29	b	610	CLA	CBB-CAB	4.32	1.51	1.30
29	b1	615	CLA	CBB-CAB	4.32	1.51	1.30
29	n1	614	CLA	CBB-CAB	4.32	1.51	1.30
48	g	605	CHL	CBB-CAB	4.32	1.51	1.30
29	G	603	CLA	CBB-CAB	4.32	1.51	1.30
29	S1	612	CLA	CBB-CAB	4.32	1.51	1.30
29	r	609	CLA	CBB-CAB	4.32	1.51	1.30
29	G1	613	CLA	CBB-CAB	4.32	1.51	1.30
48	n1	605	CHL	CBB-CAB	4.32	1.51	1.30
29	n1	603	CLA	CBB-CAB	4.32	1.51	1.30
29	y1	604	CLA	CBB-CAB	4.32	1.51	1.30
29	C	511	CLA	CBB-CAB	4.32	1.51	1.30
48	Y	601	CHL	CBB-CAB	4.32	1.51	1.30
29	r1	612	CLA	CBB-CAB	4.32	1.51	1.30
29	s1	605	CLA	CBB-CAB	4.32	1.51	1.30
29	c	508	CLA	MG-ND	-4.31	1.97	2.05
29	s1	611	CLA	MG-ND	-4.31	1.97	2.05
29	r1	610	CLA	CBB-CAB	4.31	1.51	1.30
48	G	601	CHL	CBB-CAB	4.31	1.51	1.30
29	b	604	CLA	MG-ND	-4.31	1.97	2.05
29	n1	613	CLA	CBB-CAB	4.31	1.51	1.30
29	C1	508	CLA	CBB-CAB	4.31	1.51	1.30
43	d	405	PL9	C6-C1	-4.31	1.40	1.48
29	N	602	CLA	CBB-CAB	4.31	1.51	1.30
29	c	506	CLA	CBB-CAB	4.31	1.51	1.30
29	s	609	CLA	CBB-CAB	4.31	1.51	1.30
29	R1	604	CLA	CBB-CAB	4.31	1.51	1.30
29	g1	603	CLA	CBB-CAB	4.31	1.51	1.30
29	A	410	CLA	MG-ND	-4.31	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	r	610	CLA	CBB-CAB	4.31	1.51	1.30
48	g	601	CHL	CBB-CAB	4.31	1.51	1.30
48	n	601	CHL	CBB-CAB	4.31	1.51	1.30
29	n	613	CLA	CBB-CAB	4.31	1.51	1.30
29	C1	507	CLA	CBB-CAB	4.31	1.51	1.30
29	G1	602	CLA	CBB-CAB	4.30	1.51	1.30
29	g1	612	CLA	CBB-CAB	4.30	1.51	1.30
29	A	405	CLA	CBB-CAB	4.30	1.51	1.30
48	g1	605	CHL	CBB-CAB	4.30	1.51	1.30
45	H	101	RRX	C27-C26	-4.30	1.44	1.51
29	N1	613	CLA	CBB-CAB	4.30	1.51	1.30
48	G	607	CHL	CBB-CAB	4.30	1.51	1.30
29	c1	512	CLA	CBB-CAB	4.30	1.51	1.30
29	d1	402	CLA	CBB-CAB	4.30	1.51	1.30
36	B	620	C7Z	C31-C30	4.30	1.56	1.43
29	S	605	CLA	CBB-CAB	4.30	1.51	1.30
29	s	603	CLA	CBB-CAB	4.30	1.51	1.30
29	s1	604	CLA	CBB-CAB	4.30	1.51	1.30
37	B1	623	DGD	O1G-C1A	4.30	1.45	1.33
29	B	609	CLA	MG-ND	-4.30	1.97	2.05
29	Y1	610	CLA	CBB-CAB	4.30	1.51	1.30
45	H1	101	RRX	C3-C4	4.30	1.66	1.52
48	g	607	CHL	CBB-CAB	4.30	1.51	1.30
36	b	620	C7Z	C4-C5	-4.30	1.44	1.51
29	r1	604	CLA	CBB-CAB	4.30	1.51	1.30
29	A1	407	CLA	MG-ND	-4.30	1.97	2.05
29	n1	611	CLA	CBB-CAB	4.30	1.51	1.30
29	n	612	CLA	CBB-CAB	4.30	1.51	1.30
29	A1	406	CLA	MG-ND	-4.30	1.97	2.05
29	r1	602	CLA	CBB-CAB	4.30	1.51	1.30
29	b1	613	CLA	CBB-CAB	4.30	1.51	1.30
29	g1	602	CLA	CBB-CAB	4.30	1.51	1.30
29	N	611	CLA	CBB-CAB	4.30	1.51	1.30
29	C1	501	CLA	CBB-CAB	4.30	1.51	1.30
29	y	604	CLA	CBB-CAB	4.30	1.51	1.30
29	B1	613	CLA	CBB-CAB	4.30	1.51	1.30
29	R1	602	CLA	CBB-CAB	4.30	1.51	1.30
48	s	606	CHL	CBB-CAB	4.30	1.51	1.30
48	y	601	CHL	CBB-CAB	4.30	1.51	1.30
29	B	608	CLA	CBB-CAB	4.30	1.51	1.30
29	g	612	CLA	CBB-CAB	4.30	1.51	1.30
29	C1	510	CLA	CBB-CAB	4.30	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R1	610	CLA	CBB-CAB	4.29	1.51	1.30
29	A1	405	CLA	CBB-CAB	4.29	1.51	1.30
29	B	610	CLA	CBB-CAB	4.29	1.51	1.30
29	y1	611	CLA	CBB-CAB	4.29	1.51	1.30
29	G1	610	CLA	CBB-CAB	4.29	1.51	1.30
29	c1	509	CLA	CBB-CAB	4.29	1.51	1.30
29	y1	610	CLA	CBB-CAB	4.29	1.51	1.30
29	y	610	CLA	CBB-CAB	4.29	1.51	1.30
29	S1	603	CLA	CBB-CAB	4.29	1.51	1.30
29	D1	402	CLA	CBB-CAB	4.29	1.51	1.30
29	y	613	CLA	CBB-CAB	4.29	1.51	1.30
29	Y1	613	CLA	CBB-CAB	4.29	1.51	1.30
29	C	510	CLA	CBB-CAB	4.29	1.51	1.30
29	N	612	CLA	CBB-CAB	4.29	1.51	1.30
29	C1	513	CLA	CBB-CAB	4.29	1.51	1.30
29	b1	610	CLA	CBB-CAB	4.29	1.51	1.30
29	b1	609	CLA	CBB-CAB	4.29	1.51	1.30
29	s	614	CLA	CBB-CAB	4.29	1.51	1.30
29	g1	614	CLA	CBB-CAB	4.29	1.51	1.30
29	s1	617	CLA	CBB-CAB	4.29	1.51	1.30
29	s	604	CLA	CBB-CAB	4.29	1.51	1.30
29	C	507	CLA	MG-ND	-4.29	1.97	2.05
29	S1	609	CLA	CBB-CAB	4.29	1.51	1.30
31	D	404	BCR	C16-C17	-4.29	1.30	1.43
29	S1	602	CLA	CBB-CAB	4.28	1.51	1.30
29	Y	608	CLA	CBB-CAB	4.28	1.51	1.30
29	B1	612	CLA	CBB-CAB	4.28	1.51	1.30
48	S	608	CHL	CBB-CAB	4.28	1.51	1.30
29	S	617	CLA	CBB-CAB	4.28	1.51	1.30
29	B1	608	CLA	CBB-CAB	4.28	1.51	1.30
29	b	608	CLA	CBB-CAB	4.28	1.51	1.30
29	B1	605	CLA	CBB-CAB	4.28	1.51	1.30
29	C	513	CLA	MG-ND	-4.28	1.97	2.05
29	y1	608	CLA	CBB-CAB	4.28	1.51	1.30
29	N1	611	CLA	CBB-CAB	4.28	1.51	1.30
29	y1	612	CLA	CBB-CAB	4.28	1.51	1.30
29	Y1	612	CLA	MG-ND	-4.28	1.97	2.05
29	y	608	CLA	CBB-CAB	4.28	1.51	1.30
29	a1	407	CLA	CBB-CAB	4.28	1.51	1.30
29	S1	614	CLA	MG-ND	-4.28	1.97	2.05
29	R1	603	CLA	MG-ND	-4.28	1.97	2.05
29	a1	405	CLA	CBB-CAB	4.28	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	R1	606	CHL	CBB-CAB	4.28	1.51	1.30
29	G	612	CLA	CBB-CAB	4.28	1.51	1.30
29	B	613	CLA	MG-ND	-4.28	1.97	2.05
29	n1	604	CLA	CBB-CAB	4.28	1.51	1.30
29	b	604	CLA	CBB-CAB	4.28	1.51	1.30
29	g	604	CLA	CBB-CAB	4.28	1.51	1.30
29	b	614	CLA	CBB-CAB	4.27	1.51	1.30
29	s1	609	CLA	CBB-CAB	4.27	1.51	1.30
48	y1	601	CHL	CBB-CAB	4.27	1.51	1.30
29	S	602	CLA	MG-ND	-4.27	1.97	2.05
29	Y	602	CLA	CBB-CAB	4.27	1.51	1.30
29	s	603	CLA	MG-ND	-4.27	1.97	2.05
29	N	614	CLA	CBB-CAB	4.27	1.51	1.30
29	r	612	CLA	CBB-CAB	4.27	1.51	1.30
29	S1	613	CLA	CBB-CAB	4.27	1.51	1.30
48	S1	607	CHL	CBB-CAB	4.27	1.51	1.30
29	n	611	CLA	CBB-CAB	4.27	1.51	1.30
48	S	607	CHL	CBB-CAB	4.27	1.51	1.30
29	n	614	CLA	CBB-CAB	4.27	1.51	1.30
29	S	604	CLA	CBB-CAB	4.27	1.51	1.30
48	n1	607	CHL	CBB-CAB	4.27	1.51	1.30
29	y1	603	CLA	CBB-CAB	4.27	1.51	1.30
29	g	603	CLA	CBB-CAB	4.27	1.51	1.30
29	G1	611	CLA	CBB-CAB	4.27	1.51	1.30
29	r	604	CLA	CBB-CAB	4.27	1.51	1.30
36	b	620	C7Z	C31-C30	4.27	1.56	1.43
29	C1	511	CLA	CBB-CAB	4.27	1.51	1.30
29	S	603	CLA	CBB-CAB	4.27	1.51	1.30
29	b	603	CLA	CBB-CAB	4.27	1.51	1.30
29	C1	502	CLA	CBB-CAB	4.26	1.51	1.30
29	s	617	CLA	CBB-CAB	4.26	1.51	1.30
29	b1	612	CLA	CBB-CAB	4.26	1.51	1.30
48	G	608	CHL	CBB-CAB	4.26	1.51	1.30
29	B	612	CLA	MG-ND	-4.26	1.97	2.05
29	C	508	CLA	CBB-CAB	4.26	1.51	1.30
29	R	612	CLA	CBB-CAB	4.26	1.51	1.30
48	G1	601	CHL	CBB-CAB	4.26	1.51	1.30
29	g1	604	CLA	CBB-CAB	4.26	1.51	1.30
29	s	605	CLA	CBB-CAB	4.26	1.51	1.30
29	s1	614	CLA	CBB-CAB	4.26	1.51	1.30
29	G	602	CLA	CBB-CAB	4.26	1.51	1.30
29	B	604	CLA	CBB-CAB	4.26	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	y1	607	CHL	CBB-CAB	4.26	1.51	1.30
29	c1	504	CLA	CBB-CAB	4.26	1.51	1.30
29	c	508	CLA	CBB-CAB	4.26	1.51	1.30
29	B1	617	CLA	MG-ND	-4.26	1.97	2.05
29	Y	604	CLA	CBB-CAB	4.26	1.51	1.30
48	G1	605	CHL	CBB-CAB	4.26	1.51	1.30
29	S	612	CLA	CBB-CAB	4.26	1.51	1.30
29	a1	406	CLA	CBB-CAB	4.26	1.51	1.30
29	C1	503	CLA	CBB-CAB	4.26	1.51	1.30
29	N	610	CLA	CBB-CAB	4.26	1.51	1.30
29	n	604	CLA	CBB-CAB	4.26	1.51	1.30
29	c	506	CLA	MG-ND	-4.26	1.97	2.05
29	b1	607	CLA	CBB-CAB	4.26	1.51	1.30
29	C	502	CLA	CBB-CAB	4.26	1.51	1.30
29	B1	609	CLA	CBB-CAB	4.26	1.51	1.30
31	B	618	BCR	C16-C17	-4.26	1.30	1.43
29	Y1	603	CLA	CBB-CAB	4.26	1.51	1.30
48	y	609	CHL	CBB-CAB	4.26	1.51	1.30
29	b	609	CLA	CBB-CAB	4.25	1.51	1.30
29	b1	608	CLA	MG-ND	-4.25	1.97	2.05
29	Y	611	CLA	CBB-CAB	4.25	1.51	1.30
29	r	602	CLA	CBB-CAB	4.25	1.51	1.30
29	C1	509	CLA	MG-ND	-4.25	1.97	2.05
29	c	512	CLA	CBB-CAB	4.25	1.51	1.30
29	R	602	CLA	CBB-CAB	4.25	1.51	1.30
29	N1	603	CLA	CBB-CAB	4.25	1.51	1.30
48	n1	601	CHL	CBB-CAB	4.25	1.51	1.30
29	c	507	CLA	MG-ND	-4.25	1.97	2.05
29	B	607	CLA	CBB-CAB	4.25	1.51	1.30
29	S1	617	CLA	CBB-CAB	4.25	1.51	1.30
29	S	609	CLA	CBB-CAB	4.25	1.51	1.30
29	C	507	CLA	CBB-CAB	4.25	1.51	1.30
29	g	614	CLA	CBB-CAB	4.25	1.51	1.30
29	B	602	CLA	CBB-CAB	4.25	1.51	1.30
29	r1	608	CLA	CBB-CAB	4.25	1.51	1.30
29	b1	612	CLA	MG-ND	-4.25	1.97	2.05
45	h1	101	RRX	C27-C26	-4.25	1.44	1.51
29	Y	610	CLA	CBB-CAB	4.25	1.51	1.30
29	R1	603	CLA	CBB-CAB	4.25	1.51	1.30
29	B	609	CLA	CBB-CAB	4.25	1.51	1.30
29	B1	610	CLA	CBB-CAB	4.25	1.51	1.30
29	G	610	CLA	CBB-CAB	4.24	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	615	CLA	CBB-CAB	4.24	1.51	1.30
29	N	604	CLA	CBB-CAB	4.24	1.51	1.30
29	C1	506	CLA	CBB-CAB	4.24	1.51	1.30
29	B1	603	CLA	CBB-CAB	4.24	1.51	1.30
29	B1	606	CLA	CBB-CAB	4.24	1.51	1.30
29	s1	603	CLA	CBB-CAB	4.24	1.51	1.30
29	C	503	CLA	CBB-CAB	4.24	1.51	1.30
29	n1	610	CLA	CBB-CAB	4.24	1.51	1.30
29	Y1	611	CLA	CBB-CAB	4.24	1.51	1.30
48	g1	608	CHL	CBB-CAB	4.24	1.51	1.30
29	Y	612	CLA	CBB-CAB	4.24	1.51	1.30
29	g	610	CLA	CBB-CAB	4.24	1.51	1.30
31	d	404	BCR	C16-C17	-4.24	1.30	1.43
29	R	610	CLA	CBB-CAB	4.24	1.51	1.30
29	c	507	CLA	CBB-CAB	4.24	1.51	1.30
29	R1	609	CLA	CBB-CAB	4.24	1.51	1.30
29	S1	614	CLA	CBB-CAB	4.24	1.51	1.30
29	s	613	CLA	CBB-CAB	4.24	1.51	1.30
29	c	511	CLA	CBB-CAB	4.23	1.51	1.30
48	n1	608	CHL	CBB-CAB	4.23	1.51	1.30
29	S	613	CLA	CBB-CAB	4.23	1.51	1.30
29	b	612	CLA	CBB-CAB	4.23	1.51	1.30
29	C	512	CLA	CBB-CAB	4.23	1.51	1.30
29	Y1	608	CLA	CBB-CAB	4.23	1.51	1.30
29	A	407	CLA	CBB-CAB	4.23	1.51	1.30
29	C1	509	CLA	CBB-CAB	4.23	1.51	1.30
29	c	509	CLA	CBB-CAB	4.23	1.51	1.30
29	B1	607	CLA	CBB-CAB	4.23	1.51	1.30
29	B1	615	CLA	CBB-CAB	4.23	1.51	1.30
29	G	611	CLA	CBB-CAB	4.23	1.51	1.30
29	b1	614	CLA	CBB-CAB	4.23	1.51	1.30
31	D1	404	BCR	C16-C17	-4.23	1.30	1.43
48	g1	606	CHL	CBB-CAB	4.23	1.51	1.30
29	b1	603	CLA	CBB-CAB	4.23	1.51	1.30
29	Y1	604	CLA	CBB-CAB	4.23	1.51	1.30
29	a	405	CLA	CBB-CAB	4.23	1.51	1.30
29	B	605	CLA	MG-ND	-4.23	1.97	2.05
29	R	604	CLA	CBB-CAB	4.23	1.51	1.30
29	n	602	CLA	CBB-CAB	4.23	1.51	1.30
29	S	610	CLA	CBB-CAB	4.23	1.51	1.30
29	b1	602	CLA	CBB-CAB	4.23	1.51	1.30
29	c1	502	CLA	CBB-CAB	4.23	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	611	CLA	MG-ND	-4.23	1.97	2.05
29	s1	612	CLA	MG-ND	-4.23	1.97	2.05
29	b	615	CLA	CBB-CAB	4.22	1.51	1.30
29	A1	407	CLA	CBB-CAB	4.22	1.51	1.30
29	S1	605	CLA	CBB-CAB	4.22	1.51	1.30
48	y1	605	CHL	CBB-CAB	4.22	1.51	1.30
29	C1	505	CLA	CBB-CAB	4.22	1.51	1.30
29	r1	610	CLA	MG-ND	-4.22	1.97	2.05
29	S	614	CLA	CBB-CAB	4.22	1.51	1.30
31	b1	619	BCR	C16-C17	-4.22	1.30	1.43
29	c1	505	CLA	CBB-CAB	4.22	1.51	1.30
29	c1	513	CLA	CBB-CAB	4.22	1.51	1.30
29	g	614	CLA	MG-ND	-4.22	1.97	2.05
29	a1	410	CLA	MG-ND	-4.22	1.97	2.05
29	b	607	CLA	CBB-CAB	4.22	1.51	1.30
53	r1	626	ERG	C16-C15	4.22	1.65	1.54
48	r	607	CHL	CBB-CAB	4.22	1.51	1.30
29	N1	612	CLA	CBB-CAB	4.22	1.51	1.30
29	B	611	CLA	CBB-CAB	4.22	1.51	1.30
29	N	603	CLA	CBB-CAB	4.22	1.51	1.30
48	s1	607	CHL	CBB-CAB	4.22	1.51	1.30
48	s1	601	CHL	CBB-CAB	4.21	1.51	1.30
29	Y	613	CLA	CBB-CAB	4.21	1.51	1.30
37	C1	518	DGD	O1G-C1A	4.21	1.45	1.33
29	S1	604	CLA	CBB-CAB	4.21	1.51	1.30
29	N1	604	CLA	CBB-CAB	4.21	1.51	1.30
45	H	101	RRX	C3-C4	4.21	1.65	1.52
29	C	509	CLA	CBB-CAB	4.21	1.51	1.30
29	c	513	CLA	CBB-CAB	4.21	1.51	1.30
48	Y1	606	CHL	CBB-CAB	4.21	1.51	1.30
45	H	101	RRX	C12-C13	4.21	1.55	1.45
29	S	602	CLA	CBB-CAB	4.21	1.51	1.30
37	C	519	DGD	O1G-C1A	4.21	1.45	1.33
31	C1	515	BCR	C16-C17	-4.21	1.30	1.43
51	G	623	NEX	C7-C8	4.21	1.39	1.32
29	s	612	CLA	CBB-CAB	4.21	1.51	1.30
29	c1	510	CLA	CBB-CAB	4.21	1.51	1.30
37	c1	520	DGD	O1G-C1A	4.21	1.45	1.33
29	D1	402	CLA	MG-ND	-4.21	1.97	2.05
29	b1	606	CLA	CBB-CAB	4.21	1.51	1.30
29	c1	510	CLA	MG-ND	-4.21	1.97	2.05
36	B1	620	C7Z	C11-C10	4.21	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	510	CLA	CBB-CAB	4.21	1.51	1.30
48	g	606	CHL	CBB-CAB	4.21	1.51	1.30
31	c1	514	BCR	C16-C17	-4.21	1.30	1.43
29	r1	603	CLA	CBB-CAB	4.20	1.51	1.30
29	a	407	CLA	CBB-CAB	4.20	1.51	1.30
31	C	517	BCR	C16-C17	-4.20	1.30	1.43
48	n	605	CHL	CBB-CAB	4.20	1.51	1.30
29	b	613	CLA	CBB-CAB	4.20	1.51	1.30
29	C	504	CLA	CBB-CAB	4.20	1.51	1.30
29	c1	513	CLA	MG-ND	-4.20	1.97	2.05
29	y1	614	CLA	MG-ND	-4.20	1.97	2.05
36	b1	620	C7Z	C11-C10	4.20	1.56	1.43
29	c	504	CLA	CBB-CAB	4.20	1.51	1.30
29	y	602	CLA	CBB-CAB	4.20	1.51	1.30
29	b	603	CLA	MG-ND	-4.20	1.97	2.05
29	c1	501	CLA	MG-ND	-4.20	1.97	2.05
29	N	613	CLA	CBB-CAB	4.20	1.51	1.30
29	b1	605	CLA	CBB-CAB	4.19	1.51	1.30
29	y	611	CLA	CBB-CAB	4.19	1.51	1.30
29	S1	611	CLA	CBB-CAB	4.19	1.51	1.30
29	Y1	614	CLA	CBB-CAB	4.19	1.51	1.30
29	c	503	CLA	CBB-CAB	4.19	1.51	1.30
29	C	506	CLA	CBB-CAB	4.19	1.51	1.30
43	d1	405	PL9	C7-C3	-4.19	1.47	1.51
29	B	612	CLA	CBB-CAB	4.19	1.51	1.30
29	y1	614	CLA	CBB-CAB	4.19	1.51	1.30
48	R1	607	CHL	CBB-CAB	4.19	1.51	1.30
29	Y	603	CLA	CBB-CAB	4.19	1.51	1.30
29	G	604	CLA	CBB-CAB	4.19	1.51	1.30
29	R	603	CLA	CBB-CAB	4.19	1.51	1.30
29	d	403	CLA	CBB-CAB	4.19	1.51	1.30
29	C1	504	CLA	CBB-CAB	4.19	1.51	1.30
48	y	605	CHL	CBB-CAB	4.19	1.51	1.30
37	C	518	DGD	O1G-C1A	4.19	1.45	1.33
29	G1	604	CLA	CBB-CAB	4.19	1.51	1.30
29	D	403	CLA	CBB-CAB	4.18	1.51	1.30
48	N1	609	CHL	CBB-CAB	4.18	1.51	1.30
45	h1	101	RRX	C3-C4	4.18	1.65	1.52
29	c	505	CLA	CBB-CAB	4.18	1.51	1.30
37	C1	520	DGD	O1G-C1A	4.18	1.45	1.33
29	B1	614	CLA	CBB-CAB	4.18	1.51	1.30
48	G	609	CHL	CBB-CAB	4.18	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c1	511	CLA	CBB-CAB	4.18	1.51	1.30
29	s1	610	CLA	MG-ND	-4.18	1.97	2.05
29	c	509	CLA	MG-ND	-4.18	1.97	2.05
48	Y	605	CHL	CBB-CAB	4.18	1.51	1.30
29	R1	610	CLA	MG-ND	-4.18	1.97	2.05
48	N	605	CHL	CBB-CAB	4.18	1.51	1.30
29	B1	616	CLA	CBB-CAB	4.18	1.51	1.30
29	R	609	CLA	CBB-CAB	4.18	1.51	1.30
29	y1	610	CLA	MG-ND	-4.18	1.97	2.05
29	S1	603	CLA	MG-ND	-4.18	1.97	2.05
45	h	101	RRX	C3-C4	4.18	1.65	1.52
29	S1	605	CLA	MG-ND	-4.18	1.97	2.05
29	n	603	CLA	CBB-CAB	4.18	1.51	1.30
29	C1	502	CLA	MG-ND	-4.18	1.97	2.05
29	Y1	613	CLA	MG-ND	-4.18	1.97	2.05
29	y	612	CLA	CBB-CAB	4.17	1.51	1.30
29	y	614	CLA	CBB-CAB	4.17	1.51	1.30
30	a1	408	PHO	C1D-C2D	4.17	1.44	1.39
45	H1	101	RRX	C27-C26	-4.17	1.44	1.51
48	G1	607	CHL	CBB-CAB	4.17	1.51	1.30
29	B	607	CLA	MG-ND	-4.17	1.97	2.05
29	y1	611	CLA	MG-ND	-4.17	1.97	2.05
29	A1	410	CLA	CBB-CAB	4.17	1.51	1.30
29	g1	613	CLA	CBB-CAB	4.17	1.51	1.30
29	d	402	CLA	CBB-CAB	4.17	1.50	1.30
29	B	605	CLA	CBB-CAB	4.17	1.50	1.30
29	s	602	CLA	CBB-CAB	4.17	1.50	1.30
48	G1	608	CHL	CBB-CAB	4.16	1.50	1.30
29	b	602	CLA	CBB-CAB	4.16	1.50	1.30
48	Y	609	CHL	CBB-CAB	4.16	1.50	1.30
31	b	618	BCR	C16-C17	-4.16	1.30	1.43
48	N	601	CHL	CBB-CAB	4.16	1.50	1.30
48	r	606	CHL	CBB-CAB	4.16	1.50	1.30
29	A	406	CLA	CBB-CAB	4.16	1.50	1.30
29	A	406	CLA	MG-ND	-4.16	1.97	2.05
29	s	611	CLA	CBB-CAB	4.16	1.50	1.30
29	g	603	CLA	MG-ND	-4.16	1.97	2.05
29	B1	604	CLA	MG-ND	-4.16	1.97	2.05
29	Y1	602	CLA	CBB-CAB	4.16	1.50	1.30
48	n	609	CHL	CBB-CAB	4.16	1.50	1.30
29	g	613	CLA	CBB-CAB	4.15	1.50	1.30
29	a1	407	CLA	MG-ND	-4.15	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	610	CLA	CBB-CAB	4.15	1.50	1.30
29	B	613	CLA	CBB-CAB	4.15	1.50	1.30
29	b	616	CLA	CBB-CAB	4.15	1.50	1.30
48	R	607	CHL	CBB-CAB	4.15	1.50	1.30
45	h1	101	RRX	C12-C13	4.15	1.54	1.45
29	c1	508	CLA	MG-ND	-4.15	1.97	2.05
29	c	502	CLA	CBB-CAB	4.15	1.50	1.30
29	G	613	CLA	CBB-CAB	4.15	1.50	1.30
48	r1	606	CHL	CBB-CAB	4.15	1.50	1.30
29	B	616	CLA	CBB-CAB	4.15	1.50	1.30
29	s	604	CLA	MG-ND	-4.14	1.97	2.05
31	B1	619	BCR	C16-C17	-4.14	1.30	1.43
29	b	607	CLA	MG-ND	-4.14	1.97	2.05
29	C	513	CLA	CBB-CAB	4.14	1.50	1.30
29	D	402	CLA	CBB-CAB	4.14	1.50	1.30
29	S	611	CLA	CBB-CAB	4.14	1.50	1.30
29	c	512	CLA	MG-ND	-4.14	1.97	2.05
29	B1	611	CLA	MG-ND	-4.14	1.97	2.05
29	b1	613	CLA	MG-ND	-4.14	1.97	2.05
29	B	603	CLA	CBB-CAB	4.14	1.50	1.30
29	N1	604	CLA	MG-ND	-4.13	1.97	2.05
29	B	617	CLA	CBB-CAB	4.13	1.50	1.30
29	S	603	CLA	MG-ND	-4.13	1.97	2.05
29	d	402	CLA	MG-ND	-4.13	1.97	2.05
29	c	501	CLA	CBB-CAB	4.13	1.50	1.30
48	n	607	CHL	CBB-CAB	4.13	1.50	1.30
29	B1	614	CLA	MG-ND	-4.13	1.97	2.05
29	C	501	CLA	CBB-CAB	4.13	1.50	1.30
29	b1	614	CLA	MG-ND	-4.13	1.97	2.05
29	Y	614	CLA	CBB-CAB	4.13	1.50	1.30
29	g1	613	CLA	MG-ND	-4.13	1.97	2.05
29	g	610	CLA	MG-ND	-4.13	1.97	2.05
29	D1	403	CLA	MG-ND	-4.12	1.97	2.05
29	D	402	CLA	MG-ND	-4.12	1.97	2.05
29	C1	501	CLA	MG-ND	-4.12	1.97	2.05
29	G1	604	CLA	MG-ND	-4.12	1.97	2.05
45	H1	101	RRX	C20-C21	4.12	1.56	1.43
37	c	520	DGD	O1G-C1A	4.12	1.45	1.33
48	s1	608	CHL	CBB-CAB	4.12	1.50	1.30
29	G1	602	CLA	MG-ND	-4.12	1.97	2.05
29	B	617	CLA	C1C-NC	-4.12	1.31	1.37
37	c	518	DGD	O1G-C1A	4.12	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B1	613	CLA	MG-ND	-4.12	1.97	2.05
29	b	605	CLA	CBB-CAB	4.12	1.50	1.30
29	Y1	612	CLA	CBB-CAB	4.12	1.50	1.30
29	D1	403	CLA	CBB-CAB	4.12	1.50	1.30
29	a	405	CLA	MG-ND	-4.12	1.97	2.05
29	B1	617	CLA	CBB-CAB	4.12	1.50	1.30
29	c1	512	CLA	MG-ND	-4.12	1.97	2.05
37	C	520	DGD	O1G-C1A	4.12	1.45	1.33
29	s1	611	CLA	CBB-CAB	4.12	1.50	1.30
29	C	509	CLA	MG-ND	-4.11	1.97	2.05
29	G1	611	CLA	MG-ND	-4.11	1.97	2.05
29	b	612	CLA	C1C-NC	-4.11	1.31	1.37
29	C	506	CLA	C1C-NC	-4.11	1.31	1.37
29	r	602	CLA	MG-ND	-4.11	1.97	2.05
29	C1	503	CLA	MG-ND	-4.11	1.97	2.05
29	b	617	CLA	CBB-CAB	4.11	1.50	1.30
29	B	603	CLA	MG-ND	-4.10	1.97	2.05
29	B	610	CLA	MG-ND	-4.10	1.97	2.05
53	R1	626	ERG	C16-C15	4.10	1.65	1.54
48	n	606	CHL	CBB-CAB	4.10	1.50	1.30
29	B1	606	CLA	MG-ND	-4.10	1.97	2.05
29	Y	614	CLA	MG-ND	-4.10	1.97	2.05
29	N	604	CLA	MG-ND	-4.10	1.97	2.05
29	b1	617	CLA	MG-ND	-4.10	1.97	2.05
29	C	512	CLA	MG-ND	-4.10	1.97	2.05
29	d1	402	CLA	MG-ND	-4.10	1.97	2.05
29	S1	604	CLA	MG-ND	-4.10	1.97	2.05
29	G1	610	CLA	MG-ND	-4.09	1.97	2.05
53	r	626	ERG	C16-C15	4.09	1.65	1.54
29	n	602	CLA	MG-ND	-4.09	1.97	2.05
29	a1	410	CLA	CBB-CAB	4.09	1.50	1.30
48	g	608	CHL	CBB-CAB	4.09	1.50	1.30
29	y	603	CLA	CBB-CAB	4.09	1.50	1.30
31	C1	517	BCR	C16-C17	-4.09	1.30	1.43
29	s	609	CLA	MG-ND	-4.09	1.97	2.05
31	d1	404	BCR	C16-C17	-4.09	1.30	1.43
29	C1	506	CLA	MG-ND	-4.08	1.97	2.05
29	r	603	CLA	CBB-CAB	4.08	1.50	1.30
29	A1	406	CLA	CBB-CAB	4.08	1.50	1.30
29	B1	610	CLA	MG-ND	-4.08	1.97	2.05
29	s	611	CLA	MG-ND	-4.08	1.97	2.05
29	g1	603	CLA	MG-ND	-4.08	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	N	607	CHL	CBB-CAB	4.08	1.50	1.30
48	S	606	CHL	CBB-CAB	4.08	1.50	1.30
36	B	620	C7Z	C11-C10	4.08	1.56	1.43
29	S	611	CLA	MG-ND	-4.08	1.97	2.05
29	N1	613	CLA	MG-ND	-4.08	1.97	2.05
29	C	510	CLA	MG-ND	-4.08	1.97	2.05
29	C	505	CLA	CBB-CAB	4.08	1.50	1.30
29	a	406	CLA	CBB-CAB	4.08	1.50	1.30
29	Y1	602	CLA	MG-ND	-4.07	1.97	2.05
30	a1	409	PHO	C1D-C2D	4.07	1.44	1.39
29	R1	602	CLA	MG-ND	-4.07	1.97	2.05
29	s	602	CLA	MG-ND	-4.07	1.97	2.05
29	A	410	CLA	CBB-CAB	4.07	1.50	1.30
29	N	613	CLA	MG-ND	-4.06	1.97	2.05
29	R	610	CLA	MG-ND	-4.06	1.97	2.05
29	y	608	CLA	MG-ND	-4.06	1.97	2.05
31	C1	514	BCR	C16-C17	-4.06	1.30	1.43
29	R	609	CLA	MG-ND	-4.06	1.97	2.05
48	Y	606	CHL	CBB-CAB	4.06	1.50	1.30
29	B	606	CLA	MG-ND	-4.05	1.97	2.05
29	G	604	CLA	MG-ND	-4.05	1.97	2.05
29	n	613	CLA	MG-ND	-4.05	1.97	2.05
29	B1	615	CLA	MG-ND	-4.05	1.97	2.05
29	b1	615	CLA	MG-ND	-4.05	1.97	2.05
29	s1	617	CLA	MG-ND	-4.05	1.97	2.05
29	y	613	CLA	MG-ND	-4.05	1.97	2.05
29	C	508	CLA	C1C-NC	-4.05	1.31	1.37
48	N1	606	CHL	CBB-CAB	4.04	1.50	1.30
29	Y	608	CLA	MG-ND	-4.04	1.97	2.05
37	C1	519	DGD	O1G-C1A	4.04	1.45	1.33
29	N	614	CLA	MG-ND	-4.04	1.97	2.05
45	h	101	RRX	C23-C22	4.03	1.54	1.45
29	g1	602	CLA	MG-ND	-4.03	1.97	2.05
29	c	502	CLA	MG-ND	-4.03	1.97	2.05
29	R	602	CLA	MG-ND	-4.03	1.97	2.05
29	B1	608	CLA	MG-ND	-4.03	1.97	2.05
41	c1	527	LMK	O2-C4	4.03	1.43	1.30
29	y1	603	CLA	MG-ND	-4.03	1.97	2.05
29	B	615	CLA	MG-ND	-4.03	1.97	2.05
29	S	610	CLA	MG-ND	-4.03	1.97	2.05
36	b1	620	C7Z	C15-C14	4.03	1.55	1.43
29	N1	614	CLA	MG-ND	-4.02	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A1	408	PHO	C1D-C2D	4.02	1.44	1.39
48	y	606	CHL	CBB-CAB	4.02	1.50	1.30
29	n	604	CLA	MG-ND	-4.02	1.97	2.05
29	r1	609	CLA	MG-ND	-4.02	1.97	2.05
29	a	410	CLA	MG-ND	-4.02	1.97	2.05
29	C1	512	CLA	MG-ND	-4.02	1.97	2.05
29	y	611	CLA	MG-ND	-4.02	1.97	2.05
29	n1	611	CLA	MG-ND	-4.02	1.97	2.05
29	g	612	CLA	MG-ND	-4.02	1.97	2.05
29	G	610	CLA	MG-ND	-4.02	1.97	2.05
29	g1	614	CLA	MG-ND	-4.02	1.97	2.05
41	C	527	LMK	O2-C4	4.02	1.43	1.30
48	Y	607	CHL	CBB-CAB	4.01	1.50	1.30
29	d	403	CLA	MG-ND	-4.01	1.97	2.05
29	b1	607	CLA	MG-ND	-4.01	1.97	2.05
29	a	406	CLA	MG-ND	-4.01	1.97	2.05
29	c	503	CLA	MG-ND	-4.01	1.97	2.05
45	H1	101	RRX	C15-C14	4.01	1.55	1.43
29	b	617	CLA	MG-ND	-4.01	1.97	2.05
29	C	502	CLA	MG-ND	-4.01	1.97	2.05
29	b1	609	CLA	MG-ND	-4.01	1.97	2.05
29	Y	612	CLA	MG-ND	-4.01	1.97	2.05
29	C1	510	CLA	MG-ND	-4.00	1.97	2.05
29	b	611	CLA	C1C-NC	-4.00	1.31	1.37
41	C1	527	LMK	O2-C4	4.00	1.43	1.30
29	c	510	CLA	MG-ND	-4.00	1.97	2.05
29	N1	612	CLA	MG-ND	-4.00	1.97	2.05
29	S	614	CLA	MG-ND	-4.00	1.97	2.05
29	B1	612	CLA	MG-ND	-4.00	1.97	2.05
29	a1	406	CLA	MG-ND	-4.00	1.97	2.05
29	y1	612	CLA	MG-ND	-4.00	1.97	2.05
48	s	608	CHL	CBB-CAB	4.00	1.50	1.30
29	S	612	CLA	MG-ND	-3.99	1.97	2.05
29	s	610	CLA	MG-ND	-3.99	1.97	2.05
29	S1	617	CLA	MG-ND	-3.99	1.97	2.05
29	b1	606	CLA	MG-ND	-3.99	1.97	2.05
29	c1	509	CLA	MG-ND	-3.99	1.97	2.05
29	b	606	CLA	C1C-NC	-3.99	1.31	1.37
29	r	612	CLA	MG-ND	-3.99	1.97	2.05
29	A	405	CLA	MG-ND	-3.99	1.97	2.05
29	b	612	CLA	MG-ND	-3.99	1.97	2.05
29	C1	504	CLA	MG-ND	-3.99	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y1	610	CLA	MG-ND	-3.99	1.97	2.05
29	b	611	CLA	MG-ND	-3.99	1.97	2.05
29	c	511	CLA	MG-ND	-3.99	1.97	2.05
29	s	612	CLA	MG-ND	-3.98	1.97	2.05
29	Y	613	CLA	MG-ND	-3.98	1.97	2.05
53	r1	626	ERG	C13-C17	3.98	1.62	1.55
29	a	410	CLA	CBB-CAB	3.98	1.50	1.30
48	s	607	CHL	CBB-CAB	3.98	1.50	1.30
30	A1	409	PHO	C1D-C2D	3.97	1.44	1.39
36	b	620	C7Z	C8-C9	3.97	1.54	1.45
29	G1	603	CLA	MG-ND	-3.97	1.97	2.05
29	R1	604	CLA	MG-ND	-3.97	1.97	2.05
29	b1	603	CLA	MG-ND	-3.97	1.97	2.05
29	b1	616	CLA	MG-ND	-3.97	1.97	2.05
29	A1	410	CLA	MG-ND	-3.97	1.97	2.05
29	B	617	CLA	MG-ND	-3.97	1.97	2.05
29	y	612	CLA	MG-ND	-3.96	1.97	2.05
29	g	602	CLA	MG-ND	-3.96	1.97	2.05
29	r	610	CLA	MG-ND	-3.96	1.97	2.05
29	S1	602	CLA	MG-ND	-3.96	1.97	2.05
29	b1	604	CLA	MG-ND	-3.96	1.97	2.05
29	c	505	CLA	C1C-NC	-3.96	1.31	1.37
29	Y1	604	CLA	MG-ND	-3.96	1.97	2.05
29	R	604	CLA	MG-ND	-3.96	1.97	2.05
29	B1	602	CLA	MG-ND	-3.96	1.97	2.05
29	N1	602	CLA	MG-ND	-3.96	1.97	2.05
29	S	613	CLA	MG-ND	-3.95	1.98	2.05
29	Y1	614	CLA	MG-ND	-3.95	1.98	2.05
29	b	616	CLA	MG-ND	-3.95	1.98	2.05
41	c	527	LMK	O2-C4	3.95	1.43	1.30
29	S1	612	CLA	MG-ND	-3.95	1.98	2.05
29	r1	604	CLA	MG-ND	-3.95	1.98	2.05
48	n1	606	CHL	CBB-CAB	3.95	1.49	1.30
29	B	612	CLA	C1C-NC	-3.95	1.31	1.37
45	H	101	RRX	C23-C22	3.94	1.54	1.45
48	N	606	CHL	CBB-CAB	3.94	1.49	1.30
29	S	605	CLA	MG-ND	-3.94	1.98	2.05
29	b	606	CLA	MG-ND	-3.94	1.98	2.05
36	b1	620	C7Z	C22-C21	3.94	1.67	1.54
48	G	606	CHL	CBB-CAB	3.94	1.49	1.30
31	c1	517	BCR	C16-C17	-3.94	1.31	1.43
31	b1	618	BCR	C16-C17	-3.93	1.31	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G	613	CLA	MG-ND	-3.93	1.98	2.05
29	Y1	611	CLA	MG-ND	-3.93	1.98	2.05
29	b	613	CLA	MG-ND	-3.93	1.98	2.05
29	c1	504	CLA	MG-ND	-3.93	1.98	2.05
29	A1	405	CLA	MG-ND	-3.93	1.98	2.05
29	y	602	CLA	MG-ND	-3.93	1.98	2.05
29	C1	513	CLA	MG-ND	-3.93	1.98	2.05
29	a	407	CLA	MG-ND	-3.93	1.98	2.05
29	R	608	CLA	MG-ND	-3.93	1.98	2.05
29	S1	610	CLA	MG-ND	-3.92	1.98	2.05
29	c	502	CLA	C1C-NC	-3.92	1.31	1.37
48	s	601	CHL	CBB-CAB	3.92	1.49	1.30
29	s	617	CLA	MG-ND	-3.92	1.98	2.05
29	A	410	CLA	C1C-NC	-3.92	1.31	1.37
29	b1	610	CLA	MG-ND	-3.92	1.98	2.05
29	y	604	CLA	MG-ND	-3.92	1.98	2.05
29	B	611	CLA	C1C-NC	-3.92	1.32	1.37
29	B1	603	CLA	MG-ND	-3.92	1.98	2.05
29	s1	614	CLA	MG-ND	-3.92	1.98	2.05
29	N	602	CLA	MG-ND	-3.92	1.98	2.05
29	Y	602	CLA	MG-ND	-3.92	1.98	2.05
29	n1	603	CLA	MG-ND	-3.92	1.98	2.05
48	R	606	CHL	CBB-CAB	3.92	1.49	1.30
29	n1	614	CLA	MG-ND	-3.91	1.98	2.05
29	s1	605	CLA	MG-ND	-3.91	1.98	2.05
29	N1	603	CLA	MG-ND	-3.91	1.98	2.05
29	N	612	CLA	MG-ND	-3.91	1.98	2.05
29	s	605	CLA	MG-ND	-3.91	1.98	2.05
29	c	508	CLA	C1C-NC	-3.91	1.32	1.37
53	R	626	ERG	C16-C15	3.91	1.64	1.54
29	S	609	CLA	MG-ND	-3.91	1.98	2.05
29	n1	610	CLA	MG-ND	-3.91	1.98	2.05
29	r1	602	CLA	MG-ND	-3.91	1.98	2.05
36	B1	620	C7Z	C15-C14	3.90	1.55	1.43
29	G1	602	CLA	C1C-NC	-3.90	1.32	1.37
29	y	614	CLA	MG-ND	-3.90	1.98	2.05
48	S1	601	CHL	CBB-CAB	3.90	1.49	1.30
29	G1	613	CLA	MG-ND	-3.90	1.98	2.05
29	c1	506	CLA	MG-ND	-3.90	1.98	2.05
29	n1	604	CLA	MG-ND	-3.90	1.98	2.05
29	b	605	CLA	MG-ND	-3.90	1.98	2.05
29	c1	507	CLA	MG-ND	-3.90	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y1	603	CLA	MG-ND	-3.90	1.98	2.05
29	r	609	CLA	MG-ND	-3.90	1.98	2.05
29	R	610	CLA	C1C-NC	-3.89	1.32	1.37
29	B1	605	CLA	MG-ND	-3.89	1.98	2.05
44	f	101	HEM	FE-NA	3.89	2.08	1.95
29	y1	608	CLA	MG-ND	-3.89	1.98	2.05
29	A1	406	CLA	C4B-NB	-3.89	1.33	1.37
29	n	612	CLA	MG-ND	-3.89	1.98	2.05
29	Y	610	CLA	MG-ND	-3.89	1.98	2.05
29	B	608	CLA	MG-ND	-3.89	1.98	2.05
29	G	602	CLA	MG-ND	-3.89	1.98	2.05
29	s	614	CLA	MG-ND	-3.89	1.98	2.05
29	a1	405	CLA	MG-ND	-3.88	1.98	2.05
29	c1	503	CLA	MG-ND	-3.88	1.98	2.05
36	b	620	C7Z	C11-C10	3.88	1.55	1.43
29	Y	604	CLA	MG-ND	-3.88	1.98	2.05
29	N1	610	CLA	MG-ND	-3.88	1.98	2.05
29	b	602	CLA	MG-ND	-3.88	1.98	2.05
29	d1	403	CLA	MG-ND	-3.88	1.98	2.05
29	B1	617	CLA	C1C-NC	-3.88	1.32	1.37
29	C	501	CLA	MG-ND	-3.87	1.98	2.05
29	N	611	CLA	MG-ND	-3.87	1.98	2.05
29	n	614	CLA	MG-ND	-3.87	1.98	2.05
29	s1	604	CLA	MG-ND	-3.87	1.98	2.05
36	B1	620	C7Z	C22-C21	3.87	1.66	1.54
45	h1	101	RRX	C20-C21	3.87	1.55	1.43
29	n	610	CLA	MG-ND	-3.87	1.98	2.05
29	b	614	CLA	MG-ND	-3.86	1.98	2.05
29	N	610	CLA	MG-ND	-3.86	1.98	2.05
45	h	101	RRX	C12-C13	3.86	1.54	1.45
36	b	620	C7Z	C22-C21	3.86	1.66	1.54
29	C1	502	CLA	C1C-NC	-3.86	1.32	1.37
36	B	620	C7Z	C8-C9	3.86	1.54	1.45
29	y1	602	CLA	MG-ND	-3.85	1.98	2.05
31	c1	516	BCR	C16-C17	-3.85	1.31	1.43
29	y1	604	CLA	MG-ND	-3.85	1.98	2.05
29	b	608	CLA	MG-ND	-3.85	1.98	2.05
29	R1	609	CLA	MG-ND	-3.85	1.98	2.05
29	N1	611	CLA	MG-ND	-3.85	1.98	2.05
29	B	614	CLA	MG-ND	-3.85	1.98	2.05
29	n	603	CLA	MG-ND	-3.84	1.98	2.05
29	C	503	CLA	MG-ND	-3.84	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	605	CLA	C1C-NC	-3.84	1.32	1.37
29	C1	504	CLA	C1C-NC	-3.84	1.32	1.37
29	g	611	CLA	MG-ND	-3.84	1.98	2.05
29	B1	607	CLA	MG-ND	-3.83	1.98	2.05
29	B1	606	CLA	C1C-NC	-3.83	1.32	1.37
29	b	615	CLA	MG-ND	-3.83	1.98	2.05
29	C	502	CLA	C1C-NC	-3.83	1.32	1.37
29	n1	612	CLA	MG-ND	-3.83	1.98	2.05
29	R	612	CLA	MG-ND	-3.82	1.98	2.05
29	b	610	CLA	MG-ND	-3.82	1.98	2.05
29	g1	611	CLA	MG-ND	-3.82	1.98	2.05
29	c	501	CLA	MG-ND	-3.82	1.98	2.05
36	B1	620	C7Z	C27-C26	3.82	1.58	1.45
29	b	605	CLA	C1C-NC	-3.82	1.32	1.37
29	Y	603	CLA	MG-ND	-3.81	1.98	2.05
29	b1	616	CLA	C1C-NC	-3.81	1.32	1.37
29	S1	609	CLA	MG-ND	-3.81	1.98	2.05
29	n1	613	CLA	MG-ND	-3.81	1.98	2.05
29	r	604	CLA	MG-ND	-3.80	1.98	2.05
29	A	407	CLA	MG-ND	-3.80	1.98	2.05
29	G1	602	CLA	C4B-NB	-3.80	1.33	1.37
29	g1	610	CLA	MG-ND	-3.80	1.98	2.05
29	S	613	CLA	C1C-NC	-3.80	1.32	1.37
29	b1	613	CLA	C1C-NC	-3.80	1.32	1.37
29	n	611	CLA	MG-ND	-3.80	1.98	2.05
29	G	611	CLA	MG-ND	-3.79	1.98	2.05
29	S1	610	CLA	C1C-NC	-3.79	1.32	1.37
29	Y	602	CLA	C1C-NC	-3.79	1.32	1.37
29	S	604	CLA	MG-ND	-3.79	1.98	2.05
29	C	504	CLA	MG-ND	-3.79	1.98	2.05
31	B1	618	BCR	C16-C17	-3.78	1.31	1.43
29	C1	511	CLA	MG-ND	-3.78	1.98	2.05
29	y1	613	CLA	MG-ND	-3.78	1.98	2.05
36	b1	620	C7Z	C35-C34	3.78	1.55	1.43
29	c1	511	CLA	MG-ND	-3.78	1.98	2.05
29	B	602	CLA	MG-ND	-3.78	1.98	2.05
29	A	406	CLA	C1C-NC	-3.77	1.32	1.37
45	H	101	RRX	C20-C21	3.77	1.55	1.43
29	g	604	CLA	MG-ND	-3.77	1.98	2.05
36	B1	620	C7Z	C35-C34	3.77	1.55	1.43
29	R1	608	CLA	MG-ND	-3.77	1.98	2.05
29	S	617	CLA	MG-ND	-3.77	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	613	CLA	MG-ND	-3.77	1.98	2.05
29	s1	603	CLA	MG-ND	-3.77	1.98	2.05
29	A	405	CLA	C1C-NC	-3.77	1.32	1.37
47	i	101	4RF	O18-C16	3.77	1.44	1.33
29	G1	612	CLA	C1C-NC	-3.76	1.32	1.37
29	Y	611	CLA	MG-ND	-3.76	1.98	2.05
48	S	601	CHL	CBB-CAB	3.76	1.48	1.30
29	b1	602	CLA	MG-ND	-3.76	1.98	2.05
29	B	616	CLA	MG-ND	-3.76	1.98	2.05
29	g	611	CLA	C1C-NC	-3.75	1.32	1.37
29	a1	410	CLA	C1C-NC	-3.75	1.32	1.37
29	s1	613	CLA	MG-ND	-3.75	1.98	2.05
29	c1	505	CLA	MG-ND	-3.75	1.98	2.05
29	C	504	CLA	C1C-NC	-3.75	1.32	1.37
29	S1	614	CLA	C1C-NC	-3.75	1.32	1.37
29	C	511	CLA	MG-ND	-3.74	1.98	2.05
29	g1	604	CLA	MG-ND	-3.74	1.98	2.05
29	r1	608	CLA	C1C-NC	-3.74	1.32	1.37
29	r	608	CLA	MG-ND	-3.74	1.98	2.05
29	R1	612	CLA	MG-ND	-3.74	1.98	2.05
29	D	403	CLA	MG-ND	-3.74	1.98	2.05
29	C	509	CLA	C1C-NC	-3.74	1.32	1.37
39	B1	625	DGA	OG2-CB1	3.74	1.44	1.34
29	C	505	CLA	C1C-NC	-3.74	1.32	1.37
29	C	501	CLA	C1C-NC	-3.74	1.32	1.37
29	g	610	CLA	C1C-NC	-3.74	1.32	1.37
29	r1	603	CLA	MG-ND	-3.74	1.98	2.05
29	G	614	CLA	MG-ND	-3.73	1.98	2.05
29	B1	616	CLA	MG-ND	-3.73	1.98	2.05
29	d1	402	CLA	C1C-NC	-3.73	1.32	1.37
29	R	610	CLA	C4B-NB	-3.73	1.33	1.37
29	A1	406	CLA	C1C-NC	-3.72	1.32	1.37
39	B	625	DGA	OG2-CB1	3.72	1.44	1.34
29	g	613	CLA	MG-ND	-3.72	1.98	2.05
29	A1	407	CLA	C1C-NC	-3.72	1.32	1.37
29	g	612	CLA	C1C-NC	-3.72	1.32	1.37
29	s	613	CLA	MG-ND	-3.72	1.98	2.05
29	N	603	CLA	MG-ND	-3.72	1.98	2.05
29	s1	602	CLA	MG-ND	-3.71	1.98	2.05
29	C1	501	CLA	C1C-NC	-3.71	1.32	1.37
29	A	410	CLA	C4B-NB	-3.71	1.33	1.37
29	r1	612	CLA	MG-ND	-3.71	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	620	C7Z	C21-C26	-3.71	1.48	1.53
29	A	407	CLA	C1C-NC	-3.70	1.32	1.37
36	B	620	C7Z	C22-C21	3.70	1.66	1.54
29	R	602	CLA	C1C-NC	-3.70	1.32	1.37
29	B	608	CLA	C1C-NC	-3.70	1.32	1.37
29	c	504	CLA	C1C-NC	-3.70	1.32	1.37
36	B	620	C7Z	C27-C26	3.70	1.58	1.45
36	b	620	C7Z	C15-C14	3.70	1.54	1.43
30	a	409	PHO	C1D-C2D	3.70	1.43	1.39
39	C1	524	DGA	OG2-CB1	3.69	1.44	1.34
29	y	610	CLA	MG-ND	-3.69	1.98	2.05
39	b	625	DGA	OG2-CB1	3.69	1.44	1.34
29	y	602	CLA	C1C-NC	-3.68	1.32	1.37
29	G	612	CLA	MG-ND	-3.68	1.98	2.05
29	c1	502	CLA	C1C-NC	-3.68	1.32	1.37
29	G	610	CLA	C1C-NC	-3.68	1.32	1.37
29	C	512	CLA	C1C-NC	-3.68	1.32	1.37
29	b1	617	CLA	C1C-NC	-3.67	1.32	1.37
29	D	402	CLA	C1C-NC	-3.67	1.32	1.37
29	G1	614	CLA	MG-ND	-3.67	1.98	2.05
29	R	608	CLA	C1C-NC	-3.67	1.32	1.37
29	S	614	CLA	C1C-NC	-3.67	1.32	1.37
29	y	603	CLA	MG-ND	-3.67	1.98	2.05
29	c	507	CLA	C4B-NB	-3.67	1.33	1.37
29	G	603	CLA	MG-ND	-3.66	1.98	2.05
45	H	101	RRX	C15-C14	3.66	1.54	1.43
29	a1	410	CLA	C4B-NB	-3.66	1.33	1.37
29	g1	612	CLA	MG-ND	-3.65	1.98	2.05
29	c	504	CLA	MG-ND	-3.65	1.98	2.05
29	b1	604	CLA	C1C-NC	-3.64	1.32	1.37
29	b1	612	CLA	C1C-NC	-3.64	1.32	1.37
29	B	613	CLA	C1C-NC	-3.64	1.32	1.37
29	G1	603	CLA	C1C-NC	-3.64	1.32	1.37
36	B	620	C7Z	C15-C14	3.64	1.54	1.43
45	h1	101	RRX	C15-C14	3.64	1.54	1.43
29	R	609	CLA	C1C-NC	-3.63	1.32	1.37
29	y1	610	CLA	C1C-NC	-3.63	1.32	1.37
29	b	604	CLA	C1C-NC	-3.63	1.32	1.37
29	n1	602	CLA	MG-ND	-3.63	1.98	2.05
29	G1	604	CLA	C1C-NC	-3.63	1.32	1.37
29	B	610	CLA	C1C-NC	-3.63	1.32	1.37
36	b1	620	C7Z	C27-C26	3.63	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a1	407	CLA	C1C-NC	-3.62	1.32	1.37
29	A1	405	CLA	C1C-NC	-3.62	1.32	1.37
30	A	409	PHO	C1D-C2D	3.62	1.43	1.39
39	b1	625	DGA	OG2-CB1	3.62	1.44	1.34
29	S1	609	CLA	C1C-NC	-3.62	1.32	1.37
47	K	101	4RF	O18-C16	3.62	1.43	1.33
29	A1	410	CLA	C1C-NC	-3.62	1.32	1.37
29	b	617	CLA	C1C-NC	-3.62	1.32	1.37
29	r1	608	CLA	MG-ND	-3.62	1.98	2.05
29	n1	611	CLA	C1C-NC	-3.62	1.32	1.37
29	S1	613	CLA	C1C-NC	-3.61	1.32	1.37
29	Y1	604	CLA	C1C-NC	-3.61	1.32	1.37
29	s1	610	CLA	C1C-NC	-3.61	1.32	1.37
39	j1	101	DGA	OG1-CA1	3.61	1.43	1.33
29	R1	610	CLA	C1C-NC	-3.61	1.32	1.37
29	N	610	CLA	C1C-NC	-3.61	1.32	1.37
45	h	101	RRX	C20-C21	3.61	1.54	1.43
29	G1	610	CLA	C1C-NC	-3.61	1.32	1.37
29	b	613	CLA	C1C-NC	-3.61	1.32	1.37
29	y	610	CLA	C1C-NC	-3.61	1.32	1.37
47	I1	102	4RF	O18-C16	3.60	1.43	1.33
29	S	610	CLA	C1C-NC	-3.60	1.32	1.37
29	C1	510	CLA	C1C-NC	-3.60	1.32	1.37
36	b	620	C7Z	C35-C34	3.60	1.54	1.43
29	c	507	CLA	C1C-NC	-3.59	1.32	1.37
29	s1	609	CLA	MG-ND	-3.59	1.98	2.05
29	S	604	CLA	C1C-NC	-3.59	1.32	1.37
29	b	603	CLA	C1C-NC	-3.59	1.32	1.37
45	H1	101	RRX	C11-C10	3.59	1.54	1.43
29	d	402	CLA	C1C-NC	-3.59	1.32	1.37
29	c1	504	CLA	C1C-NC	-3.58	1.32	1.37
29	a1	405	CLA	C1C-NC	-3.58	1.32	1.37
29	Y	610	CLA	C4B-NB	-3.58	1.33	1.37
29	c	506	CLA	C1C-NC	-3.58	1.32	1.37
29	a	410	CLA	C4B-NB	-3.58	1.33	1.37
29	C	507	CLA	C1C-NC	-3.58	1.32	1.37
29	B	604	CLA	C1C-NC	-3.58	1.32	1.37
29	C	506	CLA	C4B-NB	-3.58	1.33	1.37
47	k	101	4RF	O18-C16	3.58	1.43	1.33
29	S	612	CLA	C1C-NC	-3.58	1.32	1.37
29	n1	604	CLA	C1C-NC	-3.58	1.32	1.37
29	y	613	CLA	C1C-NC	-3.57	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	606	CLA	C1C-NC	-3.57	1.32	1.37
29	S1	612	CLA	C1C-NC	-3.57	1.32	1.37
29	B	615	CLA	C1C-NC	-3.56	1.32	1.37
29	Y1	614	CLA	C1C-NC	-3.56	1.32	1.37
29	N	613	CLA	C1C-NC	-3.56	1.32	1.37
47	I	102	4RF	O18-C16	3.56	1.43	1.33
39	J	101	DGA	OG2-CB1	3.56	1.44	1.34
29	C	503	CLA	C1C-NC	-3.56	1.32	1.37
29	B	613	CLA	C4B-NB	-3.55	1.33	1.37
29	G	604	CLA	C1C-NC	-3.55	1.32	1.37
29	r	609	CLA	C1C-NC	-3.55	1.32	1.37
29	n1	610	CLA	C1C-NC	-3.55	1.32	1.37
29	Y	602	CLA	C4B-NB	-3.55	1.33	1.37
29	S	612	CLA	C4B-NB	-3.55	1.33	1.37
29	s1	612	CLA	C1C-NC	-3.55	1.32	1.37
29	a	407	CLA	C1C-NC	-3.54	1.32	1.37
29	B	616	CLA	C1C-NC	-3.54	1.32	1.37
29	c	503	CLA	C1C-NC	-3.54	1.32	1.37
29	n	604	CLA	C1C-NC	-3.54	1.32	1.37
30	a1	408	PHO	C4D-CHA	3.54	1.45	1.39
29	C1	506	CLA	C1C-NC	-3.53	1.32	1.37
29	C1	511	CLA	C1C-NC	-3.53	1.32	1.37
29	N	602	CLA	C1C-NC	-3.53	1.32	1.37
29	Y1	613	CLA	C1C-NC	-3.53	1.32	1.37
29	N1	604	CLA	C1C-NC	-3.53	1.32	1.37
36	b1	620	C7Z	C38-C25	3.52	1.56	1.50
29	s	613	CLA	C1C-NC	-3.52	1.32	1.37
29	c	503	CLA	C4B-NB	-3.52	1.33	1.37
29	B1	614	CLA	C1C-NC	-3.52	1.32	1.37
29	N1	613	CLA	C1C-NC	-3.52	1.32	1.37
29	S	611	CLA	C1C-NC	-3.52	1.32	1.37
29	G	602	CLA	C1C-NC	-3.52	1.32	1.37
29	b	608	CLA	C1C-NC	-3.52	1.32	1.37
29	c1	501	CLA	C1C-NC	-3.52	1.32	1.37
36	B1	620	C7Z	C7-C6	3.52	1.57	1.45
29	b	607	CLA	C1C-NC	-3.52	1.32	1.37
29	G	612	CLA	C1C-NC	-3.51	1.32	1.37
29	b	609	CLA	C1C-NC	-3.51	1.32	1.37
29	R	602	CLA	C4B-NB	-3.51	1.33	1.37
29	y1	603	CLA	C1C-NC	-3.51	1.32	1.37
29	y1	604	CLA	C1C-NC	-3.51	1.32	1.37
44	F1	101	HEM	FE-NB	3.51	2.05	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	408	PHO	C1D-C2D	3.50	1.43	1.39
29	r	603	CLA	C1C-NC	-3.50	1.32	1.37
36	B	620	C7Z	C2-C1	3.50	1.65	1.54
29	S1	604	CLA	C1C-NC	-3.50	1.32	1.37
29	S1	605	CLA	C1C-NC	-3.50	1.32	1.37
29	S	609	CLA	C1C-NC	-3.50	1.32	1.37
29	C	509	CLA	C4B-NB	-3.50	1.33	1.37
29	S1	610	CLA	C4B-NB	-3.50	1.33	1.37
47	K1	101	4RF	O18-C16	3.50	1.43	1.33
29	Y1	602	CLA	C1C-NC	-3.50	1.32	1.37
29	C1	513	CLA	C1C-NC	-3.49	1.32	1.37
29	D1	402	CLA	C1C-NC	-3.49	1.32	1.37
29	c	511	CLA	C1C-NC	-3.49	1.32	1.37
29	c	513	CLA	C1C-NC	-3.49	1.32	1.37
29	a	406	CLA	C1C-NC	-3.49	1.32	1.37
29	Y1	610	CLA	C1C-NC	-3.49	1.32	1.37
29	d	403	CLA	C1C-NC	-3.49	1.32	1.37
29	n1	603	CLA	C1C-NC	-3.49	1.32	1.37
39	j1	101	DGA	OG2-CB1	3.49	1.44	1.34
45	H1	101	RRX	C16-C17	3.49	1.54	1.43
29	a1	406	CLA	C1C-NC	-3.48	1.32	1.37
29	g1	613	CLA	C1C-NC	-3.48	1.32	1.37
29	S	605	CLA	C1C-NC	-3.48	1.32	1.37
29	B1	602	CLA	C1C-NC	-3.48	1.32	1.37
29	c	502	CLA	C4B-NB	-3.48	1.33	1.37
29	b1	611	CLA	C4B-NB	-3.48	1.33	1.37
29	R	604	CLA	C1C-NC	-3.47	1.32	1.37
29	y	614	CLA	C1C-NC	-3.47	1.32	1.37
29	Y	603	CLA	C1C-NC	-3.47	1.32	1.37
29	b1	610	CLA	C1C-NC	-3.47	1.32	1.37
29	y	611	CLA	C1C-NC	-3.47	1.32	1.37
29	c1	505	CLA	C1C-NC	-3.47	1.32	1.37
36	B1	620	C7Z	C2-C1	3.47	1.65	1.54
29	c	510	CLA	C1C-NC	-3.47	1.32	1.37
36	b	620	C7Z	C27-C26	3.46	1.57	1.45
29	N	614	CLA	C1C-NC	-3.46	1.32	1.37
29	s	614	CLA	C1C-NC	-3.46	1.32	1.37
29	b	616	CLA	C1C-NC	-3.46	1.32	1.37
39	b1	625	DGA	OG1-CA1	3.46	1.43	1.33
29	B1	604	CLA	C1C-NC	-3.46	1.32	1.37
29	c	501	CLA	C1C-NC	-3.46	1.32	1.37
29	n	610	CLA	C1C-NC	-3.46	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A1	407	CLA	C4B-NB	-3.46	1.33	1.37
29	A	406	CLA	C4B-NB	-3.46	1.33	1.37
29	b1	605	CLA	C1C-NC	-3.46	1.32	1.37
29	N1	603	CLA	C1C-NC	-3.46	1.32	1.37
29	R1	604	CLA	C1C-NC	-3.45	1.32	1.37
29	n	603	CLA	C1C-NC	-3.45	1.32	1.37
29	c1	510	CLA	C1C-NC	-3.45	1.32	1.37
29	r	610	CLA	C1C-NC	-3.45	1.32	1.37
29	y	603	CLA	C1C-NC	-3.45	1.32	1.37
29	R1	603	CLA	C1C-NC	-3.45	1.32	1.37
29	C1	508	CLA	C1C-NC	-3.45	1.32	1.37
30	a1	409	PHO	C4D-CHA	3.45	1.45	1.39
39	j	101	DGA	OG2-CB1	3.44	1.44	1.34
29	B	609	CLA	C1C-NC	-3.44	1.32	1.37
29	B	602	CLA	C1C-NC	-3.44	1.32	1.37
29	G	611	CLA	C1C-NC	-3.44	1.32	1.37
29	n	611	CLA	C1C-NC	-3.44	1.32	1.37
39	c1	524	DGA	OG2-CB1	3.44	1.44	1.34
29	y	612	CLA	C1C-NC	-3.44	1.32	1.37
29	b	610	CLA	C1C-NC	-3.44	1.32	1.37
36	b1	620	C7Z	C7-C6	3.44	1.57	1.45
45	h	101	RRX	C15-C14	3.44	1.54	1.43
30	A1	408	PHO	C4D-CHA	3.44	1.45	1.39
29	S	602	CLA	C1C-NC	-3.43	1.32	1.37
29	b1	607	CLA	C1C-NC	-3.43	1.32	1.37
29	c1	512	CLA	C1C-NC	-3.43	1.32	1.37
29	c1	511	CLA	C1C-NC	-3.43	1.32	1.37
29	Y	613	CLA	C1C-NC	-3.43	1.32	1.37
29	C	507	CLA	C4B-NB	-3.43	1.33	1.37
29	S	602	CLA	C4B-NB	-3.43	1.33	1.37
39	J1	101	DGA	OG2-CB1	3.42	1.44	1.34
29	c	509	CLA	C1C-NC	-3.42	1.32	1.37
29	Y	612	CLA	C1C-NC	-3.42	1.32	1.37
47	i1	101	4RF	O18-C16	3.42	1.43	1.33
29	b1	615	CLA	C1C-NC	-3.42	1.32	1.37
29	C	510	CLA	C1C-NC	-3.42	1.32	1.37
29	R1	608	CLA	C1C-NC	-3.42	1.32	1.37
29	C	512	CLA	C4B-NB	-3.42	1.33	1.37
30	a	408	PHO	C1D-C2D	3.41	1.43	1.39
29	s	604	CLA	C1C-NC	-3.41	1.32	1.37
29	a	405	CLA	C1C-NC	-3.41	1.32	1.37
29	n1	613	CLA	C1C-NC	-3.41	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	N1	611	CLA	C1C-NC	-3.41	1.32	1.37
29	B	617	CLA	C4B-NB	-3.41	1.33	1.37
36	b1	620	C7Z	C2-C1	3.41	1.65	1.54
29	C1	509	CLA	C1C-NC	-3.41	1.32	1.37
29	y1	602	CLA	C1C-NC	-3.41	1.32	1.37
29	C	508	CLA	C4B-NB	-3.41	1.33	1.37
48	Y	601	CHL	C1B-NB	-3.41	1.33	1.37
29	b1	608	CLA	C1C-NC	-3.41	1.32	1.37
29	B1	605	CLA	C1C-NC	-3.41	1.32	1.37
29	b1	613	CLA	C4B-NB	-3.40	1.33	1.37
48	N1	608	CHL	C1B-NB	-3.40	1.33	1.37
29	Y	608	CLA	C1C-NC	-3.40	1.32	1.37
29	B1	612	CLA	C1C-NC	-3.40	1.32	1.37
29	c1	507	CLA	C1C-NC	-3.40	1.32	1.37
44	f1	101	HEM	FE-NA	3.40	2.06	1.95
29	n	613	CLA	C1C-NC	-3.40	1.32	1.37
29	s	609	CLA	C1C-NC	-3.40	1.32	1.37
36	B	620	C7Z	C35-C34	3.40	1.54	1.43
29	R	609	CLA	C4B-NB	-3.40	1.33	1.37
29	Y1	602	CLA	C4B-NB	-3.40	1.33	1.37
29	A	407	CLA	C4B-NB	-3.40	1.33	1.37
48	y	601	CHL	C1B-NB	-3.39	1.33	1.37
29	G	614	CLA	C1C-NC	-3.39	1.32	1.37
29	g	602	CLA	C1C-NC	-3.39	1.32	1.37
29	S1	614	CLA	C4B-NB	-3.39	1.33	1.37
29	C1	512	CLA	C1C-NC	-3.39	1.32	1.37
29	R1	612	CLA	C1C-NC	-3.39	1.32	1.37
29	y1	613	CLA	C1C-NC	-3.39	1.32	1.37
29	c1	503	CLA	C1C-NC	-3.39	1.32	1.37
47	k1	101	4RF	O18-C16	3.39	1.43	1.33
29	s1	611	CLA	C1C-NC	-3.39	1.32	1.37
29	C	513	CLA	C1C-NC	-3.39	1.32	1.37
29	N	611	CLA	C1C-NC	-3.39	1.32	1.37
29	b	603	CLA	C4B-NB	-3.39	1.33	1.37
29	B1	608	CLA	C1C-NC	-3.38	1.32	1.37
29	N	604	CLA	C1C-NC	-3.38	1.32	1.37
29	D	403	CLA	C1C-NC	-3.38	1.32	1.37
45	H	101	RRX	C11-C10	3.38	1.53	1.43
44	F1	101	HEM	FE-NA	3.37	2.06	1.95
29	c	513	CLA	C4B-NB	-3.37	1.33	1.37
29	a1	407	CLA	C4B-NB	-3.37	1.33	1.37
29	c	512	CLA	C4B-NB	-3.37	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	N	603	CLA	C1C-NC	-3.37	1.32	1.37
29	G	610	CLA	C4B-NB	-3.37	1.33	1.37
29	c	512	CLA	C1C-NC	-3.37	1.32	1.37
29	g	604	CLA	C1C-NC	-3.37	1.32	1.37
29	y	608	CLA	C1C-NC	-3.37	1.32	1.37
29	n	602	CLA	C1C-NC	-3.37	1.32	1.37
29	N1	612	CLA	C1C-NC	-3.37	1.32	1.37
29	Y	604	CLA	C1C-NC	-3.37	1.32	1.37
39	c	524	DGA	OG2-CB1	3.37	1.43	1.34
33	H1	102	LMG	C19-C18	-3.36	1.32	1.51
29	B1	615	CLA	C4B-NB	-3.36	1.33	1.37
29	g1	610	CLA	C1C-NC	-3.36	1.32	1.37
29	s	602	CLA	C1C-NC	-3.36	1.32	1.37
29	r1	604	CLA	C1C-NC	-3.36	1.32	1.37
29	b1	606	CLA	C1C-NC	-3.36	1.32	1.37
29	B1	607	CLA	C1C-NC	-3.36	1.32	1.37
29	r	604	CLA	C1C-NC	-3.35	1.32	1.37
29	s1	605	CLA	C1C-NC	-3.35	1.32	1.37
37	C	520	DGD	CAA-C9A	-3.35	1.32	1.51
29	b1	606	CLA	C4B-NB	-3.35	1.33	1.37
37	C	519	DGD	CAB-C9B	-3.35	1.32	1.51
29	c	505	CLA	C4B-NB	-3.35	1.33	1.37
29	b1	603	CLA	C1C-NC	-3.35	1.32	1.37
29	c1	510	CLA	C4B-NB	-3.35	1.33	1.37
29	r	602	CLA	C1C-NC	-3.35	1.32	1.37
39	c1	524	DGA	OG1-CA1	3.35	1.43	1.33
29	a	406	CLA	C4B-NB	-3.35	1.33	1.37
29	S	617	CLA	C1C-NC	-3.35	1.32	1.37
29	B1	615	CLA	C1C-NC	-3.35	1.32	1.37
29	N1	602	CLA	C1C-NC	-3.34	1.32	1.37
29	Y1	611	CLA	C1C-NC	-3.34	1.32	1.37
33	h	102	LMG	C19-C18	-3.34	1.32	1.51
29	g1	602	CLA	C1C-NC	-3.34	1.32	1.37
29	C	502	CLA	C4B-NB	-3.34	1.33	1.37
29	G	614	CLA	C4B-NB	-3.34	1.33	1.37
29	y	604	CLA	C1C-NC	-3.33	1.32	1.37
45	h1	101	RRX	C11-C10	3.33	1.53	1.43
29	Y1	608	CLA	C1C-NC	-3.33	1.32	1.37
29	n1	612	CLA	C1C-NC	-3.33	1.32	1.37
29	r1	609	CLA	C1C-NC	-3.33	1.32	1.37
29	G1	611	CLA	C1C-NC	-3.32	1.32	1.37
29	R	603	CLA	C1C-NC	-3.32	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	614	CLA	C1C-NC	-3.32	1.32	1.37
29	B	607	CLA	C1C-NC	-3.32	1.32	1.37
29	b	606	CLA	C4B-NB	-3.32	1.33	1.37
29	n	602	CLA	C4B-NB	-3.31	1.33	1.37
37	c1	519	DGD	CAB-C9B	-3.31	1.33	1.51
39	C	524	DGA	OG2-CB1	3.31	1.43	1.34
33	h	102	LMG	C37-C36	-3.31	1.33	1.51
29	C1	507	CLA	C1C-NC	-3.31	1.32	1.37
29	c1	513	CLA	C1C-NC	-3.31	1.32	1.37
29	B	614	CLA	C1C-NC	-3.31	1.32	1.37
33	c	523	LMG	C37-C36	-3.31	1.33	1.51
29	B1	606	CLA	C4B-NB	-3.31	1.33	1.37
29	S	610	CLA	C4B-NB	-3.31	1.33	1.37
29	C1	502	CLA	C4B-NB	-3.31	1.33	1.37
29	s1	604	CLA	C1C-NC	-3.31	1.32	1.37
33	B	622	LMG	C22-C21	-3.30	1.33	1.51
29	G	613	CLA	C1C-NC	-3.30	1.32	1.37
36	b	620	C7Z	C7-C6	3.30	1.56	1.45
37	c	518	DGD	CAB-C9B	-3.30	1.33	1.51
45	H	101	RRX	C4-C5	-3.30	1.44	1.51
29	g	613	CLA	C1C-NC	-3.30	1.32	1.37
29	g1	603	CLA	C1C-NC	-3.30	1.32	1.37
30	a	409	PHO	C4D-CHA	3.30	1.44	1.39
33	C1	521	LMG	C40-C39	-3.30	1.33	1.51
29	B1	609	CLA	C1C-NC	-3.30	1.32	1.37
37	c1	520	DGD	CAA-C9A	-3.30	1.33	1.51
48	G1	606	CHL	C1B-NB	-3.30	1.33	1.37
29	S1	617	CLA	C1C-NC	-3.30	1.32	1.37
33	b	622	LMG	C22-C21	-3.30	1.33	1.51
29	S	613	CLA	C4B-NB	-3.30	1.33	1.37
39	b	625	DGA	OG1-CA1	3.29	1.43	1.33
29	g1	602	CLA	C4B-NB	-3.29	1.33	1.37
48	s	606	CHL	C1B-NB	-3.29	1.33	1.37
39	J1	101	DGA	OG1-CA1	3.29	1.42	1.33
29	a	405	CLA	C4B-NB	-3.29	1.33	1.37
29	B1	610	CLA	C1C-NC	-3.29	1.32	1.37
37	C1	520	DGD	CAB-C9B	-3.29	1.33	1.51
29	g1	612	CLA	C1C-NC	-3.29	1.32	1.37
33	c1	523	LMG	C22-C21	-3.29	1.33	1.51
33	h1	102	LMG	C19-C18	-3.28	1.33	1.51
37	c	520	DGD	CAB-C9B	-3.28	1.33	1.51
37	C	519	DGD	CDB-CCB	-3.28	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C1	518	DGD	CAB-C9B	-3.28	1.33	1.51
33	c	521	LMG	C40-C39	-3.28	1.33	1.51
33	C1	523	LMG	C25-C24	-3.28	1.33	1.51
29	b1	609	CLA	C1C-NC	-3.28	1.32	1.37
29	N	612	CLA	C1C-NC	-3.28	1.32	1.37
37	C	520	DGD	CAB-C9B	-3.28	1.33	1.51
29	b	612	CLA	C4B-NB	-3.27	1.33	1.37
29	R1	602	CLA	C1C-NC	-3.27	1.32	1.37
29	b1	605	CLA	MG-ND	-3.27	1.99	2.05
37	C	518	DGD	CDB-CCB	-3.27	1.33	1.51
29	B1	617	CLA	C4B-NB	-3.27	1.33	1.37
29	B	611	CLA	C4B-NB	-3.27	1.33	1.37
33	C1	523	LMG	C37-C36	-3.27	1.33	1.51
33	B	622	LMG	C19-C18	-3.27	1.33	1.51
29	B1	611	CLA	C4B-NB	-3.27	1.33	1.37
29	g	603	CLA	C1C-NC	-3.27	1.32	1.37
37	C1	518	DGD	CDB-CCB	-3.27	1.33	1.51
29	c1	508	CLA	C1C-NC	-3.26	1.32	1.37
29	C1	509	CLA	C4B-NB	-3.26	1.33	1.37
29	b	615	CLA	C1C-NC	-3.26	1.32	1.37
33	H1	102	LMG	C40-C39	-3.26	1.33	1.51
37	c	519	DGD	CAB-C9B	-3.26	1.33	1.51
29	s	605	CLA	C1C-NC	-3.26	1.32	1.37
33	c	523	LMG	C40-C39	-3.26	1.33	1.51
33	c1	521	LMG	C40-C39	-3.26	1.33	1.51
29	s1	603	CLA	C1C-NC	-3.26	1.32	1.37
29	N1	610	CLA	C1C-NC	-3.26	1.32	1.37
33	H	102	LMG	C19-C18	-3.26	1.33	1.51
39	j	101	DGA	OG1-CA1	3.26	1.42	1.33
29	s1	609	CLA	C1C-NC	-3.26	1.32	1.37
33	C	523	LMG	C25-C24	-3.26	1.33	1.51
39	C	524	DGA	OG1-CA1	3.26	1.42	1.33
29	A1	405	CLA	C4B-NB	-3.26	1.33	1.37
29	G1	614	CLA	C1C-NC	-3.26	1.32	1.37
29	C1	504	CLA	C4B-NB	-3.25	1.33	1.37
45	H1	101	RRX	C24-C25	3.25	1.56	1.45
29	C1	505	CLA	C1C-NC	-3.25	1.32	1.37
33	C	523	LMG	C22-C21	-3.25	1.33	1.51
33	A	413	LMG	C19-C18	-3.25	1.33	1.51
29	Y1	604	CLA	C4B-NB	-3.25	1.33	1.37
29	Y	614	CLA	C1C-NC	-3.25	1.33	1.37
33	c1	523	LMG	C25-C24	-3.25	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C1	503	CLA	C1C-NC	-3.25	1.33	1.37
29	d	403	CLA	C4B-NB	-3.25	1.33	1.37
37	c	519	DGD	CAA-C9A	-3.25	1.33	1.51
29	s	603	CLA	C1C-NC	-3.25	1.33	1.37
37	c1	519	DGD	CDB-CCB	-3.25	1.33	1.51
33	c1	521	LMG	C22-C21	-3.25	1.33	1.51
37	C1	519	DGD	CAA-C9A	-3.25	1.33	1.51
29	C1	511	CLA	C4B-NB	-3.25	1.33	1.37
29	S	603	CLA	C1C-NC	-3.25	1.33	1.37
33	D1	411	LMG	C19-C18	-3.24	1.33	1.51
33	c1	523	LMG	C40-C39	-3.24	1.33	1.51
29	B	603	CLA	C1C-NC	-3.24	1.33	1.37
37	C1	519	DGD	CAB-C9B	-3.24	1.33	1.51
37	c1	520	DGD	CAB-C9B	-3.24	1.33	1.51
33	A1	413	LMG	C19-C18	-3.24	1.33	1.51
33	h1	102	LMG	C37-C36	-3.24	1.33	1.51
29	n1	611	CLA	C4B-NB	-3.24	1.33	1.37
47	K	101	4RF	O40-C41	3.24	1.42	1.33
29	y	612	CLA	C4B-NB	-3.24	1.33	1.37
33	C	521	LMG	C40-C39	-3.24	1.33	1.51
39	B	625	DGA	OG1-CA1	3.24	1.42	1.33
33	C	523	LMG	C37-C36	-3.24	1.33	1.51
29	Y	611	CLA	C1C-NC	-3.24	1.33	1.37
29	s1	614	CLA	C1C-NC	-3.24	1.33	1.37
29	b	602	CLA	C1C-NC	-3.24	1.33	1.37
29	n1	614	CLA	C1C-NC	-3.24	1.33	1.37
37	C	519	DGD	CDA-CCA	-3.24	1.33	1.51
29	n1	602	CLA	C1C-NC	-3.24	1.33	1.37
36	B1	620	C7Z	C38-C25	3.23	1.56	1.50
37	c1	518	DGD	CAB-C9B	-3.23	1.33	1.51
33	c	523	LMG	C43-C42	-3.23	1.33	1.51
29	S1	611	CLA	C1C-NC	-3.23	1.33	1.37
37	c	520	DGD	CAA-C9A	-3.23	1.33	1.51
33	A	413	LMG	C37-C36	-3.23	1.33	1.51
33	c1	523	LMG	C37-C36	-3.23	1.33	1.51
33	C	521	LMG	C22-C21	-3.23	1.33	1.51
33	H1	102	LMG	C37-C36	-3.23	1.33	1.51
29	c1	506	CLA	C1C-NC	-3.23	1.33	1.37
33	C1	521	LMG	C37-C36	-3.23	1.33	1.51
33	a1	413	LMG	C37-C36	-3.23	1.33	1.51
29	y1	614	CLA	C1C-NC	-3.23	1.33	1.37
29	C1	505	CLA	C4B-NB	-3.23	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	612	CLA	C4B-NB	-3.23	1.33	1.37
36	B1	620	C7Z	C21-C26	-3.23	1.49	1.53
37	c	519	DGD	CDB-CCB	-3.23	1.33	1.51
29	n	614	CLA	C1C-NC	-3.23	1.33	1.37
48	Y	607	CHL	C1B-NB	-3.23	1.33	1.37
37	C	518	DGD	CAB-C9B	-3.23	1.33	1.51
29	G	603	CLA	C1C-NC	-3.23	1.33	1.37
29	b	617	CLA	C4B-NB	-3.23	1.33	1.37
29	g1	611	CLA	C1C-NC	-3.23	1.33	1.37
33	d1	411	LMG	C22-C21	-3.23	1.33	1.51
44	f1	101	HEM	CAC-C3C	3.22	1.56	1.47
29	b1	614	CLA	C1C-NC	-3.22	1.33	1.37
33	h	102	LMG	C40-C39	-3.22	1.33	1.51
33	H	102	LMG	C37-C36	-3.22	1.33	1.51
37	c	519	DGD	CDA-CCA	-3.22	1.33	1.51
43	D1	405	PL9	C31-C29	-3.22	1.44	1.51
33	D	411	LMG	C22-C21	-3.22	1.33	1.51
33	c	523	LMG	C25-C24	-3.22	1.33	1.51
29	s	614	CLA	C4B-NB	-3.22	1.33	1.37
29	R1	602	CLA	C4B-NB	-3.22	1.33	1.37
33	C	523	LMG	C40-C39	-3.22	1.33	1.51
37	C1	520	DGD	CDB-CCB	-3.22	1.33	1.51
39	J	101	DGA	OG1-CA1	3.22	1.42	1.33
29	b1	605	CLA	C4B-NB	-3.22	1.33	1.37
29	a	410	CLA	C1C-NC	-3.22	1.33	1.37
33	b	622	LMG	C19-C18	-3.22	1.33	1.51
37	C1	519	DGD	CDA-CCA	-3.22	1.33	1.51
33	w	201	LMG	C37-C36	-3.22	1.33	1.51
29	g	610	CLA	C4B-NB	-3.22	1.33	1.37
29	B	612	CLA	C4B-NB	-3.22	1.33	1.37
37	c	518	DGD	CDB-CCB	-3.22	1.33	1.51
29	y	613	CLA	C4B-NB	-3.21	1.33	1.37
39	C1	524	DGA	OG1-CA1	3.21	1.42	1.33
29	b	613	CLA	C4B-NB	-3.21	1.33	1.37
36	b	620	C7Z	C21-C26	-3.21	1.49	1.53
33	a1	413	LMG	C19-C18	-3.21	1.33	1.51
33	H	102	LMG	C40-C39	-3.21	1.33	1.51
29	c	511	CLA	C4B-NB	-3.21	1.33	1.37
33	A	413	LMG	C40-C39	-3.21	1.33	1.51
45	h1	101	RRX	C29-C30	3.21	1.64	1.54
37	C1	520	DGD	CAA-C9A	-3.20	1.33	1.51
29	s	610	CLA	C1C-NC	-3.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	611	CLA	C1C-NC	-3.20	1.33	1.37
37	C	519	DGD	CAA-C9A	-3.20	1.33	1.51
39	c	524	DGA	OG1-CA1	3.20	1.42	1.33
29	G1	604	CLA	C4B-NB	-3.20	1.33	1.37
33	b1	622	LMG	C22-C21	-3.20	1.33	1.51
37	c1	520	DGD	CDB-CCB	-3.20	1.33	1.51
33	w1	201	LMG	C40-C39	-3.20	1.33	1.51
33	c	523	LMG	C22-C21	-3.20	1.33	1.51
29	r1	602	CLA	C1C-NC	-3.20	1.33	1.37
33	a1	413	LMG	C40-C39	-3.20	1.33	1.51
48	G1	609	CHL	C1B-NB	-3.20	1.33	1.37
37	C1	519	DGD	CDB-CCB	-3.20	1.33	1.51
29	s	612	CLA	C4B-NB	-3.20	1.33	1.37
33	C	521	LMG	C37-C36	-3.20	1.33	1.51
33	c1	523	LMG	C43-C42	-3.20	1.33	1.51
29	B1	613	CLA	C1C-NC	-3.19	1.33	1.37
33	A1	413	LMG	C40-C39	-3.19	1.33	1.51
48	R	606	CHL	C3A-C2A	-3.19	1.45	1.54
33	a	413	LMG	C37-C36	-3.19	1.33	1.51
33	a	413	LMG	C40-C39	-3.19	1.33	1.51
36	b	620	C7Z	C2-C1	3.19	1.64	1.54
29	d1	402	CLA	C4B-NB	-3.19	1.33	1.37
33	C1	521	LMG	C22-C21	-3.19	1.33	1.51
33	b1	622	LMG	C19-C18	-3.19	1.33	1.51
33	c	521	LMG	C37-C36	-3.19	1.33	1.51
33	d	411	LMG	C22-C21	-3.19	1.33	1.51
36	B	620	C7Z	C7-C6	3.19	1.56	1.45
33	d	411	LMG	C19-C18	-3.19	1.33	1.51
33	c	521	LMG	C22-C21	-3.19	1.33	1.51
33	D	411	LMG	C19-C18	-3.19	1.33	1.51
29	R1	604	CLA	C4B-NB	-3.18	1.33	1.37
33	a	413	LMG	C19-C18	-3.18	1.33	1.51
33	c1	523	LMG	C19-C18	-3.18	1.33	1.51
33	C1	523	LMG	C40-C39	-3.18	1.33	1.51
29	g1	614	CLA	C1C-NC	-3.18	1.33	1.37
29	y1	611	CLA	C1C-NC	-3.18	1.33	1.37
29	S1	609	CLA	C4B-NB	-3.18	1.33	1.37
29	c1	509	CLA	C1C-NC	-3.18	1.33	1.37
29	r	612	CLA	C1C-NC	-3.18	1.33	1.37
29	s1	613	CLA	C1C-NC	-3.18	1.33	1.37
29	S	614	CLA	C4B-NB	-3.18	1.33	1.37
29	b	605	CLA	C4B-NB	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	w1	201	LMG	C37-C36	-3.18	1.33	1.51
51	s	623	NEX	C1-C6	-3.18	1.49	1.54
37	c1	518	DGD	CDB-CCB	-3.18	1.33	1.51
29	C	510	CLA	C4B-NB	-3.18	1.33	1.37
29	y1	610	CLA	C4B-NB	-3.18	1.33	1.37
33	C	523	LMG	C19-C18	-3.18	1.33	1.51
29	C	511	CLA	C1C-NC	-3.17	1.33	1.37
33	W	201	LMG	C40-C39	-3.17	1.33	1.51
37	c1	519	DGD	CDA-CCA	-3.17	1.33	1.51
29	B	605	CLA	C4B-NB	-3.17	1.33	1.37
29	s1	602	CLA	C1C-NC	-3.17	1.33	1.37
29	C1	507	CLA	C4B-NB	-3.17	1.33	1.37
29	c	509	CLA	C4B-NB	-3.17	1.33	1.37
33	W1	201	LMG	C40-C39	-3.17	1.33	1.51
36	b	620	C7Z	C38-C25	3.17	1.56	1.50
48	N	607	CHL	C1B-NB	-3.17	1.33	1.37
33	B1	622	LMG	C22-C21	-3.17	1.33	1.51
45	h	101	RRX	C29-C30	3.17	1.64	1.54
33	C	523	LMG	C43-C42	-3.17	1.33	1.51
37	c	520	DGD	CDB-CCB	-3.17	1.33	1.51
33	d1	411	LMG	C19-C18	-3.16	1.33	1.51
33	c	521	LMG	C19-C18	-3.16	1.33	1.51
33	W	201	LMG	C37-C36	-3.16	1.33	1.51
33	c1	521	LMG	C37-C36	-3.16	1.33	1.51
33	c1	521	LMG	C19-C18	-3.16	1.33	1.51
37	c1	519	DGD	CAA-C9A	-3.16	1.33	1.51
29	b	614	CLA	C4B-NB	-3.16	1.33	1.37
29	S1	611	CLA	C4B-NB	-3.16	1.33	1.37
29	b1	607	CLA	C4B-NB	-3.16	1.33	1.37
29	s	612	CLA	C1C-NC	-3.16	1.33	1.37
29	A	405	CLA	C4B-NB	-3.16	1.33	1.37
29	B1	612	CLA	C4B-NB	-3.16	1.33	1.37
29	c	508	CLA	C4B-NB	-3.16	1.33	1.37
29	S1	603	CLA	C1C-NC	-3.16	1.33	1.37
33	C	521	LMG	C19-C18	-3.15	1.33	1.51
29	R	604	CLA	C4B-NB	-3.15	1.33	1.37
33	C1	521	LMG	C19-C18	-3.15	1.33	1.51
33	h1	102	LMG	C40-C39	-3.15	1.33	1.51
33	A1	413	LMG	C37-C36	-3.15	1.33	1.51
33	D1	411	LMG	C22-C21	-3.15	1.33	1.51
29	R1	609	CLA	C1C-NC	-3.15	1.33	1.37
29	Y	613	CLA	C4B-NB	-3.15	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C1	512	CLA	C4B-NB	-3.15	1.33	1.37
29	N	613	CLA	C4B-NB	-3.15	1.33	1.37
33	c	523	LMG	C19-C18	-3.14	1.33	1.51
29	B1	616	CLA	C1C-NC	-3.14	1.33	1.37
29	N1	611	CLA	C4B-NB	-3.14	1.33	1.37
29	Y1	612	CLA	C4B-NB	-3.14	1.33	1.37
33	w	201	LMG	C40-C39	-3.14	1.34	1.51
29	B	615	CLA	C4B-NB	-3.14	1.33	1.37
29	y	608	CLA	C4B-NB	-3.14	1.33	1.37
45	h1	101	RRX	C4-C5	-3.14	1.44	1.51
29	b	602	CLA	C4B-NB	-3.14	1.33	1.37
44	F1	101	HEM	CAB-C3B	3.14	1.56	1.47
29	s	617	CLA	C1C-NC	-3.14	1.33	1.37
29	r1	603	CLA	C1C-NC	-3.14	1.33	1.37
33	B1	622	LMG	C19-C18	-3.14	1.34	1.51
29	n	612	CLA	C1C-NC	-3.14	1.33	1.37
29	G1	613	CLA	C1C-NC	-3.14	1.33	1.37
29	G	604	CLA	C4B-NB	-3.14	1.33	1.37
29	G1	614	CLA	C4B-NB	-3.13	1.33	1.37
45	h1	101	RRX	C16-C17	3.13	1.53	1.43
29	s	610	CLA	C4B-NB	-3.13	1.33	1.37
29	b1	602	CLA	C1C-NC	-3.13	1.33	1.37
29	S1	602	CLA	C1C-NC	-3.13	1.33	1.37
29	N	614	CLA	C4B-NB	-3.13	1.33	1.37
29	B1	604	CLA	C4B-NB	-3.13	1.33	1.37
33	W1	201	LMG	C37-C36	-3.13	1.34	1.51
33	C1	523	LMG	C19-C18	-3.13	1.34	1.51
48	N1	609	CHL	C1B-NB	-3.13	1.33	1.37
29	g1	604	CLA	C1C-NC	-3.13	1.33	1.37
48	G	607	CHL	C1B-NB	-3.13	1.33	1.37
29	r1	610	CLA	C1C-NC	-3.12	1.33	1.37
29	s	609	CLA	C4B-NB	-3.12	1.33	1.37
45	H	101	RRX	C16-C17	3.12	1.53	1.43
37	C	520	DGD	CDB-CCB	-3.12	1.34	1.51
47	i1	101	4RF	O40-C41	3.12	1.42	1.33
29	B1	603	CLA	C1C-NC	-3.12	1.33	1.37
29	R1	610	CLA	C4B-NB	-3.12	1.34	1.37
33	C1	523	LMG	C43-C42	-3.12	1.34	1.51
29	y1	608	CLA	C1C-NC	-3.12	1.33	1.37
29	c	510	CLA	C4B-NB	-3.11	1.34	1.37
29	r	608	CLA	C1C-NC	-3.11	1.33	1.37
29	C1	506	CLA	C4B-NB	-3.11	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s1	617	CLA	C1C-NC	-3.11	1.33	1.37
33	C1	523	LMG	C22-C21	-3.11	1.34	1.51
29	N1	614	CLA	C1C-NC	-3.11	1.33	1.37
45	H1	101	RRX	C29-C30	3.10	1.64	1.54
29	S1	617	CLA	C4B-NB	-3.10	1.34	1.37
45	h1	101	RRX	C24-C25	3.10	1.56	1.45
44	F1	101	HEM	CAC-C3C	3.10	1.55	1.47
29	n1	604	CLA	C4B-NB	-3.09	1.34	1.37
29	N1	604	CLA	C4B-NB	-3.09	1.34	1.37
29	r	609	CLA	C4B-NB	-3.09	1.34	1.37
29	A1	410	CLA	C4B-NB	-3.09	1.34	1.37
29	B1	613	CLA	C4B-NB	-3.09	1.34	1.37
29	B1	610	CLA	C4B-NB	-3.08	1.34	1.37
53	r	626	ERG	C4-C5	3.08	1.58	1.51
29	G	611	CLA	C4B-NB	-3.08	1.34	1.37
29	B	606	CLA	C4B-NB	-3.08	1.34	1.37
29	b	616	CLA	C4B-NB	-3.08	1.34	1.37
29	y1	612	CLA	C1C-NC	-3.07	1.33	1.37
29	G	602	CLA	C4B-NB	-3.07	1.34	1.37
30	a	408	PHO	C4D-CHA	3.07	1.44	1.39
29	a	407	CLA	C4B-NB	-3.07	1.34	1.37
44	f	101	HEM	CAB-C3B	3.07	1.55	1.47
29	g	612	CLA	C4B-NB	-3.06	1.34	1.37
29	b	610	CLA	C4B-NB	-3.06	1.34	1.37
29	y	614	CLA	C4B-NB	-3.06	1.34	1.37
30	A1	409	PHO	C4D-ND	-3.06	1.34	1.38
29	B	604	CLA	C4B-NB	-3.06	1.34	1.37
29	B	609	CLA	C4B-NB	-3.06	1.34	1.37
29	B1	614	CLA	C4B-NB	-3.06	1.34	1.37
47	K1	101	4RF	O40-C41	3.06	1.42	1.33
51	R	622	NEX	C1-C6	-3.06	1.49	1.54
29	r1	604	CLA	C4B-NB	-3.06	1.34	1.37
29	C1	513	CLA	C4B-NB	-3.06	1.34	1.37
29	s	617	CLA	C4B-NB	-3.06	1.34	1.37
29	Y1	611	CLA	C4B-NB	-3.06	1.34	1.37
45	H1	101	RRX	C4-C5	-3.05	1.45	1.51
29	d1	403	CLA	C1C-NC	-3.05	1.33	1.37
29	n	613	CLA	C4B-NB	-3.05	1.34	1.37
29	S1	605	CLA	C4B-NB	-3.05	1.34	1.37
29	C	511	CLA	C4B-NB	-3.05	1.34	1.37
29	y	602	CLA	C4B-NB	-3.05	1.34	1.37
44	f1	101	HEM	FE-NC	3.04	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	H	101	RRX	C24-C25	3.04	1.55	1.45
29	Y1	603	CLA	C1C-NC	-3.04	1.33	1.37
29	g	611	CLA	C4B-NB	-3.04	1.34	1.37
29	Y1	612	CLA	C1C-NC	-3.04	1.33	1.37
29	n	603	CLA	C4B-NB	-3.04	1.34	1.37
29	C1	503	CLA	C4B-NB	-3.04	1.34	1.37
29	b1	608	CLA	C4B-NB	-3.04	1.34	1.37
29	b1	615	CLA	C4B-NB	-3.04	1.34	1.37
29	Y	603	CLA	C4B-NB	-3.04	1.34	1.37
29	s1	604	CLA	C4B-NB	-3.04	1.34	1.37
48	n	607	CHL	C1B-NB	-3.04	1.34	1.37
43	d	405	PL9	C53-C6	-3.04	1.44	1.50
30	A	408	PHO	C4D-CHA	3.03	1.44	1.39
29	B	614	CLA	C4B-NB	-3.03	1.34	1.37
29	b	607	CLA	C4B-NB	-3.03	1.34	1.37
29	b	611	CLA	C4B-NB	-3.03	1.34	1.37
29	G1	611	CLA	C4B-NB	-3.03	1.34	1.37
47	I	102	4RF	O40-C41	3.03	1.42	1.33
45	h	101	RRX	C4-C5	-3.03	1.45	1.51
29	g1	614	CLA	C4B-NB	-3.03	1.34	1.37
29	N	612	CLA	C4B-NB	-3.03	1.34	1.37
29	y	603	CLA	C4B-NB	-3.03	1.34	1.37
29	s	603	CLA	C4B-NB	-3.03	1.34	1.37
45	h	101	RRX	C11-C10	3.02	1.52	1.43
47	i	101	4RF	O40-C41	3.02	1.42	1.33
29	g	614	CLA	C1C-NC	-3.02	1.33	1.37
29	N1	603	CLA	C4B-NB	-3.02	1.34	1.37
39	B1	625	DGA	OG1-CA1	3.02	1.42	1.33
29	Y1	608	CLA	C4B-NB	-3.01	1.34	1.37
29	c1	512	CLA	C4B-NB	-3.01	1.34	1.37
29	N	604	CLA	C4B-NB	-3.01	1.34	1.37
29	b	615	CLA	C4B-NB	-3.01	1.34	1.37
29	C	501	CLA	C4B-NB	-3.01	1.34	1.37
48	y1	609	CHL	C1B-NB	-3.01	1.34	1.37
29	D1	403	CLA	C1C-NC	-3.00	1.33	1.37
29	Y	604	CLA	C4B-NB	-3.00	1.34	1.37
44	f1	101	HEM	CAB-C3B	3.00	1.55	1.47
29	y1	614	CLA	C4B-NB	-3.00	1.34	1.37
29	B1	607	CLA	C4B-NB	-3.00	1.34	1.37
48	Y1	601	CHL	C3A-C2A	-3.00	1.46	1.54
29	r1	612	CLA	C1C-NC	-3.00	1.33	1.37
47	k1	101	4RF	O40-C41	3.00	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c1	504	CLA	C4B-NB	-2.99	1.34	1.37
29	g	602	CLA	C4B-NB	-2.99	1.34	1.37
29	S1	604	CLA	C4B-NB	-2.99	1.34	1.37
47	k	101	4RF	O40-C41	2.99	1.42	1.33
29	S	617	CLA	C4B-NB	-2.99	1.34	1.37
29	a1	405	CLA	C4B-NB	-2.99	1.34	1.37
29	n	612	CLA	C4B-NB	-2.99	1.34	1.37
29	y	610	CLA	C4B-NB	-2.99	1.34	1.37
47	I1	102	4RF	O40-C41	2.99	1.42	1.33
51	G	623	NEX	C1-C6	-2.99	1.49	1.54
29	Y	612	CLA	C4B-NB	-2.99	1.34	1.37
29	g	603	CLA	C4B-NB	-2.99	1.34	1.37
48	y	607	CHL	C1B-NB	-2.98	1.34	1.37
45	h	101	RRX	C24-C25	2.98	1.55	1.45
29	D	403	CLA	C4B-NB	-2.98	1.34	1.37
29	Y1	613	CLA	C4B-NB	-2.98	1.34	1.37
29	s	604	CLA	C4B-NB	-2.98	1.34	1.37
29	N1	610	CLA	C4B-NB	-2.98	1.34	1.37
29	s	602	CLA	C4B-NB	-2.98	1.34	1.37
29	B	608	CLA	C4B-NB	-2.97	1.34	1.37
29	N1	612	CLA	C4B-NB	-2.97	1.34	1.37
29	B	610	CLA	C4B-NB	-2.97	1.34	1.37
29	Y1	610	CLA	C4B-NB	-2.97	1.34	1.37
29	B1	608	CLA	C4B-NB	-2.97	1.34	1.37
29	R	612	CLA	C1C-NC	-2.97	1.33	1.37
30	A1	408	PHO	CAC-C3C	-2.97	1.46	1.51
44	F	101	HEM	CAB-C3B	2.97	1.55	1.47
29	Y	614	CLA	C4B-NB	-2.97	1.34	1.37
29	b1	603	CLA	C4B-NB	-2.97	1.34	1.37
29	g	604	CLA	C4B-NB	-2.96	1.34	1.37
45	H	101	RRX	C29-C30	2.96	1.64	1.54
29	R	608	CLA	C4B-NB	-2.96	1.34	1.37
29	n	610	CLA	C4B-NB	-2.96	1.34	1.37
29	s1	610	CLA	C4B-NB	-2.96	1.34	1.37
44	F	101	HEM	CAC-C3C	2.96	1.55	1.47
29	c1	513	CLA	C4B-NB	-2.96	1.34	1.37
29	r	610	CLA	C4B-NB	-2.96	1.34	1.37
43	D1	405	PL9	C7-C3	-2.96	1.48	1.51
29	N1	613	CLA	C4B-NB	-2.95	1.34	1.37
29	a1	406	CLA	C4B-NB	-2.95	1.34	1.37
29	C	503	CLA	C4B-NB	-2.95	1.34	1.37
30	A	409	PHO	C4D-CHA	2.95	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S	609	CLA	C4B-NB	-2.95	1.34	1.37
29	r	604	CLA	C4B-NB	-2.95	1.34	1.37
29	y	604	CLA	C4B-NB	-2.95	1.34	1.37
29	n1	613	CLA	C4B-NB	-2.95	1.34	1.37
44	F	101	HEM	FE-ND	2.95	2.04	1.94
29	b1	617	CLA	C4B-NB	-2.95	1.34	1.37
29	C	513	CLA	C4B-NB	-2.94	1.34	1.37
29	c1	508	CLA	C4B-NB	-2.94	1.34	1.37
48	R	607	CHL	C1B-NB	-2.94	1.34	1.37
53	R1	626	ERG	C4-C5	2.94	1.58	1.51
29	c1	511	CLA	C4B-NB	-2.94	1.34	1.37
45	H1	101	RRX	C7-C6	2.94	1.55	1.45
29	b	604	CLA	C4B-NB	-2.94	1.34	1.37
29	G1	610	CLA	C4B-NB	-2.94	1.34	1.37
48	s1	608	CHL	C3A-C2A	-2.94	1.46	1.54
29	r	602	CLA	C4B-NB	-2.94	1.34	1.37
29	R1	612	CLA	C4B-NB	-2.94	1.34	1.37
29	c1	501	CLA	C4B-NB	-2.94	1.34	1.37
36	B	620	C7Z	C38-C25	2.93	1.55	1.50
29	g1	604	CLA	C4B-NB	-2.93	1.34	1.37
48	n	608	CHL	C1B-NB	-2.93	1.34	1.37
29	B	607	CLA	C4B-NB	-2.93	1.34	1.37
29	b	609	CLA	C4B-NB	-2.93	1.34	1.37
29	N	611	CLA	C4B-NB	-2.93	1.34	1.37
45	h	101	RRX	C16-C17	2.93	1.52	1.43
44	F	101	HEM	FE-NB	2.93	2.03	1.94
29	N	610	CLA	C4B-NB	-2.92	1.34	1.37
36	b1	620	C7Z	C21-C26	-2.92	1.49	1.53
29	C	505	CLA	C4B-NB	-2.92	1.34	1.37
29	C	504	CLA	C4B-NB	-2.92	1.34	1.37
29	g	613	CLA	C4B-NB	-2.92	1.34	1.37
48	N	609	CHL	C1B-NB	-2.92	1.34	1.37
54	S	625	LPX	P1-O1	2.92	1.71	1.59
29	r1	602	CLA	C4B-NB	-2.91	1.34	1.37
29	b1	610	CLA	C4B-NB	-2.91	1.34	1.37
29	S	604	CLA	C4B-NB	-2.90	1.34	1.37
48	N1	601	CHL	C1B-NB	-2.90	1.34	1.37
48	N	608	CHL	C1B-NB	-2.90	1.34	1.37
29	b1	616	CLA	C4B-NB	-2.90	1.34	1.37
29	c1	502	CLA	C4B-NB	-2.90	1.34	1.37
29	R1	603	CLA	C4B-NB	-2.90	1.34	1.37
48	S1	606	CHL	C1B-NB	-2.90	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	s	625	LPX	P1-O1	2.90	1.71	1.59
29	s1	613	CLA	C4B-NB	-2.89	1.34	1.37
47	i1	101	4RF	O21-C22	2.89	1.42	1.34
48	n1	605	CHL	C3A-C2A	-2.89	1.46	1.54
44	F	101	HEM	FE-NA	2.89	2.04	1.95
29	y	611	CLA	C4B-NB	-2.89	1.34	1.37
29	R1	609	CLA	C4B-NB	-2.89	1.34	1.37
29	r	603	CLA	C4B-NB	-2.89	1.34	1.37
29	b1	609	CLA	C4B-NB	-2.89	1.34	1.37
54	S1	625	LPX	P1-O1	2.89	1.71	1.59
52	r1	625	LMT	O3'-C3'	-2.89	1.36	1.43
45	h1	101	RRX	C7-C6	2.88	1.55	1.45
29	C1	510	CLA	C4B-NB	-2.88	1.34	1.37
29	s1	617	CLA	C4B-NB	-2.88	1.34	1.37
54	s1	625	LPX	P1-O1	2.88	1.71	1.59
29	n1	610	CLA	C4B-NB	-2.88	1.34	1.37
29	g	614	CLA	C4B-NB	-2.88	1.34	1.37
29	Y	608	CLA	C4B-NB	-2.87	1.34	1.37
29	y1	603	CLA	C4B-NB	-2.87	1.34	1.37
48	s1	601	CHL	C3A-C2A	-2.87	1.46	1.54
29	G	613	CLA	C4B-NB	-2.87	1.34	1.37
44	f	101	HEM	CAC-C3C	2.87	1.55	1.47
29	c1	506	CLA	C4B-NB	-2.87	1.34	1.37
29	Y	611	CLA	C4B-NB	-2.87	1.34	1.37
29	s	613	CLA	C4B-NB	-2.87	1.34	1.37
29	S	603	CLA	C4B-NB	-2.86	1.34	1.37
29	n1	614	CLA	C4B-NB	-2.86	1.34	1.37
29	n1	612	CLA	C4B-NB	-2.86	1.34	1.37
29	s1	603	CLA	C4B-NB	-2.86	1.34	1.37
48	G1	608	CHL	C1B-NB	-2.86	1.34	1.37
29	y1	602	CLA	C4B-NB	-2.85	1.34	1.37
52	R	625	LMT	O3'-C3'	-2.85	1.36	1.43
29	c	506	CLA	C4B-NB	-2.85	1.34	1.37
48	n	601	CHL	C3A-C2A	-2.84	1.46	1.54
29	d1	403	CLA	C4B-NB	-2.84	1.34	1.37
53	r	626	ERG	C9-C8	2.84	1.59	1.51
29	G	603	CLA	C4B-NB	-2.83	1.34	1.37
29	B	602	CLA	C4B-NB	-2.83	1.34	1.37
29	y1	608	CLA	C4B-NB	-2.83	1.34	1.37
29	D1	403	CLA	C4B-NB	-2.83	1.34	1.37
29	b1	612	CLA	C4B-NB	-2.83	1.34	1.37
52	r	625	LMT	O3'-C3'	-2.82	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G1	613	CLA	C4B-NB	-2.82	1.34	1.37
29	c1	505	CLA	C4B-NB	-2.82	1.34	1.37
29	c1	507	CLA	C4B-NB	-2.82	1.34	1.37
29	r1	610	CLA	C4B-NB	-2.82	1.34	1.37
29	s1	602	CLA	C4B-NB	-2.82	1.34	1.37
29	n	611	CLA	C4B-NB	-2.81	1.34	1.37
29	y1	611	CLA	C4B-NB	-2.81	1.34	1.37
29	r	612	CLA	C4B-NB	-2.81	1.34	1.37
29	D	402	CLA	C4B-NB	-2.81	1.34	1.37
48	n1	608	CHL	C1B-NB	-2.81	1.34	1.37
29	N	602	CLA	C4B-NB	-2.81	1.34	1.37
48	Y1	607	CHL	C3A-C2A	-2.80	1.46	1.54
29	n	604	CLA	C4B-NB	-2.80	1.34	1.37
29	R	603	CLA	C4B-NB	-2.79	1.34	1.37
29	y1	604	CLA	C4B-NB	-2.79	1.34	1.37
29	c1	503	CLA	C4B-NB	-2.79	1.34	1.37
48	Y	606	CHL	C1B-NB	-2.79	1.34	1.37
47	K	101	4RF	O21-C22	2.79	1.42	1.34
29	r1	609	CLA	C4B-NB	-2.79	1.34	1.37
30	a	408	PHO	CMC-C2C	-2.78	1.46	1.50
43	d1	405	PL9	C3-C4	-2.78	1.45	1.49
29	D1	402	CLA	C4B-NB	-2.78	1.34	1.37
51	g	623	NEX	C1-C6	-2.78	1.49	1.54
29	b1	604	CLA	C4B-NB	-2.78	1.34	1.37
29	B	603	CLA	C4B-NB	-2.78	1.34	1.37
29	Y1	603	CLA	C4B-NB	-2.78	1.34	1.37
48	y	605	CHL	C1B-NB	-2.78	1.34	1.37
29	B1	603	CLA	C4B-NB	-2.78	1.34	1.37
29	S	605	CLA	C4B-NB	-2.77	1.34	1.37
48	S1	608	CHL	C1B-NB	-2.77	1.34	1.37
29	c1	509	CLA	C4B-NB	-2.77	1.34	1.37
53	R1	626	ERG	C9-C8	2.77	1.58	1.51
29	N1	614	CLA	C4B-NB	-2.77	1.34	1.37
48	g	609	CHL	C1B-NB	-2.76	1.34	1.37
53	r1	626	ERG	C9-C8	2.76	1.58	1.51
29	s	611	CLA	C4B-NB	-2.76	1.34	1.37
30	A	409	PHO	CMC-C2C	-2.76	1.46	1.50
51	s1	623	NEX	C17-C1	-2.75	1.48	1.53
48	y1	606	CHL	C1B-NB	-2.75	1.34	1.37
29	G	612	CLA	C4B-NB	-2.75	1.34	1.37
29	s1	611	CLA	C4B-NB	-2.75	1.34	1.37
29	B1	602	CLA	C4B-NB	-2.74	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G1	603	CLA	C4B-NB	-2.74	1.34	1.37
30	A	408	PHO	C4D-ND	-2.74	1.34	1.38
53	R	626	ERG	C4-C5	2.73	1.57	1.51
48	y1	601	CHL	C1B-NB	-2.73	1.34	1.37
45	h1	101	RRX	C32-C1	2.73	1.59	1.53
29	S	611	CLA	C4B-NB	-2.73	1.34	1.37
55	Y1	627	PTY	O7-C6	-2.72	1.39	1.46
45	H	101	RRX	C7-C6	2.72	1.54	1.45
48	g1	606	CHL	C3A-C2A	-2.72	1.46	1.54
47	i	101	4RF	O21-C22	2.72	1.42	1.34
29	n1	602	CLA	C4B-NB	-2.72	1.34	1.37
29	s1	605	CLA	C4B-NB	-2.72	1.34	1.37
30	a	409	PHO	CMD-C2D	-2.71	1.46	1.51
47	k1	101	4RF	O21-C22	2.71	1.42	1.34
30	A	409	PHO	CMD-C2D	-2.71	1.46	1.51
48	n1	609	CHL	C1B-NB	-2.70	1.34	1.37
29	N1	602	CLA	C4B-NB	-2.70	1.34	1.37
44	f	101	HEM	FE-ND	2.70	2.03	1.94
45	h	101	RRX	C32-C1	2.70	1.59	1.53
29	b1	614	CLA	C4B-NB	-2.70	1.34	1.37
30	a	408	PHO	C4D-ND	-2.70	1.34	1.38
52	R1	625	LMT	O3'-C3'	-2.69	1.36	1.43
29	g1	613	CLA	C4B-NB	-2.69	1.34	1.37
48	N1	607	CHL	C1B-NB	-2.69	1.34	1.37
29	n	614	CLA	C4B-NB	-2.69	1.34	1.37
29	C1	508	CLA	C4B-NB	-2.69	1.34	1.37
48	N1	605	CHL	C1B-NB	-2.69	1.34	1.37
52	R	625	LMT	O2'-C2'	-2.69	1.36	1.43
29	c	501	CLA	C4B-NB	-2.69	1.34	1.37
50	G1	622	XAT	O24-C25	-2.68	1.42	1.46
38	S	626	3PH	O31-C31	2.68	1.41	1.33
29	B1	605	CLA	C4B-NB	-2.68	1.34	1.37
47	k	101	4RF	O21-C22	2.68	1.41	1.34
48	G1	601	CHL	C1B-NB	-2.68	1.34	1.37
47	K1	101	4RF	O21-C22	2.68	1.41	1.34
53	r1	626	ERG	C4-C5	2.68	1.57	1.51
29	g1	610	CLA	C4B-NB	-2.68	1.34	1.37
48	n	609	CHL	C1B-NB	-2.67	1.34	1.37
29	s1	609	CLA	C4B-NB	-2.66	1.34	1.37
53	R1	626	ERG	C14-C8	2.66	1.58	1.51
29	R	610	CLA	C1C-C2C	2.66	1.49	1.44
38	s	626	3PH	O31-C31	2.66	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Y1	605	CHL	C1B-NB	-2.66	1.34	1.37
30	A	408	PHO	CMC-C2C	-2.65	1.46	1.50
29	y1	613	CLA	C4B-NB	-2.65	1.34	1.37
30	a	409	PHO	CMC-C2C	-2.65	1.46	1.50
29	r1	610	CLA	C1C-C2C	2.65	1.49	1.44
29	B1	609	CLA	C4B-NB	-2.65	1.34	1.37
30	a1	409	PHO	CMC-C2C	-2.65	1.46	1.50
48	g	607	CHL	C1B-NB	-2.65	1.34	1.37
29	s	605	CLA	C4B-NB	-2.64	1.34	1.37
29	s1	614	CLA	C4B-NB	-2.63	1.34	1.37
30	a	408	PHO	CMB-C2B	-2.63	1.46	1.51
48	y1	607	CHL	C1B-NB	-2.63	1.34	1.37
48	G	609	CHL	C1B-NB	-2.62	1.34	1.37
29	N	603	CLA	C4B-NB	-2.62	1.34	1.37
29	S1	602	CLA	C4B-NB	-2.62	1.34	1.37
29	b	608	CLA	C4B-NB	-2.62	1.34	1.37
29	c	504	CLA	C4B-NB	-2.62	1.34	1.37
29	G1	612	CLA	C4B-NB	-2.61	1.34	1.37
30	A	409	PHO	C4D-ND	-2.61	1.34	1.38
52	r	625	LMT	O2'-C2'	-2.61	1.36	1.43
55	y1	627	PTY	O7-C6	-2.60	1.40	1.46
55	Y	627	PTY	O7-C8	2.60	1.41	1.35
45	H1	101	RRX	C32-C1	2.60	1.58	1.53
29	s1	612	CLA	C4B-NB	-2.60	1.34	1.37
30	a1	408	PHO	CMB-C2B	-2.60	1.46	1.51
29	c1	513	CLA	C1C-C2C	2.59	1.49	1.44
33	D1	411	LMG	C37-C36	-2.59	1.33	1.51
29	Y1	614	CLA	C4B-NB	-2.59	1.34	1.37
30	A	408	PHO	CMD-C2D	-2.59	1.46	1.51
30	A1	409	PHO	CMC-C2C	-2.59	1.46	1.50
45	h	101	RRX	C7-C6	2.59	1.54	1.45
50	g1	622	XAT	O24-C25	-2.59	1.42	1.46
48	n	606	CHL	C1B-NB	-2.59	1.34	1.37
29	y1	612	CLA	C4B-NB	-2.58	1.34	1.37
55	Y	626	PTY	O7-C6	-2.58	1.40	1.46
29	R	612	CLA	C4B-NB	-2.58	1.34	1.37
43	D	405	PL9	C7-C8	-2.58	1.46	1.50
53	R	626	ERG	C14-C8	2.58	1.58	1.51
43	D1	405	PL9	C53-C6	-2.57	1.45	1.50
48	r	607	CHL	C1B-NB	-2.57	1.34	1.37
55	y	626	PTY	O4-C30	2.57	1.40	1.33
29	g1	612	CLA	C4B-NB	-2.57	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S	607	CHL	C1B-NB	-2.56	1.34	1.37
48	N	605	CHL	C1B-NB	-2.56	1.34	1.37
30	A1	408	PHO	CMC-C2C	-2.56	1.46	1.50
44	F1	101	HEM	FE-ND	2.56	2.02	1.94
29	b1	602	CLA	C1C-C2C	2.55	1.49	1.44
52	R	625	LMT	O2B-C2B	-2.55	1.37	1.43
30	A1	409	PHO	CAC-C3C	-2.55	1.47	1.51
48	G	606	CHL	C1B-NB	-2.55	1.34	1.37
50	r	621	XAT	O24-C25	-2.54	1.42	1.46
38	b1	624	3PH	O31-C31	2.54	1.40	1.33
33	D	411	LMG	C37-C36	-2.54	1.33	1.51
48	g1	607	CHL	C1B-NB	-2.54	1.34	1.37
30	A1	408	PHO	C4D-ND	-2.54	1.35	1.38
33	d	411	LMG	C37-C36	-2.54	1.33	1.51
38	t1	101	3PH	O31-C31	2.53	1.40	1.33
29	C1	501	CLA	C4B-NB	-2.53	1.34	1.37
29	S1	613	CLA	C4B-NB	-2.53	1.34	1.37
29	S1	603	CLA	C4B-NB	-2.53	1.34	1.37
48	Y	609	CHL	C1B-NB	-2.53	1.34	1.37
29	g1	611	CLA	C4B-NB	-2.53	1.34	1.37
29	d	402	CLA	C4B-NB	-2.52	1.34	1.37
48	s1	606	CHL	C1B-NB	-2.52	1.34	1.37
48	n	605	CHL	C1B-NB	-2.52	1.34	1.37
29	B1	616	CLA	C4B-NB	-2.52	1.34	1.37
47	I1	102	4RF	O21-C22	2.52	1.41	1.34
53	R	626	ERG	C9-C8	2.52	1.58	1.51
54	S1	625	LPX	P1-O2	2.52	1.69	1.59
48	y1	605	CHL	C1B-NB	-2.52	1.34	1.37
48	g	608	CHL	C1B-NB	-2.52	1.34	1.37
30	a1	409	PHO	C4D-ND	-2.52	1.35	1.38
55	Y	626	PTY	O4-C30	2.51	1.40	1.33
29	r1	608	CLA	C4B-NB	-2.51	1.34	1.37
48	s	607	CHL	C1B-NB	-2.51	1.34	1.37
33	d1	411	LMG	C37-C36	-2.51	1.33	1.51
30	A1	408	PHO	CMB-C2B	-2.51	1.46	1.51
29	r1	612	CLA	C4B-NB	-2.51	1.34	1.37
50	g	622	XAT	O24-C25	-2.51	1.42	1.46
30	a1	408	PHO	CAC-C3C	-2.51	1.47	1.51
38	B1	624	3PH	O31-C31	2.50	1.40	1.33
55	Y1	626	PTY	O7-C8	2.50	1.41	1.34
48	Y1	601	CHL	C1B-NB	-2.50	1.34	1.37
30	a1	409	PHO	CMB-C2B	-2.50	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	b	624	3PH	O21-C2	-2.49	1.40	1.46
30	a1	408	PHO	CMC-C2C	-2.49	1.46	1.50
29	B	613	CLA	C3D-C4D	-2.49	1.38	1.44
29	n1	603	CLA	C4B-NB	-2.49	1.34	1.37
45	H	101	RRX	C32-C1	2.49	1.58	1.53
48	G1	607	CHL	C1B-NB	-2.49	1.34	1.37
48	r1	607	CHL	C1B-NB	-2.49	1.34	1.37
55	y	627	PTY	O7-C8	2.48	1.40	1.35
49	N1	621	LUT	C1-C6	-2.48	1.50	1.53
31	B	618	BCR	C1-C6	-2.48	1.50	1.53
55	y	626	PTY	O7-C6	-2.48	1.40	1.46
48	G1	605	CHL	C1B-NB	-2.48	1.34	1.37
38	T	101	3PH	O21-C21	2.48	1.41	1.34
38	S1	626	3PH	O21-C2	-2.48	1.40	1.46
30	A	409	PHO	CMB-C2B	-2.47	1.46	1.51
52	R	625	LMT	O3B-C3B	-2.47	1.37	1.43
30	a	408	PHO	CMD-C2D	-2.47	1.46	1.51
29	b1	608	CLA	C1C-C2C	2.47	1.49	1.44
29	R1	608	CLA	C4B-NB	-2.47	1.34	1.37
48	G	601	CHL	C1B-NB	-2.47	1.34	1.37
48	Y1	607	CHL	C1B-NB	-2.47	1.34	1.37
29	s1	613	CLA	C1C-C2C	2.46	1.49	1.44
31	C1	514	BCR	C12-C13	-2.46	1.40	1.45
43	d	405	PL9	C26-C24	-2.46	1.46	1.51
38	s1	626	3PH	O21-C2	-2.46	1.40	1.46
43	D	405	PL9	C53-C6	-2.46	1.45	1.50
37	b1	623	DGD	O5D-C1E	2.46	1.44	1.40
30	A1	408	PHO	CMD-C2D	-2.46	1.46	1.51
30	a1	409	PHO	CAC-C3C	-2.45	1.47	1.51
29	C	508	CLA	C3D-C4D	-2.45	1.38	1.44
30	a1	408	PHO	CMD-C2D	-2.45	1.46	1.51
31	c	515	BCR	C12-C13	-2.44	1.40	1.45
29	y1	614	CLA	C1C-C2C	2.44	1.49	1.44
48	R1	606	CHL	C1B-NB	-2.44	1.34	1.37
29	S1	603	CLA	C1C-C2C	2.44	1.49	1.44
29	d	402	CLA	C3D-C4D	-2.43	1.38	1.44
38	t	101	3PH	O31-C31	2.43	1.40	1.33
43	d	405	PL9	C46-C44	-2.43	1.46	1.51
50	y	622	XAT	O24-C25	-2.42	1.42	1.46
50	Y1	622	XAT	O24-C25	-2.42	1.42	1.46
38	T	101	3PH	O31-C31	2.42	1.40	1.33
48	n1	607	CHL	C1B-NB	-2.42	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	n	622	XAT	O24-C25	-2.42	1.42	1.46
29	R1	610	CLA	C1C-C2C	2.41	1.49	1.44
52	R1	625	LMT	O3B-C3B	-2.41	1.37	1.43
52	r	625	LMT	O3B-C3B	-2.41	1.37	1.43
29	r1	603	CLA	C4B-NB	-2.40	1.34	1.37
29	a	405	CLA	C3D-C4D	-2.40	1.38	1.44
50	G	622	XAT	O24-C25	-2.40	1.42	1.46
30	a	408	PHO	CBD-CGD	-2.39	1.49	1.52
38	S1	626	3PH	O31-C31	2.39	1.40	1.33
38	B	624	3PH	O31-C31	2.39	1.40	1.33
29	g1	603	CLA	C4B-NB	-2.39	1.34	1.37
29	b	613	CLA	C3D-C4D	-2.39	1.38	1.44
38	T1	101	3PH	O31-C31	2.39	1.40	1.33
29	r1	612	CLA	C1C-C2C	2.39	1.49	1.44
48	N	606	CHL	C1B-NB	-2.38	1.34	1.37
29	r	608	CLA	C4B-NB	-2.38	1.34	1.37
52	r	625	LMT	O2B-C2B	-2.38	1.37	1.43
29	B	616	CLA	C4B-NB	-2.38	1.34	1.37
48	y	609	CHL	C1B-NB	-2.38	1.34	1.37
29	g1	604	CLA	C1C-C2C	2.38	1.49	1.44
39	C	524	DGA	OG2-CG2	-2.38	1.40	1.46
48	r1	606	CHL	C3A-C2A	-2.38	1.47	1.54
38	s1	626	3PH	O31-C31	2.38	1.40	1.33
45	h	101	RRX	C35-C13	2.38	1.55	1.50
55	y1	626	PTY	O7-C6	-2.38	1.40	1.46
53	r1	626	ERG	C14-C8	2.37	1.57	1.51
52	r1	625	LMT	O2'-C2'	-2.37	1.37	1.43
45	h1	101	RRX	C35-C13	2.37	1.55	1.50
29	R	612	CLA	C1C-C2C	2.37	1.49	1.44
29	D	402	CLA	C3D-C4D	-2.37	1.38	1.44
36	B	620	C7Z	C20-C13	2.37	1.55	1.50
48	s1	608	CHL	C3B-C4B	2.37	1.48	1.42
29	s1	605	CLA	C1A-CHA	2.36	1.52	1.43
29	b	605	CLA	C1A-CHA	2.36	1.52	1.43
30	A1	409	PHO	C4D-CHA	2.36	1.43	1.39
29	g1	603	CLA	C1C-C2C	2.36	1.49	1.44
29	b	604	CLA	C3D-C4D	-2.36	1.38	1.44
29	s1	611	CLA	C1A-CHA	2.35	1.52	1.43
29	R1	612	CLA	C1A-CHA	2.35	1.52	1.43
30	A	408	PHO	CMB-C2B	-2.35	1.46	1.51
55	Y1	626	PTY	O7-C6	-2.35	1.40	1.46
38	b1	624	3PH	O21-C2	-2.35	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B1	620	C7Z	C20-C13	2.35	1.55	1.50
55	Y1	626	PTY	O4-C30	2.35	1.40	1.33
29	g1	602	CLA	C1C-C2C	2.35	1.49	1.44
47	I	102	4RF	O21-C22	2.35	1.40	1.34
36	b	620	C7Z	C20-C13	2.35	1.55	1.50
29	C1	503	CLA	C1C-C2C	2.35	1.49	1.44
36	b1	620	C7Z	C20-C13	2.35	1.55	1.50
38	B	624	3PH	O21-C2	-2.35	1.40	1.46
45	H1	101	RRX	C35-C13	2.34	1.55	1.50
38	b	624	3PH	O31-C31	2.34	1.40	1.33
30	A	409	PHO	CAC-C3C	-2.34	1.47	1.51
48	S	601	CHL	C3A-C2A	-2.34	1.47	1.54
29	N	604	CLA	C3D-C4D	-2.34	1.38	1.44
54	s1	625	LPX	P1-O2	2.34	1.68	1.59
48	n	601	CHL	C1B-NB	-2.34	1.34	1.37
29	G	604	CLA	C3D-C4D	-2.34	1.38	1.44
29	Y1	612	CLA	C1C-C2C	2.33	1.49	1.44
30	A1	409	PHO	CMB-C2B	-2.33	1.46	1.51
29	c	512	CLA	C1C-C2C	2.33	1.49	1.44
29	B1	603	CLA	C1A-CHA	2.33	1.52	1.43
29	n	602	CLA	C1C-C2C	2.33	1.49	1.44
48	g	601	CHL	C1B-NB	-2.33	1.34	1.37
29	c1	511	CLA	C1A-CHA	2.33	1.52	1.43
38	B1	624	3PH	O21-C2	-2.33	1.40	1.46
29	C	510	CLA	C3D-C4D	-2.33	1.38	1.44
55	y1	626	PTY	O4-C1	-2.32	1.39	1.45
48	n	605	CHL	C3A-C2A	-2.32	1.48	1.54
29	Y1	614	CLA	C3D-C4D	-2.32	1.38	1.44
29	g1	611	CLA	C1C-C2C	2.32	1.49	1.44
30	A1	409	PHO	CMD-C2D	-2.32	1.46	1.51
50	r1	621	XAT	O24-C25	-2.32	1.42	1.46
36	b1	620	C7Z	C40-C33	2.32	1.55	1.50
38	S	626	3PH	O21-C21	2.32	1.40	1.34
29	C1	507	CLA	C3D-C4D	-2.31	1.39	1.44
29	c1	505	CLA	C1A-CHA	2.31	1.52	1.43
29	B1	615	CLA	C1C-C2C	2.31	1.49	1.44
29	y1	614	CLA	C3D-C4D	-2.31	1.39	1.44
29	B1	607	CLA	C3D-C4D	-2.31	1.39	1.44
29	r1	608	CLA	C1A-CHA	2.31	1.52	1.43
29	s	609	CLA	C1A-CHA	2.31	1.52	1.43
29	Y1	608	CLA	C1C-C2C	2.30	1.49	1.44
29	n	614	CLA	C1C-C2C	2.30	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	R1	621	XAT	O24-C25	-2.30	1.42	1.46
29	R	602	CLA	C1C-C2C	2.30	1.49	1.44
29	s	603	CLA	C1A-CHA	2.30	1.52	1.43
29	r	603	CLA	C1C-C2C	2.30	1.49	1.44
55	y1	626	PTY	O4-C30	2.30	1.40	1.33
29	y1	603	CLA	C3D-C4D	-2.30	1.39	1.44
29	C	509	CLA	C3D-C4D	-2.30	1.39	1.44
48	r1	606	CHL	C1B-NB	-2.30	1.35	1.37
30	a1	409	PHO	CMD-C2D	-2.30	1.46	1.51
36	b	620	C7Z	C18-C5	2.30	1.54	1.50
55	y	627	PTY	O7-C6	-2.30	1.40	1.46
29	r	612	CLA	C1A-CHA	2.30	1.52	1.43
48	s1	607	CHL	C1B-NB	-2.29	1.35	1.37
29	N	613	CLA	C1A-CHA	2.29	1.52	1.43
29	B1	608	CLA	C1A-CHA	2.29	1.52	1.43
29	S	614	CLA	C3D-C4D	-2.29	1.39	1.44
55	y1	626	PTY	O7-C8	2.29	1.40	1.34
48	g1	606	CHL	C1B-NB	-2.29	1.35	1.37
29	S	605	CLA	C1A-CHA	2.29	1.52	1.43
29	n	611	CLA	C1A-CHA	2.29	1.52	1.43
29	c1	509	CLA	C1C-C2C	2.29	1.49	1.44
48	N	605	CHL	C3A-C2A	-2.29	1.48	1.54
48	s	601	CHL	C1B-NB	-2.29	1.35	1.37
48	g1	609	CHL	C1B-NB	-2.28	1.35	1.37
53	R1	626	ERG	C11-C9	2.28	1.57	1.53
31	C	515	BCR	C1-C6	-2.28	1.50	1.53
48	G	608	CHL	C1B-NB	-2.28	1.35	1.37
29	R	612	CLA	C1A-CHA	2.28	1.52	1.43
55	Y	627	PTY	O7-C6	-2.28	1.40	1.46
34	a1	414	SPH	C3-C4	2.28	1.53	1.50
29	y1	602	CLA	C1C-C2C	2.28	1.49	1.44
29	B	616	CLA	C3B-C4B	2.28	1.48	1.42
38	s	626	3PH	O21-C21	2.28	1.40	1.34
29	C1	513	CLA	C1C-C2C	2.28	1.49	1.44
29	S1	611	CLA	C1A-CHA	2.28	1.52	1.43
29	g	613	CLA	C1A-CHA	2.28	1.52	1.43
29	Y1	610	CLA	C1A-CHA	2.28	1.52	1.43
29	b1	602	CLA	C3B-C4B	2.27	1.48	1.42
29	G1	602	CLA	C1A-CHA	2.27	1.52	1.43
29	c	510	CLA	C3D-C4D	-2.27	1.39	1.44
29	c	506	CLA	C3D-C4D	-2.27	1.39	1.44
29	c1	510	CLA	C3D-C4D	-2.27	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	S	625	LPX	P1-O2	2.27	1.68	1.59
48	y	606	CHL	C1B-NB	-2.27	1.35	1.37
29	C1	512	CLA	C1C-C2C	2.27	1.49	1.44
29	B	607	CLA	C3D-C4D	-2.27	1.39	1.44
48	S	601	CHL	C1B-NB	-2.27	1.35	1.37
29	Y	613	CLA	C1A-CHA	2.27	1.52	1.43
29	r1	602	CLA	C1C-C2C	2.27	1.49	1.44
29	d1	403	CLA	C1C-C2C	2.27	1.49	1.44
29	g1	614	CLA	C1C-C2C	2.27	1.49	1.44
29	g1	610	CLA	C3D-C4D	-2.27	1.39	1.44
29	C	507	CLA	C1A-CHA	2.27	1.52	1.43
29	B	604	CLA	C3D-C4D	-2.26	1.39	1.44
29	s1	612	CLA	C1A-CHA	2.26	1.52	1.43
29	s1	612	CLA	C1C-C2C	2.26	1.48	1.44
38	b	624	3PH	O21-C21	2.26	1.40	1.34
48	n1	601	CHL	C1B-NB	-2.26	1.35	1.37
29	b	602	CLA	C1C-C2C	2.26	1.48	1.44
38	b	624	3PH	O31-C3	-2.26	1.40	1.45
52	R1	625	LMT	O2B-C2B	-2.26	1.37	1.43
38	T1	101	3PH	O21-C21	2.26	1.40	1.34
29	a1	407	CLA	C1A-CHA	2.26	1.52	1.43
43	d	405	PL9	C52-C5	-2.26	1.46	1.50
29	R	603	CLA	C1C-C2C	2.26	1.48	1.44
29	c	509	CLA	C3D-C4D	-2.26	1.39	1.44
29	B1	614	CLA	CHD-C1D	2.26	1.42	1.38
29	G1	613	CLA	C1C-C2C	2.26	1.48	1.44
52	r1	625	LMT	O3B-C3B	-2.26	1.37	1.43
29	G	614	CLA	C1A-CHA	2.26	1.52	1.43
29	c	513	CLA	C1C-C2C	2.26	1.48	1.44
29	B1	605	CLA	C1A-CHA	2.26	1.52	1.43
29	Y1	603	CLA	C1C-C2C	2.26	1.48	1.44
29	b1	605	CLA	C1A-CHA	2.25	1.52	1.43
48	n	608	CHL	C3A-C2A	-2.25	1.48	1.54
48	g	605	CHL	C1B-NB	-2.25	1.35	1.37
29	N	602	CLA	C1C-C2C	2.25	1.48	1.44
29	A	405	CLA	C3D-C4D	-2.25	1.39	1.44
48	g	606	CHL	C1B-NB	-2.25	1.35	1.37
29	C	506	CLA	C3D-C4D	-2.25	1.39	1.44
29	S	611	CLA	C1A-CHA	2.25	1.52	1.43
29	D1	403	CLA	C1C-C2C	2.25	1.48	1.44
51	g1	623	NEX	O24-C25	-2.25	1.43	1.46
29	b1	608	CLA	C1A-CHA	2.25	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	t1	101	3PH	O21-C2	-2.24	1.41	1.46
38	T	101	3PH	O31-C3	-2.24	1.40	1.45
29	B	616	CLA	C1A-CHA	2.24	1.52	1.43
38	b1	624	3PH	O21-C21	2.24	1.40	1.34
29	g1	611	CLA	C1A-CHA	2.24	1.52	1.43
29	B	615	CLA	C3D-C4D	-2.24	1.39	1.44
29	B1	602	CLA	C1A-CHA	2.24	1.52	1.43
30	a	409	PHO	C4D-ND	-2.24	1.35	1.38
29	N	610	CLA	C1A-CHA	2.24	1.52	1.43
29	a	406	CLA	C3D-C4D	-2.24	1.39	1.44
29	C1	502	CLA	C3D-C4D	-2.24	1.39	1.44
29	c	505	CLA	C3D-C4D	-2.24	1.39	1.44
29	b	615	CLA	C3D-C4D	-2.24	1.39	1.44
29	b1	603	CLA	C1C-C2C	2.24	1.48	1.44
29	c1	508	CLA	C1C-C2C	2.24	1.48	1.44
29	s	614	CLA	C3D-C4D	-2.24	1.39	1.44
30	a	409	PHO	CMB-C2B	-2.24	1.47	1.51
29	y	613	CLA	C1A-CHA	2.24	1.52	1.43
29	n	613	CLA	C1A-CHA	2.23	1.52	1.43
29	y	608	CLA	C3D-C4D	-2.23	1.39	1.44
29	a	407	CLA	C1A-CHA	2.23	1.52	1.43
51	n	623	NEX	C1-C6	-2.23	1.50	1.54
29	B	611	CLA	C3D-C4D	-2.23	1.39	1.44
29	B1	610	CLA	C1A-CHA	2.23	1.52	1.43
29	n1	603	CLA	C1A-CHA	2.23	1.52	1.43
29	s	605	CLA	C1A-CHA	2.23	1.52	1.43
30	a1	408	PHO	C4D-ND	-2.23	1.35	1.38
43	d	405	PL9	C7-C8	-2.23	1.47	1.50
29	r	602	CLA	C3D-C4D	-2.23	1.39	1.44
34	a	414	SPH	C3-C4	2.23	1.53	1.50
29	B	608	CLA	C1A-CHA	2.23	1.52	1.43
29	s	611	CLA	C1A-CHA	2.23	1.52	1.43
29	r1	612	CLA	C1A-CHA	2.23	1.52	1.43
53	r1	626	ERG	C11-C9	2.23	1.57	1.53
44	F	101	HEM	FE-NC	2.23	2.02	1.95
29	R1	603	CLA	C1A-CHA	2.23	1.52	1.43
29	Y1	608	CLA	C3D-C4D	-2.23	1.39	1.44
29	a1	406	CLA	C3D-C4D	-2.23	1.39	1.44
39	c	524	DGA	OG2-CG2	-2.23	1.41	1.46
48	Y	605	CHL	C1B-NB	-2.23	1.35	1.37
29	c	507	CLA	C3D-C4D	-2.22	1.39	1.44
29	S1	605	CLA	C1A-CHA	2.22	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	y1	610	CLA	C1A-CHA	2.22	1.52	1.43
29	b	616	CLA	C3D-C4D	-2.22	1.39	1.44
29	c1	501	CLA	C1A-CHA	2.22	1.52	1.43
29	C	503	CLA	C1A-CHA	2.22	1.52	1.43
29	c	512	CLA	C1A-CHA	2.22	1.52	1.43
52	R	625	LMT	O4'-C4B	-2.22	1.37	1.43
29	G1	614	CLA	C1A-CHA	2.22	1.52	1.43
29	y	604	CLA	C1A-CHA	2.22	1.52	1.43
29	y1	612	CLA	C1C-C2C	2.22	1.48	1.44
29	b	614	CLA	C1A-CHA	2.22	1.52	1.43
29	s1	609	CLA	C1A-CHA	2.22	1.52	1.43
29	s	610	CLA	C1A-CHA	2.22	1.52	1.43
29	b	608	CLA	C1A-CHA	2.22	1.52	1.43
48	S1	607	CHL	C1B-NB	-2.21	1.35	1.37
29	C1	501	CLA	C1A-CHA	2.21	1.52	1.43
29	G1	604	CLA	C1A-CHA	2.21	1.52	1.43
29	Y	614	CLA	C3D-C4D	-2.21	1.39	1.44
29	N	611	CLA	C1A-CHA	2.21	1.52	1.43
51	R	622	NEX	C18-C5	-2.21	1.49	1.52
29	N	614	CLA	C1A-CHA	2.21	1.52	1.43
48	S	606	CHL	C1B-NB	-2.21	1.35	1.37
29	R	608	CLA	C1A-CHA	2.21	1.52	1.43
29	R1	602	CLA	C1C-C2C	2.21	1.48	1.44
29	y1	612	CLA	C1A-CHA	2.21	1.52	1.43
29	R	603	CLA	C3D-C4D	-2.21	1.39	1.44
29	b1	609	CLA	C1A-CHA	2.21	1.52	1.43
29	N1	602	CLA	C3B-C4B	2.21	1.47	1.42
29	s1	613	CLA	C1A-CHA	2.21	1.52	1.43
31	C	517	BCR	C12-C13	-2.21	1.41	1.45
29	A	410	CLA	C3D-C4D	-2.21	1.39	1.44
29	b	603	CLA	C3D-C4D	-2.20	1.39	1.44
50	N	622	XAT	O24-C25	-2.20	1.43	1.46
30	A	408	PHO	CAC-C3C	-2.20	1.47	1.51
29	s1	610	CLA	C1A-CHA	2.20	1.52	1.43
29	Y1	613	CLA	C3D-C4D	-2.20	1.39	1.44
29	n	612	CLA	C1A-CHA	2.20	1.52	1.43
29	C	505	CLA	C3D-C4D	-2.20	1.39	1.44
29	g1	614	CLA	C1A-CHA	2.20	1.52	1.43
29	n	610	CLA	C1C-C2C	2.20	1.48	1.44
55	Y	626	PTY	O7-C8	2.20	1.40	1.34
29	B1	603	CLA	C1C-C2C	2.20	1.48	1.44
29	G1	613	CLA	C1A-CHA	2.20	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	S1	626	3PH	O21-C21	2.20	1.40	1.34
29	C	512	CLA	C1A-CHA	2.20	1.52	1.43
29	S	602	CLA	C3D-C4D	-2.20	1.39	1.44
38	t	101	3PH	O21-C21	2.20	1.40	1.34
29	g1	603	CLA	C3B-C4B	2.20	1.47	1.42
29	g	604	CLA	C3D-C4D	-2.20	1.39	1.44
29	n	603	CLA	C1A-CHA	2.20	1.52	1.43
51	s1	623	NEX	C4-C3	2.20	1.55	1.52
43	d	405	PL9	C21-C19	-2.20	1.46	1.51
29	n1	602	CLA	C1C-C2C	2.20	1.48	1.44
29	r1	604	CLA	C1A-CHA	2.20	1.52	1.43
43	D1	405	PL9	C7-C8	-2.19	1.47	1.50
29	Y1	602	CLA	C3D-C4D	-2.19	1.39	1.44
29	s	613	CLA	C1A-CHA	2.19	1.52	1.43
29	b1	606	CLA	C3D-C4D	-2.19	1.39	1.44
48	Y	601	CHL	C3A-C2A	-2.19	1.48	1.54
30	a	408	PHO	CAC-C3C	-2.19	1.47	1.51
38	B	624	3PH	O21-C21	2.19	1.40	1.34
29	n1	611	CLA	C1A-CHA	2.19	1.52	1.43
29	N1	602	CLA	C1C-C2C	2.19	1.48	1.44
29	R1	608	CLA	C1A-CHA	2.19	1.52	1.43
29	C	511	CLA	C1A-CHA	2.19	1.52	1.43
51	g	623	NEX	O24-C25	-2.19	1.43	1.46
29	c	511	CLA	C3D-C4D	-2.19	1.39	1.44
29	c	501	CLA	C3D-C4D	-2.19	1.39	1.44
29	G1	610	CLA	C1C-C2C	2.19	1.48	1.44
29	B1	607	CLA	C1C-C2C	2.19	1.48	1.44
52	R1	625	LMT	O1'-C1'	-2.19	1.36	1.40
29	Y1	612	CLA	C1A-CHA	2.19	1.52	1.43
30	a	409	PHO	CAC-C3C	-2.19	1.47	1.51
29	s	617	CLA	C1A-CHA	2.18	1.52	1.43
29	R	609	CLA	C3D-C4D	-2.18	1.39	1.44
29	n1	604	CLA	C1A-CHA	2.18	1.52	1.43
48	y	609	CHL	C3A-C2A	-2.18	1.48	1.54
29	y	602	CLA	C3D-C4D	-2.18	1.39	1.44
29	S1	602	CLA	C1C-C2C	2.18	1.48	1.44
29	D	402	CLA	C3B-C4B	2.18	1.47	1.42
48	N	601	CHL	C1B-NB	-2.18	1.35	1.37
48	G	605	CHL	C1B-NB	-2.18	1.35	1.37
29	S1	613	CLA	C1A-CHA	2.18	1.52	1.43
29	c1	503	CLA	C1A-CHA	2.18	1.52	1.43
29	B	609	CLA	C3D-C4D	-2.18	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	507	CLA	C3D-C4D	-2.18	1.39	1.44
52	r	625	LMT	O4'-C4B	-2.18	1.37	1.43
29	b1	602	CLA	C1A-CHA	2.18	1.52	1.43
53	r	626	ERG	C14-C8	2.18	1.57	1.51
29	N1	614	CLA	C1A-CHA	2.18	1.52	1.43
50	n1	622	XAT	O24-C25	-2.18	1.43	1.46
29	B	605	CLA	C3D-C4D	-2.18	1.39	1.44
29	N1	604	CLA	C3D-C4D	-2.18	1.39	1.44
29	b1	614	CLA	C1A-CHA	2.18	1.52	1.43
48	N	608	CHL	C3A-C2A	-2.18	1.48	1.54
29	b	607	CLA	C3D-C4D	-2.18	1.39	1.44
48	N	609	CHL	C3A-C2A	-2.18	1.48	1.54
29	s	612	CLA	C3D-C4D	-2.18	1.39	1.44
29	B	612	CLA	C3D-C4D	-2.17	1.39	1.44
29	r1	608	CLA	C3B-C4B	2.17	1.47	1.42
29	r1	609	CLA	C1C-C2C	2.17	1.48	1.44
29	c1	508	CLA	C3D-C4D	-2.17	1.39	1.44
29	c	513	CLA	C3D-C4D	-2.17	1.39	1.44
29	B	614	CLA	C1A-CHA	2.17	1.52	1.43
29	g	614	CLA	C1C-C2C	2.17	1.48	1.44
29	R1	603	CLA	C1C-C2C	2.17	1.48	1.44
29	n1	614	CLA	C1C-C2C	2.17	1.48	1.44
29	B	602	CLA	C1A-CHA	2.17	1.52	1.43
38	s	626	3PH	O21-C2	-2.17	1.41	1.46
36	B1	620	C7Z	C40-C33	2.17	1.55	1.50
38	t	101	3PH	O21-C2	-2.17	1.41	1.46
29	Y1	603	CLA	C3D-C4D	-2.17	1.39	1.44
29	g	610	CLA	C1A-CHA	2.17	1.52	1.43
29	c1	512	CLA	C1A-CHA	2.17	1.52	1.43
55	y	627	PTY	O4-C1	-2.17	1.40	1.45
48	S	608	CHL	C1B-NB	-2.17	1.35	1.37
39	c1	524	DGA	OG2-CG2	-2.17	1.41	1.46
29	g	611	CLA	C1A-CHA	2.17	1.52	1.43
29	g1	612	CLA	C1A-CHA	2.17	1.52	1.43
29	C	501	CLA	C3D-C4D	-2.17	1.39	1.44
29	D	403	CLA	C1A-CHA	2.17	1.52	1.43
29	Y	610	CLA	C1A-CHA	2.17	1.52	1.43
48	N1	606	CHL	C1B-NB	-2.17	1.35	1.37
29	Y	602	CLA	C3D-C4D	-2.17	1.39	1.44
29	C1	503	CLA	C3D-C4D	-2.17	1.39	1.44
29	Y	608	CLA	C1A-CHA	2.17	1.52	1.43
29	N1	611	CLA	CHD-C1D	2.17	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S1	610	CLA	C3D-C4D	-2.17	1.39	1.44
31	C	514	BCR	C12-C13	-2.17	1.41	1.45
29	B	603	CLA	C1A-CHA	2.17	1.52	1.43
29	S1	603	CLA	C1A-CHA	2.17	1.52	1.43
55	Y1	626	PTY	O4-C1	-2.17	1.40	1.45
29	N1	611	CLA	C3D-C4D	-2.17	1.39	1.44
29	G	611	CLA	C1A-CHA	2.17	1.52	1.43
29	s1	605	CLA	C1C-C2C	2.16	1.48	1.44
29	r	610	CLA	C1A-CHA	2.16	1.52	1.43
38	B1	624	3PH	O21-C21	2.16	1.40	1.34
29	y	614	CLA	C3D-C4D	-2.16	1.39	1.44
29	A1	406	CLA	C1A-CHA	2.16	1.52	1.43
29	A1	407	CLA	C3D-C4D	-2.16	1.39	1.44
54	s	625	LPX	P1-O2	2.16	1.68	1.59
29	G	603	CLA	C1C-C2C	2.16	1.48	1.44
29	g	614	CLA	MG-NC	2.16	2.11	2.06
29	B1	606	CLA	C1A-CHA	2.16	1.52	1.43
29	a1	405	CLA	C1A-CHA	2.16	1.52	1.43
39	j	101	DGA	OG2-CG2	-2.16	1.41	1.46
29	N1	610	CLA	C1A-CHA	2.16	1.52	1.43
29	Y	613	CLA	C3D-C4D	-2.16	1.39	1.44
29	G1	610	CLA	C3D-C4D	-2.16	1.39	1.44
29	S	612	CLA	C1A-CHA	2.16	1.52	1.43
29	R1	609	CLA	C1A-CHA	2.16	1.52	1.43
29	A	407	CLA	C1A-CHA	2.16	1.52	1.43
29	B1	613	CLA	C3D-C4D	-2.16	1.39	1.44
29	c	505	CLA	C1A-CHA	2.16	1.52	1.43
29	y1	610	CLA	C3D-C4D	-2.16	1.39	1.44
29	A1	410	CLA	C1A-CHA	2.16	1.52	1.43
50	R	621	XAT	O24-C25	-2.16	1.43	1.46
29	n	614	CLA	C1A-CHA	2.15	1.52	1.43
38	T1	101	3PH	O31-C3	-2.15	1.40	1.45
50	y1	622	XAT	O24-C25	-2.15	1.43	1.46
29	C1	507	CLA	C1C-C2C	2.15	1.48	1.44
29	b1	609	CLA	C1C-C2C	2.15	1.48	1.44
29	g1	612	CLA	C1C-C2C	2.15	1.48	1.44
29	S1	605	CLA	C1C-C2C	2.15	1.48	1.44
29	s	617	CLA	C3D-C4D	-2.15	1.39	1.44
29	B1	609	CLA	C1C-C2C	2.15	1.48	1.44
29	r1	603	CLA	C1A-CHA	2.15	1.52	1.43
29	n1	612	CLA	C1A-CHA	2.15	1.52	1.43
52	R1	625	LMT	O5B-C5B	-2.15	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	r	608	CLA	C1A-CHA	2.15	1.52	1.43
29	r	608	CLA	CHD-C1D	2.15	1.42	1.38
29	d1	402	CLA	C3D-C4D	-2.15	1.39	1.44
48	n	606	CHL	C3A-C2A	-2.15	1.48	1.54
29	B1	615	CLA	C1A-CHA	2.14	1.52	1.43
29	y	612	CLA	C1A-CHA	2.14	1.52	1.43
29	s1	603	CLA	C1A-CHA	2.14	1.52	1.43
29	b1	615	CLA	C3D-C4D	-2.14	1.39	1.44
29	Y1	611	CLA	C1A-CHA	2.14	1.52	1.43
29	b	611	CLA	C3D-C4D	-2.14	1.39	1.44
29	b	606	CLA	C3D-C4D	-2.14	1.39	1.44
29	n	604	CLA	C3D-C4D	-2.14	1.39	1.44
50	N1	622	XAT	O24-C25	-2.14	1.43	1.46
29	s	604	CLA	C3D-C4D	-2.14	1.39	1.44
29	y	603	CLA	C1A-CHA	2.14	1.52	1.43
30	A1	408	PHO	C3D-C4D	2.14	1.44	1.41
29	S	609	CLA	C1A-CHA	2.14	1.52	1.43
30	a1	409	PHO	C3D-C4D	2.14	1.44	1.41
29	b	610	CLA	C1A-CHA	2.14	1.52	1.43
29	C1	510	CLA	C1C-C2C	2.14	1.48	1.44
29	R1	609	CLA	C1C-C2C	2.14	1.48	1.44
29	c	507	CLA	C1A-CHA	2.14	1.52	1.43
29	g	610	CLA	C3D-C4D	-2.14	1.39	1.44
29	a1	410	CLA	C1A-CHA	2.14	1.52	1.43
48	n1	605	CHL	C1B-NB	-2.14	1.35	1.37
29	Y	612	CLA	C3D-C4D	-2.14	1.39	1.44
29	b	609	CLA	C3D-C4D	-2.14	1.39	1.44
29	S1	617	CLA	C1C-C2C	2.14	1.48	1.44
43	d1	405	PL9	C53-C6	-2.14	1.46	1.50
29	n	602	CLA	C3D-C4D	-2.14	1.39	1.44
29	y1	608	CLA	C3D-C4D	-2.14	1.39	1.44
45	H	101	RRX	C35-C13	2.14	1.55	1.50
29	d1	402	CLA	C1A-CHA	2.13	1.52	1.43
29	n1	612	CLA	C1C-C2C	2.13	1.48	1.44
29	s	603	CLA	C1C-C2C	2.13	1.48	1.44
29	c	503	CLA	C3D-C4D	-2.13	1.39	1.44
29	C	501	CLA	C1A-CHA	2.13	1.52	1.43
29	S	613	CLA	C3D-C4D	-2.13	1.39	1.44
29	S1	604	CLA	C1A-CHA	2.13	1.52	1.43
29	S	603	CLA	C1A-CHA	2.13	1.52	1.43
29	n1	613	CLA	C1A-CHA	2.13	1.51	1.43
29	b	617	CLA	C1A-CHA	2.13	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R1	602	CLA	C1A-CHA	2.13	1.51	1.43
29	c	513	CLA	C1A-CHA	2.13	1.51	1.43
29	c1	513	CLA	C1A-CHA	2.13	1.51	1.43
29	b	609	CLA	C1C-C2C	2.13	1.48	1.44
29	C1	513	CLA	C3D-C4D	-2.13	1.39	1.44
29	B1	614	CLA	C3D-C4D	-2.13	1.39	1.44
29	C	505	CLA	C1A-CHA	2.13	1.51	1.43
29	y1	604	CLA	C1A-CHA	2.13	1.51	1.43
29	g	603	CLA	C3D-C4D	-2.13	1.39	1.44
29	y	608	CLA	C1A-CHA	2.13	1.51	1.43
29	b	602	CLA	C1A-CHA	2.13	1.51	1.43
29	R	610	CLA	C3D-C4D	-2.13	1.39	1.44
29	B1	617	CLA	C3D-C4D	-2.13	1.39	1.44
31	b	618	BCR	C1-C6	-2.13	1.50	1.53
29	B	605	CLA	C1A-CHA	2.13	1.51	1.43
29	g	614	CLA	C1A-CHA	2.13	1.51	1.43
29	y	611	CLA	C3D-C4D	-2.13	1.39	1.44
29	C1	509	CLA	C3D-C4D	-2.13	1.39	1.44
29	S	604	CLA	C1A-CHA	2.13	1.51	1.43
51	G1	623	NEX	O24-C25	-2.12	1.43	1.46
29	Y	612	CLA	C1A-CHA	2.12	1.51	1.43
50	Y	622	XAT	O24-C25	-2.12	1.43	1.46
29	g	612	CLA	C1A-CHA	2.12	1.51	1.43
29	S	603	CLA	MG-NC	2.12	2.11	2.06
29	R	610	CLA	C3B-C4B	2.12	1.47	1.42
29	b	607	CLA	C1A-CHA	2.12	1.51	1.43
29	g1	613	CLA	C1C-C2C	2.12	1.48	1.44
29	r1	604	CLA	C1C-C2C	2.12	1.48	1.44
29	c1	508	CLA	C3B-C4B	2.12	1.47	1.42
29	c1	501	CLA	C3D-C4D	-2.12	1.39	1.44
51	n	623	NEX	O24-C25	-2.12	1.43	1.46
29	c1	505	CLA	C1C-C2C	2.12	1.48	1.44
29	G1	612	CLA	C3D-C4D	-2.12	1.39	1.44
29	G	613	CLA	C1A-CHA	2.12	1.51	1.43
29	b	612	CLA	C1A-CHA	2.12	1.51	1.43
29	b1	612	CLA	C3D-C4D	-2.12	1.39	1.44
29	R1	604	CLA	C1A-CHA	2.12	1.51	1.43
29	r	603	CLA	C1A-CHA	2.12	1.51	1.43
29	s1	605	CLA	C3D-C4D	-2.12	1.39	1.44
29	b1	612	CLA	C1A-CHA	2.12	1.51	1.43
29	y1	613	CLA	C1A-CHA	2.12	1.51	1.43
39	C1	524	DGA	CB2-CB1	2.12	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b1	604	CLA	C1C-C2C	2.12	1.48	1.44
29	N	612	CLA	C1A-CHA	2.12	1.51	1.43
29	G1	612	CLA	C1C-C2C	2.12	1.48	1.44
29	S1	609	CLA	C1A-CHA	2.12	1.51	1.43
29	C	503	CLA	C3D-C4D	-2.12	1.39	1.44
29	B1	606	CLA	C3D-C4D	-2.12	1.39	1.44
48	Y1	606	CHL	C1B-NB	-2.12	1.35	1.37
29	Y	610	CLA	C3D-C4D	-2.12	1.39	1.44
29	B	614	CLA	C1C-C2C	2.12	1.48	1.44
29	a	406	CLA	C1A-CHA	2.12	1.51	1.43
43	D1	405	PL9	C3-C4	-2.12	1.46	1.49
29	N	603	CLA	C1A-CHA	2.12	1.51	1.43
29	n1	614	CLA	C1A-CHA	2.12	1.51	1.43
29	b1	613	CLA	C1A-CHA	2.12	1.51	1.43
29	B	617	CLA	C1A-CHA	2.12	1.51	1.43
52	r1	625	LMT	O2B-C2B	-2.12	1.38	1.43
38	t1	101	3PH	O21-C21	2.11	1.40	1.34
29	B	606	CLA	C1A-CHA	2.11	1.51	1.43
29	S1	611	CLA	MG-NC	2.11	2.11	2.06
29	c1	509	CLA	C3D-C4D	-2.11	1.39	1.44
29	g1	614	CLA	MG-NC	2.11	2.11	2.06
29	C1	508	CLA	C1D-ND	-2.11	1.35	1.37
29	b	612	CLA	C3D-C4D	-2.11	1.39	1.44
29	C	506	CLA	C1A-CHA	2.11	1.51	1.43
29	B1	609	CLA	C1A-CHA	2.11	1.51	1.43
29	s1	603	CLA	C1C-C2C	2.11	1.48	1.44
29	c	508	CLA	C3D-C4D	-2.11	1.39	1.44
29	c	512	CLA	C3D-C4D	-2.11	1.39	1.44
29	C	513	CLA	C3D-C4D	-2.11	1.39	1.44
36	B	620	C7Z	C40-C33	2.11	1.55	1.50
29	y1	603	CLA	C1C-C2C	2.11	1.48	1.44
29	b	610	CLA	C3D-C4D	-2.11	1.39	1.44
29	G	610	CLA	C1A-CHA	2.11	1.51	1.43
29	d	403	CLA	C3D-C4D	-2.11	1.39	1.44
29	B1	602	CLA	C1C-C2C	2.11	1.48	1.44
29	Y1	603	CLA	C1A-CHA	2.11	1.51	1.43
29	S	612	CLA	C3D-C4D	-2.11	1.39	1.44
48	R1	607	CHL	C1B-NB	-2.11	1.35	1.37
29	s1	614	CLA	C1A-CHA	2.11	1.51	1.43
29	r1	610	CLA	C1A-CHA	2.11	1.51	1.43
29	N1	614	CLA	C3D-C4D	-2.11	1.39	1.44
29	C1	501	CLA	C3D-C4D	-2.11	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	N	612	CLA	C3D-C4D	-2.11	1.39	1.44
29	g1	602	CLA	C1A-CHA	2.11	1.51	1.43
29	d	402	CLA	C1C-C2C	2.11	1.48	1.44
48	g	601	CHL	C3A-C2A	-2.10	1.48	1.54
55	y	626	PTY	O7-C8	2.10	1.40	1.34
52	R1	625	LMT	O4'-C4B	-2.10	1.38	1.43
29	s1	605	CLA	MG-NC	2.10	2.11	2.06
36	b	620	C7Z	C10-C9	-2.10	1.33	1.35
29	Y	603	CLA	C3D-C4D	-2.10	1.39	1.44
29	r	604	CLA	C1A-CHA	2.10	1.51	1.43
29	r	609	CLA	C3D-C4D	-2.10	1.39	1.44
29	C1	511	CLA	C1A-CHA	2.10	1.51	1.43
51	y1	623	NEX	O24-C25	-2.10	1.43	1.46
29	A	406	CLA	C1A-CHA	2.10	1.51	1.43
29	b1	607	CLA	C1A-CHA	2.10	1.51	1.43
29	R	608	CLA	C3D-C4D	-2.10	1.39	1.44
55	y1	627	PTY	O7-C8	2.10	1.39	1.35
29	b1	614	CLA	MG-NC	2.10	2.11	2.06
29	b1	614	CLA	C1C-C2C	2.10	1.48	1.44
36	B1	620	C7Z	C18-C5	2.10	1.54	1.50
29	r	608	CLA	C3D-C4D	-2.10	1.39	1.44
48	r	606	CHL	C1B-NB	-2.10	1.35	1.37
29	B	615	CLA	C1A-CHA	2.10	1.51	1.43
29	c1	504	CLA	C1A-CHA	2.10	1.51	1.43
29	G	604	CLA	C1A-CHA	2.10	1.51	1.43
29	N1	612	CLA	C1A-CHA	2.10	1.51	1.43
29	s	602	CLA	C3D-C4D	-2.10	1.39	1.44
29	G	602	CLA	C1A-CHA	2.10	1.51	1.43
29	S1	617	CLA	C1A-CHA	2.10	1.51	1.43
29	b	605	CLA	C3D-C4D	-2.10	1.39	1.44
29	R	603	CLA	C1A-CHA	2.10	1.51	1.43
29	c	504	CLA	C3D-C4D	-2.10	1.39	1.44
29	R1	608	CLA	C1C-C2C	2.09	1.48	1.44
29	y1	611	CLA	C1A-CHA	2.09	1.51	1.43
48	n1	606	CHL	C1B-NB	-2.09	1.35	1.37
48	Y	609	CHL	C3D-C2D	-2.09	1.33	1.39
47	k	101	4RF	O21-C20	-2.09	1.41	1.46
29	a	410	CLA	C1A-CHA	2.09	1.51	1.43
29	S	609	CLA	C3D-C4D	-2.09	1.39	1.44
29	g	603	CLA	C1A-CHA	2.09	1.51	1.43
29	s1	609	CLA	C1C-C2C	2.09	1.48	1.44
29	y1	610	CLA	C1C-C2C	2.09	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D1	402	CLA	C3D-C4D	-2.09	1.39	1.44
29	B	607	CLA	C1A-CHA	2.09	1.51	1.43
29	C1	506	CLA	C3D-C4D	-2.09	1.39	1.44
29	C1	510	CLA	C3D-C4D	-2.09	1.39	1.44
29	y	610	CLA	C1A-CHA	2.09	1.51	1.43
52	R1	625	LMT	O5'-C5'	-2.09	1.39	1.44
29	y	603	CLA	C3D-C4D	-2.09	1.39	1.44
29	S	617	CLA	C1A-CHA	2.09	1.51	1.43
48	Y1	609	CHL	C1B-NB	-2.09	1.35	1.37
29	s	609	CLA	C3D-C4D	-2.09	1.39	1.44
29	D1	403	CLA	C1A-CHA	2.09	1.51	1.43
29	R1	610	CLA	C1A-CHA	2.09	1.51	1.43
29	C	504	CLA	C3D-C4D	-2.09	1.39	1.44
29	s	611	CLA	C1C-C2C	2.09	1.48	1.44
29	S1	612	CLA	C1A-CHA	2.09	1.51	1.43
29	A1	405	CLA	C3D-C4D	-2.09	1.39	1.44
29	r1	609	CLA	C1A-CHA	2.09	1.51	1.43
31	C	515	BCR	C12-C13	-2.09	1.41	1.45
29	N1	603	CLA	C1A-CHA	2.09	1.51	1.43
29	g1	603	CLA	C3D-C4D	-2.09	1.39	1.44
51	G	623	NEX	O24-C25	-2.09	1.43	1.46
29	S	613	CLA	C1A-CHA	2.09	1.51	1.43
29	B	617	CLA	C3D-C4D	-2.09	1.39	1.44
29	G1	611	CLA	C1A-CHA	2.09	1.51	1.43
29	g	602	CLA	C3D-C4D	-2.08	1.39	1.44
29	Y	611	CLA	C1A-CHA	2.08	1.51	1.43
29	C1	510	CLA	C1A-CHA	2.08	1.51	1.43
29	n1	613	CLA	C3D-C4D	-2.08	1.39	1.44
29	G1	603	CLA	C1A-CHA	2.08	1.51	1.43
29	d	403	CLA	C1A-CHA	2.08	1.51	1.43
29	N	603	CLA	C3D-C4D	-2.08	1.39	1.44
29	n1	612	CLA	CHD-C1D	2.08	1.42	1.38
29	B	616	CLA	C1C-C2C	2.08	1.48	1.44
29	b1	606	CLA	C1A-CHA	2.08	1.51	1.43
29	B	603	CLA	C1C-C2C	2.08	1.48	1.44
29	g	602	CLA	C1C-C2C	2.08	1.48	1.44
29	y	608	CLA	C1C-C2C	2.08	1.48	1.44
37	b	623	DGD	O5D-C1E	2.08	1.43	1.40
38	s1	626	3PH	O21-C21	2.08	1.40	1.34
29	B1	617	CLA	C1A-CHA	2.08	1.51	1.43
55	Y	627	PTY	O4-C1	-2.08	1.40	1.45
33	h	102	LMG	C22-C21	-2.08	1.32	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	g1	613	CLA	C1A-CHA	2.08	1.51	1.43
29	s1	614	CLA	C1C-C2C	2.08	1.48	1.44
30	a	408	PHO	C3D-C4D	2.08	1.44	1.41
47	I	102	4RF	O21-C20	-2.08	1.41	1.46
29	C	511	CLA	C3D-C4D	-2.08	1.39	1.44
29	S	610	CLA	C3D-C4D	-2.08	1.39	1.44
29	S	617	CLA	C3D-C4D	-2.08	1.39	1.44
29	s1	602	CLA	C3D-C4D	-2.08	1.39	1.44
29	g1	604	CLA	C1A-CHA	2.08	1.51	1.43
29	Y	608	CLA	C3D-C4D	-2.08	1.39	1.44
29	A1	410	CLA	C3D-C4D	-2.08	1.39	1.44
29	s	605	CLA	C3D-C4D	-2.08	1.39	1.44
29	D1	403	CLA	CHD-C1D	2.08	1.42	1.38
29	B	615	CLA	C1C-C2C	2.08	1.48	1.44
29	S1	604	CLA	C3D-C4D	-2.08	1.39	1.44
37	c1	518	DGD	O3G-C1D	2.08	1.43	1.40
30	a1	408	PHO	C3D-C4D	2.08	1.44	1.41
29	N	612	CLA	MG-NC	2.08	2.11	2.06
29	A	406	CLA	C3D-C4D	-2.08	1.39	1.44
29	s1	617	CLA	C1C-C2C	2.07	1.48	1.44
51	s	623	NEX	O24-C25	-2.07	1.43	1.46
29	c	501	CLA	C1A-CHA	2.07	1.51	1.43
48	S1	601	CHL	C1B-NB	-2.07	1.35	1.37
29	C	502	CLA	C1A-CHA	2.07	1.51	1.43
29	C	502	CLA	C3D-C4D	-2.07	1.39	1.44
29	g1	614	CLA	C3D-C4D	-2.07	1.39	1.44
29	Y	611	CLA	CHD-C1D	2.07	1.42	1.38
31	a1	411	BCR	C12-C13	-2.07	1.41	1.45
29	A	410	CLA	C1C-C2C	2.07	1.48	1.44
29	b	617	CLA	C3D-C4D	-2.07	1.39	1.44
29	c1	506	CLA	C1A-CHA	2.07	1.51	1.43
33	H	102	LMG	C22-C21	-2.07	1.32	1.49
51	Y1	623	NEX	C11-C10	2.07	1.49	1.43
29	Y1	602	CLA	C1A-CHA	2.07	1.51	1.43
29	C1	508	CLA	C3D-C4D	-2.07	1.39	1.44
29	G	613	CLA	C1C-C2C	2.07	1.48	1.44
29	n	610	CLA	C1A-CHA	2.07	1.51	1.43
29	S	605	CLA	C3D-C4D	-2.07	1.39	1.44
44	F	101	HEM	CMB-C2B	2.07	1.55	1.50
48	g1	608	CHL	C1B-NB	-2.07	1.35	1.37
29	r1	603	CLA	C1C-C2C	2.07	1.48	1.44
29	y	613	CLA	C3D-C4D	-2.07	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	504	CLA	C1A-CHA	2.07	1.51	1.43
29	r	608	CLA	C1C-C2C	2.07	1.48	1.44
29	d1	402	CLA	C1C-C2C	2.07	1.48	1.44
29	b1	615	CLA	C1A-CHA	2.07	1.51	1.43
29	a1	406	CLA	C1A-CHA	2.07	1.51	1.43
51	S	623	NEX	O24-C25	-2.07	1.43	1.46
29	n	610	CLA	C3D-C4D	-2.07	1.39	1.44
49	S1	621	LUT	C1-C6	-2.07	1.50	1.53
29	A	407	CLA	CHD-C1D	2.07	1.42	1.38
29	A	407	CLA	C3D-C4D	-2.06	1.39	1.44
37	c	518	DGD	CGB-CFB	-2.06	1.32	1.49
29	s	610	CLA	C1C-C2C	2.06	1.48	1.44
29	s	610	CLA	C3D-C4D	-2.06	1.39	1.44
29	c1	503	CLA	C3D-C4D	-2.06	1.39	1.44
29	g	604	CLA	C1C-C2C	2.06	1.48	1.44
29	c1	507	CLA	CHD-C1D	2.06	1.42	1.38
29	y1	602	CLA	C3B-C4B	2.06	1.47	1.42
29	a1	406	CLA	C1C-C2C	2.06	1.48	1.44
29	A1	407	CLA	CHD-C1D	2.06	1.42	1.38
44	f1	101	HEM	CMB-C2B	2.06	1.55	1.50
29	b	609	CLA	C1A-CHA	2.06	1.51	1.43
29	B1	611	CLA	C1A-CHA	2.06	1.51	1.43
29	s	602	CLA	C1C-C2C	2.06	1.48	1.44
29	B	616	CLA	C3D-C4D	-2.06	1.39	1.44
29	b1	616	CLA	C3D-C4D	-2.06	1.39	1.44
29	y1	608	CLA	C1C-C2C	2.06	1.48	1.44
29	b	606	CLA	C1A-CHA	2.06	1.51	1.43
37	c1	519	DGD	CGA-CFA	-2.06	1.33	1.49
29	b1	602	CLA	C4B-NB	-2.06	1.35	1.37
37	c1	520	DGD	CDA-CCA	-2.06	1.33	1.49
38	B	624	3PH	O31-C3	-2.06	1.40	1.45
29	B	603	CLA	C3D-C4D	-2.06	1.39	1.44
29	B1	608	CLA	C1C-C2C	2.06	1.48	1.44
29	C1	508	CLA	C1C-C2C	2.06	1.48	1.44
29	S1	611	CLA	C1C-C2C	2.06	1.48	1.44
29	S1	609	CLA	C3D-C4D	-2.06	1.39	1.44
29	s1	612	CLA	MG-NC	2.06	2.11	2.06
29	D	403	CLA	C1C-C2C	2.06	1.48	1.44
29	c1	510	CLA	C1C-C2C	2.06	1.48	1.44
29	B	609	CLA	C1A-CHA	2.06	1.51	1.43
29	G	602	CLA	C3D-C4D	-2.05	1.39	1.44
29	b1	607	CLA	C3D-C4D	-2.05	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	g	603	CLA	C1C-C2C	2.05	1.48	1.44
29	c	502	CLA	C1A-CHA	2.05	1.51	1.43
37	C	519	DGD	CGB-CFB	-2.05	1.33	1.49
29	B1	605	CLA	C3D-C4D	-2.05	1.39	1.44
29	g1	602	CLA	C3D-C4D	-2.05	1.39	1.44
29	g1	612	CLA	MG-NC	2.05	2.11	2.06
29	a	410	CLA	C3D-C4D	-2.05	1.39	1.44
48	y	606	CHL	C3A-C2A	-2.05	1.48	1.54
29	r	604	CLA	C3D-C4D	-2.05	1.39	1.44
39	J	101	DGA	OG2-CG2	-2.05	1.41	1.46
29	B1	616	CLA	C3D-C4D	-2.05	1.39	1.44
29	G1	610	CLA	C1A-CHA	2.05	1.51	1.43
48	y	601	CHL	C3A-C2A	-2.05	1.48	1.54
33	h	102	LMG	C43-C42	-2.05	1.33	1.49
29	R	602	CLA	C3D-C4D	-2.05	1.39	1.44
29	c1	513	CLA	C3D-C4D	-2.05	1.39	1.44
29	y1	611	CLA	C3D-C4D	-2.05	1.39	1.44
29	G	603	CLA	C1A-CHA	2.05	1.51	1.43
29	b1	611	CLA	C1A-CHA	2.05	1.51	1.43
29	n	604	CLA	C1A-CHA	2.05	1.51	1.43
29	N1	613	CLA	C1C-C2C	2.05	1.48	1.44
29	R1	604	CLA	C3D-C4D	-2.05	1.39	1.44
29	b1	602	CLA	MG-NC	2.05	2.11	2.06
36	B	620	C7Z	C18-C5	2.05	1.54	1.50
29	S	604	CLA	C3D-C4D	-2.05	1.39	1.44
29	Y1	611	CLA	C3D-C4D	-2.05	1.39	1.44
29	s1	612	CLA	C3D-C4D	-2.05	1.39	1.44
29	C1	509	CLA	C1A-CHA	2.05	1.51	1.43
29	y	604	CLA	C3D-C4D	-2.05	1.39	1.44
43	d	405	PL9	C16-C14	-2.05	1.47	1.51
29	n	603	CLA	C1C-C2C	2.05	1.48	1.44
29	y1	602	CLA	C3D-C4D	-2.05	1.39	1.44
29	Y	608	CLA	C1C-C2C	2.05	1.48	1.44
52	R1	625	LMT	O2'-C2'	-2.05	1.38	1.43
29	a1	410	CLA	C3D-C4D	-2.05	1.39	1.44
29	C	504	CLA	C1A-CHA	2.04	1.51	1.43
29	R	604	CLA	C3D-C4D	-2.04	1.39	1.44
29	c	503	CLA	C1A-CHA	2.04	1.51	1.43
29	S1	602	CLA	C3D-C4D	-2.04	1.39	1.44
29	d1	403	CLA	C1A-CHA	2.04	1.51	1.43
39	B1	625	DGA	CB2-CB1	2.04	1.56	1.50
29	S	603	CLA	C1C-C2C	2.04	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s1	617	CLA	C3D-C4D	-2.04	1.39	1.44
29	A1	405	CLA	C1A-CHA	2.04	1.51	1.43
37	C1	520	DGD	CGB-CFB	-2.04	1.33	1.49
29	S1	605	CLA	C3D-C4D	-2.04	1.39	1.44
34	A1	414	SPH	C3-C4	2.04	1.53	1.50
29	c1	512	CLA	C1C-C2C	2.04	1.48	1.44
29	D1	402	CLA	C3B-C4B	2.04	1.47	1.42
49	r1	620	LUT	C1-C6	-2.04	1.51	1.53
33	A1	413	LMG	C22-C21	-2.04	1.33	1.49
29	D1	403	CLA	C3D-C4D	-2.04	1.39	1.44
29	C1	505	CLA	C1A-CHA	2.04	1.51	1.43
33	C	521	LMG	C43-C42	-2.04	1.33	1.49
29	s	609	CLA	C1C-C2C	2.04	1.48	1.44
37	C1	519	DGD	CGB-CFB	-2.04	1.33	1.49
29	s1	602	CLA	C1A-CHA	2.04	1.51	1.43
37	C	520	DGD	CDA-CCA	-2.04	1.33	1.49
29	G	610	CLA	C3D-C4D	-2.04	1.39	1.44
49	g	621	LUT	C22-C21	-2.04	1.52	1.54
29	R	604	CLA	C1A-CHA	2.04	1.51	1.43
29	c1	507	CLA	C3D-C4D	-2.04	1.39	1.44
29	b	613	CLA	C1A-CHA	2.04	1.51	1.43
31	c1	517	BCR	C12-C13	-2.04	1.41	1.45
29	b	616	CLA	C1A-CHA	2.04	1.51	1.43
38	T1	101	3PH	O21-C2	-2.04	1.41	1.46
48	Y1	606	CHL	C3A-C2A	-2.04	1.48	1.54
29	g1	611	CLA	MG-NC	2.03	2.11	2.06
48	s1	608	CHL	CHC-C1C	2.03	1.42	1.38
29	R	608	CLA	CHD-C1D	2.03	1.42	1.38
29	b	615	CLA	C1C-C2C	2.03	1.48	1.44
33	A1	413	LMG	C43-C42	-2.03	1.33	1.49
29	B1	616	CLA	C1A-CHA	2.03	1.51	1.43
29	Y1	610	CLA	C3D-C4D	-2.03	1.39	1.44
29	Y	603	CLA	C1A-CHA	2.03	1.51	1.43
33	a1	413	LMG	C43-C42	-2.03	1.33	1.49
37	C	519	DGD	CGA-CFA	-2.03	1.33	1.49
29	b1	610	CLA	C3D-C4D	-2.03	1.39	1.44
33	H1	102	LMG	C22-C21	-2.03	1.33	1.49
29	a1	410	CLA	CHD-C1D	2.03	1.42	1.38
29	Y	602	CLA	CHD-C1D	2.03	1.42	1.38
33	c	521	LMG	C43-C42	-2.03	1.33	1.49
29	S	610	CLA	C1A-CHA	2.03	1.51	1.43
29	b1	610	CLA	C1A-CHA	2.03	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	606	CLA	C3D-C4D	-2.03	1.39	1.44
29	S1	614	CLA	C3D-C4D	-2.03	1.39	1.44
29	b1	610	CLA	C1C-C2C	2.03	1.48	1.44
29	R	610	CLA	C1A-CHA	2.03	1.51	1.43
29	y1	602	CLA	C1A-CHA	2.03	1.51	1.43
29	B	611	CLA	C1A-CHA	2.03	1.51	1.43
29	S	610	CLA	C1C-C2C	2.03	1.48	1.44
29	s	612	CLA	C1C-C2C	2.03	1.48	1.44
29	B1	610	CLA	C1C-C2C	2.03	1.48	1.44
48	S1	601	CHL	C3A-C2A	-2.03	1.48	1.54
29	N1	613	CLA	C1A-CHA	2.03	1.51	1.43
37	c1	518	DGD	CGB-CFB	-2.03	1.33	1.49
29	A1	406	CLA	C3D-C4D	-2.03	1.39	1.44
29	y	611	CLA	C1A-CHA	2.03	1.51	1.43
33	D	411	LMG	C25-C24	-2.03	1.33	1.49
29	r	610	CLA	C1C-C2C	2.03	1.48	1.44
29	C1	505	CLA	C1C-C2C	2.03	1.48	1.44
29	c1	503	CLA	C1C-C2C	2.03	1.48	1.44
29	B	610	CLA	C1A-CHA	2.03	1.51	1.43
29	c	508	CLA	C1A-CHA	2.03	1.51	1.43
29	R1	602	CLA	C3D-C4D	-2.03	1.39	1.44
29	Y	614	CLA	C1C-C2C	2.03	1.48	1.44
51	N1	623	NEX	C1-C6	-2.03	1.51	1.54
29	y	603	CLA	MG-NC	2.03	2.11	2.06
33	A	413	LMG	C43-C42	-2.02	1.33	1.49
30	a	408	PHO	C3B-C2B	-2.02	1.37	1.40
29	S1	617	CLA	C3D-C4D	-2.02	1.39	1.44
48	s	608	CHL	C3B-C4B	2.02	1.47	1.42
29	c1	502	CLA	C3D-C4D	-2.02	1.39	1.44
32	C	526	SQD	O47-C45	-2.02	1.41	1.46
29	c1	505	CLA	C3D-C4D	-2.02	1.39	1.44
29	b	609	CLA	C1D-ND	-2.02	1.35	1.37
38	b1	624	3PH	O31-C3	-2.02	1.40	1.45
29	a1	407	CLA	C1C-C2C	2.02	1.48	1.44
29	r	610	CLA	C3D-C4D	-2.02	1.39	1.44
29	b1	614	CLA	C3D-C4D	-2.02	1.39	1.44
29	R	612	CLA	MG-NC	2.02	2.11	2.06
33	A	413	LMG	C22-C21	-2.02	1.33	1.49
33	H	102	LMG	C43-C42	-2.02	1.33	1.49
39	j1	101	DGA	OG2-CG2	-2.02	1.41	1.46
36	b	620	C7Z	C40-C33	2.02	1.55	1.50
41	c1	527	LMK	O8-C28	2.02	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	b	622	LMG	C25-C24	-2.02	1.33	1.49
29	c1	504	CLA	C3D-C4D	-2.02	1.39	1.44
29	s1	614	CLA	MG-NC	2.02	2.11	2.06
29	C1	512	CLA	C3D-C4D	-2.02	1.39	1.44
29	n1	604	CLA	C3D-C4D	-2.02	1.39	1.44
29	R1	610	CLA	C3D-C4D	-2.02	1.39	1.44
29	s	612	CLA	C1A-CHA	2.02	1.51	1.43
29	B1	612	CLA	C1A-CHA	2.02	1.51	1.43
29	B1	614	CLA	C1A-CHA	2.02	1.51	1.43
29	Y1	602	CLA	MG-NC	2.02	2.11	2.06
55	Y1	627	PTY	O7-C8	2.02	1.39	1.35
33	h1	102	LMG	C22-C21	-2.02	1.33	1.49
29	y	610	CLA	C3D-C4D	-2.02	1.39	1.44
29	b	614	CLA	C3D-C4D	-2.02	1.39	1.44
33	a1	413	LMG	C22-C21	-2.02	1.33	1.49
29	c	511	CLA	C1A-CHA	2.02	1.51	1.43
33	C1	521	LMG	C43-C42	-2.02	1.33	1.49
29	B1	613	CLA	C1A-CHA	2.02	1.51	1.43
29	B	607	CLA	CHD-C1D	2.02	1.42	1.38
47	k	101	4RF	C19-C20	2.02	1.56	1.50
29	D	402	CLA	C1C-C2C	2.02	1.48	1.44
29	c1	509	CLA	CHD-C1D	2.02	1.42	1.38
29	Y1	613	CLA	C1A-CHA	2.02	1.51	1.43
29	G	614	CLA	MG-NC	2.02	2.11	2.06
33	a	413	LMG	C22-C21	-2.02	1.33	1.49
29	n1	602	CLA	C1A-CHA	2.01	1.51	1.43
38	S1	626	3PH	O31-C3	-2.01	1.40	1.45
29	y1	614	CLA	C1A-CHA	2.01	1.51	1.43
29	C	509	CLA	C1A-CHA	2.01	1.51	1.43
29	s1	613	CLA	MG-NC	2.01	2.11	2.06
29	r	612	CLA	C1C-C2C	2.01	1.48	1.44
37	C1	518	DGD	CGB-CFB	-2.01	1.33	1.49
48	s1	601	CHL	C1B-NB	-2.01	1.35	1.37
29	C1	504	CLA	C1A-CHA	2.01	1.51	1.43
29	N1	612	CLA	C3D-C4D	-2.01	1.39	1.44
29	b1	604	CLA	C3D-C4D	-2.01	1.39	1.44
29	b1	613	CLA	C3D-C4D	-2.01	1.39	1.44
29	A	410	CLA	C1A-CHA	2.01	1.51	1.43
29	r	602	CLA	C1A-CHA	2.01	1.51	1.43
29	N1	604	CLA	C1A-CHA	2.01	1.51	1.43
33	D1	411	LMG	C25-C24	-2.01	1.33	1.49
29	R	602	CLA	C1A-CHA	2.01	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	t	101	3PH	O31-C3	-2.01	1.40	1.45
33	c1	521	LMG	C25-C24	-2.01	1.33	1.49
29	g	604	CLA	C1A-CHA	2.01	1.51	1.43
33	B1	622	LMG	C25-C24	-2.01	1.33	1.49
29	C1	511	CLA	C3D-C4D	-2.01	1.39	1.44
37	C1	519	DGD	CGA-CFA	-2.01	1.33	1.49
37	c1	520	DGD	CGB-CFB	-2.01	1.33	1.49
31	b	619	BCR	C12-C13	-2.01	1.41	1.45
29	Y	611	CLA	C3D-C4D	-2.01	1.39	1.44
52	R	625	LMT	O1'-C1'	-2.01	1.36	1.40
37	C	518	DGD	CGB-CFB	-2.01	1.33	1.49
29	B	613	CLA	C1A-CHA	2.01	1.51	1.43
29	c	506	CLA	C1A-CHA	2.01	1.51	1.43
29	C1	503	CLA	C1A-CHA	2.01	1.51	1.43
29	S1	602	CLA	C1A-CHA	2.01	1.51	1.43
33	B	622	LMG	C25-C24	-2.01	1.33	1.49
29	Y	614	CLA	C1A-CHA	2.01	1.51	1.43
29	a	410	CLA	C1C-C2C	2.01	1.48	1.44
33	a	413	LMG	C43-C42	-2.01	1.33	1.49
29	R	609	CLA	C1A-CHA	2.01	1.51	1.43
29	S	605	CLA	CHD-C1D	2.01	1.42	1.38
29	c	512	CLA	MG-NC	2.01	2.11	2.06
29	b	604	CLA	C1A-CHA	2.01	1.51	1.43
29	y	612	CLA	C3D-C4D	-2.01	1.39	1.44
47	I1	102	4RF	C15-C16	2.01	1.56	1.50
29	B	610	CLA	C3D-C4D	-2.00	1.39	1.44
29	N	602	CLA	C1A-CHA	2.00	1.51	1.43
36	b1	620	C7Z	C18-C5	2.00	1.54	1.50
33	H1	102	LMG	C43-C42	-2.00	1.33	1.49
29	B1	606	CLA	CHD-C1D	2.00	1.42	1.38
29	B1	604	CLA	C3D-C4D	-2.00	1.39	1.44
29	R	608	CLA	MG-NC	2.00	2.11	2.06
29	c	506	CLA	CHD-C1D	2.00	1.42	1.38
29	S	602	CLA	C1A-CHA	2.00	1.51	1.43
29	s1	617	CLA	C1A-CHA	2.00	1.51	1.43
29	c1	502	CLA	CHD-C1D	2.00	1.42	1.38
29	b	603	CLA	C1A-CHA	2.00	1.51	1.43
29	y1	608	CLA	C1A-CHA	2.00	1.51	1.43
29	B1	603	CLA	MG-NC	2.00	2.11	2.06
48	g1	606	CHL	C1A-CHA	-2.00	1.34	1.43
37	C	520	DGD	CGB-CFB	-2.00	1.33	1.49

All (9056) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	L	101	LHG	O7-C7-C8	22.97	161.00	111.50
40	l	101	LHG	O7-C7-C8	22.96	160.99	111.50
29	R	609	CLA	C4-C3-C5	-22.39	77.60	115.27
38	S	626	3PH	O21-C21-C22	22.18	159.31	111.50
38	S1	626	3PH	O21-C21-C22	22.13	159.19	111.50
38	s	626	3PH	O21-C21-C22	22.09	159.10	111.50
29	R1	609	CLA	C4-C3-C5	-22.08	78.13	115.27
38	s1	626	3PH	O21-C21-C22	21.57	157.99	111.50
29	R1	609	CLA	C5-C3-C2	18.90	159.36	121.12
29	R	609	CLA	C5-C3-C2	18.45	158.44	121.12
38	s1	626	3PH	O21-C21-O22	-18.36	79.33	123.70
38	S	626	3PH	O21-C21-O22	-18.24	79.63	123.70
38	S1	626	3PH	O21-C21-O22	-18.23	79.65	123.70
38	s	626	3PH	O21-C21-O22	-18.22	79.68	123.70
40	L	101	LHG	O7-C7-O9	-17.95	80.33	123.70
40	l	101	LHG	O7-C7-O9	-17.94	80.35	123.70
50	y1	622	XAT	C37-C21-C36	-17.87	81.02	107.37
31	C	516	BCR	C10-C11-C12	17.78	178.70	123.22
31	C1	516	BCR	C10-C11-C12	17.69	178.43	123.22
31	C	515	BCR	C10-C11-C12	17.65	178.29	123.22
31	D	404	BCR	C10-C11-C12	17.60	178.14	123.22
31	b	618	BCR	C10-C11-C12	17.52	177.90	123.22
31	c	515	BCR	C10-C11-C12	17.51	177.85	123.22
50	Y1	622	XAT	C37-C21-C36	-17.50	81.55	107.37
31	B	618	BCR	C10-C11-C12	17.46	177.69	123.22
31	d	404	BCR	C10-C11-C12	17.43	177.60	123.22
31	c1	514	BCR	C10-C11-C12	17.37	177.44	123.22
31	A1	411	BCR	C10-C11-C12	17.37	177.41	123.22
31	c	514	BCR	C10-C11-C12	17.36	177.38	123.22
31	c	517	BCR	C10-C11-C12	17.26	177.08	123.22
31	C	514	BCR	C10-C11-C12	17.25	177.04	123.22
31	c	516	BCR	C10-C11-C12	17.24	177.03	123.22
31	C	517	BCR	C10-C11-C12	17.18	176.82	123.22
31	c1	516	BCR	C10-C11-C12	17.13	176.68	123.22
31	A	411	BCR	C10-C11-C12	16.95	176.10	123.22
31	a	411	BCR	C10-C11-C12	16.90	175.97	123.22
50	Y	622	XAT	C37-C21-C36	-16.76	82.65	107.37
29	R	609	CLA	C4-C3-C2	-16.69	80.87	123.68
31	b	619	BCR	C10-C11-C12	16.65	175.17	123.22
31	b1	619	BCR	C10-C11-C12	16.63	175.11	123.22
29	R1	609	CLA	C4-C3-C2	-16.54	81.25	123.68
31	B1	619	BCR	C10-C11-C12	16.39	174.36	123.22
31	B1	618	BCR	C10-C11-C12	16.33	174.17	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C1	517	BCR	C10-C11-C12	16.27	173.98	123.22
31	c1	515	BCR	C10-C11-C12	16.22	173.83	123.22
31	c1	517	BCR	C10-C11-C12	16.18	173.72	123.22
31	B1	619	BCR	C16-C15-C14	16.04	156.32	123.47
31	C1	514	BCR	C10-C11-C12	15.99	173.10	123.22
31	a1	411	BCR	C10-C11-C12	15.98	173.09	123.22
50	y	622	XAT	C37-C21-C36	-15.95	83.85	107.37
31	d1	404	BCR	C10-C11-C12	15.74	172.34	123.22
31	B	619	BCR	C10-C11-C12	15.44	171.40	123.22
31	c1	514	BCR	C16-C15-C14	15.33	154.87	123.47
31	C1	516	BCR	C16-C15-C14	15.30	154.82	123.47
31	C1	515	BCR	C16-C15-C14	15.29	154.80	123.47
31	D1	404	BCR	C11-C10-C9	15.23	149.05	127.31
31	c1	517	BCR	C16-C15-C14	15.14	154.48	123.47
31	b1	618	BCR	C10-C11-C12	14.89	169.68	123.22
31	b1	619	BCR	C11-C10-C9	14.85	148.50	127.31
31	D1	404	BCR	C10-C11-C12	14.78	169.36	123.22
31	C1	516	BCR	C11-C10-C9	14.69	148.28	127.31
31	c1	516	BCR	C11-C10-C9	14.64	148.21	127.31
31	c1	514	BCR	C11-C10-C9	14.52	148.04	127.31
31	c1	515	BCR	C16-C15-C14	14.46	153.09	123.47
31	C1	517	BCR	C11-C10-C9	14.46	147.94	127.31
31	b1	618	BCR	C16-C15-C14	14.45	153.07	123.47
31	B1	618	BCR	C11-C10-C9	14.41	147.87	127.31
31	B1	618	BCR	C16-C15-C14	14.34	152.84	123.47
31	c1	515	BCR	C11-C10-C9	14.29	147.70	127.31
31	b	618	BCR	C16-C15-C14	13.84	151.83	123.47
31	c1	516	BCR	C16-C15-C14	13.82	151.78	123.47
31	C	514	BCR	C16-C15-C14	13.76	151.65	123.47
31	a	411	BCR	C11-C10-C9	13.69	146.85	127.31
31	d1	404	BCR	C21-C20-C19	13.69	165.93	123.22
31	C	517	BCR	C21-C20-C19	13.67	165.88	123.22
31	c	516	BCR	C11-C10-C9	13.65	146.80	127.31
31	c	514	BCR	C11-C10-C9	13.63	146.77	127.31
31	B1	619	BCR	C21-C20-C19	13.52	165.40	123.22
31	c	514	BCR	C16-C15-C14	13.46	151.06	123.47
31	c1	517	BCR	C21-C20-C19	13.46	165.23	123.22
31	C1	514	BCR	C21-C20-C19	13.46	165.23	123.22
31	d1	404	BCR	C16-C15-C14	13.39	150.90	123.47
50	y1	622	XAT	C37-C21-C22	-13.39	85.72	108.98
31	C1	516	BCR	C21-C20-C19	13.36	164.91	123.22
31	C1	517	BCR	C16-C15-C14	13.28	150.68	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D1	404	BCR	C16-C15-C14	13.22	150.55	123.47
53	r	626	ERG	C15-C14-C8	-13.20	100.44	120.44
31	c	517	BCR	C21-C20-C19	13.10	164.09	123.22
31	C1	515	BCR	C10-C11-C12	12.91	163.50	123.22
50	Y	622	XAT	C37-C21-C22	-12.79	86.76	108.98
31	A	411	BCR	C11-C10-C9	12.77	145.53	127.31
31	C1	514	BCR	C16-C15-C14	12.70	149.50	123.47
50	y	622	XAT	C37-C21-C22	-12.69	86.94	108.98
31	d	404	BCR	C21-C20-C19	12.66	162.71	123.22
31	a1	411	BCR	C21-C20-C19	12.61	162.57	123.22
31	B	618	BCR	C16-C15-C14	12.60	149.29	123.47
31	C	516	BCR	C11-C10-C9	12.56	145.23	127.31
31	D	404	BCR	C21-C20-C19	12.52	162.29	123.22
31	b1	619	BCR	C16-C15-C14	12.50	149.09	123.47
31	c	517	BCR	C11-C10-C9	12.42	145.03	127.31
31	C1	517	BCR	C21-C20-C19	12.40	161.90	123.22
31	b	618	BCR	C11-C10-C9	12.38	144.97	127.31
31	A	411	BCR	C21-C20-C19	12.36	161.78	123.22
31	C	515	BCR	C16-C15-C14	12.35	148.77	123.47
31	D1	404	BCR	C21-C20-C19	12.35	161.75	123.22
53	R	626	ERG	C15-C14-C8	-12.23	101.90	120.44
31	C	517	BCR	C11-C10-C9	12.15	144.65	127.31
31	b	619	BCR	C11-C10-C9	12.04	144.49	127.31
31	a	411	BCR	C21-C20-C19	12.00	160.68	123.22
31	B	618	BCR	C11-C10-C9	11.99	144.42	127.31
31	c	515	BCR	C11-C12-C13	11.94	159.94	126.42
31	a	411	BCR	C16-C15-C14	11.92	147.88	123.47
31	C1	517	BCR	C11-C12-C13	11.84	159.68	126.42
31	d	404	BCR	C11-C12-C13	11.78	159.52	126.42
31	c	515	BCR	C16-C15-C14	11.77	147.59	123.47
31	B	619	BCR	C21-C20-C19	11.70	159.72	123.22
31	c	514	BCR	C21-C20-C19	11.69	159.71	123.22
31	A	411	BCR	C11-C12-C13	11.64	159.11	126.42
31	C	514	BCR	C11-C10-C9	11.63	143.91	127.31
31	B1	618	BCR	C21-C20-C19	11.61	159.44	123.22
38	s1	626	3PH	O22-C21-C22	-11.54	78.69	123.73
31	b1	619	BCR	C21-C20-C19	11.54	159.22	123.22
31	c1	515	BCR	C21-C20-C19	11.49	159.07	123.22
31	b	619	BCR	C11-C12-C13	11.46	158.61	126.42
31	D	404	BCR	C11-C10-C9	11.45	143.66	127.31
31	A1	411	BCR	C21-C20-C19	11.43	158.89	123.22
31	b1	618	BCR	C21-C20-C19	11.38	158.72	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	517	BCR	C11-C12-C13	11.37	158.35	126.42
31	c1	516	BCR	C21-C20-C19	11.36	158.68	123.22
31	d	404	BCR	C16-C15-C14	11.35	146.72	123.47
31	c	516	BCR	C21-C20-C19	11.32	158.54	123.22
31	A1	411	BCR	C11-C12-C13	11.32	158.21	126.42
38	S1	626	3PH	O22-C21-C22	-11.32	79.59	123.73
38	s	626	3PH	O22-C21-C22	-11.31	79.62	123.73
31	C	517	BCR	C11-C12-C13	11.28	158.10	126.42
38	S	626	3PH	O22-C21-C22	-11.27	79.75	123.73
31	b	619	BCR	C16-C15-C14	11.26	146.55	123.47
31	c	516	BCR	C16-C15-C14	11.26	146.53	123.47
50	Y1	622	XAT	C37-C21-C22	-11.21	89.51	108.98
31	c	517	BCR	C16-C15-C14	11.20	146.42	123.47
31	B1	619	BCR	C11-C10-C9	11.19	143.28	127.31
53	R1	626	ERG	C15-C14-C8	-11.16	103.52	120.44
31	a1	411	BCR	C16-C15-C14	11.14	146.30	123.47
31	C	515	BCR	C11-C10-C9	11.06	143.09	127.31
40	l	101	LHG	O9-C7-C8	-11.05	80.64	123.73
31	C	516	BCR	C21-C20-C19	11.03	157.65	123.22
31	C	516	BCR	C11-C12-C13	11.02	157.36	126.42
40	L	101	LHG	O9-C7-C8	-11.00	80.81	123.73
31	b	619	BCR	C21-C20-C19	11.00	157.54	123.22
31	d	404	BCR	C11-C10-C9	10.97	142.97	127.31
31	C	517	BCR	C16-C15-C14	10.92	145.84	123.47
31	b1	619	BCR	C11-C12-C13	10.91	157.07	126.42
31	A1	411	BCR	C11-C10-C9	10.85	142.79	127.31
29	Y	610	CLA	C4A-NA-C1A	10.80	111.56	106.71
31	D	404	BCR	C11-C12-C13	10.77	156.68	126.42
31	c1	514	BCR	C21-C20-C19	10.77	156.81	123.22
31	a1	411	BCR	C11-C12-C13	10.74	156.59	126.42
31	c1	517	BCR	C11-C10-C9	10.74	142.63	127.31
31	C1	515	BCR	C21-C20-C19	10.73	156.70	123.22
31	c	516	BCR	C11-C12-C13	10.71	156.51	126.42
31	b	618	BCR	C21-C20-C19	10.65	156.47	123.22
31	D	404	BCR	C16-C15-C14	10.64	145.26	123.47
31	C	516	BCR	C16-C15-C14	10.56	145.12	123.47
31	a	411	BCR	C11-C12-C13	10.56	156.09	126.42
31	C	514	BCR	C11-C12-C13	10.53	156.01	126.42
31	C	514	BCR	C21-C20-C19	10.52	156.03	123.22
29	b	605	CLA	C4A-NA-C1A	10.45	111.40	106.71
31	A	411	BCR	C16-C15-C14	10.41	144.80	123.47
29	b	606	CLA	C4A-NA-C1A	10.41	111.39	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	618	BCR	C11-C12-C13	10.38	155.59	126.42
31	B	618	BCR	C21-C20-C19	10.38	155.60	123.22
31	C	515	BCR	C11-C12-C13	10.33	155.43	126.42
31	B	618	BCR	C11-C12-C13	10.29	155.32	126.42
31	B1	619	BCR	C11-C12-C13	10.29	155.32	126.42
31	b1	618	BCR	C11-C12-C13	10.26	155.24	126.42
29	y1	613	CLA	C4A-NA-C1A	10.25	111.31	106.71
29	R1	610	CLA	C4A-NA-C1A	10.24	111.31	106.71
29	A	406	CLA	C4A-NA-C1A	10.23	111.31	106.71
29	g1	610	CLA	C4A-NA-C1A	10.23	111.31	106.71
29	a1	407	CLA	C4A-NA-C1A	10.22	111.30	106.71
29	s1	609	CLA	C4A-NA-C1A	10.21	111.30	106.71
29	Y1	613	CLA	C4A-NA-C1A	10.19	111.29	106.71
31	d1	404	BCR	C11-C10-C9	10.19	141.85	127.31
29	b	612	CLA	C4A-NA-C1A	10.17	111.28	106.71
29	s	613	CLA	C4A-NA-C1A	10.17	111.28	106.71
31	d1	404	BCR	C11-C12-C13	10.15	154.94	126.42
31	A1	411	BCR	C16-C15-C14	10.15	144.27	123.47
53	r1	626	ERG	C15-C14-C8	-10.14	105.07	120.44
29	y1	604	CLA	C4A-NA-C1A	10.11	111.25	106.71
29	a1	405	CLA	C4A-NA-C1A	10.08	111.24	106.71
29	B	617	CLA	C4A-NA-C1A	10.08	111.24	106.71
29	n	613	CLA	C4A-NA-C1A	10.07	111.23	106.71
31	B	619	BCR	C11-C12-C13	10.05	154.66	126.42
29	b	614	CLA	C4A-NA-C1A	10.04	111.22	106.71
29	N	610	CLA	C4A-NA-C1A	10.04	111.22	106.71
29	N	613	CLA	C4A-NA-C1A	10.04	111.22	106.71
29	b	610	CLA	C4A-NA-C1A	10.02	111.21	106.71
29	g	610	CLA	C4A-NA-C1A	10.00	111.20	106.71
29	c	513	CLA	C4A-NA-C1A	9.97	111.19	106.71
29	C1	511	CLA	C4A-NA-C1A	9.96	111.19	106.71
29	C	509	CLA	C4A-NA-C1A	9.96	111.18	106.71
29	y	603	CLA	C4A-NA-C1A	9.96	111.18	106.71
29	Y	613	CLA	C4A-NA-C1A	9.94	111.17	106.71
29	y	604	CLA	C4A-NA-C1A	9.93	111.17	106.71
29	G1	613	CLA	C4A-NA-C1A	9.93	111.17	106.71
29	S	613	CLA	C4A-NA-C1A	9.92	111.17	106.71
29	c	505	CLA	C4A-NA-C1A	9.92	111.17	106.71
29	N1	604	CLA	C4A-NA-C1A	9.92	111.17	106.71
29	b	617	CLA	C4A-NA-C1A	9.91	111.16	106.71
29	b	608	CLA	C4A-NA-C1A	9.91	111.16	106.71
29	C1	509	CLA	C4A-NA-C1A	9.91	111.16	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b1	609	CLA	C4A-NA-C1A	9.90	111.16	106.71
29	S	605	CLA	C4A-NA-C1A	9.90	111.16	106.71
29	B	606	CLA	C4A-NA-C1A	9.89	111.15	106.71
29	A1	410	CLA	C4A-NA-C1A	9.86	111.14	106.71
29	N	614	CLA	C4A-NA-C1A	9.86	111.14	106.71
31	C1	514	BCR	C11-C10-C9	9.85	141.37	127.31
29	n	603	CLA	C4A-NA-C1A	9.81	111.12	106.71
29	B	608	CLA	C4A-NA-C1A	9.78	111.10	106.71
29	B	609	CLA	C4A-NA-C1A	9.77	111.10	106.71
31	a1	411	BCR	C11-C10-C9	9.76	141.24	127.31
29	G1	614	CLA	C4A-NA-C1A	9.75	111.09	106.71
29	B	613	CLA	C4A-NA-C1A	9.75	111.09	106.71
29	g1	604	CLA	C4A-NA-C1A	9.73	111.08	106.71
29	b1	613	CLA	C4A-NA-C1A	9.73	111.08	106.71
29	C	501	CLA	C4A-NA-C1A	9.71	111.07	106.71
31	c	515	BCR	C20-C19-C18	9.70	153.67	126.42
29	C1	501	CLA	C4A-NA-C1A	9.68	111.06	106.71
29	g	613	CLA	C4A-NA-C1A	9.67	111.05	106.71
29	C	512	CLA	C4A-NA-C1A	9.64	111.04	106.71
29	N1	610	CLA	C4A-NA-C1A	9.64	111.04	106.71
29	B1	605	CLA	C4A-NA-C1A	9.64	111.04	106.71
29	N	603	CLA	C4A-NA-C1A	9.61	111.03	106.71
29	B1	617	CLA	C4A-NA-C1A	9.61	111.03	106.71
29	S1	613	CLA	C4A-NA-C1A	9.61	111.03	106.71
29	Y	603	CLA	C4A-NA-C1A	9.60	111.02	106.71
31	B	619	BCR	C16-C15-C14	9.59	143.12	123.47
29	b	613	CLA	C4A-NA-C1A	9.59	111.02	106.71
29	r	604	CLA	C4A-NA-C1A	9.59	111.02	106.71
29	g	611	CLA	C4A-NA-C1A	9.58	111.01	106.71
29	B	614	CLA	C4A-NA-C1A	9.58	111.01	106.71
29	B1	612	CLA	C4A-NA-C1A	9.58	111.01	106.71
29	N1	614	CLA	C4A-NA-C1A	9.57	111.01	106.71
29	c1	504	CLA	C4A-NA-C1A	9.57	111.01	106.71
29	n1	613	CLA	C4A-NA-C1A	9.55	111.00	106.71
29	c1	505	CLA	C4A-NA-C1A	9.54	110.99	106.71
29	y	613	CLA	C4A-NA-C1A	9.53	110.99	106.71
29	n1	610	CLA	C4A-NA-C1A	9.53	110.99	106.71
29	S	604	CLA	C4A-NA-C1A	9.52	110.99	106.71
29	a	407	CLA	C4A-NA-C1A	9.51	110.98	106.71
29	G1	604	CLA	C4A-NA-C1A	9.51	110.98	106.71
29	n1	614	CLA	C4A-NA-C1A	9.51	110.98	106.71
31	c1	514	BCR	C11-C12-C13	9.50	153.12	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c1	516	BCR	C11-C12-C13	9.50	153.10	126.42
31	C1	516	BCR	C11-C12-C13	9.50	153.09	126.42
29	r	610	CLA	C4A-NA-C1A	9.49	110.97	106.71
29	s1	611	CLA	C4A-NA-C1A	9.49	110.97	106.71
29	G1	603	CLA	C4A-NA-C1A	9.49	110.97	106.71
29	n	604	CLA	C4A-NA-C1A	9.48	110.97	106.71
29	n1	603	CLA	C4A-NA-C1A	9.48	110.97	106.71
29	G1	611	CLA	C4A-NA-C1A	9.47	110.96	106.71
31	C	515	BCR	C21-C20-C19	9.47	152.77	123.22
29	N1	603	CLA	C4A-NA-C1A	9.46	110.96	106.71
29	B	610	CLA	C4A-NA-C1A	9.44	110.95	106.71
29	A	405	CLA	C4A-NA-C1A	9.44	110.95	106.71
51	s1	623	NEX	C2-C1-C6	9.43	118.38	109.21
29	c1	511	CLA	C4A-NA-C1A	9.43	110.95	106.71
29	C	506	CLA	C4A-NA-C1A	9.43	110.94	106.71
29	N1	613	CLA	C4A-NA-C1A	9.42	110.94	106.71
29	S1	609	CLA	C4A-NA-C1A	9.39	110.93	106.71
29	B1	611	CLA	C4A-NA-C1A	9.37	110.92	106.71
29	n	611	CLA	C4A-NA-C1A	9.37	110.92	106.71
29	Y	604	CLA	C4A-NA-C1A	9.37	110.92	106.71
29	C	507	CLA	C4A-NA-C1A	9.36	110.92	106.71
29	B1	602	CLA	C4A-NA-C1A	9.36	110.91	106.71
29	c1	512	CLA	C4A-NA-C1A	9.36	110.91	106.71
30	a1	409	PHO	C4D-CHA-CBD	-9.36	104.28	108.52
29	s	611	CLA	C4A-NA-C1A	9.35	110.91	106.71
29	a	406	CLA	C4A-NA-C1A	9.35	110.91	106.71
29	c1	501	CLA	C4A-NA-C1A	9.33	110.90	106.71
29	G	611	CLA	C4A-NA-C1A	9.33	110.90	106.71
29	Y	612	CLA	C4A-NA-C1A	9.33	110.90	106.71
29	c	507	CLA	C4A-NA-C1A	9.32	110.90	106.71
29	S	617	CLA	C4A-NA-C1A	9.32	110.89	106.71
29	b1	607	CLA	C4A-NA-C1A	9.32	110.89	106.71
29	S	611	CLA	C4A-NA-C1A	9.31	110.89	106.71
29	C	513	CLA	C4A-NA-C1A	9.30	110.89	106.71
29	s	617	CLA	C4A-NA-C1A	9.29	110.88	106.71
29	b1	608	CLA	C4A-NA-C1A	9.28	110.88	106.71
29	c1	507	CLA	C4A-NA-C1A	9.27	110.87	106.71
29	c1	513	CLA	C4A-NA-C1A	9.26	110.87	106.71
29	G	603	CLA	C4A-NA-C1A	9.26	110.87	106.71
29	s	609	CLA	C4A-NA-C1A	9.26	110.87	106.71
29	g1	611	CLA	C4A-NA-C1A	9.26	110.87	106.71
29	B	602	CLA	C4A-NA-C1A	9.25	110.86	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	R1	609	CLA	C4A-NA-C1A	9.24	110.86	106.71
29	B	605	CLA	C4A-NA-C1A	9.24	110.86	106.71
29	b1	612	CLA	C4A-NA-C1A	9.23	110.86	106.71
31	c1	516	BCR	C20-C19-C18	9.23	152.35	126.42
29	A	410	CLA	C4A-NA-C1A	9.23	110.86	106.71
29	B	615	CLA	C4A-NA-C1A	9.23	110.86	106.71
29	G	602	CLA	C4A-NA-C1A	9.23	110.86	106.71
29	y	612	CLA	C4A-NA-C1A	9.23	110.86	106.71
29	B1	610	CLA	C4A-NA-C1A	9.23	110.86	106.71
29	b	615	CLA	C4A-NA-C1A	9.23	110.85	106.71
31	b1	618	BCR	C11-C10-C9	9.22	140.47	127.31
29	b1	615	CLA	C4A-NA-C1A	9.22	110.85	106.71
29	c1	506	CLA	C4A-NA-C1A	9.22	110.85	106.71
29	S	612	CLA	C4A-NA-C1A	9.20	110.84	106.71
29	y	610	CLA	C4A-NA-C1A	9.20	110.84	106.71
29	B1	615	CLA	C4A-NA-C1A	9.20	110.84	106.71
29	a	410	CLA	C4A-NA-C1A	9.20	110.84	106.71
29	G1	602	CLA	C4A-NA-C1A	9.19	110.84	106.71
29	S1	604	CLA	C4A-NA-C1A	9.19	110.84	106.71
29	G1	610	CLA	C4A-NA-C1A	9.18	110.83	106.71
29	Y	608	CLA	C4A-NA-C1A	9.18	110.83	106.71
29	S1	611	CLA	C4A-NA-C1A	9.17	110.83	106.71
29	c1	503	CLA	C4A-NA-C1A	9.17	110.83	106.71
29	n1	604	CLA	C4A-NA-C1A	9.16	110.83	106.71
29	B1	608	CLA	C4A-NA-C1A	9.16	110.82	106.71
29	B1	609	CLA	C4A-NA-C1A	9.16	110.82	106.71
29	c	502	CLA	C4A-NA-C1A	9.16	110.82	106.71
29	D	403	CLA	C4A-NA-C1A	9.15	110.82	106.71
29	C	505	CLA	C4A-NA-C1A	9.15	110.82	106.71
29	y1	612	CLA	C4A-NA-C1A	9.15	110.82	106.71
29	A1	406	CLA	C4A-NA-C1A	9.14	110.81	106.71
29	C1	502	CLA	C4A-NA-C1A	9.13	110.81	106.71
29	Y	602	CLA	C4A-NA-C1A	9.12	110.81	106.71
51	s1	623	NEX	C17-C1-C6	-9.12	102.31	110.47
31	C	515	BCR	C20-C19-C18	9.11	152.02	126.42
29	C	502	CLA	C4A-NA-C1A	9.11	110.80	106.71
29	b	602	CLA	C4A-NA-C1A	9.10	110.80	106.71
29	n	610	CLA	C4A-NA-C1A	9.10	110.80	106.71
29	s	605	CLA	C4A-NA-C1A	9.10	110.80	106.71
29	s1	605	CLA	C4A-NA-C1A	9.09	110.79	106.71
29	B1	603	CLA	C4A-NA-C1A	9.09	110.79	106.71
29	r1	609	CLA	C4A-NA-C1A	9.08	110.79	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	G	613	CLA	C4A-NA-C1A	9.08	110.79	106.71
29	b1	605	CLA	C4A-NA-C1A	9.06	110.78	106.71
29	Y1	602	CLA	C4A-NA-C1A	9.06	110.78	106.71
31	c	515	BCR	C11-C10-C9	9.05	140.22	127.31
29	S1	605	CLA	C4A-NA-C1A	9.04	110.77	106.71
29	B1	606	CLA	C4A-NA-C1A	9.04	110.77	106.71
29	G	610	CLA	C4A-NA-C1A	9.02	110.76	106.71
29	C	503	CLA	C4A-NA-C1A	9.01	110.76	106.71
29	y	608	CLA	C4A-NA-C1A	9.01	110.75	106.71
29	C1	510	CLA	C4A-NA-C1A	9.00	110.75	106.71
29	s1	614	CLA	C4A-NA-C1A	9.00	110.75	106.71
29	s1	613	CLA	C4A-NA-C1A	9.00	110.75	106.71
29	s	603	CLA	C4A-NA-C1A	8.99	110.75	106.71
29	s1	603	CLA	C4A-NA-C1A	8.99	110.75	106.71
29	g	612	CLA	C4A-NA-C1A	8.98	110.75	106.71
29	R1	608	CLA	C4A-NA-C1A	8.98	110.74	106.71
31	c1	517	BCR	C11-C12-C13	8.97	151.62	126.42
29	Y1	608	CLA	C4A-NA-C1A	8.97	110.74	106.71
29	b1	606	CLA	C4A-NA-C1A	8.97	110.74	106.71
29	G1	612	CLA	C4A-NA-C1A	8.96	110.74	106.71
29	c	504	CLA	C4A-NA-C1A	8.96	110.73	106.71
31	c	515	BCR	C21-C20-C19	8.95	151.16	123.22
29	S1	612	CLA	C4A-NA-C1A	8.95	110.73	106.71
31	A1	411	BCR	C20-C19-C18	8.95	151.56	126.42
29	R1	612	CLA	C4A-NA-C1A	8.95	110.73	106.71
29	a1	410	CLA	C4A-NA-C1A	8.95	110.73	106.71
29	A1	405	CLA	C4A-NA-C1A	8.94	110.72	106.71
31	c1	514	BCR	C20-C19-C18	8.94	151.53	126.42
29	g1	612	CLA	C4A-NA-C1A	8.94	110.72	106.71
29	Y1	612	CLA	C4A-NA-C1A	8.93	110.72	106.71
29	N1	612	CLA	C4A-NA-C1A	8.92	110.72	106.71
29	S1	617	CLA	C4A-NA-C1A	8.92	110.72	106.71
29	b	607	CLA	C4A-NA-C1A	8.91	110.71	106.71
31	B1	618	BCR	C20-C19-C18	8.91	151.44	126.42
29	n1	611	CLA	C4A-NA-C1A	8.91	110.71	106.71
31	C1	515	BCR	C20-C19-C18	8.91	151.44	126.42
29	c	512	CLA	C4A-NA-C1A	8.90	110.71	106.71
29	R	609	CLA	C4A-NA-C1A	8.90	110.71	106.71
29	R1	604	CLA	C4A-NA-C1A	8.87	110.70	106.71
31	C	514	BCR	C20-C19-C18	8.87	151.33	126.42
29	S1	610	CLA	C4A-NA-C1A	8.87	110.69	106.71
31	C1	514	BCR	C11-C12-C13	8.86	151.32	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S1	614	CLA	C4A-NA-C1A	8.86	110.69	106.71
29	a	405	CLA	C4A-NA-C1A	8.85	110.69	106.71
29	c	511	CLA	C4A-NA-C1A	8.85	110.69	106.71
29	A	407	CLA	C4A-NA-C1A	8.85	110.68	106.71
29	R	610	CLA	C4A-NA-C1A	8.85	110.68	106.71
29	b1	603	CLA	C4A-NA-C1A	8.84	110.68	106.71
29	r1	608	CLA	C4A-NA-C1A	8.83	110.68	106.71
29	g1	614	CLA	C4A-NA-C1A	8.83	110.68	106.71
29	r1	604	CLA	C4A-NA-C1A	8.83	110.68	106.71
29	b	609	CLA	C4A-NA-C1A	8.83	110.67	106.71
31	B1	618	BCR	C11-C12-C13	8.83	151.21	126.42
31	D1	404	BCR	C11-C12-C13	8.82	151.20	126.42
29	y	614	CLA	C4A-NA-C1A	8.82	110.67	106.71
29	Y1	610	CLA	C4A-NA-C1A	8.81	110.67	106.71
29	R	612	CLA	C4A-NA-C1A	8.79	110.66	106.71
29	c	509	CLA	C4A-NA-C1A	8.79	110.66	106.71
31	b	618	BCR	C20-C19-C18	8.79	151.12	126.42
29	C	511	CLA	C4A-NA-C1A	8.79	110.66	106.71
29	y1	611	CLA	C4A-NA-C1A	8.79	110.66	106.71
29	b1	604	CLA	C4A-NA-C1A	8.77	110.65	106.71
29	N1	602	CLA	C4A-NA-C1A	8.76	110.65	106.71
29	N	602	CLA	C4A-NA-C1A	8.76	110.64	106.71
29	s1	617	CLA	C4A-NA-C1A	8.76	110.64	106.71
29	C1	505	CLA	C4A-NA-C1A	8.75	110.64	106.71
29	c	503	CLA	C4A-NA-C1A	8.75	110.64	106.71
29	g1	613	CLA	C4A-NA-C1A	8.75	110.64	106.71
29	N	604	CLA	C4A-NA-C1A	8.74	110.63	106.71
29	C1	506	CLA	C4A-NA-C1A	8.73	110.63	106.71
29	B	603	CLA	C4A-NA-C1A	8.72	110.63	106.71
29	C	504	CLA	C4A-NA-C1A	8.72	110.62	106.71
29	B	612	CLA	C4A-NA-C1A	8.71	110.62	106.71
29	B1	607	CLA	C4A-NA-C1A	8.70	110.62	106.71
29	c	501	CLA	C4A-NA-C1A	8.70	110.62	106.71
29	b	603	CLA	C4A-NA-C1A	8.69	110.61	106.71
29	c	510	CLA	C4A-NA-C1A	8.68	110.61	106.71
29	R1	602	CLA	C4A-NA-C1A	8.68	110.61	106.71
29	y1	610	CLA	C4A-NA-C1A	8.68	110.61	106.71
29	G	614	CLA	C4A-NA-C1A	8.66	110.60	106.71
29	r	603	CLA	C4A-NA-C1A	8.66	110.60	106.71
29	Y	611	CLA	C4A-NA-C1A	8.61	110.58	106.71
29	b	611	CLA	C4A-NA-C1A	8.61	110.58	106.71
29	r	612	CLA	C4A-NA-C1A	8.61	110.58	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S	614	CLA	C4A-NA-C1A	8.60	110.57	106.71
29	S	602	CLA	C4A-NA-C1A	8.60	110.57	106.71
29	c	506	CLA	C4A-NA-C1A	8.59	110.57	106.71
29	R	604	CLA	C4A-NA-C1A	8.58	110.56	106.71
29	b1	617	CLA	C4A-NA-C1A	8.57	110.56	106.71
29	n	614	CLA	C4A-NA-C1A	8.57	110.56	106.71
29	B	604	CLA	C4A-NA-C1A	8.55	110.55	106.71
29	Y	614	CLA	C4A-NA-C1A	8.54	110.55	106.71
29	D1	402	CLA	C4A-NA-C1A	8.54	110.55	106.71
31	b1	618	BCR	C20-C19-C18	8.54	150.40	126.42
29	s	604	CLA	C4A-NA-C1A	8.53	110.54	106.71
29	B	616	CLA	C4A-NA-C1A	8.52	110.54	106.71
29	G	612	CLA	C4A-NA-C1A	8.51	110.53	106.71
29	d1	402	CLA	C4A-NA-C1A	8.51	110.53	106.71
29	R	608	CLA	C4A-NA-C1A	8.51	110.53	106.71
29	s	612	CLA	C4A-NA-C1A	8.50	110.53	106.71
29	C1	504	CLA	C4A-NA-C1A	8.49	110.52	106.71
29	S1	602	CLA	C4A-NA-C1A	8.48	110.52	106.71
29	S1	603	CLA	C4A-NA-C1A	8.48	110.52	106.71
29	R1	603	CLA	C4A-NA-C1A	8.47	110.52	106.71
29	b1	610	CLA	C4A-NA-C1A	8.47	110.52	106.71
29	N	611	CLA	C4A-NA-C1A	8.46	110.51	106.71
29	B1	616	CLA	C4A-NA-C1A	8.45	110.51	106.71
29	R	603	CLA	C4A-NA-C1A	8.43	110.50	106.71
29	Y1	604	CLA	C4A-NA-C1A	8.43	110.50	106.71
29	r1	603	CLA	C4A-NA-C1A	8.43	110.50	106.71
29	s1	610	CLA	C4A-NA-C1A	8.42	110.49	106.71
29	b	604	CLA	C4A-NA-C1A	8.42	110.49	106.71
29	s	602	CLA	C4A-NA-C1A	8.39	110.48	106.71
31	c1	515	BCR	C20-C19-C18	8.38	149.95	126.42
29	G	604	CLA	C4A-NA-C1A	8.37	110.47	106.71
31	B	618	BCR	C20-C19-C18	8.36	149.90	126.42
29	r	609	CLA	C4A-NA-C1A	8.36	110.46	106.71
29	g1	602	CLA	C4A-NA-C1A	8.35	110.46	106.71
29	s1	604	CLA	C4A-NA-C1A	8.34	110.46	106.71
29	N1	611	CLA	C4A-NA-C1A	8.31	110.44	106.71
29	s1	612	CLA	C4A-NA-C1A	8.31	110.44	106.71
29	g	603	CLA	C4A-NA-C1A	8.30	110.44	106.71
31	c1	515	BCR	C11-C12-C13	8.30	149.72	126.42
29	c	508	CLA	C4A-NA-C1A	8.29	110.43	106.71
29	S	609	CLA	C4A-NA-C1A	8.29	110.43	106.71
29	d	402	CLA	C4A-NA-C1A	8.29	110.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D	402	CLA	C4A-NA-C1A	8.29	110.43	106.71
29	S	610	CLA	C4A-NA-C1A	8.28	110.43	106.71
29	g	614	CLA	C4A-NA-C1A	8.28	110.43	106.71
29	y1	603	CLA	C4A-NA-C1A	8.27	110.42	106.71
31	b1	619	BCR	C20-C19-C18	8.26	149.63	126.42
29	b	616	CLA	C4A-NA-C1A	8.25	110.42	106.71
29	B	611	CLA	C4A-NA-C1A	8.25	110.42	106.71
29	Y1	603	CLA	C4A-NA-C1A	8.25	110.41	106.71
29	y1	602	CLA	C4A-NA-C1A	8.24	110.41	106.71
31	C	516	BCR	C20-C19-C18	8.24	149.57	126.42
29	B	607	CLA	C4A-NA-C1A	8.24	110.41	106.71
29	B1	613	CLA	C4A-NA-C1A	8.23	110.41	106.71
29	b1	616	CLA	C4A-NA-C1A	8.23	110.41	106.71
29	s	614	CLA	C4A-NA-C1A	8.23	110.40	106.71
29	C1	512	CLA	C4A-NA-C1A	8.23	110.40	106.71
29	n1	602	CLA	C4A-NA-C1A	8.20	110.39	106.71
29	y1	608	CLA	C4A-NA-C1A	8.19	110.39	106.71
29	r1	602	CLA	C4A-NA-C1A	8.19	110.39	106.71
29	g	602	CLA	C4A-NA-C1A	8.18	110.39	106.71
29	a1	406	CLA	C4A-NA-C1A	8.16	110.37	106.71
31	b	619	BCR	C20-C19-C18	8.16	149.33	126.42
29	Y1	611	CLA	C4A-NA-C1A	8.14	110.37	106.71
29	r1	610	CLA	C4A-NA-C1A	8.14	110.37	106.71
29	r	608	CLA	C4A-NA-C1A	8.14	110.36	106.71
31	c	514	BCR	C11-C12-C13	8.13	149.25	126.42
29	s1	602	CLA	C4A-NA-C1A	8.12	110.36	106.71
29	d1	403	CLA	C4A-NA-C1A	8.11	110.35	106.71
29	y	611	CLA	C4A-NA-C1A	8.10	110.35	106.71
29	B1	614	CLA	C4A-NA-C1A	8.05	110.33	106.71
29	b1	602	CLA	C4A-NA-C1A	8.05	110.33	106.71
29	y1	614	CLA	C4A-NA-C1A	8.05	110.32	106.71
29	r1	612	CLA	C4A-NA-C1A	8.04	110.32	106.71
29	c1	509	CLA	C4A-NA-C1A	8.01	110.31	106.71
29	C1	508	CLA	C4A-NA-C1A	8.00	110.30	106.71
29	c1	502	CLA	C4A-NA-C1A	8.00	110.30	106.71
29	b1	611	CLA	C4A-NA-C1A	7.98	110.29	106.71
31	c	516	BCR	C20-C19-C18	7.97	148.80	126.42
41	C	527	LMK	O2-C4-O3	-7.94	106.07	124.09
29	b1	614	CLA	C4A-NA-C1A	7.94	110.27	106.71
29	C1	503	CLA	C4A-NA-C1A	7.93	110.27	106.71
29	g1	603	CLA	C4A-NA-C1A	7.93	110.27	106.71
29	S	603	CLA	C4A-NA-C1A	7.92	110.27	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	N	612	CLA	C4A-NA-C1A	7.85	110.23	106.71
29	n	612	CLA	C4A-NA-C1A	7.85	110.23	106.71
29	R	602	CLA	C4A-NA-C1A	7.82	110.22	106.71
29	A1	407	CLA	C4A-NA-C1A	7.82	110.22	106.71
41	C1	527	LMK	O2-C4-O3	-7.82	106.33	124.09
29	n1	612	CLA	C4A-NA-C1A	7.82	110.22	106.71
29	C	510	CLA	C4A-NA-C1A	7.81	110.22	106.71
29	D1	403	CLA	C4A-NA-C1A	7.77	110.20	106.71
29	d	403	CLA	C4A-NA-C1A	7.75	110.19	106.71
29	y	602	CLA	C4A-NA-C1A	7.70	110.17	106.71
29	g	604	CLA	C4A-NA-C1A	7.69	110.16	106.71
29	Y1	614	CLA	C4A-NA-C1A	7.69	110.16	106.71
31	c	514	BCR	C20-C19-C18	7.67	147.97	126.42
29	C1	513	CLA	C4A-NA-C1A	7.65	110.15	106.71
31	a	411	BCR	C20-C19-C18	7.63	147.85	126.42
30	A1	409	PHO	C4D-CHA-CBD	-7.61	105.07	108.52
31	C1	517	BCR	C20-C19-C18	7.58	147.71	126.42
50	Y	622	XAT	C36-C21-C22	7.57	122.14	108.98
29	B	609	CLA	O2D-CGD-CBD	7.56	124.70	111.27
50	Y1	622	XAT	C37-C21-C26	-7.53	89.71	110.05
43	D1	405	PL9	C7-C3-C4	7.53	123.00	116.88
45	h	101	RRX	C33-C5-C6	-7.50	116.10	124.53
30	A1	408	PHO	C4D-CHA-CBD	-7.46	105.14	108.52
50	y	622	XAT	C37-C21-C26	-7.44	89.96	110.05
30	A	409	PHO	C4D-CHA-CBD	-7.42	105.16	108.52
29	s1	602	CLA	O2D-CGD-CBD	7.41	124.43	111.27
31	B	619	BCR	C11-C10-C9	7.40	137.87	127.31
29	r	602	CLA	C4A-NA-C1A	7.40	110.03	106.71
29	n	602	CLA	C4A-NA-C1A	7.38	110.03	106.71
29	c1	508	CLA	C4A-NA-C1A	7.37	110.02	106.71
49	s1	621	LUT	C21-C26-C27	7.36	122.00	112.70
29	c1	510	CLA	C4A-NA-C1A	7.36	110.01	106.71
29	C	508	CLA	C4A-NA-C1A	7.35	110.01	106.71
31	B	619	BCR	C20-C19-C18	7.33	146.99	126.42
29	C1	507	CLA	C4A-NA-C1A	7.32	110.00	106.71
29	s	610	CLA	C4A-NA-C1A	7.32	110.00	106.71
31	A	411	BCR	C20-C19-C18	7.30	146.93	126.42
45	h1	101	RRX	C33-C5-C6	-7.30	116.33	124.53
29	a	407	CLA	O2D-CGD-CBD	7.26	124.17	111.27
50	Y	622	XAT	C37-C21-C26	-7.25	90.47	110.05
30	a	408	PHO	C4D-CHA-CBD	-7.24	105.24	108.52
45	H	101	RRX	C38-C26-C25	-7.24	116.40	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	R	626	ERG	C14-C13-C17	7.22	107.42	99.72
29	B1	604	CLA	C4A-NA-C1A	7.21	109.95	106.71
31	D1	404	BCR	C20-C19-C18	7.19	146.61	126.42
45	h	101	RRX	C38-C26-C25	-7.17	116.47	124.53
31	a1	411	BCR	C20-C19-C18	7.16	146.53	126.42
29	g1	610	CLA	CMD-C2D-C1D	7.15	137.31	124.71
29	r	604	CLA	O2A-C1-C2	7.14	125.68	108.97
29	R1	604	CLA	O2A-C1-C2	7.12	125.61	108.97
29	R	604	CLA	O2A-C1-C2	7.10	125.57	108.97
50	y1	622	XAT	C36-C21-C22	7.07	121.26	108.98
36	b	620	C7Z	C15-C14-C13	-7.05	117.25	127.31
36	b1	620	C7Z	C2-C3-C4	7.05	119.95	110.30
49	Y1	621	LUT	C21-C26-C27	7.04	121.60	112.70
50	Y1	622	XAT	C36-C21-C22	7.02	121.18	108.98
45	H1	101	RRX	C38-C26-C25	-7.00	116.67	124.53
31	D	404	BCR	C20-C19-C18	6.96	145.96	126.42
39	c	524	DGA	CDB-CCB-CBB	-6.94	79.17	114.42
29	Y1	614	CLA	CMD-C2D-C1D	6.90	136.87	124.71
49	s1	621	LUT	C35-C34-C33	-6.84	117.55	127.31
31	C1	514	BCR	C20-C19-C18	6.79	145.50	126.42
45	h1	101	RRX	C38-C26-C25	-6.75	116.94	124.53
29	a1	407	CLA	O2D-CGD-CBD	6.74	123.25	111.27
29	S	602	CLA	O2D-CGD-CBD	6.69	123.16	111.27
29	S1	610	CLA	CMD-C2D-C1D	6.69	136.50	124.71
29	R1	609	CLA	O2A-C1-C2	6.68	126.20	108.64
39	B	625	DGA	CDB-CCB-CBB	-6.68	80.54	114.42
53	r	626	ERG	C14-C13-C17	6.65	106.82	99.72
29	n1	614	CLA	O2A-C1-C2	6.64	124.50	108.97
29	B1	603	CLA	O2A-C1-C2	6.64	126.08	108.64
39	C	524	DGA	CDB-CCB-CBB	-6.63	80.78	114.42
30	A	408	PHO	C4D-CHA-CBD	-6.62	105.52	108.52
31	C	517	BCR	C20-C19-C18	6.62	145.02	126.42
39	C1	524	DGA	CDB-CCB-CBB	-6.62	80.84	114.42
51	s1	623	NEX	C19-C9-C10	-6.61	113.66	122.92
50	y1	622	XAT	C37-C21-C26	-6.60	92.22	110.05
39	b	625	DGA	CDB-CCB-CBB	-6.59	80.95	114.42
29	a	406	CLA	CMD-C2D-C1D	6.59	136.32	124.71
49	g1	621	LUT	C35-C34-C33	-6.58	117.91	127.31
31	d	404	BCR	C20-C19-C18	6.58	144.90	126.42
51	G	623	NEX	C2-C1-C6	6.57	115.60	109.21
31	c	517	BCR	C20-C19-C18	6.56	144.84	126.42
29	Y1	602	CLA	O2D-CGD-CBD	6.55	122.91	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	R	612	CLA	O2A-C1-C2	6.54	125.84	108.64
29	a	405	CLA	O2A-C1-C2	6.54	125.83	108.64
51	s	623	NEX	C2-C1-C6	6.54	115.56	109.21
50	y	622	XAT	C36-C21-C22	6.53	120.32	108.98
31	B1	619	BCR	C20-C19-C18	6.51	144.70	126.42
29	g1	614	CLA	CMD-C2D-C1D	6.49	136.16	124.71
31	c1	515	BCR	C15-C14-C13	-6.45	118.11	127.31
41	c	527	LMK	O2-C4-O3	-6.43	109.49	124.09
29	B1	614	CLA	CMD-C2D-C1D	6.42	136.03	124.71
41	c1	527	LMK	O2-C4-O3	-6.42	109.51	124.09
39	b1	625	DGA	CDB-CCB-CBB	-6.42	81.86	114.42
29	s1	603	CLA	O2D-CGD-CBD	6.40	122.64	111.27
31	c1	517	BCR	C20-C19-C18	6.40	144.38	126.42
29	Y	604	CLA	O2D-CGD-CBD	6.39	122.63	111.27
29	b1	612	CLA	O2D-CGD-CBD	6.39	122.63	111.27
29	b	609	CLA	O2D-CGD-CBD	6.39	122.62	111.27
29	R1	602	CLA	O2A-C1-C2	6.36	125.34	108.64
29	a1	406	CLA	CMD-C2D-C1D	6.35	135.91	124.71
53	r1	626	ERG	C12-C13-C14	6.35	117.34	107.27
39	B1	625	DGA	CDB-CCB-CBB	-6.35	82.20	114.42
39	c1	524	DGA	CDB-CCB-CBB	-6.32	82.34	114.42
29	B1	612	CLA	O2A-C1-C2	6.32	125.23	108.64
49	g1	621	LUT	C21-C26-C27	6.31	120.68	112.70
49	R1	620	LUT	C21-C26-C27	6.31	120.68	112.70
50	Y	622	XAT	C31-C30-C29	-6.31	118.31	127.31
51	R	622	NEX	C2-C1-C6	6.31	115.34	109.21
53	R1	626	ERG	C1-C2-C3	6.29	118.54	110.47
49	r1	620	LUT	C21-C26-C27	6.29	120.65	112.70
29	N1	604	CLA	CMD-C2D-C1D	6.26	135.74	124.71
29	s1	604	CLA	CMD-C2D-C1D	6.25	135.73	124.71
29	N1	604	CLA	O2A-C1-C2	6.25	125.06	108.64
50	n	622	XAT	C31-C30-C29	-6.24	118.41	127.31
45	h	101	RRX	C24-C25-C26	-6.23	106.37	121.46
29	B1	607	CLA	CMD-C2D-C1D	6.23	135.69	124.71
49	S1	620	LUT	C21-C26-C27	6.21	120.56	112.70
49	N1	621	LUT	C21-C26-C27	6.21	120.55	112.70
29	c1	504	CLA	O2A-C1-C2	6.18	124.89	108.64
29	C1	511	CLA	CMD-C2D-C1D	6.18	135.61	124.71
29	a1	405	CLA	CMD-C2D-C1D	6.18	135.60	124.71
29	G1	614	CLA	O2A-C1-C2	6.16	123.37	108.97
53	R1	626	ERG	C14-C13-C17	6.15	106.28	99.72
29	b	614	CLA	CMD-C2D-C1D	6.15	135.54	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C1	501	CLA	O2A-C1-C2	6.14	124.78	108.64
29	r1	603	CLA	O2A-C1-C2	6.14	124.77	108.64
31	d1	404	BCR	C20-C19-C18	6.14	143.66	126.42
45	H	101	RRX	C23-C22-C21	-6.13	109.53	118.94
49	r1	620	LUT	C35-C34-C33	-6.13	118.56	127.31
29	N	604	CLA	O2D-CGD-CBD	6.10	122.11	111.27
53	r1	626	ERG	C14-C13-C17	6.10	106.23	99.72
36	b1	620	C7Z	C38-C25-C26	-6.10	117.68	124.53
29	Y	614	CLA	CMD-C2D-C1D	6.09	135.45	124.71
29	c	513	CLA	O2A-C1-C2	6.09	124.64	108.64
29	S	605	CLA	O2D-CGD-CBD	6.09	122.09	111.27
29	s	602	CLA	O2D-CGD-CBD	6.09	122.08	111.27
49	y1	620	LUT	C7-C8-C9	-6.08	117.04	126.23
29	A	407	CLA	O2A-C1-C2	6.08	124.60	108.64
29	B1	613	CLA	CMD-C2D-C1D	6.08	135.42	124.71
53	R	626	ERG	C1-C2-C3	6.07	118.26	110.47
51	y	623	NEX	C17-C1-C6	-6.07	105.04	110.47
29	A1	405	CLA	O2A-C1-C2	6.07	124.58	108.64
29	R1	610	CLA	O2D-CGD-CBD	6.06	122.04	111.27
29	B1	609	CLA	O2D-CGD-CBD	6.06	122.04	111.27
29	y	603	CLA	O2D-CGD-CBD	6.06	122.03	111.27
49	y1	621	LUT	C7-C8-C9	-6.06	117.08	126.23
49	y1	621	LUT	C11-C10-C9	-6.05	118.68	127.31
29	S1	609	CLA	CMD-C2D-C1D	6.05	135.37	124.71
29	S1	603	CLA	O2D-CGD-CBD	6.05	122.01	111.27
50	R	621	XAT	C31-C30-C29	-6.05	118.68	127.31
31	c1	517	BCR	C15-C14-C13	-6.05	118.68	127.31
29	B1	607	CLA	O2D-CGD-CBD	6.04	122.00	111.27
29	N1	603	CLA	O2A-C1-C2	6.04	124.50	108.64
29	N	604	CLA	CMD-C2D-C1D	6.03	135.35	124.71
29	r	610	CLA	CMD-C2D-C1D	6.03	135.34	124.71
50	N	622	XAT	O4-C5-C4	-6.03	108.85	113.38
45	H	101	RRX	C24-C23-C22	6.02	135.34	126.23
49	R	620	LUT	C21-C26-C27	6.02	120.31	112.70
29	N1	611	CLA	CMD-C2D-C1D	6.01	135.31	124.71
29	S	614	CLA	CMD-C2D-C1D	6.01	135.30	124.71
29	C	504	CLA	O2A-C1-C2	6.01	124.42	108.64
29	C	505	CLA	O2D-CGD-CBD	6.00	121.93	111.27
31	C1	515	BCR	C11-C12-C13	6.00	143.27	126.42
29	r	608	CLA	CMD-C2D-C1D	6.00	135.28	124.71
29	S1	604	CLA	O2A-C1-C2	6.00	124.39	108.64
51	S1	623	NEX	C17-C1-C6	-5.99	105.11	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n1	613	CLA	O2A-C1-C2	5.99	124.37	108.64
29	A	410	CLA	O2D-CGD-CBD	5.99	121.91	111.27
29	B1	606	CLA	CMD-C2D-C1D	5.98	135.25	124.71
29	r1	612	CLA	CMD-C2D-C1D	5.98	135.25	124.71
29	B1	611	CLA	O2D-CGD-CBD	5.98	121.89	111.27
29	y1	608	CLA	CMD-C2D-C1D	5.97	135.23	124.71
29	B1	616	CLA	CMD-C2D-C1D	5.96	135.22	124.71
45	h	101	RRX	C23-C22-C21	-5.96	109.79	118.94
29	S1	602	CLA	O2D-CGD-CBD	5.95	121.85	111.27
29	B	605	CLA	O2D-CGD-CBD	5.95	121.84	111.27
29	b1	609	CLA	O2D-CGD-CBD	5.95	121.84	111.27
29	c	501	CLA	CMD-C2D-C1D	5.94	135.19	124.71
29	a	407	CLA	O2A-C1-C2	5.94	122.86	108.97
29	c	504	CLA	O2A-C1-C2	5.94	124.25	108.64
29	c	506	CLA	CMD-C2D-C1D	5.94	135.18	124.71
29	D	403	CLA	O2D-CGD-CBD	5.94	121.82	111.27
45	h	101	RRX	C24-C23-C22	5.94	135.21	126.23
29	s	610	CLA	O2A-C1-C2	5.93	124.23	108.64
29	A	405	CLA	CMD-C2D-C1D	5.93	135.16	124.71
53	r	626	ERG	C12-C13-C14	5.93	116.67	107.27
29	g	602	CLA	O2A-C1-C2	5.92	124.21	108.64
29	n	614	CLA	O2A-C1-C2	5.92	122.81	108.97
29	C	509	CLA	CMD-C2D-C1D	5.92	135.15	124.71
45	H	101	RRX	C24-C25-C26	-5.92	107.12	121.46
29	N1	614	CLA	O2A-C1-C2	5.92	122.81	108.97
29	C1	512	CLA	CMD-C2D-C1D	5.92	135.14	124.71
29	g1	610	CLA	O2A-C1-C2	5.92	124.18	108.64
29	a1	406	CLA	O2A-C1-C2	5.92	124.18	108.64
29	C1	513	CLA	CMD-C2D-C1D	5.92	135.14	124.71
36	B	620	C7Z	C18-C5-C6	-5.91	117.89	124.53
29	s1	609	CLA	O2A-C1-C2	5.91	124.18	108.64
29	b	611	CLA	CMD-C2D-C1D	5.91	135.13	124.71
50	n1	622	XAT	C31-C30-C29	-5.91	118.88	127.31
29	g	603	CLA	O2A-C1-C2	5.90	124.15	108.64
29	R	608	CLA	O2A-C1-C2	5.90	124.14	108.64
29	c1	503	CLA	CMD-C2D-C1D	5.90	135.11	124.71
29	c1	511	CLA	CMD-C2D-C1D	5.90	135.11	124.71
49	g1	620	LUT	C35-C34-C33	-5.90	118.89	127.31
29	c	505	CLA	O2D-CGD-CBD	5.90	121.75	111.27
29	b	603	CLA	O2A-C1-C2	5.90	124.13	108.64
29	n	610	CLA	O2A-C1-C2	5.90	124.13	108.64
29	G	613	CLA	CMD-C2D-C1D	5.89	135.10	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	405	CLA	O2A-C1-C2	5.89	124.12	108.64
29	G	614	CLA	CMD-C2D-C1D	5.89	135.10	124.71
29	y	604	CLA	O2D-CGD-CBD	5.89	121.74	111.27
29	C	509	CLA	O2D-CGD-CBD	5.89	121.73	111.27
29	B	606	CLA	CMD-C2D-C1D	5.89	135.09	124.71
29	c1	510	CLA	CMD-C2D-C1D	5.89	135.09	124.71
45	H	101	RRX	C11-C10-C9	-5.89	118.91	127.31
50	r1	621	XAT	O4-C5-C4	-5.88	108.97	113.38
29	r1	604	CLA	O2A-C1-C2	5.87	122.71	108.97
29	b1	615	CLA	CMD-C2D-C1D	5.87	135.06	124.71
49	y1	620	LUT	C21-C26-C27	5.87	120.12	112.70
29	c	502	CLA	O2D-CGD-CBD	5.87	121.70	111.27
29	c1	501	CLA	O2A-C1-C2	5.86	124.04	108.64
29	S1	602	CLA	O2A-C1-C2	5.86	124.03	108.64
29	n1	602	CLA	CMD-C2D-C1D	5.86	135.03	124.71
29	c1	507	CLA	O2A-C1-C2	5.85	124.01	108.64
29	C	502	CLA	O2A-C1-C2	5.85	124.00	108.64
29	R1	608	CLA	CMD-C2D-C1D	5.84	135.01	124.71
29	G	602	CLA	CMD-C2D-C1D	5.84	135.00	124.71
29	b1	608	CLA	O2A-C1-C2	5.84	123.97	108.64
29	G1	613	CLA	O2A-C1-C2	5.84	123.97	108.64
36	b1	620	C7Z	C15-C14-C13	-5.84	118.98	127.31
50	g	622	XAT	C31-C30-C29	-5.84	118.98	127.31
29	b1	605	CLA	O2D-CGD-CBD	5.84	121.64	111.27
29	S1	612	CLA	O2D-CGD-CBD	5.83	121.63	111.27
29	c	502	CLA	O2A-C1-C2	5.83	123.96	108.64
36	B1	620	C7Z	C35-C34-C33	-5.83	118.99	127.31
29	s1	610	CLA	O2A-C1-C2	5.83	123.95	108.64
29	C1	505	CLA	O2D-CGD-CBD	5.83	121.62	111.27
29	n	604	CLA	O2A-C1-C2	5.82	123.93	108.64
29	c1	508	CLA	O2A-C1-C2	5.82	123.93	108.64
49	N	621	LUT	C21-C26-C27	5.82	120.05	112.70
29	r	610	CLA	O2A-C1-C2	5.81	123.91	108.64
29	B1	605	CLA	CMD-C2D-C1D	5.81	134.95	124.71
29	G	611	CLA	O2D-CGD-CBD	5.81	121.59	111.27
29	g	611	CLA	O2A-C1-C2	5.81	123.89	108.64
29	S	604	CLA	O2A-C1-C2	5.80	123.89	108.64
29	n	614	CLA	CMD-C2D-C1D	5.80	134.94	124.71
29	s	602	CLA	O2A-C1-C2	5.80	123.88	108.64
50	n	622	XAT	C15-C14-C13	-5.80	119.04	127.31
29	D1	402	CLA	O2D-CGD-CBD	5.79	121.56	111.27
29	c1	506	CLA	O2D-CGD-CBD	5.79	121.56	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	g	604	CLA	O2A-C1-C2	5.79	122.50	108.97
29	a1	410	CLA	O2D-CGD-CBD	5.79	121.55	111.27
29	s1	604	CLA	O2A-C1-C2	5.79	123.85	108.64
36	B	620	C7Z	C11-C10-C9	-5.78	119.05	127.31
29	s	603	CLA	O2D-CGD-CBD	5.78	121.54	111.27
50	g	622	XAT	O4-C5-C4	-5.78	109.04	113.38
29	n	610	CLA	O2D-CGD-CBD	5.78	121.54	111.27
29	G	614	CLA	O2A-C1-C2	5.78	122.49	108.97
29	c1	504	CLA	CMD-C2D-C1D	5.78	134.90	124.71
29	b	613	CLA	O2D-CGD-CBD	5.78	121.54	111.27
49	S	620	LUT	C21-C26-C25	5.78	121.77	111.42
29	C1	506	CLA	CMD-C2D-C1D	5.78	134.89	124.71
49	r	620	LUT	C21-C26-C25	5.77	121.76	111.42
29	c	501	CLA	O2D-CGD-CBD	5.77	121.52	111.27
29	b	607	CLA	O2D-CGD-CBD	5.77	121.52	111.27
29	c1	507	CLA	CMD-C2D-C1D	5.77	134.88	124.71
29	C	510	CLA	CMD-C2D-C1D	5.77	134.88	124.71
29	y1	614	CLA	CMD-C2D-C1D	5.77	134.88	124.71
29	d	403	CLA	CMD-C2D-C1D	5.77	134.88	124.71
29	B	607	CLA	CMD-C2D-C1D	5.76	134.87	124.71
29	G	602	CLA	O2D-CGD-CBD	5.76	121.51	111.27
29	r1	602	CLA	O2D-CGD-CBD	5.76	121.51	111.27
29	g	604	CLA	CMD-C2D-C1D	5.76	134.87	124.71
29	C	512	CLA	O2D-CGD-CBD	5.76	121.50	111.27
29	c	510	CLA	CMD-C2D-C1D	5.76	134.86	124.71
29	c	509	CLA	CMD-C2D-C1D	5.76	134.86	124.71
49	G1	621	LUT	C21-C26-C27	5.75	119.97	112.70
29	G	604	CLA	O2A-C1-C2	5.75	122.42	108.97
29	b1	613	CLA	CMD-C2D-C1D	5.75	134.85	124.71
29	N	614	CLA	O2A-C1-C2	5.75	122.41	108.97
29	N	612	CLA	O2D-CGD-CBD	5.75	121.48	111.27
29	c1	505	CLA	O2D-CGD-CBD	5.74	121.48	111.27
36	b	620	C7Z	C11-C10-C9	-5.74	119.12	127.31
29	b1	607	CLA	O2D-CGD-CBD	5.74	121.47	111.27
50	R	621	XAT	C15-C14-C13	-5.74	119.12	127.31
31	C1	515	BCR	C11-C10-C9	5.74	135.50	127.31
29	Y1	604	CLA	O2D-CGD-CBD	5.73	121.46	111.27
29	B1	615	CLA	CMD-C2D-C1D	5.73	134.81	124.71
29	D	403	CLA	O2A-C1-C2	5.73	123.70	108.64
29	R1	610	CLA	O2A-C1-C2	5.73	123.70	108.64
29	d	402	CLA	O2A-C1-C2	5.73	123.70	108.64
45	h	101	RRX	C21-C20-C19	-5.73	105.33	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	612	CLA	O2D-CGD-CBD	5.73	121.45	111.27
29	Y	613	CLA	CMD-C2D-C1D	5.73	134.81	124.71
29	n1	611	CLA	O2A-C1-C2	5.73	122.36	108.97
29	S	612	CLA	O2D-CGD-CBD	5.72	121.43	111.27
29	R	608	CLA	CMD-C2D-C1D	5.72	134.79	124.71
29	b	603	CLA	CMD-C2D-C1D	5.72	134.79	124.71
53	R	626	ERG	C12-C13-C14	5.70	116.32	107.27
31	C1	516	BCR	C20-C19-C18	5.70	142.44	126.42
29	S	604	CLA	CMD-C2D-C1D	5.70	134.76	124.71
29	c1	513	CLA	O2A-C1-C2	5.70	123.62	108.64
50	G	622	XAT	C15-C14-C13	-5.69	119.19	127.31
29	s	614	CLA	CMD-C2D-C1D	5.69	134.75	124.71
29	s1	610	CLA	CMD-C2D-C1D	5.69	134.74	124.71
29	Y	613	CLA	O2D-CGD-CBD	5.69	121.37	111.27
29	b	613	CLA	CMD-C2D-C1D	5.68	134.73	124.71
29	G1	613	CLA	CMD-C2D-C1D	5.68	134.73	124.71
29	c	506	CLA	O2A-C1-C2	5.68	123.57	108.64
29	C1	502	CLA	O2A-C1-C2	5.68	123.56	108.64
29	Y1	613	CLA	CMD-C2D-C1D	5.68	134.72	124.71
29	R	602	CLA	O2D-CGD-CBD	5.67	121.35	111.27
29	B	613	CLA	O2D-CGD-CBD	5.67	121.34	111.27
29	D1	403	CLA	O2D-CGD-CBD	5.67	121.34	111.27
29	b	615	CLA	O2A-C1-C2	5.67	123.54	108.64
29	r	604	CLA	CMD-C2D-C1D	5.67	134.70	124.71
29	R	612	CLA	CMD-C2D-C1D	5.67	134.70	124.71
29	G1	604	CLA	CMD-C2D-C1D	5.66	134.69	124.71
29	G1	602	CLA	O2A-C1-C2	5.66	123.51	108.64
29	B1	614	CLA	O2A-C1-C2	5.66	123.51	108.64
29	S1	614	CLA	O2D-CGD-CBD	5.66	121.32	111.27
29	B1	602	CLA	CMD-C2D-C1D	5.66	134.68	124.71
29	b1	602	CLA	CMD-C2D-C1D	5.66	134.68	124.71
29	B1	606	CLA	O2A-C1-C2	5.65	123.49	108.64
29	d1	402	CLA	O2D-CGD-CBD	5.65	121.31	111.27
29	b	602	CLA	CMD-C2D-C1D	5.65	134.67	124.71
29	y1	612	CLA	O2D-CGD-CBD	5.65	121.31	111.27
29	D1	402	CLA	O2A-C1-C2	5.65	123.49	108.64
29	Y1	602	CLA	CMD-C2D-C1D	5.65	134.67	124.71
29	C1	503	CLA	CMD-C2D-C1D	5.65	134.67	124.71
30	a	409	PHO	C4D-CHA-CBD	-5.65	105.96	108.52
29	G1	610	CLA	CMD-C2D-C1D	5.64	134.66	124.71
29	g	613	CLA	O2A-C1-C2	5.64	123.46	108.64
29	B	606	CLA	O2D-CGD-CBD	5.63	121.28	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	g	614	CLA	O2A-C1-C2	5.63	122.14	108.97
29	a	410	CLA	O2D-CGD-CBD	5.63	121.27	111.27
29	G	610	CLA	CMD-C2D-C1D	5.63	134.63	124.71
29	y1	613	CLA	CMD-C2D-C1D	5.63	134.63	124.71
29	r	609	CLA	O2A-C1-C2	5.63	123.42	108.64
29	N1	602	CLA	O2A-C1-C2	5.63	123.42	108.64
29	d1	403	CLA	CMD-C2D-C1D	5.63	134.63	124.71
51	N1	623	NEX	C5-C4-C3	5.62	118.40	111.75
29	G1	602	CLA	CMD-C2D-C1D	5.62	134.61	124.71
29	s1	602	CLA	O2A-C1-C2	5.61	123.39	108.64
45	H	101	RRX	C21-C20-C19	-5.61	105.71	123.22
29	a	410	CLA	O2A-C1-C2	5.61	123.38	108.64
29	B1	603	CLA	CMD-C2D-C1D	5.61	134.59	124.71
29	y1	603	CLA	CMD-C2D-C1D	5.61	134.59	124.71
29	y	608	CLA	CMD-C2D-C1D	5.60	134.59	124.71
29	S1	613	CLA	CMD-C2D-C1D	5.60	134.59	124.71
29	B1	613	CLA	O2A-C1-C2	5.60	123.36	108.64
29	c1	503	CLA	O2D-CGD-CBD	5.60	121.22	111.27
29	a	406	CLA	O2A-C1-C2	5.60	123.36	108.64
29	y	610	CLA	CMD-C2D-C1D	5.60	134.58	124.71
29	R	610	CLA	O2D-CGD-CBD	5.60	121.22	111.27
29	y1	602	CLA	CMD-C2D-C1D	5.60	134.58	124.71
29	B	615	CLA	CMD-C2D-C1D	5.60	134.58	124.71
49	S	621	LUT	C21-C26-C27	5.60	119.78	112.70
29	Y1	610	CLA	CMD-C2D-C1D	5.60	134.58	124.71
29	C1	509	CLA	CMD-C2D-C1D	5.60	134.57	124.71
29	N	603	CLA	CMD-C2D-C1D	5.59	134.57	124.71
29	G1	603	CLA	CMD-C2D-C1D	5.59	134.57	124.71
29	C1	504	CLA	O2A-C1-C2	5.59	123.33	108.64
29	Y1	603	CLA	CMD-C2D-C1D	5.59	134.57	124.71
29	C	507	CLA	O2D-CGD-CBD	5.59	121.20	111.27
29	g	610	CLA	CMD-C2D-C1D	5.59	134.56	124.71
29	S1	602	CLA	CMD-C2D-C1D	5.59	134.56	124.71
29	b	615	CLA	O2D-CGD-CBD	5.59	121.20	111.27
49	y1	621	LUT	C35-C34-C33	-5.59	119.34	127.31
29	B	611	CLA	O2A-C1-C2	5.59	123.32	108.64
29	y	614	CLA	CMD-C2D-C1D	5.58	134.55	124.71
37	B	623	DGD	O2G-C1B-C2B	5.58	123.53	111.50
29	s	614	CLA	O2D-CGD-CBD	5.58	121.18	111.27
49	N	620	LUT	C21-C26-C25	5.58	121.41	111.42
29	y	602	CLA	O2D-CGD-CBD	5.58	121.18	111.27
29	N1	603	CLA	CMD-C2D-C1D	5.58	134.54	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C1	508	CLA	O2A-C1-C2	5.57	123.28	108.64
49	n1	621	LUT	C21-C26-C27	5.57	119.74	112.70
29	R	604	CLA	CMD-C2D-C1D	5.57	134.53	124.71
29	b	605	CLA	CMD-C2D-C1D	5.57	134.53	124.71
29	B	612	CLA	O2A-C1-C2	5.57	123.26	108.64
29	d	402	CLA	CMD-C2D-C1D	5.56	134.52	124.71
29	Y1	610	CLA	O2A-C1-C2	5.56	123.25	108.64
29	N	610	CLA	CMD-C2D-C1D	5.56	134.50	124.71
29	n	611	CLA	CMD-C2D-C1D	5.56	134.50	124.71
29	N	603	CLA	O2A-C1-C2	5.55	123.22	108.64
29	c1	512	CLA	O2A-C1-C2	5.55	123.22	108.64
29	a	407	CLA	CMD-C2D-C1D	5.55	134.50	124.71
29	b1	605	CLA	CMD-C2D-C1D	5.55	134.50	124.71
50	g1	622	XAT	C15-C14-C13	-5.55	119.39	127.31
29	B1	607	CLA	O2A-C1-C2	5.55	123.22	108.64
29	g1	612	CLA	CMD-C2D-C1D	5.55	134.49	124.71
50	g1	622	XAT	C31-C30-C29	-5.55	119.39	127.31
29	n1	613	CLA	CMD-C2D-C1D	5.55	134.49	124.71
29	s1	602	CLA	CMD-C2D-C1D	5.55	134.49	124.71
29	Y	611	CLA	CMD-C2D-C1D	5.54	134.49	124.71
29	g1	614	CLA	O2A-C1-C2	5.54	121.93	108.97
29	s	605	CLA	CMD-C2D-C1D	5.54	134.48	124.71
50	g	622	XAT	C15-C14-C13	-5.54	119.40	127.31
29	b	606	CLA	CMD-C2D-C1D	5.54	134.48	124.71
29	b	610	CLA	O2D-CGD-CBD	5.54	121.11	111.27
29	g1	602	CLA	CMD-C2D-C1D	5.54	134.47	124.71
29	G1	610	CLA	O2D-CGD-CBD	5.54	121.11	111.27
29	Y1	611	CLA	CMD-C2D-C1D	5.54	134.47	124.71
29	C	501	CLA	CMD-C2D-C1D	5.54	134.47	124.71
29	y	611	CLA	O2A-C1-C2	5.54	123.19	108.64
29	Y1	611	CLA	O2D-CGD-CBD	5.53	121.10	111.27
29	C1	505	CLA	O2A-C1-C2	5.53	123.17	108.64
29	r1	603	CLA	CMD-C2D-C1D	5.53	134.46	124.71
49	n	620	LUT	C21-C26-C25	5.53	121.32	111.42
29	N	604	CLA	O2A-C1-C2	5.52	123.16	108.64
29	r	604	CLA	O2D-CGD-CBD	5.52	121.08	111.27
29	G	612	CLA	CMD-C2D-C1D	5.52	134.45	124.71
50	N1	622	XAT	C31-C30-C29	-5.52	119.43	127.31
29	C	513	CLA	O2D-CGD-CBD	5.52	121.08	111.27
29	r	609	CLA	CMD-C2D-C1D	5.52	134.44	124.71
29	D1	403	CLA	CMD-C2D-C1D	5.52	134.44	124.71
29	d1	402	CLA	CMD-C2D-C1D	5.52	134.44	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	617	CLA	O2D-CGD-CBD	5.52	121.07	111.27
29	s1	613	CLA	CMD-C2D-C1D	5.52	134.43	124.71
29	r	612	CLA	O2D-CGD-CBD	5.51	121.06	111.27
29	b	615	CLA	CMD-C2D-C1D	5.51	134.43	124.71
29	g1	613	CLA	O2A-C1-C2	5.51	123.12	108.64
29	G	604	CLA	CMD-C2D-C1D	5.51	134.42	124.71
50	N	622	XAT	C31-C30-C29	-5.51	119.45	127.31
29	B	602	CLA	CMD-C2D-C1D	5.51	134.42	124.71
30	a1	408	PHO	C4D-CHA-CBD	-5.50	106.03	108.52
29	G1	604	CLA	O2D-CGD-CBD	5.50	121.05	111.27
29	r	612	CLA	O2A-C1-C2	5.50	123.09	108.64
29	n	604	CLA	O2D-CGD-CBD	5.50	121.04	111.27
49	g	621	LUT	C21-C26-C27	5.50	119.65	112.70
29	b1	610	CLA	CMD-C2D-C1D	5.50	134.40	124.71
50	Y1	622	XAT	C15-C14-C13	-5.50	119.47	127.31
29	Y	610	CLA	CMD-C2D-C1D	5.50	134.40	124.71
29	D	402	CLA	O2A-C1-C2	5.49	123.07	108.64
29	G	610	CLA	O2A-C1-C2	5.49	123.07	108.64
29	n1	604	CLA	CMD-C2D-C1D	5.49	134.39	124.71
29	S	605	CLA	CMD-C2D-C1D	5.49	134.39	124.71
29	c	507	CLA	O2D-CGD-CBD	5.49	121.03	111.27
29	y1	610	CLA	O2A-C1-C2	5.49	123.06	108.64
29	g	603	CLA	CMD-C2D-C1D	5.49	134.39	124.71
49	r	620	LUT	C11-C10-C9	-5.49	119.48	127.31
29	D	402	CLA	CMD-C2D-C1D	5.49	134.38	124.71
29	Y1	604	CLA	CMD-C2D-C1D	5.49	134.38	124.71
29	s	604	CLA	CMD-C2D-C1D	5.48	134.38	124.71
29	c	510	CLA	O2A-C1-C2	5.48	123.04	108.64
29	c	513	CLA	O2D-CGD-CBD	5.48	121.00	111.27
49	n1	621	LUT	C35-C34-C33	-5.48	119.49	127.31
29	b1	613	CLA	O2D-CGD-CBD	5.48	121.00	111.27
29	C	508	CLA	CMD-C2D-C1D	5.48	134.37	124.71
29	C1	501	CLA	CMD-C2D-C1D	5.48	134.37	124.71
42	d1	401	BCT	O2-C-O1	5.47	133.74	119.55
29	s	604	CLA	O2D-CGD-CBD	5.47	120.99	111.27
29	c1	508	CLA	CMD-C2D-C1D	5.47	134.35	124.71
51	Y1	623	NEX	C38-C25-C24	5.47	120.43	114.28
29	n1	603	CLA	CMD-C2D-C1D	5.47	134.35	124.71
36	B1	620	C7Z	C38-C25-C26	-5.47	118.39	124.53
29	C1	502	CLA	O2D-CGD-CBD	5.47	120.98	111.27
45	H	101	RRX	C37-C22-C23	5.47	126.69	118.08
29	c1	509	CLA	CMD-C2D-C1D	5.47	134.35	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	N	602	CLA	O2D-CGD-CBD	5.46	120.97	111.27
29	C	506	CLA	CMD-C2D-C1D	5.46	134.33	124.71
29	S	609	CLA	CMD-C2D-C1D	5.46	134.33	124.71
29	S	617	CLA	O2A-C1-C2	5.46	122.97	108.64
29	r1	608	CLA	CMD-C2D-C1D	5.45	134.32	124.71
49	Y1	621	LUT	C21-C26-C25	5.45	121.18	111.42
29	C	503	CLA	O2D-CGD-CBD	5.45	120.95	111.27
29	s	617	CLA	O2D-CGD-CBD	5.45	120.95	111.27
29	y1	604	CLA	O2D-CGD-CBD	5.45	120.95	111.27
29	b	605	CLA	O2D-CGD-CBD	5.45	120.95	111.27
29	C1	512	CLA	O2A-C1-C2	5.45	122.95	108.64
29	y1	610	CLA	CMD-C2D-C1D	5.45	134.31	124.71
29	b1	606	CLA	CMD-C2D-C1D	5.45	134.31	124.71
29	y	613	CLA	O2D-CGD-CBD	5.44	120.94	111.27
29	s	613	CLA	O2A-C1-C2	5.44	122.93	108.64
29	G1	611	CLA	O2A-C1-C2	5.44	122.93	108.64
29	B	608	CLA	CMD-C2D-C1D	5.44	134.29	124.71
29	b1	613	CLA	O2A-C1-C2	5.43	122.92	108.64
29	Y	603	CLA	CMD-C2D-C1D	5.43	134.29	124.71
29	s	613	CLA	CMD-C2D-C1D	5.43	134.29	124.71
29	n1	612	CLA	CMD-C2D-C1D	5.43	134.28	124.71
29	R	610	CLA	CMD-C2D-C1D	5.43	134.28	124.71
49	g	620	LUT	C21-C26-C27	5.43	119.56	112.70
29	D	403	CLA	CMD-C2D-C1D	5.43	134.28	124.71
29	b1	612	CLA	CMD-C2D-C1D	5.43	134.28	124.71
29	A1	407	CLA	O2D-CGD-CBD	5.42	120.91	111.27
29	g1	612	CLA	O2D-CGD-CBD	5.42	120.90	111.27
29	A1	410	CLA	O2D-CGD-CBD	5.42	120.90	111.27
29	d	403	CLA	O2D-CGD-CBD	5.42	120.90	111.27
29	n1	602	CLA	O2D-CGD-CBD	5.42	120.90	111.27
29	a1	410	CLA	O2A-C1-C2	5.42	122.87	108.64
29	c	504	CLA	CMD-C2D-C1D	5.41	134.25	124.71
29	g	603	CLA	O2D-CGD-CBD	5.41	120.89	111.27
29	B1	612	CLA	CMD-C2D-C1D	5.41	134.25	124.71
29	S1	604	CLA	CMD-C2D-C1D	5.41	134.25	124.71
29	C1	507	CLA	CMD-C2D-C1D	5.41	134.25	124.71
29	S	605	CLA	O2A-C1-C2	5.41	122.85	108.64
50	N	622	XAT	C15-C14-C13	-5.41	119.59	127.31
29	N	612	CLA	CMD-C2D-C1D	5.41	134.24	124.71
29	B	617	CLA	O2D-CGD-CBD	5.41	120.88	111.27
29	y1	611	CLA	O2A-C1-C2	5.40	122.84	108.64
49	y	621	LUT	C21-C26-C27	5.40	119.53	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C1	509	CLA	O2D-CGD-CBD	5.40	120.87	111.27
29	N1	604	CLA	O2D-CGD-CBD	5.40	120.86	111.27
29	n1	603	CLA	O2D-CGD-CBD	5.40	120.86	111.27
36	B1	620	C7Z	C11-C10-C9	-5.40	119.61	127.31
29	y1	611	CLA	O2D-CGD-CBD	5.40	120.86	111.27
29	c	507	CLA	CMD-C2D-C1D	5.40	134.23	124.71
29	C	506	CLA	O2D-CGD-CBD	5.40	120.86	111.27
29	G	602	CLA	O2A-C1-C2	5.40	122.81	108.64
29	c1	501	CLA	CMD-C2D-C1D	5.39	134.22	124.71
29	C	502	CLA	O2D-CGD-CBD	5.39	120.85	111.27
29	Y	603	CLA	O2D-CGD-CBD	5.39	120.85	111.27
29	r1	612	CLA	O2A-C1-C2	5.39	122.81	108.64
31	D1	404	BCR	C35-C13-C12	5.39	126.58	118.08
29	y1	613	CLA	O2D-CGD-CBD	5.39	120.85	111.27
29	R1	612	CLA	O2A-C1-C2	5.39	122.80	108.64
51	s1	623	NEX	C4-C3-C2	5.39	121.18	110.77
29	D1	402	CLA	CMD-C2D-C1D	5.39	134.21	124.71
29	B	613	CLA	CMD-C2D-C1D	5.39	134.21	124.71
29	R1	604	CLA	CMD-C2D-C1D	5.39	134.21	124.71
29	y1	612	CLA	CMD-C2D-C1D	5.39	134.21	124.71
29	b1	610	CLA	O2A-C1-C2	5.39	122.79	108.64
29	g1	610	CLA	O2D-CGD-CBD	5.39	120.84	111.27
49	g	620	LUT	C15-C14-C13	-5.38	119.62	127.31
29	n1	611	CLA	CMD-C2D-C1D	5.38	134.20	124.71
29	s1	614	CLA	O2D-CGD-CBD	5.38	120.83	111.27
29	n1	614	CLA	O2D-CGD-CBD	5.38	120.83	111.27
29	Y1	612	CLA	O2D-CGD-CBD	5.38	120.83	111.27
29	s	605	CLA	O2A-C1-C2	5.38	122.77	108.64
29	C	507	CLA	O2A-C1-C2	5.38	122.77	108.64
29	c1	506	CLA	O2A-C1-C2	5.38	122.77	108.64
29	s	605	CLA	O2D-CGD-CBD	5.38	120.82	111.27
49	y	620	LUT	C21-C26-C25	5.38	121.05	111.42
29	A	407	CLA	CMD-C2D-C1D	5.38	134.19	124.71
29	g	611	CLA	O2D-CGD-CBD	5.37	120.82	111.27
29	Y	612	CLA	O2D-CGD-CBD	5.37	120.82	111.27
29	Y	608	CLA	O2A-C1-C2	5.37	122.76	108.64
29	c	511	CLA	CMD-C2D-C1D	5.37	134.18	124.71
45	h	101	RRX	C34-C9-C8	5.37	126.54	118.08
29	s	610	CLA	CMD-C2D-C1D	5.37	134.18	124.71
29	b1	604	CLA	CMD-C2D-C1D	5.37	134.18	124.71
36	b	620	C7Z	C38-C25-C26	-5.37	118.50	124.53
29	r1	609	CLA	O2A-C1-C2	5.37	122.74	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b1	606	CLA	O2A-C1-C2	5.37	122.74	108.64
49	Y	621	LUT	C21-C26-C25	5.36	121.03	111.42
29	N	613	CLA	O2A-C1-C2	5.36	122.73	108.64
29	d	402	CLA	O2D-CGD-CBD	5.36	120.80	111.27
49	g1	621	LUT	C11-C10-C9	-5.36	119.66	127.31
29	c1	508	CLA	O2D-CGD-CBD	5.36	120.79	111.27
29	N	603	CLA	O2D-CGD-CBD	5.36	120.79	111.27
29	c1	504	CLA	O2D-CGD-CBD	5.36	120.78	111.27
29	c1	511	CLA	O2A-C1-C2	5.35	122.71	108.64
29	n	614	CLA	O2D-CGD-CBD	5.35	120.78	111.27
29	y	612	CLA	O2D-CGD-CBD	5.35	120.77	111.27
29	c1	513	CLA	O2D-CGD-CBD	5.35	120.77	111.27
29	s	617	CLA	CMD-C2D-C1D	5.35	134.14	124.71
29	Y1	603	CLA	O2A-C1-C2	5.35	122.69	108.64
29	s1	605	CLA	O2A-C1-C2	5.35	122.69	108.64
29	B	604	CLA	O2A-C1-C2	5.35	122.68	108.64
29	N1	610	CLA	O2A-C1-C2	5.35	122.68	108.64
29	B	606	CLA	O2A-C1-C2	5.34	122.68	108.64
29	n	612	CLA	CMD-C2D-C1D	5.34	134.13	124.71
29	S1	617	CLA	O2A-C1-C2	5.34	122.68	108.64
29	B	605	CLA	CMD-C2D-C1D	5.34	134.13	124.71
29	y1	604	CLA	CMD-C2D-C1D	5.34	134.13	124.71
29	g1	611	CLA	O2D-CGD-CBD	5.34	120.76	111.27
29	g1	604	CLA	CMD-C2D-C1D	5.34	134.13	124.71
29	n	611	CLA	O2A-C1-C2	5.34	121.45	108.97
29	r1	608	CLA	O2A-C1-C2	5.34	122.66	108.64
29	b1	604	CLA	O2A-C1-C2	5.33	122.65	108.64
29	s	612	CLA	O2D-CGD-CBD	5.33	120.75	111.27
29	b1	614	CLA	CMD-C2D-C1D	5.33	134.11	124.71
29	s1	614	CLA	CMD-C2D-C1D	5.33	134.11	124.71
29	G	603	CLA	O2A-C1-C2	5.33	122.64	108.64
29	n	602	CLA	CMD-C2D-C1D	5.33	134.10	124.71
29	B1	602	CLA	O2D-CGD-CBD	5.33	120.73	111.27
49	n	621	LUT	C21-C26-C25	5.33	120.96	111.42
29	N	610	CLA	O2A-C1-C2	5.32	122.63	108.64
29	c	509	CLA	O2D-CGD-CBD	5.32	120.72	111.27
29	S1	609	CLA	O2D-CGD-CBD	5.32	120.72	111.27
49	y	621	LUT	C22-C23-C24	-5.32	105.69	111.74
29	C	503	CLA	CMD-C2D-C1D	5.32	134.09	124.71
45	h1	101	RRX	C21-C20-C19	-5.32	106.62	123.22
29	c	503	CLA	CMD-C2D-C1D	5.32	134.08	124.71
29	y1	610	CLA	O2D-CGD-CBD	5.32	120.71	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	614	CLA	CMD-C2D-C1D	5.31	134.07	124.71
29	C1	501	CLA	O2D-CGD-CBD	5.31	120.71	111.27
49	s	621	LUT	C21-C26-C27	5.31	119.42	112.70
51	G1	623	NEX	C2-C1-C6	5.31	114.37	109.21
50	n1	622	XAT	C15-C14-C13	-5.31	119.73	127.31
29	S1	617	CLA	O2D-CGD-CBD	5.31	120.70	111.27
49	n1	621	LUT	C21-C26-C25	5.31	120.93	111.42
29	s1	603	CLA	O2A-C1-C2	5.31	122.58	108.64
49	s	621	LUT	C21-C26-C25	5.31	120.92	111.42
29	r	612	CLA	CMD-C2D-C1D	5.31	134.06	124.71
29	C	510	CLA	O2D-CGD-CBD	5.31	120.70	111.27
29	b1	603	CLA	O2D-CGD-CBD	5.30	120.69	111.27
29	G	603	CLA	CMD-C2D-C1D	5.30	134.06	124.71
29	b1	611	CLA	O2D-CGD-CBD	5.30	120.69	111.27
29	S	602	CLA	O2A-C1-C2	5.30	122.57	108.64
49	g	621	LUT	C22-C23-C24	-5.30	105.71	111.74
29	c	510	CLA	O2D-CGD-CBD	5.30	120.69	111.27
49	G1	620	LUT	C21-C26-C25	5.30	120.91	111.42
29	r1	603	CLA	O2D-CGD-CBD	5.30	120.68	111.27
29	B	608	CLA	O2A-C1-C2	5.30	122.56	108.64
29	B	610	CLA	O2D-CGD-CBD	5.29	120.68	111.27
29	A1	410	CLA	CMD-C2D-C1D	5.29	134.04	124.71
29	b1	610	CLA	O2D-CGD-CBD	5.29	120.67	111.27
29	d	403	CLA	O2A-C1-C2	5.29	122.55	108.64
29	s1	603	CLA	CMD-C2D-C1D	5.29	134.04	124.71
29	N1	611	CLA	O2D-CGD-CBD	5.29	120.67	111.27
29	G1	602	CLA	O2D-CGD-CBD	5.29	120.67	111.27
49	s1	620	LUT	C21-C26-C27	5.29	119.39	112.70
29	s1	613	CLA	O2A-C1-C2	5.29	122.53	108.64
29	S1	617	CLA	CMD-C2D-C1D	5.29	134.03	124.71
29	b	608	CLA	CMD-C2D-C1D	5.28	134.02	124.71
29	a	405	CLA	CMD-C2D-C1D	5.28	134.02	124.71
29	G	603	CLA	O2D-CGD-CBD	5.28	120.65	111.27
29	b	608	CLA	O2A-C1-C2	5.28	122.51	108.64
29	g1	603	CLA	O2A-C1-C2	5.28	122.51	108.64
29	B	604	CLA	O2D-CGD-CBD	5.28	120.65	111.27
29	b	610	CLA	CMD-C2D-C1D	5.28	134.01	124.71
29	S	609	CLA	O2D-CGD-CBD	5.28	120.64	111.27
29	b	612	CLA	CMD-C2D-C1D	5.27	134.01	124.71
49	g	620	LUT	C31-C30-C29	-5.27	119.78	127.31
29	c	508	CLA	O2A-C1-C2	5.27	122.49	108.64
49	r1	620	LUT	C11-C10-C9	-5.27	119.79	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n	610	CLA	CMD-C2D-C1D	5.27	134.00	124.71
49	G	621	LUT	C21-C26-C27	5.27	119.36	112.70
29	r1	610	CLA	O2A-C1-C2	5.27	122.48	108.64
29	s1	609	CLA	CMD-C2D-C1D	5.27	134.00	124.71
29	n1	602	CLA	O2A-C1-C2	5.27	122.47	108.64
37	b	623	DGD	O2G-C1B-C2B	5.26	122.85	111.50
49	g	621	LUT	C21-C26-C25	5.26	120.85	111.42
29	g1	613	CLA	O2D-CGD-CBD	5.26	120.62	111.27
29	S1	605	CLA	O2A-C1-C2	5.26	122.47	108.64
29	s1	605	CLA	O2D-CGD-CBD	5.26	120.62	111.27
29	g	611	CLA	CMD-C2D-C1D	5.26	133.98	124.71
29	b1	617	CLA	CMD-C2D-C1D	5.26	133.98	124.71
29	s1	617	CLA	CMD-C2D-C1D	5.25	133.97	124.71
29	r	602	CLA	CMD-C2D-C1D	5.25	133.97	124.71
29	N	614	CLA	O2D-CGD-CBD	5.25	120.59	111.27
29	b1	609	CLA	O2A-C1-C2	5.25	122.43	108.64
29	C	511	CLA	CMD-C2D-C1D	5.25	133.96	124.71
29	N	611	CLA	CMD-C2D-C1D	5.25	133.96	124.71
49	y1	621	LUT	C22-C23-C24	-5.25	105.77	111.74
29	N1	613	CLA	CMD-C2D-C1D	5.24	133.95	124.71
29	G	611	CLA	O2A-C1-C2	5.24	122.41	108.64
49	G	621	LUT	C21-C26-C25	5.24	120.81	111.42
49	N1	621	LUT	C21-C26-C25	5.24	120.80	111.42
29	B1	616	CLA	O2A-C1-C2	5.24	122.40	108.64
29	g1	602	CLA	O2D-CGD-CBD	5.24	120.57	111.27
49	r	620	LUT	C7-C8-C9	-5.23	118.33	126.23
49	y1	621	LUT	C21-C26-C27	5.23	119.31	112.70
29	b	606	CLA	O2A-C1-C2	5.23	122.38	108.64
29	b1	603	CLA	O2A-C1-C2	5.23	122.38	108.64
29	A	406	CLA	CMD-C2D-C1D	5.23	133.93	124.71
29	c	512	CLA	O2D-CGD-CBD	5.23	120.56	111.27
29	g	610	CLA	O2D-CGD-CBD	5.23	120.56	111.27
29	S	617	CLA	O2D-CGD-CBD	5.23	120.56	111.27
29	S1	610	CLA	O2A-C1-C2	5.23	122.37	108.64
29	Y	604	CLA	CMD-C2D-C1D	5.23	133.93	124.71
29	B	607	CLA	O2D-CGD-CBD	5.22	120.55	111.27
49	g1	621	LUT	C21-C26-C25	5.22	120.78	111.42
29	S1	603	CLA	O2A-C1-C2	5.22	122.36	108.64
29	y1	608	CLA	O2D-CGD-CBD	5.22	120.55	111.27
29	C1	507	CLA	O2A-C1-C2	5.22	122.36	108.64
29	Y	602	CLA	O2A-C1-C2	5.22	122.34	108.64
29	R1	612	CLA	CMD-C2D-C1D	5.22	133.91	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	N1	614	CLA	O2D-CGD-CBD	5.21	120.53	111.27
49	N	621	LUT	C21-C26-C25	5.21	120.76	111.42
29	b	607	CLA	CMD-C2D-C1D	5.21	133.90	124.71
29	N1	612	CLA	CMD-C2D-C1D	5.21	133.90	124.71
50	N1	622	XAT	C15-C14-C13	-5.21	119.88	127.31
29	G	604	CLA	O2D-CGD-CBD	5.21	120.53	111.27
29	C	505	CLA	CMD-C2D-C1D	5.21	133.89	124.71
29	B	613	CLA	O2A-C1-C2	5.21	122.32	108.64
29	b1	605	CLA	O2A-C1-C2	5.20	122.31	108.64
29	B1	611	CLA	O2A-C1-C2	5.20	122.31	108.64
29	A1	406	CLA	CMD-C2D-C1D	5.20	133.88	124.71
49	S	620	LUT	C15-C14-C13	-5.20	119.89	127.31
50	y1	622	XAT	C31-C30-C29	-5.20	119.89	127.31
29	s1	605	CLA	CMD-C2D-C1D	5.20	133.87	124.71
29	G1	610	CLA	O2A-C1-C2	5.20	122.29	108.64
29	y	610	CLA	O2D-CGD-CBD	5.20	120.50	111.27
29	y	614	CLA	O2D-CGD-CBD	5.20	120.50	111.27
29	b	604	CLA	O2D-CGD-CBD	5.20	120.50	111.27
29	C1	506	CLA	O2A-C1-C2	5.19	122.28	108.64
29	b1	604	CLA	O2D-CGD-CBD	5.19	120.50	111.27
29	S1	613	CLA	O2A-C1-C2	5.19	122.28	108.64
29	b1	611	CLA	CMD-C2D-C1D	5.19	133.86	124.71
29	C	504	CLA	CMD-C2D-C1D	5.19	133.86	124.71
29	G1	614	CLA	CMD-C2D-C1D	5.19	133.86	124.71
29	n	612	CLA	O2D-CGD-CBD	5.19	120.49	111.27
29	G1	612	CLA	O2D-CGD-CBD	5.19	120.49	111.27
29	B1	616	CLA	O2D-CGD-CBD	5.19	120.48	111.27
29	C1	502	CLA	CMD-C2D-C1D	5.19	133.85	124.71
29	y1	612	CLA	O2A-C1-C2	5.18	122.26	108.64
29	n1	614	CLA	CMD-C2D-C1D	5.18	133.85	124.71
29	s1	611	CLA	CMD-C2D-C1D	5.18	133.85	124.71
29	B	605	CLA	O2A-C1-C2	5.18	122.25	108.64
29	b	616	CLA	O2D-CGD-CBD	5.18	120.47	111.27
29	Y1	610	CLA	O2D-CGD-CBD	5.18	120.47	111.27
29	R1	602	CLA	CMD-C2D-C1D	5.18	133.84	124.71
29	C1	504	CLA	O2D-CGD-CBD	5.18	120.47	111.27
29	A1	405	CLA	CMD-C2D-C1D	5.18	133.84	124.71
29	y1	602	CLA	O2A-C1-C2	5.18	122.24	108.64
29	r1	604	CLA	CMD-C2D-C1D	5.17	133.83	124.71
29	G	610	CLA	O2D-CGD-CBD	5.17	120.45	111.27
29	s	612	CLA	CMD-C2D-C1D	5.17	133.82	124.71
29	N	611	CLA	O2D-CGD-CBD	5.17	120.45	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	614	CLA	O2A-C1-C2	5.17	122.22	108.64
49	s1	620	LUT	C21-C26-C25	5.16	120.67	111.42
29	r	608	CLA	O2D-CGD-CBD	5.16	120.44	111.27
29	s	602	CLA	CMD-C2D-C1D	5.16	133.81	124.71
29	Y	613	CLA	O2A-C1-C2	5.16	122.20	108.64
29	C1	510	CLA	CMD-C2D-C1D	5.16	133.81	124.71
29	Y	610	CLA	O2D-CGD-CBD	5.16	120.44	111.27
29	b1	609	CLA	CMD-C2D-C1D	5.16	133.81	124.71
29	S1	603	CLA	CMD-C2D-C1D	5.16	133.81	124.71
49	r1	620	LUT	C7-C8-C9	-5.16	118.44	126.23
29	b	607	CLA	O2A-C1-C2	5.15	122.18	108.64
29	n1	612	CLA	O2D-CGD-CBD	5.15	120.42	111.27
45	h	101	RRX	C8-C9-C10	-5.15	111.03	118.94
29	G1	603	CLA	O2A-C1-C2	5.15	122.17	108.64
29	B1	608	CLA	O2A-C1-C2	5.15	122.17	108.64
29	b1	611	CLA	O2A-C1-C2	5.15	122.17	108.64
29	b1	616	CLA	O2D-CGD-CBD	5.15	120.42	111.27
29	s	603	CLA	O2A-C1-C2	5.15	122.17	108.64
29	c	504	CLA	O2D-CGD-CBD	5.15	120.41	111.27
29	c1	511	CLA	O2D-CGD-CBD	5.15	120.41	111.27
29	b	604	CLA	CMD-C2D-C1D	5.14	133.78	124.71
29	R1	609	CLA	C1-C2-C3	-5.14	117.15	126.04
29	b	612	CLA	O2A-C1-C2	5.14	122.15	108.64
29	D1	403	CLA	O2A-C1-C2	5.14	122.15	108.64
49	G	620	LUT	C21-C26-C25	5.14	120.62	111.42
31	b1	618	BCR	C30-C25-C26	-5.14	115.38	122.61
29	R	609	CLA	O2D-CGD-CBD	5.14	120.39	111.27
50	y	622	XAT	C7-C8-C9	-5.13	117.56	125.53
50	Y	622	XAT	C15-C14-C13	-5.13	119.98	127.31
29	y1	611	CLA	CMD-C2D-C1D	5.13	133.76	124.71
29	r	602	CLA	O2D-CGD-CBD	5.13	120.38	111.27
29	B	611	CLA	CMD-C2D-C1D	5.13	133.75	124.71
29	N	611	CLA	O2A-C1-C2	5.13	120.96	108.97
29	r	603	CLA	O2D-CGD-CBD	5.12	120.37	111.27
29	C	504	CLA	O2D-CGD-CBD	5.12	120.37	111.27
29	S	603	CLA	CMD-C2D-C1D	5.12	133.74	124.71
29	c1	501	CLA	O2D-CGD-CBD	5.12	120.37	111.27
36	b1	620	C7Z	C35-C34-C33	-5.12	120.00	127.31
29	B	611	CLA	O2D-CGD-CBD	5.12	120.36	111.27
29	c	506	CLA	O2D-CGD-CBD	5.12	120.36	111.27
29	n	603	CLA	O2D-CGD-CBD	5.12	120.36	111.27
29	B	616	CLA	O2D-CGD-CBD	5.11	120.36	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s1	614	CLA	O2A-C1-C2	5.11	122.07	108.64
29	C	502	CLA	CMD-C2D-C1D	5.11	133.72	124.71
29	N1	611	CLA	O2A-C1-C2	5.11	120.92	108.97
29	r1	609	CLA	CMD-C2D-C1D	5.11	133.72	124.71
29	B1	603	CLA	O2D-CGD-CBD	5.11	120.34	111.27
29	n1	610	CLA	O2D-CGD-CBD	5.11	120.34	111.27
50	y1	622	XAT	C15-C14-C13	-5.10	120.03	127.31
29	b1	611	CLA	C2C-C1C-NC	5.10	114.75	109.97
29	Y	602	CLA	CMD-C2D-C1D	5.10	133.71	124.71
29	y	603	CLA	CMD-C2D-C1D	5.10	133.71	124.71
36	b	620	C7Z	C18-C5-C6	-5.10	118.80	124.53
29	c	501	CLA	O2A-C1-C2	5.10	122.04	108.64
29	s	609	CLA	CMD-C2D-C1D	5.10	133.70	124.71
29	C	505	CLA	O2A-C1-C2	5.10	122.04	108.64
29	B1	604	CLA	CMD-C2D-C1D	5.10	133.70	124.71
29	B	615	CLA	O2D-CGD-CBD	5.10	120.33	111.27
29	b	608	CLA	O2D-CGD-CBD	5.10	120.33	111.27
49	n1	620	LUT	C21-C26-C25	5.10	120.55	111.42
29	g	612	CLA	CMD-C2D-C1D	5.10	133.69	124.71
50	y	622	XAT	C31-C30-C29	-5.09	120.04	127.31
29	C1	511	CLA	O2A-C1-C2	5.09	122.02	108.64
29	B1	605	CLA	O2A-C1-C2	5.09	122.02	108.64
29	G1	611	CLA	CMD-C2D-C1D	5.09	133.69	124.71
29	s	610	CLA	O2D-CGD-CBD	5.09	120.32	111.27
29	b1	617	CLA	O2D-CGD-CBD	5.09	120.31	111.27
29	c1	506	CLA	CMD-C2D-C1D	5.09	133.69	124.71
29	S1	613	CLA	O2D-CGD-CBD	5.09	120.31	111.27
29	C1	506	CLA	O2D-CGD-CBD	5.09	120.31	111.27
29	B	616	CLA	CMD-C2D-C1D	5.09	133.68	124.71
45	H1	101	RRX	C24-C23-C22	5.09	133.92	126.23
49	Y1	621	LUT	C7-C8-C9	-5.09	118.55	126.23
51	g1	623	NEX	C2-C1-C6	5.08	114.15	109.21
49	s	620	LUT	C21-C26-C25	5.08	120.53	111.42
49	r	620	LUT	C21-C26-C27	5.08	119.13	112.70
29	g	614	CLA	O2D-CGD-CBD	5.08	120.30	111.27
29	B	602	CLA	O2D-CGD-CBD	5.08	120.29	111.27
29	C	507	CLA	CMD-C2D-C1D	5.08	133.66	124.71
55	y	627	PTY	O7-C8-C11	5.08	120.43	111.09
29	G1	613	CLA	O2D-CGD-CBD	5.07	120.29	111.27
29	G	613	CLA	O2A-C1-C2	5.07	121.97	108.64
29	R1	602	CLA	O2D-CGD-CBD	5.07	120.28	111.27
29	c1	505	CLA	CMD-C2D-C1D	5.07	133.66	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	R1	608	CLA	O2A-C1-C2	5.07	121.97	108.64
29	b	606	CLA	O2D-CGD-CBD	5.07	120.28	111.27
29	B	609	CLA	O2A-C1-C2	5.07	121.97	108.64
49	N	621	LUT	C22-C23-C24	-5.07	105.97	111.74
29	y	602	CLA	CMD-C2D-C1D	5.07	133.65	124.71
53	r	626	ERG	C18-C13-C12	-5.07	102.58	110.59
29	Y1	608	CLA	CMD-C2D-C1D	5.07	133.65	124.71
29	b1	612	CLA	O2A-C1-C2	5.07	121.96	108.64
29	c	508	CLA	CMD-C2D-C1D	5.07	133.64	124.71
29	g	602	CLA	CMD-C2D-C1D	5.07	133.64	124.71
29	Y	608	CLA	CMD-C2D-C1D	5.06	133.64	124.71
29	G1	614	CLA	O2D-CGD-CBD	5.06	120.27	111.27
29	S1	605	CLA	CMD-C2D-C1D	5.06	133.63	124.71
29	N	610	CLA	O2D-CGD-CBD	5.06	120.26	111.27
45	h	101	RRX	C37-C22-C23	5.06	126.05	118.08
29	g	602	CLA	O2D-CGD-CBD	5.06	120.26	111.27
29	R	610	CLA	O2A-C1-C2	5.06	121.93	108.64
29	Y	602	CLA	O2D-CGD-CBD	5.06	120.26	111.27
29	c	512	CLA	O2A-C1-C2	5.06	121.93	108.64
29	C1	503	CLA	O2D-CGD-CBD	5.06	120.25	111.27
29	b1	602	CLA	O2A-C1-C2	5.05	121.92	108.64
29	G	611	CLA	CMD-C2D-C1D	5.05	133.62	124.71
29	c1	507	CLA	O2D-CGD-CBD	5.05	120.25	111.27
29	N1	614	CLA	CMD-C2D-C1D	5.05	133.62	124.71
29	Y1	614	CLA	O2A-C1-C2	5.05	121.91	108.64
29	B	604	CLA	CMD-C2D-C1D	5.05	133.61	124.71
29	b1	603	CLA	CMD-C2D-C1D	5.05	133.61	124.71
29	B	603	CLA	O2A-C1-C2	5.05	121.89	108.64
36	B	620	C7Z	C21-C26-C25	-5.04	115.51	122.61
31	b1	618	BCR	C15-C14-C13	-5.04	120.12	127.31
29	R	612	CLA	O2D-CGD-CBD	5.04	120.22	111.27
29	b	616	CLA	CMD-C2D-C1D	5.04	133.59	124.71
29	C1	503	CLA	O2A-C1-C2	5.04	121.88	108.64
49	s1	621	LUT	C21-C26-C25	5.04	120.44	111.42
29	B	610	CLA	CMD-C2D-C1D	5.04	133.59	124.71
29	B	612	CLA	O2D-CGD-CBD	5.04	120.22	111.27
49	N1	620	LUT	C22-C23-C24	-5.04	106.01	111.74
51	y	623	NEX	C38-C25-C24	5.04	119.95	114.28
50	Y1	622	XAT	C31-C30-C29	-5.04	120.12	127.31
49	y1	621	LUT	C21-C26-C25	5.03	120.44	111.42
29	b1	616	CLA	CMD-C2D-C1D	5.03	133.59	124.71
29	b1	615	CLA	O2D-CGD-CBD	5.03	120.21	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	g1	613	CLA	CMD-C2D-C1D	5.03	133.58	124.71
29	c	505	CLA	CMD-C2D-C1D	5.03	133.58	124.71
29	B	609	CLA	CMD-C2D-C1D	5.03	133.58	124.71
29	B	617	CLA	CMD-C2D-C1D	5.03	133.57	124.71
51	Y1	623	NEX	O24-C25-C24	-5.03	109.61	113.38
36	b	620	C7Z	C27-C28-C29	-5.02	118.64	126.23
29	B	603	CLA	O2D-CGD-CBD	5.02	120.20	111.27
43	d1	405	PL9	C7-C3-C4	5.02	120.96	116.88
49	Y1	621	LUT	C35-C34-C33	-5.02	120.14	127.31
29	d1	402	CLA	O2A-C1-C2	5.02	121.83	108.64
29	n	613	CLA	O2A-C1-C2	5.02	121.82	108.64
29	B	607	CLA	O2A-C1-C2	5.02	121.82	108.64
29	Y	614	CLA	O2D-CGD-CBD	5.02	120.18	111.27
51	s	623	NEX	C38-C25-C24	5.02	119.92	114.28
29	c	503	CLA	O2D-CGD-CBD	5.01	120.18	111.27
29	N	614	CLA	CMD-C2D-C1D	5.01	133.55	124.71
29	S	610	CLA	O2A-C1-C2	5.01	121.81	108.64
29	y1	603	CLA	O2A-C1-C2	5.01	121.81	108.64
50	N	622	XAT	O24-C25-C24	5.01	117.14	113.38
29	s	617	CLA	O2A-C1-C2	5.01	121.80	108.64
29	n1	604	CLA	O2A-C1-C2	5.01	121.79	108.64
29	N1	610	CLA	CMD-C2D-C1D	5.01	133.53	124.71
29	S	610	CLA	CMD-C2D-C1D	5.01	133.53	124.71
29	S1	611	CLA	O2D-CGD-CBD	5.00	120.15	111.27
29	C	511	CLA	O2D-CGD-CBD	5.00	120.15	111.27
31	C1	516	BCR	C15-C14-C13	-5.00	120.18	127.31
29	S	614	CLA	O2D-CGD-CBD	5.00	120.15	111.27
29	b1	607	CLA	O2A-C1-C2	5.00	121.76	108.64
29	C	510	CLA	O2A-C1-C2	4.99	121.76	108.64
29	S1	604	CLA	O2D-CGD-CBD	4.99	120.14	111.27
29	B	617	CLA	O2A-C1-C2	4.99	121.75	108.64
29	R1	608	CLA	O2D-CGD-CBD	4.99	120.14	111.27
55	Y	627	PTY	O7-C8-C11	4.99	120.27	111.09
29	S	613	CLA	CMD-C2D-C1D	4.99	133.51	124.71
49	n1	620	LUT	C21-C26-C27	4.99	119.01	112.70
29	a1	407	CLA	O2A-C1-C2	4.99	120.63	108.97
29	B1	604	CLA	O2D-CGD-CBD	4.99	120.13	111.27
29	R1	604	CLA	O2D-CGD-CBD	4.98	120.12	111.27
29	B1	608	CLA	CMD-C2D-C1D	4.98	133.50	124.71
29	y1	608	CLA	O2A-C1-C2	4.98	121.73	108.64
29	b1	606	CLA	O2D-CGD-CBD	4.98	120.12	111.27
29	b1	608	CLA	CMD-C2D-C1D	4.98	133.50	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	508	CLA	O2A-C1-C2	4.98	121.73	108.64
29	s1	610	CLA	O2D-CGD-CBD	4.98	120.12	111.27
29	c1	503	CLA	O2A-C1-C2	4.98	121.72	108.64
50	r	621	XAT	O4-C5-C4	-4.98	109.64	113.38
29	b1	617	CLA	O2A-C1-C2	4.98	121.71	108.64
29	y1	602	CLA	O2D-CGD-CBD	4.97	120.11	111.27
29	R	608	CLA	O2D-CGD-CBD	4.97	120.11	111.27
50	N	622	XAT	C18-C5-C4	4.97	119.87	114.28
29	C1	513	CLA	O2D-CGD-CBD	4.97	120.10	111.27
50	G	622	XAT	C31-C30-C29	-4.97	120.22	127.31
29	g	614	CLA	CMD-C2D-C1D	4.97	133.47	124.71
29	Y	612	CLA	CMD-C2D-C1D	4.97	133.47	124.71
48	s1	608	CHL	CHD-C1D-ND	-4.97	119.89	124.45
29	S	617	CLA	CMD-C2D-C1D	4.97	133.47	124.71
45	H1	101	RRX	C15-C14-C13	-4.97	120.22	127.31
29	Y	611	CLA	O2D-CGD-CBD	4.97	120.09	111.27
29	d1	403	CLA	O2A-C1-C2	4.97	121.69	108.64
29	y	604	CLA	CMD-C2D-C1D	4.97	133.46	124.71
29	b1	608	CLA	O2D-CGD-CBD	4.96	120.09	111.27
29	d1	403	CLA	O2D-CGD-CBD	4.96	120.08	111.27
29	s1	609	CLA	O2D-CGD-CBD	4.96	120.08	111.27
29	Y1	613	CLA	O2D-CGD-CBD	4.96	120.08	111.27
29	c1	502	CLA	O2D-CGD-CBD	4.95	120.07	111.27
49	s1	621	LUT	C31-C30-C29	-4.95	120.24	127.31
29	y	611	CLA	O2D-CGD-CBD	4.95	120.06	111.27
29	Y1	613	CLA	O2A-C1-C2	4.95	121.64	108.64
51	g1	623	NEX	C38-C25-C24	4.95	119.84	114.28
29	S	611	CLA	CMD-C2D-C1D	4.94	133.43	124.71
29	n1	610	CLA	O2A-C1-C2	4.94	121.63	108.64
29	B	603	CLA	CMD-C2D-C1D	4.94	133.42	124.71
29	y1	614	CLA	O2D-CGD-CBD	4.94	120.04	111.27
29	b	614	CLA	O2D-CGD-CBD	4.94	120.04	111.27
29	Y	614	CLA	O2A-C1-C2	4.94	121.61	108.64
29	N1	603	CLA	O2D-CGD-CBD	4.93	120.03	111.27
29	C1	504	CLA	CMD-C2D-C1D	4.93	133.41	124.71
29	R	602	CLA	O2A-C1-C2	4.93	121.60	108.64
29	c	507	CLA	O2A-C1-C2	4.93	121.60	108.64
29	s	609	CLA	O2D-CGD-CBD	4.93	120.03	111.27
29	s1	604	CLA	O2D-CGD-CBD	4.93	120.03	111.27
29	R	603	CLA	O2A-C1-C2	4.93	121.59	108.64
49	y	621	LUT	C21-C26-C25	4.93	120.25	111.42
29	y	604	CLA	O2A-C1-C2	4.93	121.59	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	603	CLA	O2D-CGD-CBD	4.93	120.02	111.27
29	A1	407	CLA	O2A-C1-C2	4.93	121.58	108.64
29	r1	610	CLA	O2D-CGD-CBD	4.92	120.01	111.27
29	y1	604	CLA	O2A-C1-C2	4.92	121.57	108.64
29	r1	612	CLA	O2D-CGD-CBD	4.92	120.01	111.27
29	y1	603	CLA	O2D-CGD-CBD	4.92	120.01	111.27
29	c1	512	CLA	CMD-C2D-C1D	4.92	133.38	124.71
29	Y1	614	CLA	O2D-CGD-CBD	4.92	120.00	111.27
29	n	603	CLA	CMD-C2D-C1D	4.91	133.37	124.71
29	n	613	CLA	O2D-CGD-CBD	4.91	119.99	111.27
29	S	613	CLA	O2A-C1-C2	4.91	121.54	108.64
29	n	604	CLA	CMD-C2D-C1D	4.91	133.37	124.71
29	a	410	CLA	CMD-C2D-C1D	4.91	133.36	124.71
29	r1	602	CLA	O2A-C1-C2	4.91	121.53	108.64
51	g1	623	NEX	C31-C30-C29	4.91	134.31	127.31
29	R	603	CLA	O2D-CGD-CBD	4.90	119.98	111.27
39	C1	524	DGA	OG2-CB1-CB2	4.90	122.07	111.50
29	B1	617	CLA	O2A-C1-C2	4.90	121.52	108.64
29	B1	610	CLA	CMD-C2D-C1D	4.90	133.35	124.71
53	R1	626	ERG	C12-C13-C14	4.90	115.04	107.27
29	y1	614	CLA	O2A-C1-C2	4.90	121.52	108.64
29	y	603	CLA	O2A-C1-C2	4.90	121.51	108.64
29	A1	407	CLA	CMD-C2D-C1D	4.90	133.35	124.71
29	R1	612	CLA	O2D-CGD-CBD	4.90	119.97	111.27
50	G1	622	XAT	C18-C5-C4	4.89	119.78	114.28
29	g	604	CLA	O2D-CGD-CBD	4.89	119.96	111.27
29	C1	512	CLA	O2D-CGD-CBD	4.89	119.96	111.27
49	G1	621	LUT	C11-C10-C9	-4.89	120.33	127.31
29	g1	604	CLA	O2A-C1-C2	4.89	120.41	108.97
29	Y	608	CLA	O2D-CGD-CBD	4.89	119.96	111.27
29	S	614	CLA	O2A-C1-C2	4.89	121.47	108.64
29	n	602	CLA	O2A-C1-C2	4.88	121.47	108.64
29	S	612	CLA	CMD-C2D-C1D	4.88	133.31	124.71
36	b	620	C7Z	C35-C34-C33	-4.88	120.35	127.31
48	Y	605	CHL	CHD-C1D-ND	-4.88	119.97	124.45
29	R	604	CLA	O2D-CGD-CBD	4.88	119.94	111.27
50	n	622	XAT	O24-C25-C24	4.88	117.05	113.38
29	n1	613	CLA	CAA-C2A-C3A	-4.88	99.42	112.78
29	g1	603	CLA	CMD-C2D-C1D	4.88	133.31	124.71
36	B1	620	C7Z	C21-C26-C25	-4.88	115.75	122.61
29	g	613	CLA	O2D-CGD-CBD	4.87	119.93	111.27
55	y1	627	PTY	O7-C8-C11	4.87	120.06	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y1	604	CLA	O2A-C1-C2	4.87	121.44	108.64
29	n	613	CLA	CAA-C2A-C3A	-4.87	99.44	112.78
49	g	620	LUT	C21-C26-C25	4.87	120.14	111.42
29	S1	614	CLA	O2A-C1-C2	4.87	121.43	108.64
29	S	604	CLA	O2D-CGD-CBD	4.87	119.92	111.27
29	c	511	CLA	O2D-CGD-CBD	4.86	119.91	111.27
29	A	410	CLA	O2A-C1-C2	4.86	121.41	108.64
29	Y	603	CLA	O2A-C1-C2	4.86	121.40	108.64
29	a1	410	CLA	CMD-C2D-C1D	4.85	133.27	124.71
29	c1	510	CLA	O2D-CGD-CBD	4.85	119.89	111.27
29	N	602	CLA	CMD-C2D-C1D	4.85	133.26	124.71
29	Y1	608	CLA	O2D-CGD-CBD	4.85	119.88	111.27
29	S	613	CLA	O2D-CGD-CBD	4.84	119.88	111.27
49	N1	620	LUT	C21-C26-C25	4.84	120.09	111.42
29	b1	607	CLA	CMD-C2D-C1D	4.84	133.25	124.71
48	N1	601	CHL	C4A-NA-C1A	4.84	108.88	106.71
51	y1	623	NEX	C38-C25-C24	4.84	119.72	114.28
50	n1	622	XAT	C18-C5-C4	4.84	119.72	114.28
29	r1	608	CLA	O2D-CGD-CBD	4.84	119.86	111.27
29	g	610	CLA	O2A-C1-C2	4.84	121.34	108.64
29	S	603	CLA	O2A-C1-C2	4.83	121.34	108.64
29	c1	502	CLA	CMD-C2D-C1D	4.83	133.23	124.71
29	a1	405	CLA	O2D-CGD-CBD	4.83	119.86	111.27
36	b1	620	C7Z	C1-C6-C5	-4.83	115.81	122.61
33	a1	413	LMG	O7-C10-C11	4.83	121.91	111.50
29	s1	611	CLA	O2A-C1-C2	4.83	121.33	108.64
29	B	616	CLA	O2A-C1-C2	4.83	121.33	108.64
29	B1	602	CLA	O2A-C1-C2	4.83	121.32	108.64
29	g1	604	CLA	O2D-CGD-CBD	4.83	119.84	111.27
29	s1	611	CLA	O2D-CGD-CBD	4.82	119.84	111.27
29	c	502	CLA	CMD-C2D-C1D	4.82	133.21	124.71
31	c	515	BCR	C12-C13-C14	-4.82	111.54	118.94
40	g1	624	LHG	O7-C7-C8	4.82	121.89	111.50
29	y	608	CLA	O2A-C1-C2	4.82	121.30	108.64
29	s	609	CLA	O2A-C1-C2	4.82	121.29	108.64
29	s	611	CLA	O2A-C1-C2	4.81	121.28	108.64
29	C1	507	CLA	O2D-CGD-CBD	4.81	119.82	111.27
50	G	622	XAT	C18-C5-C4	4.81	119.69	114.28
29	r	603	CLA	O2A-C1-C2	4.80	121.26	108.64
29	r	610	CLA	O2D-CGD-CBD	4.80	119.80	111.27
29	s1	617	CLA	O2D-CGD-CBD	4.80	119.80	111.27
49	N1	620	LUT	C21-C26-C27	4.80	118.77	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	Y1	622	XAT	C38-C25-C24	4.80	119.68	114.28
29	Y1	612	CLA	CMD-C2D-C1D	4.80	133.16	124.71
29	A	410	CLA	CMD-C2D-C1D	4.79	133.16	124.71
29	r	609	CLA	O2D-CGD-CBD	4.79	119.78	111.27
29	B1	611	CLA	CMD-C2D-C1D	4.79	133.16	124.71
29	Y	612	CLA	O2A-C1-C2	4.79	121.22	108.64
29	c1	502	CLA	O2A-C1-C2	4.79	121.22	108.64
29	s	604	CLA	O2A-C1-C2	4.79	121.21	108.64
49	Y1	621	LUT	C35-C15-C14	-4.79	113.67	123.47
37	b1	623	DGD	O2G-C1B-C2B	4.78	121.81	111.50
29	r1	602	CLA	CMD-C2D-C1D	4.78	133.14	124.71
29	B	610	CLA	O2A-C1-C2	4.78	121.20	108.64
49	Y1	620	LUT	C21-C26-C25	4.78	119.98	111.42
49	Y1	621	LUT	C22-C23-C24	-4.78	106.30	111.74
29	N	602	CLA	O2A-C1-C2	4.78	121.20	108.64
29	B1	617	CLA	CMD-C2D-C1D	4.78	133.14	124.71
49	Y	620	LUT	C21-C26-C25	4.78	119.97	111.42
29	S	611	CLA	O2D-CGD-CBD	4.78	119.75	111.27
36	B1	620	C7Z	C15-C14-C13	-4.77	120.50	127.31
50	r	621	XAT	C18-C5-C4	4.77	119.65	114.28
29	n1	611	CLA	O2D-CGD-CBD	4.77	119.75	111.27
29	C1	505	CLA	CMD-C2D-C1D	4.77	133.12	124.71
29	S1	611	CLA	O2A-C1-C2	4.77	121.17	108.64
49	G1	621	LUT	C21-C26-C25	4.77	119.96	111.42
29	B1	612	CLA	O2D-CGD-CBD	4.77	119.74	111.27
29	C1	510	CLA	O2D-CGD-CBD	4.77	119.74	111.27
49	S1	621	LUT	C21-C26-C25	4.77	119.95	111.42
29	R	603	CLA	CMD-C2D-C1D	4.76	133.11	124.71
29	N1	613	CLA	O2D-CGD-CBD	4.76	119.73	111.27
38	b	624	3PH	O21-C21-C22	4.76	121.77	111.50
29	g	613	CLA	CMD-C2D-C1D	4.76	133.10	124.71
29	S1	611	CLA	CMD-C2D-C1D	4.76	133.10	124.71
50	G	622	XAT	C38-C25-C24	4.76	119.63	114.28
29	B1	617	CLA	O2D-CGD-CBD	4.76	119.72	111.27
50	n1	622	XAT	C7-C8-C9	-4.75	118.15	125.53
50	R	621	XAT	O24-C25-C24	4.75	116.95	113.38
29	C	501	CLA	O2D-CGD-CBD	4.75	119.72	111.27
49	g1	620	LUT	C21-C26-C25	4.75	119.93	111.42
29	R1	610	CLA	C1-C2-C3	-4.75	117.83	126.04
40	L1	101	LHG	O7-C7-C8	4.75	121.74	111.50
29	y	612	CLA	CMD-C2D-C1D	4.75	133.08	124.71
43	d	405	PL9	C7-C3-C4	4.75	120.74	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s	603	CLA	CMD-C2D-C1D	4.75	133.08	124.71
30	a1	409	PHO	C2B-C1B-NB	-4.74	106.25	109.53
29	y	602	CLA	O2A-C1-C2	4.74	121.09	108.64
29	C	513	CLA	O2A-C1-C2	4.74	121.08	108.64
49	s	620	LUT	C21-C26-C27	4.74	118.69	112.70
29	Y1	611	CLA	O2A-C1-C2	4.74	121.08	108.64
29	G1	604	CLA	O2A-C1-C2	4.73	120.04	108.97
49	N1	621	LUT	C18-C5-C6	-4.73	119.21	124.53
51	g	623	NEX	C38-C25-C24	4.73	119.60	114.28
29	Y	604	CLA	O2A-C1-C2	4.73	121.06	108.64
43	D	405	PL9	C7-C3-C4	4.73	120.72	116.88
29	S1	614	CLA	CMD-C2D-C1D	4.72	133.04	124.71
29	b1	614	CLA	O2D-CGD-CBD	4.72	119.66	111.27
29	s1	612	CLA	O2D-CGD-CBD	4.72	119.66	111.27
29	a1	405	CLA	O2A-C1-C2	4.72	121.05	108.64
50	n	622	XAT	C18-C5-C4	4.71	119.58	114.28
48	Y	609	CHL	CHD-C1D-ND	-4.71	120.12	124.45
29	Y1	602	CLA	O2A-C1-C2	4.71	121.02	108.64
29	N1	612	CLA	O2D-CGD-CBD	4.71	119.64	111.27
29	y	613	CLA	CMD-C2D-C1D	4.71	133.01	124.71
29	a1	406	CLA	O2D-CGD-CBD	4.71	119.64	111.27
45	h1	101	RRX	C24-C25-C26	-4.71	110.06	121.46
50	y	622	XAT	C18-C5-C4	4.71	119.58	114.28
29	N	613	CLA	O2D-CGD-CBD	4.70	119.63	111.27
29	B1	606	CLA	O2D-CGD-CBD	4.70	119.63	111.27
29	D	402	CLA	O2D-CGD-CBD	4.70	119.63	111.27
29	R	609	CLA	CMD-C2D-C1D	4.70	133.00	124.71
51	y1	623	NEX	C31-C30-C29	4.70	134.02	127.31
45	h1	101	RRX	C37-C22-C23	4.70	125.49	118.08
29	b	605	CLA	O2A-C1-C2	4.70	120.99	108.64
29	C	512	CLA	O2A-C1-C2	4.70	120.99	108.64
29	N1	610	CLA	O2D-CGD-CBD	4.70	119.62	111.27
33	b	622	LMG	O7-C10-C11	4.70	121.63	111.50
29	B1	605	CLA	O2D-CGD-CBD	4.70	119.61	111.27
29	g1	602	CLA	O2A-C1-C2	4.70	120.98	108.64
33	B	622	LMG	O7-C10-C11	4.70	121.62	111.50
29	A1	406	CLA	O2D-CGD-CBD	4.70	119.61	111.27
29	y	612	CLA	O2A-C1-C2	4.69	120.97	108.64
50	N	622	XAT	C38-C25-C24	4.69	119.56	114.28
29	y	610	CLA	O2A-C1-C2	4.69	120.97	108.64
29	s	611	CLA	CMD-C2D-C1D	4.69	132.98	124.71
29	B1	604	CLA	O2A-C1-C2	4.69	120.96	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	406	CLA	O2D-CGD-CBD	4.68	119.59	111.27
50	r1	621	XAT	C38-C25-C24	4.68	119.55	114.28
29	B	614	CLA	O2D-CGD-CBD	4.68	119.59	111.27
29	b1	602	CLA	O2D-CGD-CBD	4.68	119.58	111.27
29	s	613	CLA	O2D-CGD-CBD	4.68	119.58	111.27
29	Y1	603	CLA	O2D-CGD-CBD	4.68	119.58	111.27
51	s	623	NEX	C16-C1-C6	-4.67	106.29	110.47
29	A1	405	CLA	O2D-CGD-CBD	4.67	119.57	111.27
29	b1	616	CLA	O2A-C1-C2	4.67	120.91	108.64
49	Y	621	LUT	C22-C23-C24	-4.67	106.43	111.74
29	b	611	CLA	O2A-C1-C2	4.67	120.90	108.64
33	a	413	LMG	O7-C10-C11	4.66	121.55	111.50
49	S	621	LUT	C21-C26-C25	4.66	119.77	111.42
29	c1	505	CLA	O2A-C1-C2	4.66	120.89	108.64
31	b	618	BCR	C33-C5-C4	4.66	122.57	113.62
29	y	611	CLA	CMD-C2D-C1D	4.66	132.93	124.71
31	B1	619	BCR	C15-C14-C13	-4.66	120.66	127.31
43	D1	405	PL9	C7-C3-C2	-4.66	117.18	123.30
49	R	620	LUT	C35-C34-C33	-4.66	120.67	127.31
45	H	101	RRX	C4-C5-C6	-4.65	115.98	122.73
48	n	609	CHL	CMA-C3A-C4A	4.65	124.27	111.77
50	Y1	622	XAT	C7-C8-C9	-4.65	118.32	125.53
29	B	612	CLA	CMD-C2D-C1D	4.65	132.90	124.71
51	r	622	NEX	C27-C28-C29	-4.65	118.32	125.53
29	c	508	CLA	O2D-CGD-CBD	4.64	119.52	111.27
51	N	623	NEX	C38-C25-C24	4.64	119.50	114.28
29	Y1	612	CLA	O2A-C1-C2	4.64	120.84	108.64
29	A	406	CLA	O2D-CGD-CBD	4.64	119.51	111.27
29	C	503	CLA	O2A-C1-C2	4.64	120.83	108.64
29	b	616	CLA	O2A-C1-C2	4.64	120.83	108.64
50	R1	621	XAT	C38-C25-C24	4.64	119.50	114.28
29	b	602	CLA	O2A-C1-C2	4.64	120.82	108.64
29	B1	613	CLA	O2D-CGD-CBD	4.64	119.51	111.27
31	b	618	BCR	C33-C5-C6	-4.64	119.32	124.53
29	S	609	CLA	O2A-C1-C2	4.63	120.81	108.64
29	A	407	CLA	O2D-CGD-CBD	4.63	119.50	111.27
50	g	622	XAT	C38-C25-C24	4.63	119.48	114.28
29	S	602	CLA	CMD-C2D-C1D	4.63	132.87	124.71
29	n1	604	CLA	O2D-CGD-CBD	4.62	119.48	111.27
29	b	609	CLA	O2A-C1-C2	4.62	120.79	108.64
33	A	413	LMG	O7-C10-C11	4.62	121.46	111.50
29	B	608	CLA	O2D-CGD-CBD	4.62	119.47	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	611	CLA	O2D-CGD-CBD	4.61	119.46	111.27
29	r1	609	CLA	O2D-CGD-CBD	4.61	119.46	111.27
29	R	609	CLA	O2A-C1-C2	4.61	120.75	108.64
36	b	620	C7Z	C7-C8-C9	-4.61	119.27	126.23
29	R1	603	CLA	O2A-C1-C2	4.61	120.74	108.64
51	n	623	NEX	C38-C25-C24	4.60	119.46	114.28
29	b	604	CLA	O2A-C1-C2	4.60	120.72	108.64
29	g1	603	CLA	O2D-CGD-CBD	4.60	119.44	111.27
29	N1	602	CLA	CMD-C2D-C1D	4.60	132.81	124.71
50	N1	622	XAT	O4-C5-C4	-4.60	109.93	113.38
29	R1	609	CLA	CMD-C2D-C1D	4.59	132.81	124.71
51	R1	622	NEX	C2-C1-C6	4.59	113.68	109.21
29	B1	614	CLA	O2D-CGD-CBD	4.59	119.42	111.27
51	S	623	NEX	C38-C25-C24	4.59	119.44	114.28
29	b	602	CLA	O2D-CGD-CBD	4.59	119.42	111.27
29	y	608	CLA	O2D-CGD-CBD	4.59	119.42	111.27
50	Y	622	XAT	C38-C25-C24	4.58	119.43	114.28
37	B1	623	DGD	O2G-C1B-C2B	4.58	121.37	111.50
31	C1	515	BCR	C15-C14-C13	-4.58	120.78	127.31
33	w1	201	LMG	O7-C10-C11	4.58	121.37	111.50
31	C1	516	BCR	C33-C5-C6	-4.58	119.39	124.53
29	n	613	CLA	CMD-C2D-C1D	4.57	132.78	124.71
29	b1	615	CLA	O2A-C1-C2	4.57	120.66	108.64
53	r1	626	ERG	C13-C17-C20	-4.57	113.53	119.43
45	H	101	RRX	C33-C5-C6	-4.57	119.39	124.53
49	S1	621	LUT	C35-C34-C33	-4.57	120.78	127.31
29	B	602	CLA	O2A-C1-C2	4.57	120.64	108.64
49	g1	621	LUT	C22-C23-C24	-4.57	106.54	111.74
29	y	613	CLA	O2A-C1-C2	4.57	120.64	108.64
29	N	613	CLA	CMD-C2D-C1D	4.57	132.76	124.71
33	h	102	LMG	O7-C10-C11	4.57	121.34	111.50
29	R	602	CLA	CMD-C2D-C1D	4.57	132.76	124.71
55	Y1	627	PTY	O7-C8-C11	4.57	119.49	111.09
51	Y	623	NEX	C38-C25-C24	4.56	119.42	114.28
45	h1	101	RRX	C24-C23-C22	4.56	133.12	126.23
29	n	602	CLA	O2D-CGD-CBD	4.55	119.36	111.27
29	B1	608	CLA	O2D-CGD-CBD	4.55	119.36	111.27
33	w	201	LMG	O7-C10-C11	4.55	121.31	111.50
29	s1	602	CLA	C1-C2-C3	-4.55	118.18	126.04
51	Y1	623	NEX	C38-C25-C26	-4.54	114.65	122.26
29	c1	509	CLA	O2D-CGD-CBD	4.54	119.34	111.27
45	h	101	RRX	C1-C6-C5	-4.54	116.22	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	y1	621	LUT	C3-C4-C5	-4.54	102.81	111.85
53	R	626	ERG	C18-C13-C12	-4.54	103.42	110.59
29	s	614	CLA	O2A-C1-C2	4.54	120.56	108.64
29	r	602	CLA	O2A-C1-C2	4.53	120.55	108.64
29	n	611	CLA	O2D-CGD-CBD	4.53	119.32	111.27
51	r1	622	NEX	C17-C1-C6	-4.53	106.42	110.47
29	A	405	CLA	O2D-CGD-CBD	4.53	119.31	111.27
29	G	612	CLA	O2D-CGD-CBD	4.52	119.31	111.27
29	N1	613	CLA	O2A-C1-C2	4.52	120.52	108.64
29	r	608	CLA	O2A-C1-C2	4.52	120.52	108.64
45	h	101	RRX	C16-C17-C18	-4.52	120.86	127.31
29	B	614	CLA	O2A-C1-C2	4.52	120.50	108.64
29	r1	610	CLA	CMD-C2D-C1D	4.52	132.67	124.71
29	y	614	CLA	O2A-C1-C2	4.51	120.50	108.64
51	r1	622	NEX	C2-C1-C6	4.51	113.60	109.21
29	g1	611	CLA	O2A-C1-C2	4.51	120.50	108.64
29	b	617	CLA	O2A-C1-C2	4.51	120.49	108.64
33	W	201	LMG	O7-C10-C11	4.51	121.22	111.50
36	B1	620	C7Z	C22-C23-C24	4.51	116.48	110.30
48	y1	601	CHL	CHD-C1D-ND	-4.51	120.31	124.45
29	b1	616	CLA	C2C-C1C-NC	4.51	114.20	109.97
50	g	622	XAT	C18-C5-C4	4.51	119.35	114.28
29	C	506	CLA	O2A-C1-C2	4.50	120.47	108.64
36	B	620	C7Z	C38-C25-C26	-4.50	119.47	124.53
36	B1	620	C7Z	C2-C3-C4	4.50	116.47	110.30
29	C	513	CLA	CMD-C2D-C1D	4.50	132.64	124.71
30	A1	409	PHO	C2B-C1B-NB	-4.50	106.42	109.53
29	B1	610	CLA	O2D-CGD-CBD	4.50	119.26	111.27
40	Y1	624	LHG	O7-C7-C8	4.50	121.19	111.50
50	y	622	XAT	C36-C21-C26	4.49	122.18	110.05
29	S	611	CLA	O2A-C1-C2	4.49	120.44	108.64
40	c	525	LHG	O7-C7-C8	4.49	121.18	111.50
29	b1	614	CLA	O2A-C1-C2	4.48	120.42	108.64
29	N1	604	CLA	C1-C2-C3	-4.48	118.29	126.04
38	t	101	3PH	O21-C21-C22	4.48	121.16	111.50
51	R	622	NEX	C16-C1-C6	-4.48	106.46	110.47
50	N1	622	XAT	C18-C5-C4	4.48	119.32	114.28
29	R1	609	CLA	O2D-CGD-CBD	4.47	119.21	111.27
36	b1	620	C7Z	C7-C8-C9	-4.47	119.48	126.23
50	r	621	XAT	C38-C25-C24	4.47	119.31	114.28
29	G	614	CLA	O2D-CGD-CBD	4.47	119.20	111.27
49	G1	621	LUT	C15-C14-C13	-4.46	120.94	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n1	613	CLA	O2D-CGD-CBD	4.46	119.20	111.27
29	c1	512	CLA	O2D-CGD-CBD	4.46	119.20	111.27
29	Y	610	CLA	O2A-C1-C2	4.46	120.36	108.64
50	g1	622	XAT	C38-C25-C24	4.46	119.30	114.28
29	G1	611	CLA	O2D-CGD-CBD	4.46	119.19	111.27
29	a	406	CLA	C1-C2-C3	-4.45	118.34	126.04
29	s1	617	CLA	O2A-C1-C2	4.45	120.34	108.64
29	R1	610	CLA	CMD-C2D-C1D	4.45	132.56	124.71
29	S1	609	CLA	O2A-C1-C2	4.45	120.33	108.64
29	n1	603	CLA	O2A-C1-C2	4.45	120.32	108.64
31	C	516	BCR	C33-C5-C6	-4.45	119.53	124.53
29	N1	602	CLA	O2D-CGD-CBD	4.45	119.17	111.27
40	s	624	LHG	O7-C7-C8	4.45	121.08	111.50
29	C	508	CLA	O2D-CGD-CBD	4.45	119.17	111.27
29	g	603	CLA	C1-C2-C3	-4.45	118.35	126.04
49	N1	621	LUT	C22-C23-C24	-4.44	106.68	111.74
49	Y	621	LUT	C21-C26-C27	4.44	118.32	112.70
36	b1	620	C7Z	C27-C28-C29	-4.43	119.55	126.23
29	c	511	CLA	O2A-C1-C2	4.43	120.27	108.64
29	C	501	CLA	O2A-C1-C2	4.42	120.25	108.64
49	Y1	620	LUT	C21-C26-C27	4.42	118.28	112.70
51	R	622	NEX	C38-C25-C24	4.41	119.25	114.28
53	R1	626	ERG	C2-C1-C10	4.41	122.30	112.74
49	Y	620	LUT	C21-C26-C27	4.41	118.28	112.70
29	r1	604	CLA	O2D-CGD-CBD	4.41	119.10	111.27
29	r1	602	CLA	CMA-C3A-C4A	4.41	123.61	111.77
49	G1	620	LUT	C21-C26-C27	4.40	118.27	112.70
53	R	626	ERG	C2-C1-C10	4.40	122.28	112.74
40	n	624	LHG	O7-C7-C8	4.40	120.99	111.50
45	h	101	RRX	C10-C11-C12	-4.40	109.49	123.22
45	h	101	RRX	C15-C14-C13	-4.39	121.04	127.31
51	r1	622	NEX	C19-C9-C10	-4.39	116.77	122.92
39	J1	101	DGA	OG2-CB1-CB2	4.39	120.96	111.50
49	R	620	LUT	C11-C10-C9	-4.38	121.05	127.31
29	s	611	CLA	O2D-CGD-CBD	4.38	119.06	111.27
29	C1	509	CLA	O2A-C1-C2	4.38	120.15	108.64
50	Y1	622	XAT	C36-C21-C26	4.38	121.87	110.05
36	b	620	C7Z	C31-C30-C29	-4.38	121.06	127.31
40	S1	624	LHG	O7-C7-C8	4.37	120.92	111.50
48	S	601	CHL	C3B-C4B-NB	-4.37	106.46	110.52
29	C	509	CLA	O2A-C1-C2	4.37	120.11	108.64
51	Y	623	NEX	C2-C1-C6	4.36	113.45	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	h1	101	RRX	C7-C8-C9	4.36	132.83	126.23
50	Y	622	XAT	C7-C8-C9	-4.36	118.76	125.53
29	c1	513	CLA	CMD-C2D-C1D	4.36	132.40	124.71
29	B1	609	CLA	O2A-C1-C2	4.35	120.08	108.64
38	B1	624	3PH	O21-C21-C22	4.35	120.88	111.50
29	S1	610	CLA	O2D-CGD-CBD	4.35	119.00	111.27
55	y	626	PTY	O7-C8-C11	4.35	120.87	111.50
49	n	620	LUT	C15-C14-C13	-4.35	121.11	127.31
50	n1	622	XAT	C38-C25-C24	4.35	119.17	114.28
40	D	408	LHG	O7-C7-C8	4.34	120.86	111.50
29	S1	612	CLA	CMD-C2D-C1D	4.34	132.36	124.71
40	N1	624	LHG	O7-C7-C8	4.34	120.85	111.50
48	g	605	CHL	C4A-NA-C1A	4.34	108.66	106.71
36	B	620	C7Z	C35-C34-C33	-4.33	121.12	127.31
31	b	618	BCR	C1-C6-C5	-4.33	116.51	122.61
48	y1	609	CHL	C4B-CHC-C1C	4.33	136.61	126.34
29	G	613	CLA	O2D-CGD-CBD	4.33	118.97	111.27
49	s1	620	LUT	C22-C23-C24	-4.33	106.81	111.74
29	c	503	CLA	O2A-C1-C2	4.33	120.01	108.64
30	A1	408	PHO	C2B-C1B-NB	-4.33	106.54	109.53
29	b	605	CLA	C2C-C1C-NC	4.32	114.02	109.97
31	b1	618	BCR	C1-C6-C5	-4.32	116.52	122.61
29	g	612	CLA	O2D-CGD-CBD	4.32	118.95	111.27
50	Y1	622	XAT	O4-C5-C4	-4.32	110.14	113.38
29	C1	501	CLA	C1-C2-C3	-4.32	118.57	126.04
31	B	618	BCR	C33-C5-C4	4.32	121.91	113.62
29	a	405	CLA	O2D-CGD-CBD	4.31	118.93	111.27
29	Y	611	CLA	O2A-C1-C2	4.31	119.97	108.64
49	G	620	LUT	C35-C34-C33	-4.31	121.16	127.31
29	C	512	CLA	CMD-C2D-C1D	4.31	132.31	124.71
48	n1	605	CHL	CHD-C1D-ND	-4.31	120.50	124.45
29	B1	615	CLA	O2D-CGD-CBD	4.31	118.92	111.27
29	g1	614	CLA	O2D-CGD-CBD	4.30	118.91	111.27
38	B	624	3PH	O21-C21-C22	4.30	120.77	111.50
51	R	622	NEX	C5-C6-C1	4.30	123.96	119.70
29	B1	611	CLA	C2C-C1C-NC	4.30	114.00	109.97
29	C	511	CLA	O2A-C1-C2	4.30	119.93	108.64
49	R1	620	LUT	C7-C8-C9	-4.29	119.75	126.23
29	n	603	CLA	O2A-C1-C2	4.29	119.92	108.64
29	y1	613	CLA	O2A-C1-C2	4.29	119.91	108.64
29	A	406	CLA	O2A-C1-C2	4.29	119.91	108.64
40	d1	408	LHG	O7-C7-C8	4.29	120.75	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	R1	622	NEX	C38-C25-C24	4.29	119.10	114.28
40	y	624	LHG	O7-C7-C8	4.29	120.74	111.50
49	Y1	620	LUT	C35-C34-C33	-4.29	121.19	127.31
30	A	409	PHO	C2B-C1B-NB	-4.28	106.57	109.53
49	N1	620	LUT	C7-C8-C9	-4.28	119.76	126.23
29	R1	603	CLA	CMD-C2D-C1D	4.28	132.26	124.71
33	W1	201	LMG	O7-C10-C11	4.28	120.72	111.50
49	G	621	LUT	C22-C23-C24	-4.28	106.88	111.74
50	R1	621	XAT	C31-C30-C29	-4.27	121.21	127.31
29	a1	407	CLA	CMD-C2D-C1D	4.27	132.25	124.71
50	G	622	XAT	O4-C5-C4	-4.27	110.17	113.38
53	r	626	ERG	C4-C5-C10	4.27	122.09	116.42
29	C1	510	CLA	O2A-C1-C2	4.27	119.85	108.64
29	S1	605	CLA	O2D-CGD-CBD	4.27	118.85	111.27
45	h	101	RRX	C7-C6-C5	-4.26	111.13	121.46
48	g	606	CHL	CHD-C1D-ND	-4.26	120.54	124.45
50	N1	622	XAT	C38-C25-C24	4.26	119.08	114.28
29	S	610	CLA	O2D-CGD-CBD	4.26	118.84	111.27
48	n1	601	CHL	CHD-C1D-ND	-4.26	120.54	124.45
50	N	622	XAT	C7-C8-C9	-4.26	118.92	125.53
29	c1	510	CLA	O2A-C1-C2	4.26	119.82	108.64
29	y1	611	CLA	C1-C2-C3	-4.26	118.68	126.04
29	B	615	CLA	O2A-C1-C2	4.26	119.82	108.64
53	R1	626	ERG	C2-C3-C4	4.26	116.14	110.31
45	h	101	RRX	C7-C8-C9	4.25	132.66	126.23
29	b	609	CLA	CMD-C2D-C1D	4.25	132.21	124.71
50	y	622	XAT	C15-C14-C13	-4.25	121.24	127.31
48	r1	607	CHL	CHD-C1D-ND	-4.25	120.55	124.45
29	C	506	CLA	C2C-C1C-NC	4.25	113.95	109.97
49	N	621	LUT	C15-C14-C13	-4.24	121.26	127.31
40	C	525	LHG	O7-C7-C8	4.24	120.64	111.50
49	n1	620	LUT	C15-C14-C13	-4.24	121.26	127.31
29	c	513	CLA	CMD-C2D-C1D	4.24	132.18	124.71
40	G	624	LHG	O7-C7-C8	4.24	120.63	111.50
29	S1	617	CLA	C1-C2-C3	-4.24	119.90	126.75
39	B1	625	DGA	OG2-CB1-CB2	4.24	120.63	111.50
29	c	505	CLA	O2A-C1-C2	4.24	119.77	108.64
33	C1	521	LMG	O7-C10-C11	4.23	120.62	111.50
29	C1	508	CLA	CMD-C2D-C1D	4.23	132.17	124.71
40	Y	624	LHG	O7-C7-C8	4.22	120.60	111.50
49	s1	621	LUT	C11-C10-C9	-4.22	121.28	127.31
40	n1	624	LHG	O7-C7-C8	4.22	120.59	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	521	LMG	O7-C10-C11	4.21	120.58	111.50
51	s1	623	NEX	C38-C25-C24	4.21	119.02	114.28
29	b1	612	CLA	C1-C2-C3	-4.21	118.76	126.04
29	R1	610	CLA	C2D-C1D-ND	4.21	113.20	110.10
29	B1	614	CLA	C2C-C1C-NC	4.21	113.91	109.97
48	g1	609	CHL	CHD-C1D-ND	-4.20	120.59	124.45
49	g1	621	LUT	C7-C8-C9	-4.20	119.89	126.23
49	G	620	LUT	C7-C8-C9	-4.20	119.89	126.23
45	H1	101	RRX	C24-C25-C26	-4.19	111.30	121.46
33	c	523	LMG	O7-C10-C11	4.19	120.54	111.50
49	G	620	LUT	C21-C26-C27	4.19	118.00	112.70
31	B	618	BCR	C1-C6-C5	-4.19	116.71	122.61
48	n	605	CHL	CHD-C1D-ND	-4.19	120.60	124.45
31	c1	515	BCR	C33-C5-C6	-4.19	119.83	124.53
45	h1	101	RRX	C34-C9-C8	4.18	124.67	118.08
40	D	410	LHG	O7-C7-C8	4.18	120.52	111.50
29	a	406	CLA	CHD-C1D-ND	-4.18	120.61	124.45
51	R1	622	NEX	C31-C30-C29	4.18	133.28	127.31
51	G1	623	NEX	C38-C25-C24	4.18	118.98	114.28
29	R	608	CLA	C2C-C1C-NC	4.18	113.89	109.97
45	H1	101	RRX	C11-C10-C9	-4.18	121.35	127.31
29	b1	604	CLA	CMA-C3A-C4A	4.17	122.99	111.77
29	C1	504	CLA	C1-C2-C3	-4.17	118.83	126.04
47	i1	101	4RF	O21-C22-C24	4.17	120.49	111.50
50	y1	622	XAT	C18-C5-C4	4.17	118.97	114.28
49	Y	621	LUT	C35-C34-C33	-4.17	121.36	127.31
51	S1	623	NEX	C27-C28-C29	-4.17	119.06	125.53
29	B1	603	CLA	C1-C2-C3	-4.17	118.83	126.04
50	y1	622	XAT	C7-C8-C9	-4.17	119.07	125.53
39	j1	101	DGA	OG2-CB1-CB2	4.16	120.47	111.50
48	N	601	CHL	CHD-C1D-ND	-4.16	120.63	124.45
49	r1	620	LUT	C15-C14-C13	-4.16	121.37	127.31
50	r1	621	XAT	C32-C33-C34	4.15	125.31	118.94
51	G	623	NEX	C17-C1-C6	-4.15	106.76	110.47
29	c1	505	CLA	C1-C2-C3	-4.15	118.86	126.04
29	r	610	CLA	C1-C2-C3	-4.15	118.86	126.04
36	B	620	C7Z	C31-C30-C29	-4.15	121.39	127.31
29	C1	508	CLA	O2D-CGD-CBD	4.14	118.63	111.27
29	Y1	608	CLA	C1-C2-C3	-4.14	120.05	126.75
51	y1	623	NEX	O24-C25-C24	-4.14	110.27	113.38
36	B	620	C7Z	C7-C8-C9	-4.14	119.98	126.23
49	y1	620	LUT	C21-C26-C25	4.14	118.84	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	r	620	LUT	C35-C34-C33	-4.14	121.40	127.31
40	d1	409	LHG	O7-C7-C8	4.13	120.41	111.50
29	s1	613	CLA	O2D-CGD-CBD	4.13	118.61	111.27
48	g	609	CHL	CHD-C1D-ND	-4.13	120.66	124.45
49	G1	621	LUT	C35-C34-C33	-4.13	121.42	127.31
48	g	605	CHL	CHD-C1D-ND	-4.12	120.66	124.45
29	R1	603	CLA	O2D-CGD-CBD	4.12	118.59	111.27
29	C1	511	CLA	O2D-CGD-CBD	4.12	118.59	111.27
29	c	507	CLA	C2C-C1C-NC	4.11	113.83	109.97
50	R1	621	XAT	C18-C5-C4	4.11	118.91	114.28
53	R	626	ERG	C2-C3-C4	4.11	115.94	110.31
29	B1	610	CLA	O2A-C1-C2	4.11	119.42	108.64
48	N	605	CHL	CHD-C1D-ND	-4.10	120.68	124.45
50	r1	621	XAT	C18-C5-C4	4.10	118.90	114.28
29	G1	612	CLA	CMD-C2D-C1D	4.10	131.94	124.71
29	C1	513	CLA	O2A-C1-C2	4.10	119.41	108.64
48	N1	605	CHL	CHD-C1D-ND	-4.10	120.69	124.45
51	G1	623	NEX	C39-C29-C30	-4.10	117.19	122.92
48	n1	609	CHL	CHD-C1D-ND	-4.10	120.69	124.45
48	R1	607	CHL	C2C-C3C-C4C	4.09	109.41	106.49
45	h1	101	RRX	C7-C6-C5	-4.09	111.55	121.46
50	r	621	XAT	C15-C14-C13	-4.09	121.47	127.31
31	c	516	BCR	C33-C5-C6	-4.09	119.93	124.53
31	C1	515	BCR	C33-C5-C6	-4.09	119.93	124.53
50	Y	622	XAT	C18-C5-C4	4.08	118.87	114.28
48	g1	605	CHL	CHD-C1D-ND	-4.08	120.70	124.45
29	c	513	CLA	CAA-C2A-C3A	-4.07	101.62	112.78
30	a	408	PHO	C2B-C1B-NB	-4.07	106.72	109.53
31	B1	619	BCR	C33-C5-C6	-4.07	119.96	124.53
29	n1	604	CLA	C1-C2-C3	-4.07	119.01	126.04
39	J	101	DGA	OG2-CB1-CB2	4.06	120.26	111.50
50	y1	622	XAT	C19-C9-C10	-4.06	117.23	122.92
33	h1	102	LMG	O7-C10-C11	4.05	120.24	111.50
29	g1	611	CLA	CMD-C2D-C1D	4.05	131.86	124.71
37	c1	518	DGD	O2G-C1B-C2B	4.05	120.23	111.50
29	B	614	CLA	C2D-C1D-ND	4.05	113.09	110.10
50	Y1	622	XAT	C18-C5-C4	4.05	118.84	114.28
49	G1	621	LUT	C31-C30-C29	-4.05	121.53	127.31
29	n	610	CLA	CAA-C2A-C3A	-4.05	101.69	112.78
38	t1	101	3PH	O21-C21-C22	4.05	120.23	111.50
29	a1	406	CLA	C1-C2-C3	-4.05	119.04	126.04
49	n	621	LUT	C21-C26-C27	4.05	117.82	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	b1	624	3PH	O21-C21-C22	4.05	120.23	111.50
53	R	626	ERG	C7-C6-C5	-4.05	116.10	123.20
51	S1	623	NEX	C38-C25-C24	4.05	118.83	114.28
29	a1	405	CLA	CHD-C1D-ND	-4.05	120.73	124.45
29	n1	602	CLA	CHD-C1D-ND	-4.05	120.74	124.45
33	c	521	LMG	O7-C10-C11	4.04	120.22	111.50
45	H1	101	RRX	C30-C25-C26	-4.04	116.92	122.61
49	R1	620	LUT	C35-C34-C33	-4.04	121.54	127.31
32	m1	101	SQD	O7-S-C6	-4.04	102.13	106.94
50	r	621	XAT	O24-C25-C24	4.04	116.42	113.38
29	G1	602	CLA	C2C-C1C-NC	4.04	113.76	109.97
33	A1	413	LMG	O7-C10-C11	4.04	120.21	111.50
33	c1	521	LMG	O7-C10-C11	4.04	120.21	111.50
37	C	519	DGD	O2G-C1B-C2B	4.04	120.20	111.50
37	c	518	DGD	O2G-C1B-C2B	4.04	120.20	111.50
49	R	620	LUT	C21-C26-C25	4.04	118.65	111.42
45	H1	101	RRX	C21-C20-C19	-4.04	110.62	123.22
50	R1	621	XAT	C15-C14-C13	-4.04	121.55	127.31
49	R1	620	LUT	C11-C10-C9	-4.03	121.55	127.31
40	s1	624	LHG	O7-C7-C8	4.03	120.19	111.50
29	n1	610	CLA	CMD-C2D-C1D	4.03	131.81	124.71
29	B1	609	CLA	CMD-C2D-C1D	4.03	131.81	124.71
51	G	623	NEX	C38-C25-C24	4.03	118.81	114.28
49	Y1	621	LUT	C11-C10-C9	-4.03	121.56	127.31
51	r	622	NEX	C38-C25-C24	4.03	118.81	114.28
40	d	410	LHG	O7-C7-C8	4.03	120.18	111.50
53	r	626	ERG	C7-C6-C5	-4.02	116.14	123.20
49	g1	621	LUT	C31-C30-C29	-4.02	121.57	127.31
49	S1	620	LUT	C21-C26-C25	4.02	118.62	111.42
49	r1	620	LUT	C31-C30-C29	-4.02	121.57	127.31
45	H1	101	RRX	C7-C8-C9	-4.02	120.17	126.23
48	Y	609	CHL	C4B-CHC-C1C	4.02	135.87	126.34
49	n	620	LUT	C11-C10-C9	-4.01	121.59	127.31
29	b	610	CLA	O2A-C1-C2	4.01	119.17	108.64
29	A1	407	CLA	C2C-C1C-NC	4.01	113.73	109.97
29	c	509	CLA	O2A-C1-C2	4.01	119.17	108.64
29	B1	602	CLA	C2C-C1C-NC	4.01	113.73	109.97
48	y	605	CHL	CHD-C1D-ND	-4.01	120.77	124.45
51	r1	622	NEX	C38-C25-C24	4.01	118.79	114.28
39	c	524	DGA	OG2-CB1-CB2	4.01	120.14	111.50
39	b1	625	DGA	OG2-CB1-CB2	4.01	120.13	111.50
29	N1	612	CLA	C2C-C1C-NC	4.01	113.72	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	408	PHO	C2B-C1B-NB	-4.00	106.76	109.53
50	n	622	XAT	C6-C7-C8	-4.00	117.53	125.99
32	c	526	SQD	O7-S-C6	-4.00	102.18	106.94
31	b1	618	BCR	C27-C26-C25	-4.00	116.92	122.73
29	b	617	CLA	CMD-C2D-C1D	3.99	131.75	124.71
48	n	601	CHL	C2C-C3C-C4C	3.99	109.33	106.49
29	c	501	CLA	CHD-C1D-ND	-3.99	120.79	124.45
38	T	101	3PH	O21-C21-C22	3.99	120.10	111.50
39	c1	524	DGA	OG2-CB1-CB2	3.99	120.09	111.50
50	r	621	XAT	C6-C7-C8	-3.98	117.57	125.99
45	H	101	RRX	C15-C14-C13	-3.98	121.62	127.31
29	G1	611	CLA	C1-C2-C3	-3.98	119.15	126.04
48	S1	607	CHL	CHD-C1D-ND	-3.98	120.79	124.45
31	c1	517	BCR	C36-C18-C17	-3.98	117.35	122.92
29	R1	612	CLA	C2C-C1C-NC	3.98	113.70	109.97
49	S	621	LUT	C22-C23-C24	-3.98	107.21	111.74
29	R	610	CLA	C4B-CHC-C1C	3.98	135.77	126.34
29	C	508	CLA	C1-C2-C3	-3.98	119.16	126.04
50	R1	621	XAT	C7-C8-C9	-3.97	119.37	125.53
48	r	607	CHL	CHD-C1D-ND	-3.97	120.81	124.45
31	c1	517	BCR	C19-C18-C17	3.97	125.03	118.94
50	y1	622	XAT	C38-C25-C24	3.97	118.74	114.28
37	C1	519	DGD	O2G-C1B-C2B	3.96	120.03	111.50
49	s1	621	LUT	C7-C8-C9	-3.96	120.25	126.23
50	G1	622	XAT	C27-C28-C29	3.96	131.67	125.53
40	D1	410	LHG	O7-C7-C8	3.95	120.02	111.50
36	b1	620	C7Z	C22-C23-C24	3.95	115.72	110.30
29	D1	402	CLA	C1-C2-C3	-3.95	119.21	126.04
51	r	622	NEX	C2-C1-C6	3.95	113.05	109.21
48	G1	601	CHL	CHD-C1D-ND	-3.95	120.83	124.45
29	S	603	CLA	O2D-CGD-CBD	3.95	118.28	111.27
33	H	102	LMG	O7-C10-C11	3.95	120.01	111.50
29	G1	613	CLA	CMA-C3A-C4A	3.94	122.37	111.77
49	n	620	LUT	C31-C30-C29	-3.94	121.69	127.31
48	G	606	CHL	CHD-C1D-ND	-3.94	120.83	124.45
49	y	620	LUT	C35-C34-C33	-3.94	121.69	127.31
29	B1	615	CLA	O2A-C1-C2	3.94	118.99	108.64
29	s	617	CLA	CMA-C3A-C4A	3.94	122.36	111.77
50	y	622	XAT	C38-C25-C24	3.94	118.71	114.28
47	I	102	4RF	O21-C22-C24	3.93	119.98	111.50
48	g1	601	CHL	CHD-C1D-ND	-3.93	120.84	124.45
48	Y	609	CHL	C4D-CHA-C1A	3.93	126.03	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	B1	620	C7Z	C1-C6-C5	-3.93	117.08	122.61
51	Y1	623	NEX	C31-C30-C29	3.93	132.92	127.31
48	g	609	CHL	C1-O2A-CGA	3.93	126.75	116.44
37	c	520	DGD	O2G-C1B-C2B	3.93	119.97	111.50
29	R	609	CLA	CMA-C3A-C4A	3.93	122.33	111.77
33	b1	622	LMG	O7-C10-C11	3.92	119.96	111.50
29	Y	602	CLA	C2C-C1C-NC	3.92	113.64	109.97
51	Y	623	NEX	C17-C1-C6	-3.92	106.97	110.47
37	c1	519	DGD	O2G-C1B-C2B	3.92	119.94	111.50
29	s1	612	CLA	CMD-C2D-C1D	3.91	131.61	124.71
50	Y1	622	XAT	O24-C25-C38	-3.91	110.37	115.06
29	A	406	CLA	C2C-C1C-NC	3.91	113.64	109.97
31	C1	515	BCR	C23-C24-C25	-3.91	116.22	127.20
29	A1	406	CLA	O2A-C1-C2	3.91	118.90	108.64
40	G1	624	LHG	O7-C7-C8	3.91	119.92	111.50
29	A1	406	CLA	C2C-C1C-NC	3.91	113.63	109.97
29	r1	602	CLA	C1-C2-C3	-3.90	119.29	126.04
40	S	624	LHG	O7-C7-C8	3.90	119.92	111.50
29	C	507	CLA	C2C-C1C-NC	3.90	113.63	109.97
50	r	621	XAT	C31-C30-C29	-3.90	121.74	127.31
29	C1	513	CLA	CAA-C2A-C3A	-3.90	102.11	112.78
48	s	608	CHL	CHD-C1D-ND	-3.89	120.88	124.45
31	A1	411	BCR	C33-C5-C6	-3.89	120.16	124.53
29	Y	608	CLA	C1-C2-C3	-3.89	120.46	126.75
49	S1	621	LUT	C18-C5-C6	-3.89	120.16	124.53
29	C	508	CLA	CHD-C1D-ND	-3.89	120.88	124.45
49	y1	620	LUT	C11-C10-C9	-3.89	121.76	127.31
48	g	605	CHL	C2C-C3C-C4C	3.89	109.26	106.49
29	b1	613	CLA	C2C-C1C-NC	3.88	113.61	109.97
39	j	101	DGA	OG2-CB1-CB2	3.88	119.87	111.50
29	G1	603	CLA	O2D-CGD-CBD	3.88	118.17	111.27
48	N1	609	CHL	C4B-CHC-C1C	3.88	135.54	126.34
31	C	515	BCR	C33-C5-C4	3.88	121.07	113.62
31	C1	516	BCR	C27-C26-C25	-3.88	117.10	122.73
39	C	524	DGA	OG2-CB1-CB2	3.88	119.86	111.50
29	b1	615	CLA	OBD-CAD-C3D	-3.88	119.19	128.52
49	G	621	LUT	C11-C10-C9	-3.88	121.78	127.31
49	n	620	LUT	C7-C8-C9	-3.87	120.38	126.23
29	B	612	CLA	C1-C2-C3	-3.87	119.34	126.04
29	b1	617	CLA	C2C-C1C-NC	3.87	113.60	109.97
37	c	519	DGD	O2G-C1B-C2B	3.87	119.85	111.50
29	b	613	CLA	O2A-C1-C2	3.87	118.81	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S1	621	LUT	C22-C23-C24	-3.87	107.33	111.74
40	N	624	LHG	O7-C7-C8	3.87	119.84	111.50
48	n	601	CHL	C3C-C4C-NC	-3.87	106.23	110.57
49	S	621	LUT	C35-C34-C33	-3.87	121.79	127.31
29	A1	410	CLA	O2A-C1-C2	3.87	118.80	108.64
29	g1	610	CLA	C1-C2-C3	-3.87	119.36	126.04
48	N1	606	CHL	C3B-C4B-NB	-3.87	106.93	110.52
47	k1	101	4RF	O21-C22-C24	3.87	119.83	111.50
29	b1	604	CLA	C1-C2-C3	-3.87	119.36	126.04
49	s	620	LUT	C22-C23-C24	-3.86	107.34	111.74
29	S	602	CLA	C2C-C1C-NC	3.86	113.59	109.97
48	g	605	CHL	C3C-C4C-NC	-3.86	106.24	110.57
48	Y	607	CHL	C4A-NA-C1A	3.86	108.44	106.71
29	n	602	CLA	C1-C2-C3	-3.86	119.37	126.04
48	g1	605	CHL	C2C-C3C-C4C	3.86	109.24	106.49
32	b	621	SQD	O7-S-C6	-3.86	102.35	106.94
50	n	622	XAT	C38-C25-C24	3.86	118.62	114.28
29	S	603	CLA	CMA-C3A-C4A	3.85	122.13	111.77
48	n	609	CHL	CHD-C1D-ND	-3.85	120.91	124.45
40	C1	525	LHG	O7-C7-C8	3.85	119.80	111.50
49	n1	621	LUT	C11-C10-C9	-3.85	121.81	127.31
50	G	622	XAT	C19-C9-C10	-3.85	117.53	122.92
49	n	620	LUT	C35-C34-C33	-3.85	121.81	127.31
32	c1	526	SQD	O7-S-C6	-3.85	102.36	106.94
51	Y1	623	NEX	C20-C13-C14	-3.85	117.53	122.92
33	C	523	LMG	O7-C10-C11	3.85	119.79	111.50
49	g1	620	LUT	C18-C5-C6	-3.85	120.21	124.53
29	c1	502	CLA	C2C-C1C-NC	3.85	113.58	109.97
29	b1	612	CLA	O2D-CGD-O1D	-3.84	116.32	123.84
37	C1	520	DGD	O2G-C1B-C2B	3.84	119.78	111.50
48	G1	601	CHL	C3C-C4C-NC	-3.84	106.26	110.57
29	c1	504	CLA	C2C-C1C-NC	3.84	113.57	109.97
29	y	608	CLA	C1-C2-C3	-3.84	120.54	126.75
40	D1	409	LHG	O7-C7-C8	3.84	119.78	111.50
49	Y	621	LUT	C15-C14-C13	-3.84	121.83	127.31
29	c	502	CLA	C1-C2-C3	-3.84	119.40	126.04
51	N	623	NEX	C27-C28-C29	-3.84	119.57	125.53
29	y	614	CLA	CHD-C1D-ND	-3.84	120.93	124.45
30	a	409	PHO	CMB-C2B-C3B	3.83	131.85	124.68
50	N1	622	XAT	C40-C33-C34	-3.83	117.56	122.92
50	G1	622	XAT	C7-C8-C9	-3.83	119.59	125.53
29	g1	610	CLA	CHD-C1D-ND	-3.83	120.94	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	N	601	CHL	C1-C2-C3	-3.83	119.42	126.04
29	N1	604	CLA	C2C-C1C-NC	3.83	113.56	109.97
31	c1	516	BCR	C33-C5-C6	-3.83	120.23	124.53
48	S	608	CHL	CHD-C1D-ND	-3.83	120.94	124.45
31	B1	618	BCR	C36-C18-C17	-3.83	117.56	122.92
50	Y	622	XAT	C36-C21-C26	3.82	120.37	110.05
29	S1	610	CLA	CHD-C1D-ND	-3.82	120.94	124.45
51	s	623	NEX	O24-C25-C24	-3.82	110.51	113.38
29	S	605	CLA	C2C-C1C-NC	3.82	113.55	109.97
29	c	504	CLA	C1-C2-C3	-3.82	119.44	126.04
50	r1	621	XAT	C31-C30-C29	-3.82	121.86	127.31
48	Y1	601	CHL	CHD-C1D-ND	-3.82	120.95	124.45
29	c1	513	CLA	C2D-C1D-ND	3.82	112.92	110.10
31	B	618	BCR	C23-C24-C25	-3.82	116.48	127.20
29	c	512	CLA	CMD-C2D-C1D	3.82	131.44	124.71
29	C	513	CLA	CAA-C2A-C3A	-3.81	102.34	112.78
31	b1	618	BCR	C4-C5-C6	-3.81	117.20	122.73
31	d1	404	BCR	C8-C9-C10	3.81	124.79	118.94
29	A	407	CLA	C2C-C1C-NC	3.81	113.54	109.97
36	B	620	C7Z	C15-C14-C13	-3.81	121.87	127.31
48	g	607	CHL	CHD-C1D-ND	-3.81	120.95	124.45
31	D1	404	BCR	C35-C13-C14	-3.81	117.59	122.92
53	R1	626	ERG	C18-C13-C12	-3.81	104.58	110.59
40	c1	525	LHG	O7-C7-C8	3.81	119.70	111.50
48	n	606	CHL	C1-C2-C3	-3.81	119.46	126.04
40	g	624	LHG	O7-C7-C8	3.80	119.70	111.50
29	a1	407	CLA	C2D-C1D-ND	3.80	112.91	110.10
36	B	620	C7Z	C1-C6-C5	-3.80	117.26	122.61
43	d1	405	PL9	C7-C3-C2	-3.80	118.30	123.30
29	c	506	CLA	CHD-C1D-ND	-3.80	120.97	124.45
50	N1	622	XAT	C6-C7-C8	-3.79	117.97	125.99
50	n	622	XAT	C7-C8-C9	-3.79	119.65	125.53
29	a1	410	CLA	C2C-C1C-NC	3.79	113.52	109.97
29	Y1	608	CLA	O2A-C1-C2	3.79	118.59	108.64
48	r1	607	CHL	C2C-C3C-C4C	3.79	109.19	106.49
38	T1	101	3PH	O21-C21-C22	3.79	119.66	111.50
48	N1	609	CHL	CHB-C1B-NB	-3.79	120.25	124.26
45	H	101	RRX	C2-C1-C6	3.79	116.31	110.48
48	N1	608	CHL	CHD-C1D-ND	-3.78	120.98	124.45
29	Y1	602	CLA	C2C-C1C-NC	3.78	113.52	109.97
30	A	408	PHO	CMB-C2B-C3B	3.78	131.76	124.68
55	Y1	626	PTY	O7-C8-C11	3.78	119.65	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S	620	LUT	C2-C3-C4	-3.78	105.13	110.30
48	N1	605	CHL	C1-C2-C3	-3.78	119.50	126.04
40	D	409	LHG	O7-C7-C8	3.78	119.65	111.50
47	i	101	4RF	O21-C22-C24	3.78	119.65	111.50
36	B	620	C7Z	C35-C15-C14	-3.78	115.73	123.47
48	y	609	CHL	CHD-C1D-ND	-3.78	120.98	124.45
29	c	508	CLA	CHD-C1D-ND	-3.77	120.99	124.45
48	s1	601	CHL	C4B-CHC-C1C	3.77	135.28	126.34
29	B	616	CLA	C2D-C1D-ND	3.77	112.88	110.10
51	n1	623	NEX	C19-C9-C10	-3.77	117.64	122.92
29	b	614	CLA	CHD-C1D-ND	-3.77	120.99	124.45
51	n1	623	NEX	C39-C29-C30	-3.77	117.65	122.92
50	y1	622	XAT	C36-C21-C26	3.76	120.21	110.05
30	a1	408	PHO	C2B-C1B-NB	-3.76	106.93	109.53
48	y	601	CHL	CHD-C1D-ND	-3.76	121.00	124.45
49	G1	620	LUT	C15-C14-C13	-3.76	121.94	127.31
48	y1	607	CHL	CHD-C1D-ND	-3.76	121.00	124.45
32	a1	412	SQD	O7-S-C6	-3.76	102.47	106.94
51	R1	622	NEX	C27-C28-C29	-3.76	119.69	125.53
48	g	601	CHL	CHD-C1D-ND	-3.76	121.00	124.45
29	a	405	CLA	CHD-C1D-ND	-3.76	121.00	124.45
51	s	623	NEX	C27-C28-C29	-3.76	119.70	125.53
36	B1	620	C7Z	C27-C28-C29	-3.76	120.56	126.23
47	I1	102	4RF	O21-C22-C24	3.76	119.60	111.50
53	r1	626	ERG	C2-C1-C10	3.76	120.88	112.74
29	c	504	CLA	CHD-C1D-ND	-3.76	121.00	124.45
32	B	621	SQD	O7-S-C6	-3.76	102.48	106.94
29	B1	609	CLA	C1-C2-C3	-3.75	119.55	126.04
29	C1	509	CLA	C2C-C1C-NC	3.75	113.49	109.97
48	N	601	CHL	C3C-C4C-NC	-3.75	106.37	110.57
49	y	620	LUT	C15-C14-C13	-3.75	121.96	127.31
29	b1	605	CLA	C1-C2-C3	-3.75	119.56	126.04
50	g	622	XAT	C26-C27-C28	-3.75	118.07	125.99
48	S	606	CHL	CHD-C1D-ND	-3.75	121.01	124.45
48	r1	607	CHL	C3C-C4C-NC	-3.74	106.37	110.57
29	s1	604	CLA	C1-C2-C3	-3.74	119.57	126.04
29	s1	609	CLA	C2D-C1D-ND	3.74	112.86	110.10
29	g	610	CLA	CHD-C1D-ND	-3.74	121.02	124.45
51	y	623	NEX	C27-C28-C29	-3.74	119.72	125.53
29	y	603	CLA	C2C-C1C-NC	3.74	113.48	109.97
55	y1	626	PTY	O7-C8-C11	3.74	119.56	111.50
51	y1	623	NEX	C5-C4-C3	3.74	116.17	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	611	CLA	C2C-C1C-NC	3.74	113.47	109.97
37	C	520	DGD	O2G-C1B-C2B	3.74	119.56	111.50
48	Y	601	CHL	CHD-C1D-ND	-3.73	121.02	124.45
48	n1	605	CHL	C2C-C3C-C4C	3.73	109.15	106.49
37	C1	518	DGD	O2G-C1B-C2B	3.73	119.55	111.50
53	r1	626	ERG	C18-C13-C14	-3.73	104.19	110.24
29	s	617	CLA	C1-C2-C3	-3.73	120.71	126.75
48	N	608	CHL	CHD-C1D-ND	-3.73	121.03	124.45
49	g	620	LUT	C7-C8-C9	-3.73	120.60	126.23
49	S1	621	LUT	C1-C6-C5	-3.73	117.36	122.61
29	N	604	CLA	C1-C2-C3	-3.73	119.59	126.04
29	B	606	CLA	C1-C2-C3	-3.73	119.60	126.04
29	B	605	CLA	C1-C2-C3	-3.73	119.60	126.04
29	C1	506	CLA	C2C-C1C-NC	3.73	113.46	109.97
48	n1	601	CHL	C2C-C3C-C4C	3.72	109.14	106.49
44	F1	101	HEM	CAD-CBD-CGD	-3.72	105.60	113.60
48	n1	605	CHL	C3C-C4C-NC	-3.72	106.40	110.57
48	s1	608	CHL	C3B-C4B-NB	-3.72	107.07	110.52
49	N1	621	LUT	C38-C25-C24	-3.72	115.61	123.56
30	A1	409	PHO	C4A-C3A-C2A	-3.72	99.30	102.84
32	C	526	SQD	O7-S-C6	-3.71	102.53	106.94
33	d1	411	LMG	O7-C10-C11	3.71	119.50	111.50
32	M	101	SQD	O7-S-C6	-3.71	102.53	106.94
36	B	620	C7Z	C2-C3-C4	3.71	115.38	110.30
50	Y	622	XAT	C38-C25-C26	-3.71	116.05	122.26
36	B	620	C7Z	C22-C23-C24	3.71	115.38	110.30
49	s	621	LUT	C22-C23-C24	-3.71	107.52	111.74
49	g	620	LUT	C22-C23-C24	-3.70	107.53	111.74
53	R	626	ERG	C16-C17-C13	3.70	108.31	103.84
29	A	406	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
29	y1	602	CLA	C2D-C1D-ND	3.70	112.83	110.10
48	n	601	CHL	CHD-C1D-ND	-3.70	121.05	124.45
48	g1	608	CHL	CHD-C1D-ND	-3.70	121.05	124.45
49	R1	620	LUT	C15-C14-C13	-3.70	122.03	127.31
49	r1	620	LUT	C18-C5-C6	-3.70	120.37	124.53
29	N	602	CLA	C2D-C1D-ND	3.70	112.83	110.10
29	c	510	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
51	g	623	NEX	C5-C6-C1	3.70	123.37	119.70
51	G	623	NEX	C27-C28-C29	-3.70	119.79	125.53
29	n	613	CLA	CBA-CAA-C2A	3.70	124.78	113.86
49	s1	620	LUT	C11-C10-C9	-3.70	122.03	127.31
51	n1	623	NEX	C31-C30-C29	3.69	132.58	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s1	605	CLA	C2C-C1C-NC	3.69	113.43	109.97
49	r1	620	LUT	C21-C26-C25	3.69	118.03	111.42
50	r1	621	XAT	C15-C14-C13	-3.69	122.04	127.31
48	g1	607	CHL	C1-C2-C3	-3.69	119.67	126.04
32	a	412	SQD	O7-S-C6	-3.69	102.56	106.94
48	N	601	CHL	C2C-C3C-C4C	3.69	109.12	106.49
55	Y	626	PTY	O7-C8-C11	3.68	119.44	111.50
49	N1	620	LUT	C15-C14-C13	-3.68	122.05	127.31
51	N1	623	NEX	C38-C25-C24	3.68	118.42	114.28
29	N	614	CLA	C2C-C1C-NC	3.68	113.42	109.97
29	c	510	CLA	C1-C2-C3	-3.68	119.67	126.04
29	g	611	CLA	C2C-C1C-NC	3.68	113.42	109.97
49	s1	620	LUT	C1-C6-C5	-3.68	117.43	122.61
48	R	606	CHL	CHD-C1D-ND	-3.68	121.07	124.45
48	s	601	CHL	C3C-C4C-NC	-3.68	106.45	110.57
48	n1	609	CHL	CMA-C3A-C4A	3.68	121.66	111.77
48	R1	607	CHL	C2B-C1B-NB	-3.68	107.77	110.23
32	b1	626	SQD	O7-S-C6	-3.68	102.57	106.94
29	S	613	CLA	C2C-C1C-NC	3.68	113.42	109.97
29	B	611	CLA	C2C-C1C-NC	3.67	113.41	109.97
29	g1	602	CLA	CMA-C3A-C4A	3.67	121.64	111.77
29	n	614	CLA	CHD-C1D-ND	-3.67	121.08	124.45
51	y1	623	NEX	C2-C1-C6	3.67	112.78	109.21
48	y1	609	CHL	CHD-C4C-C3C	3.67	130.24	124.84
33	B1	622	LMG	O7-C10-C11	3.67	119.41	111.50
48	y	609	CHL	C2C-C3C-C4C	3.67	109.10	106.49
29	b	614	CLA	C1-C2-C3	-3.66	119.70	126.04
29	B	609	CLA	C1-C2-C3	-3.66	119.71	126.04
29	s	610	CLA	C1-C2-C3	-3.66	119.71	126.04
29	C1	511	CLA	C2C-C1C-NC	3.66	113.40	109.97
51	n1	623	NEX	C38-C25-C24	3.66	118.40	114.28
31	b1	618	BCR	C33-C5-C4	3.66	120.65	113.62
32	B1	626	SQD	O7-S-C6	-3.66	102.59	106.94
48	N1	608	CHL	C3C-C4C-NC	-3.66	106.47	110.57
29	c1	508	CLA	C1-C2-C3	-3.66	119.71	126.04
45	H1	101	RRX	C1-C6-C5	-3.66	117.46	122.61
53	r1	626	ERG	C7-C6-C5	-3.66	116.78	123.20
51	g	623	NEX	O24-C25-C38	-3.66	110.67	115.06
29	G	613	CLA	C1-C2-C3	-3.66	119.72	126.04
29	r	609	CLA	CHD-C1D-ND	-3.66	121.09	124.45
48	Y	601	CHL	C1-C2-C3	-3.65	119.72	126.04
48	G1	608	CHL	CHD-C1D-ND	-3.65	121.10	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	g1	606	CHL	C2B-C1B-NB	-3.65	107.78	110.23
33	c1	523	LMG	O7-C10-C11	3.65	119.37	111.50
31	a1	411	BCR	C33-C5-C4	3.65	120.63	113.62
29	s1	617	CLA	C1-C2-C3	-3.65	120.85	126.75
48	S	601	CHL	CHD-C1D-ND	-3.65	121.10	124.45
29	n1	603	CLA	C2C-C1C-NC	3.65	113.39	109.97
48	N	609	CHL	CMA-C3A-C4A	3.65	121.58	111.77
48	y1	607	CHL	C4A-NA-C1A	3.65	108.34	106.71
48	G	607	CHL	CHD-C1D-ND	-3.64	121.11	124.45
51	g	623	NEX	C27-C28-C29	-3.64	119.88	125.53
29	n	602	CLA	C2C-C1C-NC	3.64	113.38	109.97
29	Y1	613	CLA	CMA-C3A-C4A	3.64	121.55	111.77
50	g	622	XAT	C6-C7-C8	-3.64	118.30	125.99
48	n1	607	CHL	CMA-C3A-C4A	3.63	121.53	111.77
48	G1	601	CHL	C2C-C3C-C4C	3.63	109.08	106.49
29	G1	612	CLA	C2D-C1D-ND	3.63	112.78	110.10
29	y	610	CLA	CHD-C1D-ND	-3.63	121.12	124.45
48	n1	606	CHL	C3B-C4B-NB	-3.63	107.15	110.52
32	A1	412	SQD	O7-S-C6	-3.63	102.63	106.94
48	N	606	CHL	C3B-C4B-NB	-3.63	107.15	110.52
53	r	626	ERG	C1-C10-C5	3.63	115.39	108.75
29	c1	511	CLA	C2C-C1C-NC	3.63	113.37	109.97
40	y1	624	LHG	O7-C7-C8	3.62	119.31	111.50
48	S	607	CHL	C2C-C3C-C4C	3.62	109.07	106.49
48	n	607	CHL	CHD-C1D-ND	-3.62	121.13	124.45
32	M1	101	SQD	O7-S-C6	-3.62	102.64	106.94
29	a	407	CLA	C2C-C1C-NC	3.62	113.36	109.97
48	g1	605	CHL	C3C-C4C-NC	-3.62	106.51	110.57
32	A	412	SQD	O7-S-C6	-3.62	102.64	106.94
48	S1	608	CHL	C4A-NA-C1A	3.62	108.33	106.71
49	n	621	LUT	C22-C23-C24	-3.62	107.62	111.74
37	C	518	DGD	O2G-C1B-C2B	3.61	119.29	111.50
43	d	405	PL9	C7-C3-C2	-3.61	118.55	123.30
32	m	101	SQD	O7-S-C6	-3.61	102.65	106.94
48	s	606	CHL	C3C-C4C-NC	-3.61	106.52	110.57
29	B1	609	CLA	C2C-C1C-NC	3.61	113.35	109.97
31	c	515	BCR	C35-C13-C12	3.61	123.76	118.08
49	y	621	LUT	C15-C14-C13	-3.61	122.16	127.31
36	b	620	C7Z	C11-C12-C13	-3.61	116.28	126.42
31	c1	517	BCR	C33-C5-C6	-3.61	120.48	124.53
29	b1	606	CLA	C2C-C1C-NC	3.61	113.35	109.97
48	s	606	CHL	C2C-C3C-C4C	3.61	109.06	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	N1	611	CLA	C2C-C1C-NC	3.60	113.35	109.97
29	s	605	CLA	C2C-C1C-NC	3.60	113.35	109.97
29	g1	604	CLA	C2D-C1D-ND	3.60	112.76	110.10
51	G	623	NEX	C39-C29-C30	-3.60	117.88	122.92
48	N1	609	CHL	C3C-C4C-NC	-3.60	106.53	110.57
29	A1	406	CLA	C1-C2-C3	-3.60	119.82	126.04
29	C1	511	CLA	C1-C2-C3	-3.60	119.82	126.04
48	N1	608	CHL	C2C-C3C-C4C	3.60	109.05	106.49
29	n1	602	CLA	C2D-C1D-ND	3.59	112.75	110.10
51	R1	622	NEX	C38-C25-C26	-3.59	116.24	122.26
49	n1	621	LUT	C22-C23-C24	-3.59	107.65	111.74
29	y	612	CLA	C2D-C1D-ND	3.59	112.75	110.10
40	d1	410	LHG	O7-C7-C8	3.59	119.23	111.50
48	N1	601	CHL	C4B-CHC-C1C	3.59	134.84	126.34
40	d	409	LHG	O7-C7-C8	3.59	119.23	111.50
32	B	626	SQD	O7-S-C6	-3.58	102.68	106.94
29	B	615	CLA	OBD-CAD-C3D	-3.58	119.90	128.52
50	y1	622	XAT	C18-C5-C6	-3.58	116.26	122.26
31	B	618	BCR	C33-C5-C6	-3.58	120.50	124.53
51	g1	623	NEX	C39-C29-C30	-3.58	117.91	122.92
48	g	601	CHL	C2C-C3C-C4C	3.58	109.04	106.49
29	S	602	CLA	O2A-CGA-CBA	3.58	123.14	111.91
29	g	612	CLA	C2C-C1C-NC	3.58	113.33	109.97
50	y1	622	XAT	C38-C25-C26	-3.58	116.26	122.26
29	A1	410	CLA	CHD-C1D-ND	-3.58	121.17	124.45
29	D	402	CLA	C3B-C4B-NB	-3.58	107.20	110.52
29	D	402	CLA	C2D-C1D-ND	3.58	112.74	110.10
51	R	622	NEX	C27-C28-C29	-3.58	119.98	125.53
48	y	606	CHL	C3B-C4B-NB	-3.58	107.20	110.52
48	N1	609	CHL	CMA-C3A-C4A	3.58	121.38	111.77
29	s1	612	CLA	C2C-C1C-NC	3.57	113.32	109.97
48	R	607	CHL	C3C-C4C-NC	-3.57	106.56	110.57
31	A	411	BCR	C35-C13-C12	3.57	123.71	118.08
29	c1	509	CLA	O2A-C1-C2	3.57	118.02	108.64
29	s1	617	CLA	CHD-C1D-ND	-3.57	121.17	124.45
41	c1	527	LMK	O3-C4-C3	-3.57	110.73	122.98
29	b	606	CLA	C1-C2-C3	-3.57	119.87	126.04
29	c1	510	CLA	C1-C2-C3	-3.57	119.87	126.04
29	N1	603	CLA	C2C-C1C-NC	3.57	113.32	109.97
29	b	611	CLA	CHD-C1D-ND	-3.57	121.17	124.45
51	r1	622	NEX	C27-C28-C29	-3.57	119.99	125.53
29	A	406	CLA	C1-C2-C3	-3.57	119.87	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	n	609	CHL	C4D-CHA-C1A	3.57	125.59	121.25
45	h1	101	RRX	C15-C14-C13	-3.57	122.22	127.31
29	R	610	CLA	C2D-C1D-ND	3.56	112.73	110.10
29	D1	403	CLA	C1-C2-C3	-3.56	119.88	126.04
36	b1	620	C7Z	C11-C10-C9	-3.56	122.22	127.31
29	y	608	CLA	C2C-C1C-NC	3.56	113.31	109.97
48	y1	605	CHL	CHD-C1D-ND	-3.56	121.18	124.45
51	S	623	NEX	C5-C4-C3	3.56	115.96	111.75
31	D1	404	BCR	C36-C18-C17	-3.56	117.94	122.92
50	G1	622	XAT	C15-C14-C13	-3.56	122.23	127.31
50	G1	622	XAT	C38-C25-C24	3.56	118.28	114.28
29	b1	612	CLA	C2D-C1D-ND	3.56	112.73	110.10
29	N	611	CLA	C2C-C1C-NC	3.56	113.30	109.97
29	N1	610	CLA	C2D-C1D-ND	3.56	112.72	110.10
48	N1	609	CHL	CHD-C1D-ND	-3.55	121.19	124.45
29	d	403	CLA	CHD-C1D-ND	-3.55	121.19	124.45
48	n1	609	CHL	C4B-CHC-C1C	3.55	134.76	126.34
48	n	605	CHL	C3C-C4C-NC	-3.55	106.59	110.57
29	Y1	614	CLA	CMD-C2D-C3D	-3.55	119.45	127.61
31	B	619	BCR	C33-C5-C4	3.55	120.44	113.62
31	C	516	BCR	C36-C18-C17	-3.55	117.95	122.92
48	N1	605	CHL	C4B-CHC-C1C	3.55	134.75	126.34
31	C1	517	BCR	C37-C22-C21	-3.55	117.95	122.92
48	N1	601	CHL	CHD-C1D-ND	-3.55	121.19	124.45
29	C1	510	CLA	C2D-C1D-ND	3.55	112.72	110.10
48	s1	608	CHL	C1-O2A-CGA	3.55	125.75	116.44
29	b	614	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
31	B	618	BCR	C4-C5-C6	-3.55	117.58	122.73
31	C	515	BCR	C23-C24-C25	-3.55	117.24	127.20
32	B1	621	SQD	O7-S-C6	-3.54	102.73	106.94
29	A1	407	CLA	C1-C2-C3	-3.54	121.02	126.75
49	R	620	LUT	C18-C5-C6	-3.54	120.55	124.53
48	G1	609	CHL	CHD-C1D-ND	-3.54	121.20	124.45
29	G1	604	CLA	C2C-C1C-NC	3.54	113.29	109.97
51	S	623	NEX	C39-C29-C30	-3.54	117.96	122.92
48	N1	609	CHL	C4A-NA-C1A	3.54	108.30	106.71
50	g1	622	XAT	C18-C5-C4	3.54	118.27	114.28
30	A	409	PHO	CMB-C2B-C3B	3.54	131.31	124.68
40	D1	408	LHG	O7-C7-C8	3.54	119.13	111.50
48	S	607	CHL	C3C-C4C-NC	-3.54	106.60	110.57
29	C1	513	CLA	CHD-C1D-ND	-3.54	121.20	124.45
48	s	601	CHL	C3B-C4B-NB	-3.54	107.23	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y	611	CLA	CHD-C1D-ND	-3.54	121.20	124.45
29	Y1	611	CLA	CHD-C1D-ND	-3.53	121.21	124.45
49	S	620	LUT	C10-C11-C12	-3.53	112.19	123.22
29	r1	608	CLA	C2C-C1C-NC	3.53	113.28	109.97
48	y	607	CHL	CHD-C1D-ND	-3.53	121.21	124.45
29	s	613	CLA	CHD-C1D-ND	-3.53	121.21	124.45
29	y1	602	CLA	CHD-C1D-ND	-3.53	121.21	124.45
29	B1	612	CLA	C1-C2-C3	-3.53	119.94	126.04
29	N1	611	CLA	CHD-C1D-ND	-3.53	121.21	124.45
49	g1	620	LUT	C21-C26-C27	3.53	117.16	112.70
29	G1	603	CLA	C2D-C1D-ND	3.53	112.70	110.10
29	G1	613	CLA	C1-C2-C3	-3.53	119.94	126.04
48	R	606	CHL	C3B-C4B-NB	-3.53	107.24	110.52
29	b1	612	CLA	CMA-C3A-C4A	3.53	121.25	111.77
29	D1	402	CLA	C2D-C1D-ND	3.53	112.70	110.10
50	Y1	622	XAT	C26-C27-C28	-3.53	118.54	125.99
49	n1	621	LUT	C7-C8-C9	-3.53	120.91	126.23
48	r	607	CHL	C2C-C3C-C4C	3.53	109.00	106.49
48	Y1	606	CHL	C1-O2A-CGA	3.52	125.68	116.44
29	r	603	CLA	CMD-C2D-C1D	3.52	130.91	124.71
33	D1	411	LMG	O7-C10-C11	3.52	119.08	111.50
48	g	609	CHL	CMA-C3A-C4A	3.51	121.22	111.77
29	R	602	CLA	CMA-C3A-C4A	3.51	121.22	111.77
49	G	620	LUT	C15-C14-C13	-3.51	122.30	127.31
48	g1	607	CHL	C4A-NA-C1A	3.51	108.28	106.71
29	S1	611	CLA	C2C-C1C-NC	3.51	113.26	109.97
48	n1	607	CHL	C2C-C3C-C4C	3.51	108.99	106.49
29	c	508	CLA	C1-C2-C3	-3.51	119.98	126.04
29	n1	613	CLA	CBA-CAA-C2A	3.51	124.21	113.86
40	d	408	LHG	O7-C7-C8	3.50	119.05	111.50
29	g	611	CLA	CHD-C1D-ND	-3.50	121.24	124.45
29	N1	613	CLA	CHD-C1D-ND	-3.50	121.24	124.45
29	Y1	614	CLA	CHD-C1D-ND	-3.50	121.24	124.45
51	N1	623	NEX	C38-C25-C26	-3.50	116.40	122.26
29	C1	508	CLA	C1-C2-C3	-3.50	120.00	126.04
33	C1	523	LMG	O7-C10-C11	3.49	119.03	111.50
49	s1	621	LUT	C18-C5-C6	-3.49	120.61	124.53
53	r1	626	ERG	C14-C8-C7	-3.49	117.50	124.38
48	N	605	CHL	C3C-C4C-NC	-3.49	106.66	110.57
29	B	603	CLA	C1-C2-C3	-3.49	120.01	126.04
49	y1	620	LUT	C18-C5-C6	-3.49	120.61	124.53
29	A	407	CLA	CHD-C1D-ND	-3.49	121.25	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	y1	604	CLA	CHD-C1D-ND	-3.49	121.25	124.45
29	c	507	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
29	S	613	CLA	CMA-C3A-C4A	3.49	121.14	111.77
29	s	614	CLA	C1-C2-C3	-3.49	120.01	126.04
48	G	606	CHL	C3C-C4C-NC	-3.48	106.66	110.57
48	n	609	CHL	C4B-CHC-C1C	3.48	134.60	126.34
48	N1	609	CHL	C2C-C3C-C4C	3.48	108.97	106.49
48	n1	606	CHL	CHD-C1D-ND	-3.48	121.25	124.45
48	G	606	CHL	CMA-C3A-C4A	3.48	121.13	111.77
29	c1	511	CLA	CHD-C1D-ND	-3.48	121.25	124.45
29	S	602	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
31	C1	514	BCR	C19-C18-C17	3.48	124.28	118.94
49	S1	620	LUT	C35-C15-C14	-3.48	116.34	123.47
29	C1	503	CLA	CMA-C3A-C4A	3.48	121.13	111.77
45	H	101	RRX	C7-C8-C9	-3.48	120.98	126.23
29	S	604	CLA	CHD-C1D-ND	-3.48	121.26	124.45
29	G	610	CLA	C1-C2-C3	-3.48	120.03	126.04
29	D	403	CLA	CHD-C1D-ND	-3.48	121.26	124.45
48	N1	607	CHL	CHD-C1D-ND	-3.48	121.26	124.45
29	g	610	CLA	CAA-C2A-C3A	-3.48	103.26	112.78
29	C	509	CLA	C2C-C1C-NC	3.48	113.23	109.97
31	A	411	BCR	C12-C13-C14	-3.48	113.61	118.94
29	n1	611	CLA	C2C-C1C-NC	3.48	113.23	109.97
29	s	613	CLA	C2D-C1D-ND	3.48	112.67	110.10
31	C1	515	BCR	C34-C9-C10	-3.47	118.06	122.92
48	g1	606	CHL	C3B-C4B-NB	-3.47	107.30	110.52
29	S	613	CLA	C1-C2-C3	-3.47	120.04	126.04
31	C	517	BCR	C28-C27-C26	-3.47	107.88	114.08
48	G	601	CHL	C3C-C4C-NC	-3.47	106.68	110.57
45	h1	101	RRX	C4-C5-C6	-3.47	117.70	122.73
29	r	612	CLA	C2C-C1C-NC	3.47	113.22	109.97
29	g	613	CLA	C2D-C1D-ND	3.47	112.66	110.10
48	s	608	CHL	C3B-C4B-NB	-3.47	107.30	110.52
41	c	527	LMK	O3-C4-C3	-3.47	111.09	122.98
29	r1	610	CLA	C3B-C4B-NB	-3.46	107.30	110.52
49	R1	620	LUT	C18-C5-C6	-3.46	120.64	124.53
29	b1	616	CLA	C1-C2-C3	-3.46	120.05	126.04
31	B1	619	BCR	C33-C5-C4	3.46	120.27	113.62
49	S	620	LUT	C22-C23-C24	-3.46	107.80	111.74
45	h	101	RRX	C20-C21-C22	3.46	132.25	127.31
48	S1	607	CHL	C2C-C3C-C4C	3.46	108.95	106.49
29	C	501	CLA	CHD-C1D-ND	-3.46	121.28	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	s	601	CHL	CHD-C1D-ND	-3.45	121.28	124.45
29	s	617	CLA	C2C-C1C-NC	3.45	113.21	109.97
29	N1	603	CLA	CHD-C1D-ND	-3.45	121.28	124.45
48	r1	607	CHL	C4B-CHC-C1C	3.45	134.53	126.34
49	s	620	LUT	C15-C14-C13	-3.45	122.38	127.31
31	c	517	BCR	C3-C4-C5	-3.45	107.91	114.08
50	n1	622	XAT	C38-C25-C26	-3.45	116.48	122.26
29	B	606	CLA	CHD-C1D-ND	-3.45	121.28	124.45
29	y1	610	CLA	C1-C2-C3	-3.45	120.08	126.04
29	b	612	CLA	C1-C2-C3	-3.45	120.08	126.04
29	n	610	CLA	CHD-C1D-ND	-3.45	121.29	124.45
29	g1	613	CLA	CMA-C3A-C4A	3.45	121.04	111.77
29	g	603	CLA	C2C-C1C-NC	3.44	113.20	109.97
48	n	605	CHL	C3B-C4B-NB	-3.44	107.32	110.52
29	S	612	CLA	C2C-C1C-NC	3.44	113.20	109.97
48	G	609	CHL	CHD-C1D-ND	-3.44	121.29	124.45
29	b	610	CLA	C2D-C1D-ND	3.44	112.64	110.10
45	h1	101	RRX	C23-C22-C21	-3.44	113.66	118.94
29	y1	613	CLA	CHD-C1D-ND	-3.44	121.29	124.45
48	s	606	CHL	CHD-C1D-ND	-3.44	121.29	124.45
49	s	621	LUT	C10-C11-C12	-3.44	112.48	123.22
29	a	405	CLA	C2D-C1D-ND	3.44	112.64	110.10
29	r	603	CLA	C2D-C1D-ND	3.44	112.64	110.10
29	S1	617	CLA	CMA-C3A-C4A	3.44	121.02	111.77
29	c	501	CLA	C1-C2-C3	-3.44	120.09	126.04
29	B1	607	CLA	CHD-C1D-ND	-3.44	121.29	124.45
48	G1	608	CHL	C2C-C3C-C4C	3.44	108.94	106.49
29	b1	605	CLA	C2D-C1D-ND	3.44	112.64	110.10
48	G	601	CHL	CHB-C4A-NA	3.44	129.26	124.51
48	Y	605	CHL	C3C-C4C-NC	-3.44	106.72	110.57
48	y	606	CHL	CHD-C1D-ND	-3.44	121.30	124.45
29	C	508	CLA	CAC-C3C-C4C	3.43	129.27	124.81
48	g1	601	CHL	C2C-C3C-C4C	3.43	108.94	106.49
29	b1	603	CLA	C1-C2-C3	-3.43	120.10	126.04
48	n1	608	CHL	CMA-C3A-C4A	3.43	121.00	111.77
29	Y	610	CLA	C2D-C1D-ND	3.43	112.63	110.10
29	B	605	CLA	C2C-C1C-NC	3.43	113.19	109.97
29	Y1	604	CLA	C2C-C1C-NC	3.43	113.19	109.97
48	R1	607	CHL	C3C-C4C-NC	-3.43	106.72	110.57
49	Y1	620	LUT	C2-C3-C4	-3.43	105.61	110.30
29	G1	611	CLA	C2C-C1C-NC	3.43	113.19	109.97
29	b	615	CLA	C1-C2-C3	-3.43	120.11	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	g1	612	CLA	C2C-C1C-NC	3.43	113.19	109.97
31	d1	404	BCR	C4-C5-C6	-3.43	117.75	122.73
29	C	512	CLA	C2C-C1C-NC	3.43	113.19	109.97
29	G	612	CLA	C2C-C1C-NC	3.43	113.19	109.97
48	s1	608	CHL	C3C-C4C-NC	-3.43	106.73	110.57
48	y	605	CHL	C3C-C4C-NC	-3.43	106.73	110.57
29	c1	513	CLA	C1-C2-C3	-3.43	120.12	126.04
29	Y	612	CLA	C2D-C1D-ND	3.43	112.63	110.10
29	G1	603	CLA	CHD-C1D-ND	-3.43	121.31	124.45
48	r1	607	CHL	C4A-NA-C1A	3.43	108.25	106.71
29	G1	610	CLA	C2D-C1D-ND	3.42	112.63	110.10
29	C	510	CLA	C1-C2-C3	-3.42	120.12	126.04
29	Y1	608	CLA	C2D-C1D-ND	3.42	112.63	110.10
29	Y1	612	CLA	C2D-C1D-ND	3.42	112.63	110.10
29	g1	614	CLA	C2C-C1C-NC	3.42	113.18	109.97
29	N1	610	CLA	C1-C2-C3	-3.42	120.13	126.04
29	Y	608	CLA	C2C-C1C-NC	3.42	113.18	109.97
29	y	612	CLA	C2C-C1C-NC	3.42	113.18	109.97
29	N1	602	CLA	C1-C2-C3	-3.42	120.13	126.04
48	g	606	CHL	CMA-C3A-C4A	3.42	120.96	111.77
29	R	603	CLA	C1-C2-C3	-3.42	120.13	126.04
48	y	606	CHL	C1-O2A-CGA	3.42	125.42	116.44
29	B1	608	CLA	C2C-C1C-NC	3.42	113.17	109.97
29	b1	604	CLA	C2D-C1D-ND	3.42	112.62	110.10
29	g1	613	CLA	C2D-C1D-ND	3.42	112.62	110.10
29	n1	610	CLA	CAA-C2A-C3A	-3.42	103.42	112.78
29	c	504	CLA	C2D-C1D-ND	3.42	112.62	110.10
48	N1	601	CHL	C2C-C3C-C4C	3.42	108.92	106.49
29	S1	604	CLA	C2C-C1C-NC	3.41	113.17	109.97
29	a	406	CLA	C2C-C1C-NC	3.41	113.17	109.97
33	D	411	LMG	O7-C10-C11	3.41	118.86	111.50
29	B	609	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
48	g	609	CHL	C2B-C1B-NB	-3.41	107.94	110.23
29	R1	610	CLA	O1D-CGD-CBD	-3.41	117.51	124.48
29	b1	604	CLA	CHD-C1D-ND	-3.41	121.32	124.45
29	n	603	CLA	C2D-C1D-ND	3.41	112.62	110.10
49	S	621	LUT	C2-C3-C4	-3.41	105.64	110.30
29	N1	613	CLA	CMA-C3A-C4A	3.41	120.93	111.77
49	y1	620	LUT	C35-C34-C33	-3.41	122.45	127.31
29	b	606	CLA	CHD-C1D-ND	-3.41	121.32	124.45
31	B	619	BCR	C36-C18-C17	-3.41	118.15	122.92
29	S	617	CLA	C2C-C1C-NC	3.41	113.16	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	g	606	CHL	C4D-CHA-C1A	3.41	125.39	121.25
29	G	610	CLA	CHD-C1D-ND	-3.40	121.33	124.45
29	y	613	CLA	C1-C2-C3	-3.40	120.16	126.04
29	s1	610	CLA	C1-C2-C3	-3.40	120.16	126.04
48	y	609	CHL	C3C-C4C-NC	-3.40	106.76	110.57
29	b	614	CLA	C2C-C1C-NC	3.40	113.16	109.97
29	Y	602	CLA	C1-C2-C3	-3.40	120.17	126.04
29	G1	603	CLA	C2C-C1C-NC	3.40	113.16	109.97
29	y	602	CLA	C1-C2-C3	-3.40	120.17	126.04
45	H1	101	RRX	C4-C5-C6	-3.40	117.80	122.73
29	R	604	CLA	C2C-C1C-NC	3.40	113.15	109.97
29	c1	501	CLA	C2C-C1C-NC	3.40	113.15	109.97
39	B	625	DGA	OG2-CB1-CB2	3.40	118.82	111.50
29	c1	503	CLA	CHD-C1D-ND	-3.40	121.33	124.45
29	b1	602	CLA	C3B-C4B-NB	-3.40	107.36	110.52
29	G	612	CLA	C2D-C1D-ND	3.40	112.61	110.10
29	c1	510	CLA	CHD-C1D-ND	-3.40	121.33	124.45
39	b	625	DGA	OG2-CB1-CB2	3.39	118.81	111.50
51	y	623	NEX	C2-C1-C6	3.39	112.51	109.21
29	c	506	CLA	C2C-C1C-NC	3.39	113.15	109.97
48	n	606	CHL	C3C-C4C-NC	-3.39	106.77	110.57
29	s	610	CLA	C3B-C4B-NB	-3.39	107.37	110.52
48	G1	609	CHL	C4B-CHC-C1C	3.39	134.38	126.34
29	N	603	CLA	CHD-C1D-ND	-3.39	121.34	124.45
29	s1	614	CLA	C2C-C1C-NC	3.39	113.15	109.97
29	n	614	CLA	CMA-C3A-C4A	3.39	120.88	111.77
29	c1	508	CLA	CHD-C1D-ND	-3.39	121.34	124.45
48	Y1	605	CHL	CHD-C1D-ND	-3.39	121.34	124.45
31	c1	515	BCR	C33-C5-C4	3.39	120.12	113.62
29	S1	617	CLA	C2C-C1C-NC	3.39	113.14	109.97
48	S1	601	CHL	C3B-C4B-NB	-3.39	107.37	110.52
29	R	612	CLA	C1-O2A-CGA	3.39	125.33	116.44
49	s1	620	LUT	C15-C14-C13	-3.39	122.48	127.31
29	B1	613	CLA	C2C-C1C-NC	3.38	113.14	109.97
48	S1	606	CHL	CHD-C1D-ND	-3.38	121.34	124.45
50	r1	621	XAT	C26-C27-C28	-3.38	118.84	125.99
29	c1	510	CLA	C2C-C1C-NC	3.38	113.14	109.97
48	n	605	CHL	C2C-C3C-C4C	3.38	108.90	106.49
48	N1	606	CHL	CHD-C1D-ND	-3.38	121.35	124.45
29	C1	512	CLA	CHD-C1D-ND	-3.38	121.35	124.45
29	r	608	CLA	CHD-C1D-ND	-3.38	121.35	124.45
29	s1	609	CLA	CHD-C1D-ND	-3.38	121.35	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	516	BCR	C19-C18-C17	3.38	124.12	118.94
29	C1	504	CLA	C2C-C1C-NC	3.38	113.14	109.97
42	D1	401	BCT	O2-C-O1	-3.38	110.79	119.55
49	n1	621	LUT	C3-C4-C5	-3.38	105.13	111.85
48	Y	606	CHL	C3B-C4B-NB	-3.37	107.38	110.52
29	C	502	CLA	C2C-C1C-NC	3.37	113.13	109.97
48	g	606	CHL	C3B-C4B-NB	-3.37	107.39	110.52
29	c	503	CLA	CHD-C1D-ND	-3.37	121.36	124.45
29	B	605	CLA	CMA-C3A-C4A	3.37	120.83	111.77
49	N	620	LUT	C11-C10-C9	-3.37	122.50	127.31
49	y	620	LUT	C22-C23-C24	-3.37	107.91	111.74
29	G	611	CLA	C2C-C1C-NC	3.37	113.13	109.97
48	Y1	605	CHL	CMA-C3A-C4A	3.37	120.82	111.77
29	c1	503	CLA	CMA-C3A-C4A	3.37	120.82	111.77
48	N1	601	CHL	C3C-C4C-NC	-3.37	106.80	110.57
29	S	605	CLA	C1-C2-C3	-3.37	121.31	126.75
29	A	405	CLA	CHD-C1D-ND	-3.37	121.36	124.45
48	r	606	CHL	CHD-C1D-ND	-3.37	121.36	124.45
29	s	604	CLA	C2C-C1C-NC	3.37	113.12	109.97
48	n	606	CHL	C3B-C4B-NB	-3.37	107.39	110.52
31	d1	404	BCR	C15-C14-C13	-3.36	122.51	127.31
29	D	403	CLA	C1-C2-C3	-3.36	120.22	126.04
49	y	620	LUT	C21-C26-C27	3.36	116.95	112.70
48	y	601	CHL	C1-C2-C3	-3.36	120.22	126.04
29	G1	613	CLA	C2D-C1D-ND	3.36	112.58	110.10
49	s1	620	LUT	C7-C8-C9	-3.36	121.15	126.23
36	b	620	C7Z	C38-C25-C24	3.36	120.59	114.36
29	B	614	CLA	CHD-C1D-ND	-3.36	121.36	124.45
29	N1	610	CLA	CHD-C1D-ND	-3.36	121.36	124.45
32	b	626	SQD	O7-S-C6	-3.36	102.94	106.94
29	A	407	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
31	d1	404	BCR	C36-C18-C17	-3.36	118.21	122.92
48	g1	601	CHL	C4B-CHC-C1C	3.36	134.31	126.34
32	b1	621	SQD	O7-S-C6	-3.36	102.95	106.94
29	s	603	CLA	C2C-C1C-NC	3.36	113.12	109.97
29	g	614	CLA	C2C-C1C-NC	3.36	113.12	109.97
29	B	615	CLA	C1-C2-C3	-3.36	120.24	126.04
51	Y	623	NEX	C27-C28-C29	-3.36	120.32	125.53
48	y1	607	CHL	C3C-C4C-NC	-3.36	106.81	110.57
33	d	411	LMG	O7-C10-C11	3.36	118.73	111.50
31	d1	404	BCR	C33-C5-C4	3.35	120.06	113.62
52	r	625	LMT	O5B-C1B-C2B	3.35	117.45	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	k	101	4RF	O21-C22-C24	3.35	118.73	111.50
29	b	603	CLA	C1-C2-C3	-3.35	120.25	126.04
37	c1	520	DGD	O2G-C1B-C2B	3.35	118.72	111.50
29	b	615	CLA	CHD-C1D-ND	-3.35	121.37	124.45
50	R	621	XAT	C38-C25-C24	3.35	118.05	114.28
29	s1	604	CLA	CHD-C1D-ND	-3.35	121.38	124.45
48	Y1	609	CHL	CHD-C1D-ND	-3.35	121.38	124.45
29	n1	610	CLA	C2D-C1D-ND	3.35	112.57	110.10
48	g	607	CHL	CMA-C3A-C4A	3.35	120.77	111.77
51	R1	622	NEX	C39-C29-C30	-3.35	118.23	122.92
29	g1	610	CLA	CMD-C2D-C3D	-3.35	119.92	127.61
48	y1	601	CHL	C1-O2A-CGA	3.34	125.22	116.44
29	s1	605	CLA	C1-C2-C3	-3.34	121.34	126.75
31	C	517	BCR	C34-C9-C10	-3.34	118.24	122.92
29	c	502	CLA	C2C-C1C-NC	3.34	113.11	109.97
48	y	607	CHL	C2C-C3C-C4C	3.34	108.87	106.49
50	g1	622	XAT	C7-C8-C9	-3.34	120.34	125.53
29	B1	604	CLA	CHD-C1D-ND	-3.34	121.38	124.45
29	C1	508	CLA	CHD-C1D-ND	-3.34	121.38	124.45
43	d1	405	PL9	C7-C8-C9	-3.34	121.23	126.79
29	a	410	CLA	C2C-C1C-NC	3.34	113.10	109.97
47	K1	101	4RF	O21-C22-C24	3.34	118.70	111.50
48	g1	608	CHL	C3C-C4C-NC	-3.34	106.82	110.57
29	n	604	CLA	C2D-C1D-ND	3.34	112.57	110.10
29	n	603	CLA	C1-C2-C3	-3.34	120.27	126.04
49	Y	620	LUT	C10-C11-C12	-3.34	112.79	123.22
29	B1	615	CLA	C2D-C1D-ND	3.34	112.56	110.10
48	y	601	CHL	C4B-CHC-C1C	3.34	134.26	126.34
29	N1	613	CLA	C2C-C1C-NC	3.34	113.10	109.97
29	r1	603	CLA	CHD-C1D-ND	-3.34	121.39	124.45
29	d1	403	CLA	C1-C2-C3	-3.34	120.27	126.04
48	g1	606	CHL	C3C-C4C-NC	-3.34	106.83	110.57
29	G	613	CLA	CHD-C1D-ND	-3.34	121.39	124.45
48	Y	605	CHL	C2C-C3C-C4C	3.33	108.87	106.49
31	C	515	BCR	C4-C5-C6	-3.33	117.89	122.73
48	g	601	CHL	C3C-C4C-NC	-3.33	106.83	110.57
29	s1	602	CLA	CHD-C1D-ND	-3.33	121.39	124.45
48	s	608	CHL	C1-C2-C3	-3.33	120.28	126.04
49	N	620	LUT	C35-C34-C33	-3.33	122.55	127.31
29	b1	611	CLA	C4B-CHC-C1C	3.33	134.24	126.34
29	Y1	608	CLA	CMA-C3A-C4A	3.33	120.73	111.77
29	R	604	CLA	CHD-C1D-ND	-3.33	121.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C1	510	CLA	CHD-C1D-ND	-3.33	121.39	124.45
49	g	621	LUT	C15-C14-C13	-3.33	122.56	127.31
49	G	621	LUT	C7-C8-C9	-3.33	121.20	126.23
49	G	620	LUT	C11-C10-C9	-3.33	122.56	127.31
29	B1	615	CLA	CHD-C1D-ND	-3.33	121.40	124.45
48	s1	601	CHL	C3B-C4B-NB	-3.33	107.43	110.52
45	H1	101	RRX	C37-C22-C23	3.33	123.32	118.08
43	d	405	PL9	C7-C8-C9	-3.32	121.26	126.79
48	g	606	CHL	C4B-CHC-C1C	3.32	134.22	126.34
29	N1	602	CLA	CAA-C2A-C3A	-3.32	103.69	112.78
29	C	502	CLA	C1-C2-C3	-3.32	120.30	126.04
29	C	501	CLA	CMA-C3A-C4A	3.32	120.70	111.77
29	Y1	614	CLA	C2C-C1C-NC	3.32	113.08	109.97
48	N	606	CHL	C4B-CHC-C1C	3.32	134.21	126.34
48	g1	608	CHL	C2C-C3C-C4C	3.32	108.86	106.49
31	d	404	BCR	C1-C6-C5	-3.32	117.94	122.61
48	s1	601	CHL	CHD-C1D-ND	-3.32	121.41	124.45
29	a1	407	CLA	C2C-C1C-NC	3.32	113.08	109.97
47	K	101	4RF	O21-C22-C24	3.32	118.65	111.50
49	g1	620	LUT	C15-C14-C13	-3.31	122.58	127.31
48	R	606	CHL	CHB-C4A-NA	3.31	129.09	124.51
49	G	621	LUT	C35-C15-C14	-3.31	116.69	123.47
48	n1	601	CHL	C3C-C4C-NC	-3.31	106.86	110.57
29	g1	612	CLA	CHD-C1D-ND	-3.31	121.41	124.45
29	g	611	CLA	C1-C2-C3	-3.31	120.31	126.04
48	g1	601	CHL	C3C-C4C-NC	-3.31	106.86	110.57
30	a	409	PHO	C2B-C1B-NB	-3.31	107.24	109.53
29	B	602	CLA	C2C-C1C-NC	3.31	113.08	109.97
29	N	613	CLA	C2C-C1C-NC	3.31	113.08	109.97
29	Y	611	CLA	C2C-C1C-NC	3.31	113.08	109.97
31	A	411	BCR	C33-C5-C6	-3.31	120.81	124.53
48	G1	605	CHL	C2C-C3C-C4C	3.31	108.85	106.49
33	d	411	LMG	O8-C28-C29	3.31	122.30	111.91
48	n1	607	CHL	CHD-C1D-ND	-3.31	121.41	124.45
29	N	613	CLA	CMA-C3A-C4A	3.31	120.67	111.77
29	S1	609	CLA	CHD-C1D-ND	-3.31	121.41	124.45
49	y1	621	LUT	C35-C15-C14	-3.31	116.70	123.47
47	K	101	4RF	O40-C41-C43	3.31	122.29	111.91
50	g	622	XAT	C38-C25-C26	-3.31	116.72	122.26
29	S1	614	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
29	S	614	CLA	CHD-C1D-ND	-3.31	121.42	124.45
48	g1	606	CHL	CHD-C1D-ND	-3.31	121.42	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	S1	607	CHL	C3C-C4C-NC	-3.31	106.86	110.57
31	A1	411	BCR	C33-C5-C4	3.31	119.97	113.62
29	C1	506	CLA	CHD-C1D-ND	-3.31	121.42	124.45
31	D	404	BCR	C38-C26-C25	-3.31	120.82	124.53
51	S	623	NEX	C27-C28-C29	-3.31	120.40	125.53
48	r	607	CHL	C3C-C4C-NC	-3.31	106.86	110.57
29	s1	609	CLA	C2C-C1C-NC	3.30	113.07	109.97
29	C	513	CLA	C2D-C1D-ND	3.30	112.54	110.10
29	b	613	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
29	S	602	CLA	CAA-C2A-C3A	-3.30	103.73	112.78
29	S	611	CLA	C2C-C1C-NC	3.30	113.07	109.97
29	C	510	CLA	CHD-C1D-ND	-3.30	121.42	124.45
29	y	602	CLA	CHD-C1D-ND	-3.30	121.42	124.45
29	n	612	CLA	C2C-C1C-NC	3.30	113.06	109.97
29	b1	606	CLA	C1-C2-C3	-3.30	120.34	126.04
29	C1	511	CLA	CHD-C1D-ND	-3.30	121.42	124.45
29	b	612	CLA	CHD-C1D-ND	-3.29	121.43	124.45
29	B1	616	CLA	CHD-C1D-ND	-3.29	121.43	124.45
31	C1	516	BCR	C38-C26-C27	3.29	119.94	113.62
29	d	403	CLA	CAA-C2A-C3A	-3.29	103.76	112.78
48	G	608	CHL	CMA-C3A-C4A	3.29	120.62	111.77
29	B1	616	CLA	C2C-C1C-NC	3.29	113.06	109.97
29	y1	603	CLA	C2C-C1C-NC	3.29	113.06	109.97
48	s1	606	CHL	C2C-C3C-C4C	3.29	108.83	106.49
29	g	604	CLA	CHD-C1D-ND	-3.29	121.43	124.45
29	A	407	CLA	C1-C2-C3	-3.29	121.43	126.75
31	d1	404	BCR	C1-C6-C5	-3.29	117.98	122.61
29	b1	614	CLA	OBD-CAD-C3D	-3.29	120.61	128.52
29	r1	612	CLA	CHD-C1D-ND	-3.29	121.43	124.45
31	C1	514	BCR	C36-C18-C17	-3.29	118.32	122.92
53	R	626	ERG	C17-C20-C22	-3.29	104.01	110.27
48	g1	605	CHL	CMA-C3A-C4A	3.29	120.61	111.77
29	R	609	CLA	CAA-C2A-C3A	-3.29	103.78	112.78
29	S	605	CLA	O2D-CGD-O1D	-3.29	117.42	123.84
29	n1	614	CLA	C2C-C1C-NC	3.28	113.05	109.97
31	B	619	BCR	C23-C24-C25	-3.28	117.99	127.20
48	G1	605	CHL	C3C-C4C-NC	-3.28	106.89	110.57
29	R1	609	CLA	CAA-C2A-C3A	-3.28	103.80	112.78
49	Y	620	LUT	C22-C23-C24	-3.28	108.01	111.74
29	s	617	CLA	CHD-C1D-ND	-3.28	121.44	124.45
29	B1	605	CLA	C2C-C1C-NC	3.28	113.04	109.97
31	a1	411	BCR	C23-C24-C25	-3.28	118.00	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B1	606	CLA	CHD-C1D-ND	-3.28	121.44	124.45
29	n	611	CLA	C2C-C1C-NC	3.27	113.04	109.97
50	R	621	XAT	C18-C5-C4	3.27	117.96	114.28
48	y	607	CHL	C3C-C4C-NC	-3.27	106.90	110.57
49	N	620	LUT	C21-C26-C27	3.27	116.84	112.70
29	B	603	CLA	C2C-C1C-NC	3.27	113.04	109.97
49	S	620	LUT	C21-C26-C27	3.27	116.84	112.70
29	n1	602	CLA	C1-C2-C3	-3.27	120.38	126.04
29	G	612	CLA	CHD-C1D-ND	-3.27	121.45	124.45
29	G1	603	CLA	C1-C2-C3	-3.27	120.38	126.04
29	R1	602	CLA	C1-C2-C3	-3.27	120.38	126.04
51	Y	623	NEX	C38-C25-C26	-3.27	116.78	122.26
29	N	610	CLA	C2D-C1D-ND	3.27	112.52	110.10
48	s	607	CHL	C3C-C4C-NC	-3.27	106.90	110.57
48	s	601	CHL	C2C-C3C-C4C	3.27	108.82	106.49
29	Y	608	CLA	CHD-C1D-ND	-3.27	121.45	124.45
29	G1	604	CLA	OBD-CAD-C3D	-3.27	120.65	128.52
40	S1	624	LHG	C5-O7-C7	-3.27	109.74	117.79
29	Y	603	CLA	C1-C2-C3	-3.27	120.39	126.04
29	B	609	CLA	C2D-C1D-ND	3.27	112.51	110.10
49	G1	620	LUT	C35-C34-C33	-3.27	122.64	127.31
49	N1	621	LUT	C7-C8-C9	-3.27	121.30	126.23
29	Y	602	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
29	B1	611	CLA	C4B-CHC-C1C	3.27	134.09	126.34
50	n1	622	XAT	C18-C5-C6	-3.27	116.78	122.26
31	c	515	BCR	C23-C24-C25	-3.27	118.02	127.20
29	b	603	CLA	CHD-C1D-ND	-3.27	121.45	124.45
29	G1	614	CLA	C2C-C1C-NC	3.27	113.03	109.97
29	Y	610	CLA	CAA-C2A-C3A	-3.27	103.83	112.78
29	D1	403	CLA	CHD-C1D-ND	-3.27	121.45	124.45
29	B	616	CLA	C3B-C4B-NB	-3.27	107.49	110.52
29	y1	611	CLA	CMA-C3A-C4A	3.26	120.55	111.77
29	G1	613	CLA	CHD-C1D-ND	-3.26	121.45	124.45
29	d1	403	CLA	CHD-C1D-ND	-3.26	121.45	124.45
48	G1	607	CHL	CHD-C1D-ND	-3.26	121.45	124.45
29	a1	406	CLA	C2C-C1C-NC	3.26	113.03	109.97
48	Y1	609	CHL	C1-C2-C3	-3.26	120.40	126.04
40	D1	409	LHG	C5-O7-C7	-3.26	109.76	117.79
32	C1	526	SQD	O7-S-C6	-3.26	103.06	106.94
29	R1	608	CLA	C2C-C1C-NC	3.26	113.03	109.97
29	r1	610	CLA	C1-C2-C3	-3.26	120.40	126.04
48	s1	607	CHL	C4A-NA-C1A	3.26	108.17	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	620	C7Z	C1-C6-C5	-3.26	118.02	122.61
50	R	621	XAT	C7-C8-C9	-3.26	120.47	125.53
48	g	608	CHL	CHD-C1D-ND	-3.26	121.46	124.45
49	R	620	LUT	C15-C14-C13	-3.26	122.66	127.31
48	N	605	CHL	C2C-C3C-C4C	3.26	108.81	106.49
29	r	610	CLA	CHD-C1D-ND	-3.26	121.46	124.45
31	B1	618	BCR	C33-C5-C6	-3.26	120.87	124.53
49	S1	620	LUT	C35-C34-C33	-3.26	122.66	127.31
29	N1	603	CLA	CMA-C3A-C4A	3.26	120.53	111.77
29	y	610	CLA	C1-C2-C3	-3.26	120.41	126.04
29	s	604	CLA	CHD-C1D-ND	-3.26	121.46	124.45
29	R1	610	CLA	CHD-C1D-ND	-3.26	121.46	124.45
29	y	610	CLA	C2D-C1D-ND	3.26	112.50	110.10
45	h	101	RRX	C15-C16-C17	-3.26	116.80	123.47
51	G	623	NEX	O24-C25-C38	-3.26	111.15	115.06
29	r1	604	CLA	C2D-C1D-ND	3.26	112.50	110.10
29	c	505	CLA	C1-C2-C3	-3.25	120.41	126.04
29	G	604	CLA	C2C-C1C-NC	3.25	113.02	109.97
53	r1	626	ERG	C18-C13-C12	-3.25	105.45	110.59
31	C1	516	BCR	C35-C13-C14	-3.25	118.36	122.92
48	s1	601	CHL	CMA-C3A-C4A	3.25	120.52	111.77
50	G	622	XAT	C7-C8-C9	-3.25	120.48	125.53
31	A	411	BCR	C23-C24-C25	-3.25	118.07	127.20
29	d	402	CLA	C3B-C4B-NB	-3.25	107.50	110.52
49	g1	621	LUT	C31-C32-C33	-3.25	117.28	126.42
29	C	507	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
30	a	409	PHO	O2D-CGD-O1D	-3.25	117.48	123.84
45	h1	101	RRX	C30-C25-C26	-3.25	118.04	122.61
29	s	603	CLA	C1-C2-C3	-3.25	120.42	126.04
29	b	615	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
29	B	613	CLA	C2C-C1C-NC	3.25	113.02	109.97
29	a	410	CLA	CHD-C1D-ND	-3.25	121.47	124.45
51	n1	623	NEX	C40-C33-C34	-3.25	118.37	122.92
29	Y	614	CLA	CHD-C1D-ND	-3.24	121.47	124.45
51	s1	623	NEX	C31-C30-C29	3.24	131.94	127.31
50	R1	621	XAT	O4-C5-C4	-3.24	110.94	113.38
29	G1	612	CLA	C2C-C1C-NC	3.24	113.01	109.97
29	s1	611	CLA	C2C-C1C-NC	3.24	113.01	109.97
29	Y1	610	CLA	CMA-C3A-C4A	3.24	120.49	111.77
29	c1	507	CLA	CHD-C1D-ND	-3.24	121.47	124.45
29	g1	613	CLA	C2C-C1C-NC	3.24	113.01	109.97
29	n	604	CLA	C1-C2-C3	-3.24	120.44	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A1	405	CLA	CHD-C1D-ND	-3.24	121.48	124.45
48	N1	609	CHL	CHD-C4C-C3C	3.24	129.60	124.84
50	g	622	XAT	C19-C9-C10	-3.24	118.38	122.92
29	Y	613	CLA	C2C-C1C-NC	3.24	113.01	109.97
29	S1	612	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
29	A1	410	CLA	C2D-C1D-ND	3.24	112.49	110.10
29	n1	613	CLA	C2C-C1C-NC	3.24	113.01	109.97
48	n1	606	CHL	C2C-C3C-C4C	3.24	108.80	106.49
29	y1	612	CLA	C2D-C1D-ND	3.24	112.49	110.10
48	G	605	CHL	CHB-C4A-NA	3.24	128.99	124.51
48	N	609	CHL	CHD-C1D-ND	-3.24	121.48	124.45
29	C	503	CLA	C1-C2-C3	-3.24	120.44	126.04
49	S	621	LUT	C10-C11-C12	-3.24	113.12	123.22
29	C	503	CLA	CMA-C3A-C4A	3.24	120.47	111.77
48	N	606	CHL	CHD-C1D-ND	-3.24	121.48	124.45
49	n	620	LUT	C21-C26-C27	3.23	116.79	112.70
49	G	621	LUT	C35-C34-C33	-3.23	122.69	127.31
48	r	606	CHL	C4A-NA-C1A	3.23	108.16	106.71
29	r	602	CLA	CHD-C1D-ND	-3.23	121.48	124.45
48	N1	608	CHL	CMA-C3A-C4A	3.23	120.47	111.77
29	G	602	CLA	CMA-C3A-C4A	3.23	120.46	111.77
29	g1	603	CLA	C3B-C4B-NB	-3.23	107.52	110.52
29	B1	617	CLA	C1-C2-C3	-3.23	120.45	126.04
29	C	504	CLA	CHD-C1D-ND	-3.23	121.48	124.45
29	N	610	CLA	CHD-C1D-ND	-3.23	121.48	124.45
29	g	611	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
29	C1	507	CLA	C2C-C1C-NC	3.23	113.00	109.97
29	b	605	CLA	C1-C2-C3	-3.23	120.45	126.04
49	Y	620	LUT	C35-C34-C33	-3.23	122.70	127.31
48	n1	606	CHL	C4B-CHC-C1C	3.23	134.00	126.34
50	r1	621	XAT	C18-C5-C6	-3.23	116.85	122.26
29	n1	612	CLA	C2C-C1C-NC	3.23	113.00	109.97
29	B1	611	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
30	a1	408	PHO	C2D-C1D-ND	-3.23	107.30	109.53
29	a	410	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
29	Y	602	CLA	CHD-C1D-ND	-3.23	121.49	124.45
29	a1	405	CLA	C2D-C1D-ND	3.23	112.48	110.10
48	N	605	CHL	C3B-C4B-NB	-3.23	107.52	110.52
48	g1	601	CHL	CMA-C3A-C4A	3.23	120.44	111.77
29	B1	606	CLA	C2C-C1C-NC	3.22	112.99	109.97
29	S1	605	CLA	CMA-C3A-C4A	3.22	120.44	111.77
50	Y1	622	XAT	C40-C33-C34	-3.22	118.41	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	n	607	CHL	C3C-C4C-NC	-3.22	106.96	110.57
29	R1	602	CLA	C2C-C1C-NC	3.22	112.99	109.97
29	c1	512	CLA	C2C-C1C-NC	3.22	112.99	109.97
29	r1	609	CLA	CMA-C3A-C4A	3.22	120.43	111.77
48	N1	609	CHL	C1-O2A-CGA	3.22	124.89	116.44
49	Y	620	LUT	C15-C14-C13	-3.22	122.71	127.31
29	s1	603	CLA	CMA-C3A-C4A	3.22	120.43	111.77
29	C1	512	CLA	C1-C2-C3	-3.22	120.47	126.04
49	n1	620	LUT	C7-C8-C9	-3.22	121.37	126.23
29	A	407	CLA	C1-O2A-CGA	3.22	124.89	116.44
29	Y1	612	CLA	C2C-C1C-NC	3.22	112.99	109.97
51	n	623	NEX	C27-C28-C29	-3.22	120.54	125.53
48	g1	609	CHL	C3C-C4C-NC	-3.22	106.96	110.57
49	N	620	LUT	C7-C8-C9	-3.22	121.37	126.23
29	B1	616	CLA	C1-C2-C3	-3.22	120.48	126.04
29	r1	610	CLA	C2D-C1D-ND	3.22	112.47	110.10
29	S1	613	CLA	CHD-C1D-ND	-3.22	121.50	124.45
48	y	606	CHL	C3C-C4C-NC	-3.22	106.97	110.57
29	Y	614	CLA	CMA-C3A-C4A	3.22	120.41	111.77
48	n1	607	CHL	C3C-C4C-NC	-3.21	106.97	110.57
49	N1	621	LUT	C35-C34-C33	-3.21	122.72	127.31
49	Y1	621	LUT	C30-C31-C32	-3.21	113.19	123.22
51	s1	623	NEX	C39-C29-C30	-3.21	118.42	122.92
42	D	401	BCT	O2-C-O1	-3.21	111.22	119.55
29	c1	507	CLA	C2C-C1C-NC	3.21	112.98	109.97
29	y	604	CLA	C1-C2-C3	-3.21	120.49	126.04
48	Y1	606	CHL	C3C-C4C-NC	-3.21	106.97	110.57
51	N	623	NEX	C5-C4-C3	3.21	115.55	111.75
48	G	605	CHL	C2C-C3C-C4C	3.21	108.78	106.49
29	s1	603	CLA	C2D-C1D-ND	3.21	112.47	110.10
45	H	101	RRX	C8-C7-C6	-3.21	118.19	127.20
48	S	606	CHL	C4B-CHC-C1C	3.21	133.95	126.34
29	y1	604	CLA	C2C-C1C-NC	3.21	112.98	109.97
53	R1	626	ERG	C13-C17-C20	-3.21	115.29	119.43
29	Y	613	CLA	CMA-C3A-C4A	3.21	120.39	111.77
29	C	512	CLA	C2D-C1D-ND	3.21	112.47	110.10
31	b	618	BCR	C15-C14-C13	-3.20	122.74	127.31
29	N	613	CLA	C1-C2-C3	-3.20	120.50	126.04
29	S1	602	CLA	O2A-CGA-CBA	3.20	121.96	111.91
33	D1	411	LMG	O8-C28-C29	3.20	121.96	111.91
48	Y1	605	CHL	C2C-C3C-C4C	3.20	108.77	106.49
48	Y1	609	CHL	C2C-C3C-C4C	3.20	108.77	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	505	CLA	CHD-C1D-ND	-3.20	121.51	124.45
33	W1	201	LMG	O8-C28-C29	3.20	121.95	111.91
31	c	514	BCR	C38-C26-C25	-3.20	120.93	124.53
29	c1	504	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
51	N	623	NEX	C39-C29-C30	-3.20	118.44	122.92
29	n	602	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
45	H1	101	RRX	C33-C5-C6	-3.20	120.94	124.53
29	S	614	CLA	C1-C2-C3	-3.20	120.51	126.04
48	y	601	CHL	C3C-C4C-NC	-3.20	106.98	110.57
29	n	610	CLA	C2D-C1D-ND	3.20	112.46	110.10
51	s1	623	NEX	O24-C25-C38	-3.20	111.22	115.06
29	s1	602	CLA	O1D-CGD-CBD	-3.20	117.94	124.48
29	a	405	CLA	C1-O2A-CGA	3.20	124.83	116.44
31	d1	404	BCR	C19-C18-C17	3.20	123.85	118.94
29	g1	613	CLA	CHD-C1D-ND	-3.20	121.52	124.45
29	Y	612	CLA	C2C-C1C-NC	3.20	112.97	109.97
29	S1	605	CLA	C2C-C1C-NC	3.20	112.97	109.97
29	G1	610	CLA	O2A-CGA-CBA	3.20	121.94	111.91
34	A1	414	SPH	C3-C4-C5	-3.20	117.66	124.79
29	B	614	CLA	C1-C2-C3	-3.20	120.52	126.04
48	G	607	CHL	C4B-CHC-C1C	3.19	133.92	126.34
48	s1	607	CHL	C3C-C4C-NC	-3.19	106.99	110.57
29	s	609	CLA	C2C-C1C-NC	3.19	112.97	109.97
29	g1	602	CLA	CHD-C1D-ND	-3.19	121.52	124.45
29	B1	608	CLA	CMA-C3A-C4A	3.19	120.36	111.77
40	n1	624	LHG	C5-O7-C7	-3.19	109.93	117.79
29	S1	613	CLA	C1-C2-C3	-3.19	120.52	126.04
31	C1	517	BCR	C36-C18-C17	-3.19	118.45	122.92
36	b1	620	C7Z	C31-C30-C29	-3.19	122.75	127.31
43	D	405	PL9	C7-C8-C9	-3.19	121.48	126.79
48	s1	606	CHL	C3C-C4C-NC	-3.19	106.99	110.57
29	B	606	CLA	C2C-C1C-NC	3.19	112.96	109.97
51	N1	623	NEX	C39-C29-C30	-3.19	118.45	122.92
49	n1	621	LUT	C35-C15-C14	-3.19	116.94	123.47
31	B1	618	BCR	C19-C18-C17	3.19	123.84	118.94
29	n	613	CLA	C2C-C1C-NC	3.19	112.96	109.97
29	B	610	CLA	C2D-C1D-ND	3.19	112.46	110.10
48	Y	609	CHL	C3C-C4C-NC	-3.19	106.99	110.57
50	G1	622	XAT	O24-C25-C24	3.19	115.78	113.38
48	Y	609	CHL	C3B-C4B-NB	-3.19	107.56	110.52
29	Y1	613	CLA	C1-C2-C3	-3.19	120.53	126.04
29	r1	602	CLA	CHD-C1D-ND	-3.19	121.52	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	s	623	NEX	C39-C29-C30	-3.19	118.45	122.92
29	S1	614	CLA	C2D-C1D-ND	3.19	112.45	110.10
48	y	606	CHL	C2C-C3C-C4C	3.19	108.76	106.49
49	S	621	LUT	C18-C5-C6	-3.19	120.95	124.53
48	g	608	CHL	CMA-C3A-C4A	3.19	120.35	111.77
50	n1	622	XAT	O24-C25-C24	3.19	115.78	113.38
29	s1	603	CLA	C2C-C1C-NC	3.19	112.96	109.97
29	y1	602	CLA	C1-C2-C3	-3.19	120.53	126.04
29	B1	614	CLA	CMD-C2D-C3D	-3.19	120.28	127.61
48	g1	607	CHL	CHB-C4A-NA	3.19	128.92	124.51
49	G1	620	LUT	C22-C23-C24	-3.19	108.11	111.74
52	r	625	LMT	C3B-C4B-C5B	-3.19	104.56	110.24
48	y	605	CHL	C4B-CHC-C1C	3.18	133.89	126.34
48	n1	607	CHL	C1-O2A-CGA	3.18	124.80	116.44
31	b	618	BCR	C4-C5-C6	-3.18	118.11	122.73
43	D	405	PL9	C7-C3-C2	-3.18	119.11	123.30
48	g	607	CHL	C1-C2-C3	-3.18	120.54	126.04
29	s1	602	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
29	C	504	CLA	C1-O2A-CGA	3.18	124.80	116.44
29	C1	509	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
29	S	617	CLA	C1-O2A-CGA	3.18	124.79	116.44
29	B	608	CLA	C2D-C1D-ND	3.18	112.45	110.10
29	S	610	CLA	C2D-C1D-ND	3.18	112.45	110.10
29	D1	402	CLA	CHD-C1D-ND	-3.18	121.53	124.45
48	S1	606	CHL	C4B-CHC-C1C	3.18	133.88	126.34
29	N1	612	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
29	s	614	CLA	CHD-C1D-ND	-3.18	121.53	124.45
29	c	510	CLA	C2C-C1C-NC	3.18	112.95	109.97
49	S1	620	LUT	C22-C23-C24	-3.18	108.12	111.74
29	B1	609	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
29	G	603	CLA	C2D-C1D-ND	3.18	112.45	110.10
29	Y1	603	CLA	C2C-C1C-NC	3.18	112.95	109.97
29	N1	602	CLA	C2D-C1D-ND	3.18	112.44	110.10
29	b1	614	CLA	C3B-C4B-NB	-3.18	107.57	110.52
29	R1	604	CLA	CHD-C1D-ND	-3.18	121.53	124.45
29	B1	615	CLA	C2C-C1C-NC	3.17	112.95	109.97
29	c	509	CLA	C2C-C1C-NC	3.17	112.94	109.97
51	N	623	NEX	C31-C30-C29	3.17	131.83	127.31
48	N1	607	CHL	C3C-C4C-NC	-3.17	107.02	110.57
29	R1	612	CLA	C1-C2-C3	-3.17	120.56	126.04
29	c1	511	CLA	CMA-C3A-C4A	3.17	120.29	111.77
48	Y1	601	CHL	C4B-CHC-C1C	3.17	133.85	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	603	CLA	C2C-C1C-NC	3.17	112.94	109.97
29	D	402	CLA	CHD-C1D-ND	-3.17	121.54	124.45
29	N	612	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
31	D1	404	BCR	C19-C18-C17	3.17	123.80	118.94
29	c	511	CLA	CMA-C3A-C4A	3.17	120.28	111.77
29	n1	611	CLA	C2D-C1D-ND	3.17	112.44	110.10
29	n	611	CLA	CHD-C1D-ND	-3.17	121.55	124.45
29	r	602	CLA	C6-C5-C3	-3.17	105.16	113.45
29	S1	602	CLA	C2D-C1D-ND	3.16	112.44	110.10
29	c	510	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	N1	613	CLA	C2D-C1D-ND	3.16	112.44	110.10
29	n1	603	CLA	C1C-C2C-C3C	-3.16	103.63	106.96
29	R	612	CLA	C2C-C1C-NC	3.16	112.94	109.97
48	r1	606	CHL	C3B-C4B-NB	-3.16	107.58	110.52
51	R1	622	NEX	C17-C1-C6	-3.16	107.64	110.47
48	R	607	CHL	C2C-C3C-C4C	3.16	108.74	106.49
29	B1	602	CLA	CMA-C3A-C4A	3.16	120.27	111.77
49	y	621	LUT	C38-C25-C24	-3.16	116.80	123.56
48	Y	601	CHL	CMA-C3A-C4A	3.16	120.27	111.77
29	s	610	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	R	602	CLA	C4B-CHC-C1C	3.16	133.84	126.34
29	B	602	CLA	C1C-C2C-C3C	-3.16	103.63	106.96
29	B1	612	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	d	403	CLA	CMA-C3A-C4A	3.16	120.26	111.77
48	r1	606	CHL	CHB-C4A-NA	3.16	128.88	124.51
29	B	610	CLA	C2C-C1C-NC	3.16	112.93	109.97
34	y1	625	SPH	C3-C4-C5	-3.16	117.75	124.79
29	R	603	CLA	C3B-C4B-NB	-3.16	107.58	110.52
29	C	503	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	S1	617	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	c	505	CLA	C2C-C1C-NC	3.16	112.93	109.97
29	R1	610	CLA	C1D-ND-C4D	-3.16	104.09	106.33
48	g	606	CHL	C3C-C4C-NC	-3.16	107.03	110.57
31	C	515	BCR	C8-C7-C6	-3.16	118.33	127.20
31	D	404	BCR	C19-C18-C17	3.16	123.78	118.94
29	S1	603	CLA	C2C-C1C-NC	3.16	112.93	109.97
49	N1	620	LUT	C18-C5-C6	-3.16	120.98	124.53
48	Y1	606	CHL	CHD-C1D-ND	-3.16	121.55	124.45
50	G	622	XAT	C26-C27-C28	-3.16	119.32	125.99
29	c1	506	CLA	C2C-C1C-NC	3.16	112.93	109.97
50	N	622	XAT	C38-C25-C26	-3.15	116.97	122.26
29	s1	614	CLA	CHD-C1D-ND	-3.15	121.56	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	s	606	CHL	CHB-C4A-NA	3.15	128.87	124.51
29	b1	615	CLA	CHD-C1D-ND	-3.15	121.56	124.45
29	d	403	CLA	C2C-C1C-NC	3.15	112.92	109.97
29	R1	604	CLA	C2C-C1C-NC	3.15	112.92	109.97
29	c	512	CLA	C2C-C1C-NC	3.15	112.92	109.97
29	y1	611	CLA	C2C-C1C-NC	3.15	112.92	109.97
29	b1	602	CLA	C2D-C1D-ND	3.15	112.43	110.10
48	s	607	CHL	CMA-C3A-C4A	3.15	120.24	111.77
29	c1	506	CLA	CHD-C1D-ND	-3.15	121.56	124.45
29	c1	506	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
29	y	613	CLA	C2C-C1C-NC	3.15	112.92	109.97
29	n	610	CLA	O2A-CGA-CBA	3.15	121.79	111.91
48	G1	607	CHL	CMA-C3A-C4A	3.15	120.24	111.77
29	S1	604	CLA	CHD-C1D-ND	-3.15	121.56	124.45
29	R	610	CLA	CMA-C3A-C4A	3.15	120.23	111.77
48	s	607	CHL	CHB-C4A-NA	3.15	128.86	124.51
29	c	513	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
29	R	610	CLA	CMC-C2C-C1C	3.15	129.83	125.04
29	B	612	CLA	CHD-C1D-ND	-3.15	121.56	124.45
48	G	601	CHL	CHD-C1D-ND	-3.15	121.56	124.45
29	B1	605	CLA	CMA-C3A-C4A	3.15	120.23	111.77
53	R	626	ERG	C1-C10-C5	3.15	114.51	108.75
29	r	609	CLA	C1-C2-C3	-3.15	120.60	126.04
29	A	405	CLA	CAC-C3C-C4C	3.15	128.89	124.81
29	n1	610	CLA	CMA-C3A-C4A	3.15	120.23	111.77
29	C	513	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
29	B1	605	CLA	CHD-C1D-ND	-3.14	121.56	124.45
29	r1	609	CLA	C2C-C1C-NC	3.14	112.92	109.97
29	a	407	CLA	O1D-CGD-CBD	-3.14	118.05	124.48
49	g	620	LUT	C31-C32-C33	-3.14	117.58	126.42
48	s	601	CHL	CHB-C4A-NA	3.14	128.86	124.51
29	y	614	CLA	C2D-C1D-ND	3.14	112.42	110.10
29	y1	613	CLA	C2D-C1D-ND	3.14	112.42	110.10
29	S	617	CLA	CHD-C1D-ND	-3.14	121.56	124.45
29	n1	613	CLA	CHD-C1D-ND	-3.14	121.56	124.45
29	r	602	CLA	CMA-C3A-C4A	3.14	120.22	111.77
48	Y1	607	CHL	C1-O2A-CGA	3.14	124.69	116.44
31	C	517	BCR	C37-C22-C21	-3.14	118.52	122.92
31	d	404	BCR	C34-C9-C10	-3.14	118.52	122.92
29	n1	602	CLA	C1D-ND-C4D	-3.14	104.10	106.33
44	F1	101	HEM	C1C-CHC-C4B	-3.14	119.29	126.06
49	S	620	LUT	C30-C31-C32	-3.14	113.42	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	g1	621	LUT	C35-C15-C14	-3.14	117.05	123.47
29	N	604	CLA	CHD-C1D-ND	-3.14	121.57	124.45
48	y1	607	CHL	C2C-C3C-C4C	3.14	108.73	106.49
49	g	620	LUT	C15-C35-C34	-3.14	117.05	123.47
42	d	401	BCT	O2-C-O1	-3.14	111.41	119.55
48	G	609	CHL	CMA-C3A-C4A	3.14	120.20	111.77
40	l	101	LHG	O8-C23-C24	3.14	121.75	111.91
29	Y1	603	CLA	C1-C2-C3	-3.14	120.62	126.04
29	B1	607	CLA	CMD-C2D-C3D	-3.14	120.40	127.61
48	G1	608	CHL	C3B-C4B-NB	-3.13	107.61	110.52
48	g1	601	CHL	C4D-CHA-C1A	3.13	125.06	121.25
48	G	601	CHL	C2C-C3C-C4C	3.13	108.72	106.49
49	g1	620	LUT	C31-C32-C33	-3.13	117.62	126.42
33	a1	413	LMG	C8-O7-C10	-3.13	110.08	117.79
29	c1	513	CLA	C3B-C4B-NB	-3.13	107.61	110.52
50	N1	622	XAT	C28-C29-C30	3.13	123.75	118.94
29	r1	603	CLA	C1-C2-C3	-3.13	120.63	126.04
29	b	606	CLA	C2C-C1C-NC	3.13	112.91	109.97
29	b	616	CLA	C2D-C1D-ND	3.13	112.41	110.10
31	c	515	BCR	C33-C5-C6	-3.13	121.01	124.53
29	S1	603	CLA	C3B-C4B-NB	-3.13	107.61	110.52
29	B	615	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
29	g	612	CLA	CMA-C3A-C4A	3.13	120.18	111.77
48	S1	606	CHL	C3C-C4C-NC	-3.13	107.06	110.57
49	N1	620	LUT	C38-C25-C24	-3.13	116.86	123.56
29	B1	602	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
29	y	603	CLA	CHD-C1D-ND	-3.13	121.58	124.45
51	r1	622	NEX	C5-C6-C1	3.13	122.80	119.70
29	g1	612	CLA	C2D-C1D-ND	3.13	112.41	110.10
29	A1	410	CLA	C2C-C1C-NC	3.13	112.90	109.97
29	C	510	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
29	A1	406	CLA	CMA-C3A-C4A	3.13	120.17	111.77
29	a	407	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
48	G1	601	CHL	C4B-CHC-C1C	3.13	133.75	126.34
29	G	613	CLA	CMA-C3A-C4A	3.12	120.17	111.77
49	S1	620	LUT	C18-C5-C6	-3.12	121.02	124.53
51	n1	623	NEX	C20-C13-C14	-3.12	118.55	122.92
48	n	607	CHL	CHB-C4A-NA	3.12	128.83	124.51
48	s1	606	CHL	CHB-C4A-NA	3.12	128.83	124.51
48	N	601	CHL	CMA-C3A-C4A	3.12	120.17	111.77
53	R1	626	ERG	C7-C6-C5	-3.12	117.72	123.20
29	B1	617	CLA	CMA-C3A-C4A	3.12	120.16	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s1	613	CLA	CMA-C3A-C4A	3.12	120.16	111.77
49	r	620	LUT	C22-C23-C24	-3.12	108.19	111.74
31	A1	411	BCR	C23-C24-C25	-3.12	118.44	127.20
45	h1	101	RRX	C36-C18-C19	3.12	122.99	118.08
49	G1	620	LUT	C31-C30-C29	-3.12	122.86	127.31
48	N1	606	CHL	C2C-C3C-C4C	3.12	108.71	106.49
29	b1	611	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
29	A1	410	CLA	CMA-C3A-C4A	3.12	120.15	111.77
48	Y1	609	CHL	C3C-C4C-NC	-3.12	107.08	110.57
48	Y1	605	CHL	C3C-C4C-NC	-3.12	107.08	110.57
48	y1	605	CHL	C3C-C4C-NC	-3.12	107.08	110.57
51	g1	623	NEX	C17-C1-C6	-3.12	107.68	110.47
33	c1	521	LMG	O8-C28-C29	3.11	121.68	111.91
29	G	614	CLA	CMA-C3A-C4A	3.11	120.14	111.77
29	N1	604	CLA	CHD-C1D-ND	-3.11	121.59	124.45
29	b	602	CLA	C3B-C4B-NB	-3.11	107.63	110.52
29	y	613	CLA	CMA-C3A-C4A	3.11	120.14	111.77
31	a	411	BCR	C23-C24-C25	-3.11	118.46	127.20
29	c	509	CLA	CHD-C1D-ND	-3.11	121.59	124.45
31	C	515	BCR	C33-C5-C6	-3.11	121.03	124.53
29	c1	509	CLA	C2C-C1C-NC	3.11	112.89	109.97
45	h	101	RRX	C4-C5-C6	-3.11	118.22	122.73
29	B1	613	CLA	CMD-C2D-C3D	-3.11	120.46	127.61
29	y	604	CLA	C2D-C1D-ND	3.11	112.40	110.10
48	G	606	CHL	C3B-C4B-NB	-3.11	107.63	110.52
29	y1	604	CLA	CMA-C3A-C4A	3.11	120.13	111.77
48	R	607	CHL	CMA-C3A-C4A	3.11	120.13	111.77
31	d	404	BCR	C38-C26-C25	-3.11	121.04	124.53
29	n	614	CLA	C2D-C1D-ND	3.11	112.39	110.10
29	B1	614	CLA	CHD-C1D-ND	-3.11	121.60	124.45
29	c	502	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
29	b1	611	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
29	a1	405	CLA	C2C-C1C-NC	3.11	112.88	109.97
29	n1	613	CLA	C1-C2-C3	-3.11	120.67	126.04
48	R1	606	CHL	CHB-C4A-NA	3.11	128.81	124.51
31	B1	618	BCR	C38-C26-C25	-3.11	121.04	124.53
48	s1	607	CHL	CHB-C4A-NA	3.11	128.81	124.51
51	y1	623	NEX	C20-C13-C14	-3.10	118.57	122.92
49	S	620	LUT	C35-C15-C14	-3.10	117.11	123.47
48	S1	601	CHL	CMA-C3A-C4A	3.10	120.12	111.77
29	y	611	CLA	C1-C2-C3	-3.10	120.67	126.04
29	r1	604	CLA	C2C-C1C-NC	3.10	112.88	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	609	CLA	O1D-CGD-CBD	-3.10	118.14	124.48
49	n	620	LUT	C18-C5-C6	-3.10	121.04	124.53
29	S	604	CLA	C2D-C1D-ND	3.10	112.39	110.10
29	s	605	CLA	C1-C2-C3	-3.10	121.73	126.75
29	Y	610	CLA	CHD-C1D-ND	-3.10	121.60	124.45
29	G1	603	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
29	R	608	CLA	C1-O2A-CGA	3.10	124.58	116.44
29	B1	611	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
29	G	614	CLA	CHD-C1D-ND	-3.10	121.61	124.45
29	G1	610	CLA	CHD-C1D-ND	-3.10	121.61	124.45
48	g1	609	CHL	C4B-CHC-C1C	3.10	133.69	126.34
29	y	608	CLA	CMA-C3A-C4A	3.10	120.10	111.77
47	I1	102	4RF	O18-C16-C15	3.10	121.64	111.91
29	N	602	CLA	CMA-C3A-C4A	3.10	120.10	111.77
29	n	602	CLA	C4B-CHC-C1C	3.10	133.69	126.34
29	b	617	CLA	C1-C2-C3	-3.10	120.68	126.04
29	C1	502	CLA	C2C-C1C-NC	3.10	112.88	109.97
48	S	607	CHL	CHD-C1D-ND	-3.10	121.61	124.45
48	S	608	CHL	C3C-C4C-NC	-3.10	107.10	110.57
29	C	501	CLA	C2C-C1C-NC	3.10	112.87	109.97
29	b1	603	CLA	C2D-C1D-ND	3.10	112.39	110.10
31	C1	516	BCR	C28-C27-C26	-3.10	108.55	114.08
29	A1	405	CLA	C1-C2-C3	-3.10	120.69	126.04
29	s1	617	CLA	C2C-C1C-NC	3.10	112.87	109.97
29	n	602	CLA	CMC-C2C-C1C	3.10	129.75	125.04
48	S	606	CHL	C3B-C4B-NB	-3.09	107.64	110.52
48	G	608	CHL	CHD-C1D-ND	-3.09	121.61	124.45
49	s	621	LUT	C38-C25-C24	-3.09	116.94	123.56
29	c1	504	CLA	CHD-C1D-ND	-3.09	121.61	124.45
48	S1	608	CHL	CHD-C1D-ND	-3.09	121.61	124.45
45	h1	101	RRX	C19-C18-C17	-3.09	114.20	118.94
48	G1	606	CHL	C1-O2A-CGA	3.09	124.56	116.44
29	b	610	CLA	CHD-C1D-ND	-3.09	121.61	124.45
29	A	410	CLA	CHD-C1D-ND	-3.09	121.61	124.45
29	s1	617	CLA	CMA-C3A-C4A	3.09	120.08	111.77
31	C1	514	BCR	C15-C14-C13	-3.09	122.90	127.31
29	R	612	CLA	CHD-C1D-ND	-3.09	121.61	124.45
50	N	622	XAT	C6-C7-C8	-3.09	119.46	125.99
29	C	508	CLA	CMB-C2B-C1B	-3.09	120.67	125.37
29	s	603	CLA	CMA-C3A-C4A	3.09	120.07	111.77
29	N	610	CLA	C1-C2-C3	-3.09	120.70	126.04
48	n	601	CHL	CMA-C3A-C4A	3.09	120.07	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	R1	621	XAT	C38-C25-C26	-3.09	117.08	122.26
49	S1	621	LUT	C15-C14-C13	-3.09	122.90	127.31
29	N1	603	CLA	C1-O2A-CGA	3.09	124.54	116.44
31	a1	411	BCR	C8-C7-C6	-3.09	118.53	127.20
33	c	521	LMG	O8-C28-C29	3.09	121.59	111.91
29	y	612	CLA	CHD-C1D-ND	-3.09	121.62	124.45
29	R1	608	CLA	CHD-C1D-ND	-3.09	121.62	124.45
48	Y	609	CHL	C1-C2-C3	-3.09	120.71	126.04
48	s	607	CHL	C4A-NA-C1A	3.09	108.09	106.71
29	A	406	CLA	CHD-C1D-ND	-3.08	121.62	124.45
50	N1	622	XAT	O24-C25-C24	3.08	115.70	113.38
31	b1	619	BCR	C33-C5-C4	3.08	119.54	113.62
29	a1	406	CLA	CHD-C1D-ND	-3.08	121.62	124.45
51	n	623	NEX	C26-C27-C28	-3.08	119.47	125.99
29	C	511	CLA	CHD-C1D-ND	-3.08	121.62	124.45
29	g1	614	CLA	CHD-C1D-ND	-3.08	121.62	124.45
29	B	614	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
48	y	605	CHL	C2C-C3C-C4C	3.08	108.69	106.49
29	D	402	CLA	C1D-ND-C4D	-3.08	104.15	106.33
29	B	609	CLA	C2C-C1C-NC	3.08	112.86	109.97
29	Y	610	CLA	O2A-CGA-CBA	3.08	121.57	111.91
48	Y	605	CHL	C3B-C4B-NB	-3.08	107.66	110.52
30	A	409	PHO	O2D-CGD-O1D	-3.08	117.82	123.84
29	G1	610	CLA	CMA-C3A-C4A	3.08	120.05	111.77
29	C	505	CLA	C2C-C1C-NC	3.08	112.86	109.97
29	b1	609	CLA	C2C-C1C-NC	3.08	112.86	109.97
29	G	611	CLA	CHD-C1D-ND	-3.08	121.63	124.45
48	G	606	CHL	C2C-C3C-C4C	3.08	108.68	106.49
29	g	612	CLA	C2D-C1D-ND	3.08	112.37	110.10
29	G1	611	CLA	CMA-C3A-C4A	3.08	120.04	111.77
29	S1	609	CLA	C2D-C1D-ND	3.07	112.37	110.10
29	s	602	CLA	C3B-C4B-NB	-3.07	107.66	110.52
29	G	602	CLA	CHD-C1D-ND	-3.07	121.63	124.45
51	y1	623	NEX	C31-C32-C33	3.07	135.05	126.42
29	g	610	CLA	C1-C2-C3	-3.07	120.73	126.04
39	c1	524	DGA	OG1-CA1-CA2	3.07	121.55	111.91
29	N	611	CLA	CHD-C1D-ND	-3.07	121.63	124.45
29	Y	604	CLA	CHD-C1D-ND	-3.07	121.63	124.45
29	c	502	CLA	CHD-C1D-ND	-3.07	121.63	124.45
29	c	511	CLA	CHD-C1D-ND	-3.07	121.63	124.45
29	s1	614	CLA	C1-C2-C3	-3.07	120.73	126.04
31	a1	411	BCR	C4-C5-C6	-3.07	118.27	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	612	CLA	C2C-C1C-NC	3.07	112.85	109.97
29	s1	603	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
29	C1	501	CLA	C2D-C1D-ND	3.07	112.37	110.10
30	a	408	PHO	CMB-C2B-C3B	3.07	130.42	124.68
48	s	608	CHL	C3C-C4C-NC	-3.07	107.13	110.57
48	g	609	CHL	C2C-C3C-C4C	3.07	108.68	106.49
51	G1	623	NEX	C27-C28-C29	-3.07	120.77	125.53
29	s1	603	CLA	CHD-C1D-ND	-3.07	121.63	124.45
51	G1	623	NEX	C31-C30-C29	3.07	131.69	127.31
29	s	605	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
51	R	622	NEX	C39-C29-C30	-3.07	118.62	122.92
29	B1	610	CLA	C2D-C1D-ND	3.07	112.36	110.10
31	C	517	BCR	C19-C18-C17	3.07	123.65	118.94
29	B1	606	CLA	C1-C2-C3	-3.07	120.74	126.04
51	r	622	NEX	C39-C29-C30	-3.07	118.63	122.92
29	c	507	CLA	CHD-C1D-ND	-3.07	121.64	124.45
29	C	507	CLA	C1-C2-C3	-3.07	120.74	126.04
29	Y	603	CLA	C2D-C1D-ND	3.07	112.36	110.10
49	N1	621	LUT	C16-C1-C6	-3.07	105.33	110.30
48	n1	609	CHL	C4D-CHA-C1A	3.07	124.98	121.25
48	S	607	CHL	CMA-C3A-C4A	3.07	120.01	111.77
29	g	613	CLA	C1-C2-C3	-3.06	120.74	126.04
48	Y	605	CHL	C4B-CHC-C1C	3.06	133.60	126.34
29	r1	602	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
29	G	614	CLA	C2C-C1C-NC	3.06	112.84	109.97
29	S	609	CLA	C2C-C1C-NC	3.06	112.84	109.97
29	b	616	CLA	C3B-C4B-NB	-3.06	107.67	110.52
48	N	607	CHL	CHB-C4A-NA	3.06	128.75	124.51
29	Y1	608	CLA	CMC-C2C-C1C	3.06	129.70	125.04
29	a	406	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
29	a	407	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
29	R	602	CLA	C2D-C1D-ND	3.06	112.36	110.10
29	g	611	CLA	C2D-C1D-ND	3.06	112.36	110.10
48	R	606	CHL	C4B-CHC-C1C	3.06	133.60	126.34
31	d1	404	BCR	C34-C9-C10	-3.06	118.63	122.92
29	b1	606	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
29	g1	612	CLA	CMA-C3A-C4A	3.06	120.00	111.77
31	C1	514	BCR	C38-C26-C25	-3.06	121.09	124.53
29	A	410	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
31	D	404	BCR	C36-C18-C17	-3.06	118.64	122.92
29	b1	614	CLA	CHD-C1D-ND	-3.06	121.64	124.45
29	c1	502	CLA	C1-C2-C3	-3.06	120.75	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b1	615	CLA	C2C-C1C-NC	3.06	112.84	109.97
36	B	620	C7Z	C8-C7-C6	-3.06	118.61	127.20
29	b	606	CLA	C2D-C1D-ND	3.06	112.36	110.10
29	C1	503	CLA	C1-C2-C3	-3.06	120.75	126.04
29	B	604	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
51	y	623	NEX	C20-C13-C14	-3.06	118.64	122.92
29	g	613	CLA	C2C-C1C-NC	3.06	112.84	109.97
29	S	603	CLA	C1-C2-C3	-3.06	120.75	126.04
29	R1	608	CLA	C2D-C1D-ND	3.06	112.36	110.10
29	b	611	CLA	C1-C2-C3	-3.06	120.76	126.04
49	G1	621	LUT	C7-C8-C9	-3.06	121.62	126.23
29	b1	603	CLA	CHD-C1D-ND	-3.06	121.64	124.45
31	a1	411	BCR	C33-C5-C6	-3.06	121.10	124.53
49	s	621	LUT	C18-C5-C6	-3.06	121.10	124.53
48	N1	601	CHL	CHB-C4A-NA	3.06	128.74	124.51
48	g1	607	CHL	C1-O2A-CGA	3.06	124.46	116.44
29	s1	610	CLA	CAC-C3C-C4C	3.06	128.78	124.81
31	d	404	BCR	C19-C18-C17	3.06	123.63	118.94
51	Y1	623	NEX	C39-C29-C30	-3.06	118.64	122.92
29	g1	614	CLA	CMA-C3A-C4A	3.06	119.98	111.77
29	S1	610	CLA	CMD-C2D-C3D	-3.05	120.59	127.61
29	B	604	CLA	C2C-C1C-NC	3.05	112.83	109.97
29	y1	608	CLA	C2C-C1C-NC	3.05	112.83	109.97
29	a1	410	CLA	OBD-CAD-C3D	-3.05	121.17	128.52
47	I	102	4RF	O40-C41-C43	3.05	121.49	111.91
50	r	621	XAT	C18-C5-C6	-3.05	117.14	122.26
29	g1	603	CLA	C2C-C1C-NC	3.05	112.83	109.97
48	Y1	606	CHL	CHB-C4A-NA	3.05	128.73	124.51
29	y1	602	CLA	C1D-ND-C4D	-3.05	104.17	106.33
29	D1	403	CLA	C2C-C1C-NC	3.05	112.83	109.97
48	Y1	601	CHL	C1-C2-C3	-3.05	120.77	126.04
29	s1	614	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
48	s1	608	CHL	C4B-CHC-C1C	3.05	133.58	126.34
29	c1	505	CLA	CHD-C1D-ND	-3.05	121.65	124.45
29	R	610	CLA	C3B-C4B-NB	-3.05	107.69	110.52
29	C1	513	CLA	C2D-C1D-ND	3.05	112.35	110.10
45	H	101	RRX	C16-C17-C18	-3.05	122.96	127.31
48	S1	606	CHL	C2C-C3C-C4C	3.05	108.66	106.49
51	s1	623	NEX	C40-C33-C34	-3.05	118.65	122.92
45	H	101	RRX	C15-C16-C17	-3.05	117.23	123.47
29	c	502	CLA	CMA-C3A-C4A	3.05	119.97	111.77
29	g1	604	CLA	CHD-C1D-ND	-3.05	121.65	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	r1	608	CLA	C1-O2A-CGA	3.05	124.44	116.44
29	S	603	CLA	C2C-C1C-NC	3.05	112.83	109.97
29	c1	510	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
29	s1	613	CLA	CHD-C1D-ND	-3.05	121.65	124.45
29	y1	611	CLA	C7-C6-C5	-3.05	105.09	113.36
51	g	623	NEX	C31-C30-C29	3.05	131.66	127.31
48	Y1	609	CHL	CHB-C4A-NA	3.05	128.72	124.51
29	b	602	CLA	C2D-C1D-ND	3.05	112.35	110.10
29	N	613	CLA	O2A-CGA-CBA	3.04	121.46	111.91
29	B	617	CLA	C2C-C1C-NC	3.04	112.82	109.97
29	n	603	CLA	CBC-CAC-C3C	-3.04	104.04	112.43
29	C1	507	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
51	n	623	NEX	C39-C29-C30	-3.04	118.66	122.92
29	c	507	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
29	y1	608	CLA	CHD-C1D-ND	-3.04	121.66	124.45
29	S1	612	CLA	C2D-C1D-ND	3.04	112.35	110.10
45	h1	101	RRX	C15-C16-C17	-3.04	117.24	123.47
48	S1	601	CHL	C2C-C3C-C4C	3.04	108.66	106.49
29	B1	614	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
29	S	612	CLA	C2D-C1D-ND	3.04	112.34	110.10
29	S1	603	CLA	C2D-C1D-ND	3.04	112.34	110.10
48	n1	609	CHL	C3C-C4C-NC	-3.04	107.16	110.57
29	c1	509	CLA	CHD-C1D-ND	-3.04	121.66	124.45
48	G1	605	CHL	CHD-C1D-ND	-3.04	121.66	124.45
49	n1	620	LUT	C35-C34-C33	-3.04	122.97	127.31
29	s1	605	CLA	CMA-C3A-C4A	3.04	119.94	111.77
29	Y1	608	CLA	C3B-C4B-NB	-3.04	107.69	110.52
29	R1	603	CLA	C2C-C1C-NC	3.04	112.82	109.97
29	c1	508	CLA	CMA-C3A-C4A	3.04	119.94	111.77
29	Y	604	CLA	C2D-C1D-ND	3.04	112.34	110.10
29	B1	610	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
29	S	603	CLA	C3B-C4B-NB	-3.04	107.70	110.52
51	S1	623	NEX	C39-C29-C30	-3.04	118.67	122.92
29	b	602	CLA	CHD-C1D-ND	-3.04	121.66	124.45
29	C1	507	CLA	CHD-C1D-ND	-3.04	121.66	124.45
29	B1	608	CLA	C2D-C1D-ND	3.04	112.34	110.10
29	A	410	CLA	C2C-C1C-NC	3.04	112.82	109.97
48	N	601	CHL	CHB-C4A-NA	3.04	128.71	124.51
29	N1	603	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
29	S	617	CLA	C1-C2-C3	-3.04	121.84	126.75
29	r1	603	CLA	CMA-C3A-C4A	3.04	119.93	111.77
29	S1	613	CLA	C2D-C1D-ND	3.04	112.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	517	BCR	C23-C22-C21	3.04	123.60	118.94
29	Y1	604	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
29	A1	406	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
48	N1	607	CHL	C2C-C3C-C4C	3.03	108.65	106.49
48	G	608	CHL	C2B-C1B-NB	-3.03	108.20	110.23
48	S1	608	CHL	C4B-CHC-C1C	3.03	133.53	126.34
29	c1	511	CLA	C1-C2-C3	-3.03	120.80	126.04
33	H1	102	LMG	O7-C10-C11	3.03	118.04	111.50
29	G	613	CLA	C2C-C1C-NC	3.03	112.81	109.97
29	G	612	CLA	CMA-C3A-C4A	3.03	119.92	111.77
48	n1	601	CHL	CMA-C3A-C4A	3.03	119.92	111.77
36	B1	620	C7Z	C7-C8-C9	-3.03	121.65	126.23
29	Y	613	CLA	C1-C2-C3	-3.03	120.80	126.04
48	n1	607	CHL	C1-C2-C3	-3.03	120.80	126.04
48	n	601	CHL	C3B-C4B-NB	-3.03	107.70	110.52
48	G1	606	CHL	C4B-CHC-C1C	3.03	133.53	126.34
29	Y	613	CLA	CHD-C1D-ND	-3.03	121.67	124.45
51	g1	623	NEX	C38-C25-C26	-3.03	117.18	122.26
29	b1	613	CLA	C1-C2-C3	-3.03	120.80	126.04
49	S	621	LUT	C7-C8-C9	-3.03	121.66	126.23
29	s1	611	CLA	C3B-C4B-NB	-3.03	107.70	110.52
29	B1	603	CLA	C2C-C1C-NC	3.03	112.81	109.97
29	a1	407	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
48	n	601	CHL	CHB-C4A-NA	3.03	128.70	124.51
48	N	609	CHL	C4B-CHC-C1C	3.03	133.52	126.34
29	b	608	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
49	S1	621	LUT	C21-C26-C27	3.03	116.53	112.70
45	H1	101	RRX	C33-C5-C4	3.03	119.43	113.62
29	R1	608	CLA	C1-C2-C3	-3.03	120.81	126.04
29	B	608	CLA	C2C-C1C-NC	3.03	112.81	109.97
29	r1	602	CLA	C2D-C1D-ND	3.03	112.33	110.10
30	A1	409	PHO	C1A-C2A-C3A	-3.03	99.96	102.84
48	g	608	CHL	C4B-CHC-C1C	3.03	133.51	126.34
48	n1	606	CHL	C3C-C4C-NC	-3.03	107.18	110.57
29	b	607	CLA	O2A-CGA-CBA	3.03	121.40	111.91
29	b	603	CLA	C1-O2A-CGA	3.02	124.38	116.44
29	c1	505	CLA	C2D-C1D-ND	3.02	112.33	110.10
29	G1	612	CLA	C3B-C4B-NB	-3.02	107.71	110.52
29	S1	611	CLA	CMA-C3A-C4A	3.02	119.90	111.77
29	Y1	608	CLA	C2C-C1C-NC	3.02	112.81	109.97
29	g	602	CLA	CHD-C1D-ND	-3.02	121.67	124.45
29	s	612	CLA	CHD-C1D-ND	-3.02	121.67	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	y1	603	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
29	S1	602	CLA	CHD-C1D-ND	-3.02	121.68	124.45
29	Y	603	CLA	C2C-C1C-NC	3.02	112.80	109.97
48	Y	607	CHL	C3C-C4C-NC	-3.02	107.18	110.57
49	S	621	LUT	C15-C14-C13	-3.02	123.00	127.31
29	g1	614	CLA	CMD-C2D-C3D	-3.02	120.67	127.61
34	y	625	SPH	C3-C4-C5	-3.02	118.05	124.79
29	A1	405	CLA	C2C-C1C-NC	3.02	112.80	109.97
29	c1	503	CLA	C2C-C1C-NC	3.02	112.80	109.97
45	H	101	RRX	C30-C29-C28	-3.02	106.82	113.64
51	g	623	NEX	C1-C2-C3	3.02	120.46	113.64
29	r1	612	CLA	C1-C2-C3	-3.02	120.82	126.04
29	R1	609	CLA	C2C-C1C-NC	3.02	112.80	109.97
49	s1	620	LUT	C19-C9-C10	-3.02	118.70	122.92
48	y	601	CHL	CHC-C1C-NC	3.02	128.78	124.20
49	y	620	LUT	C2-C3-C4	-3.02	106.17	110.30
29	a1	410	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
49	g	621	LUT	C31-C30-C29	-3.02	123.01	127.31
48	G	605	CHL	C3C-C4C-NC	-3.01	107.19	110.57
29	r	604	CLA	CHD-C1D-ND	-3.01	121.68	124.45
29	y	608	CLA	CHD-C1D-ND	-3.01	121.68	124.45
48	N1	607	CHL	CMA-C3A-C4A	3.01	119.87	111.77
48	y1	607	CHL	C4B-CHC-C1C	3.01	133.49	126.34
29	b1	609	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
48	r1	607	CHL	C4D-CHA-C1A	3.01	124.92	121.25
29	Y	603	CLA	CHD-C1D-ND	-3.01	121.69	124.45
29	s1	617	CLA	C2D-C1D-ND	3.01	112.32	110.10
29	g	614	CLA	C2D-C1D-ND	3.01	112.32	110.10
51	r	622	NEX	C40-C33-C34	-3.01	118.71	122.92
29	s1	611	CLA	C1-C2-C3	-3.01	120.84	126.04
29	n1	603	CLA	CMA-C3A-C4A	3.01	119.86	111.77
29	B	602	CLA	C2D-C1D-ND	3.01	112.32	110.10
29	s	612	CLA	C2D-C1D-ND	3.01	112.32	110.10
29	y1	610	CLA	C2C-C1C-NC	3.01	112.79	109.97
29	S	605	CLA	CHD-C1D-ND	-3.01	121.69	124.45
29	R	612	CLA	C2D-C1D-ND	3.01	112.32	110.10
31	C	514	BCR	C12-C13-C14	-3.01	114.33	118.94
48	Y	607	CHL	CMA-C3A-C4A	3.01	119.85	111.77
29	G	602	CLA	C1-C2-C3	-3.01	120.84	126.04
29	B	602	CLA	CHD-C1D-ND	-3.01	121.69	124.45
29	C1	501	CLA	CHD-C1D-ND	-3.01	121.69	124.45
51	g	623	NEX	C39-C29-C30	-3.01	118.71	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b1	607	CLA	C1-C2-C3	-3.01	120.84	126.04
29	b1	608	CLA	C1-O2A-CGA	3.01	124.33	116.44
29	B1	611	CLA	C2D-C1D-ND	3.01	112.32	110.10
29	r1	609	CLA	CHD-C1D-ND	-3.01	121.69	124.45
29	S	602	CLA	C1C-C2C-C3C	-3.01	103.80	106.96
29	b1	603	CLA	C2C-C1C-NC	3.00	112.79	109.97
49	s1	621	LUT	C35-C15-C14	-3.00	117.32	123.47
29	R1	609	CLA	C2D-C1D-ND	3.00	112.32	110.10
29	g1	603	CLA	C2D-C1D-ND	3.00	112.32	110.10
48	G1	605	CHL	CHB-C4A-NA	3.00	128.67	124.51
48	y	605	CHL	CMA-C3A-C4A	3.00	119.84	111.77
48	G	608	CHL	C3B-C4B-NB	-3.00	107.73	110.52
29	b	611	CLA	C2D-C1D-ND	3.00	112.32	110.10
49	s	620	LUT	C38-C25-C24	-3.00	117.14	123.56
53	r	626	ERG	C19-C10-C1	-3.00	104.69	109.43
50	y	622	XAT	C19-C9-C10	-3.00	118.72	122.92
29	N	614	CLA	C1C-C2C-C3C	-3.00	103.80	106.96
29	a1	410	CLA	C1-C2-C3	-3.00	120.85	126.04
29	b	611	CLA	C1C-C2C-C3C	-3.00	103.80	106.96
29	s	602	CLA	C2D-C1D-ND	3.00	112.31	110.10
29	c1	505	CLA	C3B-C4B-NB	-3.00	107.73	110.52
40	s1	624	LHG	O8-C23-C24	3.00	121.32	111.91
29	B	611	CLA	CHD-C1D-ND	-3.00	121.70	124.45
48	g	608	CHL	C3C-C4C-NC	-3.00	107.21	110.57
50	r1	621	XAT	C19-C9-C10	-3.00	118.72	122.92
51	n	623	NEX	C31-C30-C29	3.00	131.59	127.31
52	R	625	LMT	C3'-C4'-C5'	-3.00	104.05	110.93
48	Y1	609	CHL	C1-O2A-CGA	3.00	124.31	116.44
30	a	408	PHO	O1D-CGD-CBD	3.00	129.73	124.74
48	G1	609	CHL	CMA-C3A-C4A	3.00	119.83	111.77
48	N1	607	CHL	C1-O2A-CGA	3.00	124.31	116.44
29	N	602	CLA	C1D-ND-C4D	-3.00	104.21	106.33
48	S1	601	CHL	C4B-CHC-C1C	3.00	133.45	126.34
29	B1	614	CLA	C1-C2-C3	-3.00	120.86	126.04
29	B1	612	CLA	CAC-C3C-C4C	3.00	128.70	124.81
29	y	604	CLA	CHD-C1D-ND	-3.00	121.70	124.45
29	n1	610	CLA	C2C-C1C-NC	3.00	112.78	109.97
38	b1	624	3PH	O31-C31-C32	3.00	121.31	111.91
29	N	614	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	B	619	BCR	C4-C5-C6	-2.99	118.38	122.73
29	N1	614	CLA	C2C-C1C-NC	2.99	112.78	109.97
29	y1	613	CLA	C2C-C1C-NC	2.99	112.78	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	603	CLA	CMA-C3A-C4A	2.99	119.82	111.77
29	b	608	CLA	CHD-C1D-ND	-2.99	121.70	124.45
51	s	623	NEX	C31-C30-C29	2.99	131.58	127.31
50	G1	622	XAT	C40-C33-C34	-2.99	118.73	122.92
29	a	406	CLA	CMD-C2D-C3D	-2.99	120.73	127.61
49	s	620	LUT	C10-C11-C12	-2.99	113.88	123.22
36	B1	620	C7Z	C23-C24-C25	2.99	117.81	111.85
29	Y	614	CLA	C3B-C4B-NB	-2.99	107.74	110.52
48	Y	607	CHL	C2C-C3C-C4C	2.99	108.62	106.49
29	B1	616	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
29	B	608	CLA	CHD-C1D-ND	-2.99	121.70	124.45
29	B1	608	CLA	CHD-C1D-ND	-2.99	121.70	124.45
29	G	602	CLA	C2C-C1C-NC	2.99	112.77	109.97
29	A	406	CLA	C2D-C1D-ND	2.99	112.31	110.10
29	B	607	CLA	CHD-C1D-ND	-2.99	121.71	124.45
29	r1	604	CLA	CHD-C1D-ND	-2.99	121.71	124.45
48	Y1	606	CHL	C3B-C4B-NB	-2.99	107.74	110.52
29	n	613	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
49	S	621	LUT	C35-C15-C14	-2.99	117.35	123.47
29	R	609	CLA	CHD-C1D-ND	-2.99	121.71	124.45
29	Y1	610	CLA	CHD-C1D-ND	-2.99	121.71	124.45
48	G1	608	CHL	C3C-C4C-NC	-2.99	107.22	110.57
29	B1	607	CLA	O1D-CGD-CBD	-2.99	118.37	124.48
52	R	625	LMT	C3B-C4B-C5B	-2.99	104.91	110.24
48	N1	605	CHL	CHB-C4A-NA	2.99	128.64	124.51
29	a	407	CLA	CHD-C1D-ND	-2.99	121.71	124.45
48	N	601	CHL	C3B-C4B-NB	-2.99	107.74	110.52
48	y1	606	CHL	CMA-C3A-C4A	2.99	119.80	111.77
29	S1	612	CLA	C2C-C1C-NC	2.99	112.77	109.97
48	S	608	CHL	CMA-C3A-C4A	2.99	119.80	111.77
29	s	613	CLA	C2C-C1C-NC	2.99	112.77	109.97
37	b1	623	DGD	O5D-C6D-C5D	2.99	114.57	109.05
29	B1	611	CLA	C1-C2-C3	-2.99	120.88	126.04
29	B	611	CLA	C1C-C2C-C3C	-2.99	103.82	106.96
48	Y	606	CHL	CHD-C1D-ND	-2.98	121.71	124.45
55	Y1	627	PTY	C6-O7-C8	-2.98	112.33	117.90
29	n1	604	CLA	C2C-C1C-NC	2.98	112.77	109.97
29	n1	614	CLA	CAA-C2A-C3A	-2.98	104.61	112.78
29	Y1	604	CLA	CHD-C1D-ND	-2.98	121.71	124.45
49	n1	620	LUT	C22-C23-C24	-2.98	108.34	111.74
29	D1	402	CLA	C3B-C4B-NB	-2.98	107.75	110.52
50	G1	622	XAT	O24-C25-C38	-2.98	111.48	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A1	407	CLA	CMA-C3A-C4A	2.98	119.79	111.77
48	S1	608	CHL	C3C-C4C-NC	-2.98	107.23	110.57
29	B	611	CLA	C4B-CHC-C1C	2.98	133.41	126.34
45	h	101	RRX	C33-C5-C4	2.98	119.34	113.62
29	G	603	CLA	C1-C2-C3	-2.98	120.89	126.04
31	B	619	BCR	C33-C5-C6	-2.98	121.18	124.53
29	B	615	CLA	CHD-C1D-ND	-2.98	121.72	124.45
48	S1	601	CHL	CHD-C1D-ND	-2.98	121.72	124.45
29	s	611	CLA	C2C-C1C-NC	2.98	112.76	109.97
29	C1	510	CLA	C1-C2-C3	-2.98	120.89	126.04
48	y1	605	CHL	C3B-C4B-NB	-2.98	107.75	110.52
48	n1	605	CHL	C4B-CHC-C1C	2.98	133.40	126.34
31	d	404	BCR	C4-C5-C6	-2.98	118.41	122.73
29	s	611	CLA	CMA-C3A-C4A	2.98	119.78	111.77
29	N	612	CLA	C3B-C4B-NB	-2.98	107.75	110.52
29	B	616	CLA	CHD-C1D-ND	-2.98	121.72	124.45
29	D	403	CLA	C2D-C1D-ND	2.98	112.30	110.10
29	g	610	CLA	C2D-C1D-ND	2.98	112.30	110.10
29	y1	604	CLA	C2D-C1D-ND	2.98	112.30	110.10
48	y	601	CHL	CMA-C3A-C4A	2.98	119.77	111.77
49	S	620	LUT	C38-C25-C24	-2.98	117.19	123.56
49	Y1	620	LUT	C7-C8-C9	-2.98	121.74	126.23
29	c	501	CLA	C3B-C4B-NB	-2.98	107.75	110.52
29	G1	611	CLA	C2D-C1D-ND	2.98	112.30	110.10
48	Y1	606	CHL	C2C-C3C-C4C	2.98	108.61	106.49
36	B	620	C7Z	C27-C28-C29	-2.98	121.74	126.23
53	r	626	ERG	C14-C8-C7	-2.98	118.52	124.38
29	Y1	603	CLA	CHD-C1D-ND	-2.98	121.72	124.45
51	n1	623	NEX	C27-C28-C29	-2.97	120.91	125.53
48	S	606	CHL	C3C-C4C-NC	-2.97	107.23	110.57
48	s1	601	CHL	C4D-CHA-C1A	2.97	124.87	121.25
31	B	619	BCR	C37-C22-C23	2.97	122.76	118.08
29	S	611	CLA	C3B-C4B-NB	-2.97	107.76	110.52
29	B	605	CLA	O2A-CGA-CBA	2.97	121.23	111.91
29	g	602	CLA	O2A-CGA-CBA	2.97	121.23	111.91
29	d1	403	CLA	CMA-C3A-C4A	2.97	119.76	111.77
49	y	620	LUT	C11-C10-C9	-2.97	123.07	127.31
29	a	405	CLA	C1D-ND-C4D	-2.97	104.22	106.33
48	S1	606	CHL	C2B-C1B-NB	-2.97	108.24	110.23
29	y1	612	CLA	C1-C2-C3	-2.97	120.90	126.04
29	C	501	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
29	g	613	CLA	CHD-C1D-ND	-2.97	121.72	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	y1	610	CLA	C2D-C1D-ND	2.97	112.29	110.10
49	s1	620	LUT	C18-C5-C6	-2.97	121.19	124.53
48	g	601	CHL	C3B-C4B-NB	-2.97	107.76	110.52
29	b	605	CLA	C11-C12-C13	-2.97	106.32	115.92
29	R1	612	CLA	C2D-C1D-ND	2.97	112.29	110.10
48	y1	609	CHL	CHB-C4A-NA	2.97	128.62	124.51
49	y	620	LUT	C38-C25-C24	-2.97	117.21	123.56
29	b	607	CLA	C1-C2-C3	-2.97	120.91	126.04
48	N1	608	CHL	CHB-C4A-NA	2.97	128.62	124.51
29	n1	614	CLA	CHD-C1D-ND	-2.97	121.73	124.45
29	b1	615	CLA	C1-C2-C3	-2.97	120.91	126.04
49	s1	620	LUT	C38-C25-C24	-2.97	117.21	123.56
48	y1	607	CHL	CHB-C4A-NA	2.97	128.61	124.51
48	R	607	CHL	CHD-C4C-C3C	2.97	129.20	124.84
48	y	609	CHL	C4B-CHC-C1C	2.96	133.37	126.34
49	r	620	LUT	C15-C14-C13	-2.96	123.08	127.31
48	y	609	CHL	CMA-C3A-C4A	2.96	119.74	111.77
53	r	626	ERG	C2-C1-C10	2.96	119.16	112.74
29	C	507	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
29	y	612	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
29	R1	612	CLA	CMA-C3A-C4A	2.96	119.74	111.77
48	G1	608	CHL	CMA-C3A-C4A	2.96	119.73	111.77
29	b	617	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
29	r1	609	CLA	C2D-C1D-ND	2.96	112.29	110.10
29	R	609	CLA	C2C-C1C-NC	2.96	112.75	109.97
31	c	517	BCR	C19-C18-C17	2.96	123.49	118.94
50	y	622	XAT	C38-C25-C26	-2.96	117.30	122.26
29	n	613	CLA	CMA-C3A-C4A	2.96	119.73	111.77
48	N	608	CHL	C3C-C4C-NC	-2.96	107.25	110.57
48	g1	607	CHL	CMA-C3A-C4A	2.96	119.73	111.77
29	b1	602	CLA	CHD-C1D-ND	-2.96	121.73	124.45
48	N	609	CHL	C3C-C4C-NC	-2.96	107.25	110.57
29	s	602	CLA	O2A-CGA-CBA	2.96	121.19	111.91
45	H	101	RRX	C20-C21-C22	2.96	131.53	127.31
50	r1	621	XAT	C27-C28-C29	2.96	130.12	125.53
29	n	610	CLA	O1D-CGD-CBD	-2.96	118.43	124.48
29	n	611	CLA	C2D-C1D-ND	2.96	112.28	110.10
51	G1	623	NEX	C17-C1-C6	-2.96	107.83	110.47
48	r	607	CHL	C4B-CHC-C1C	2.96	133.35	126.34
29	y	610	CLA	O2A-CGA-CBA	2.96	121.19	111.91
29	a1	407	CLA	CMA-C3A-C4A	2.96	119.72	111.77
51	r	622	NEX	C19-C9-C10	-2.96	118.78	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	Y	607	CHL	CHB-C4A-NA	2.95	128.60	124.51
29	Y1	602	CLA	O1D-CGD-CBD	-2.95	118.44	124.48
51	R1	622	NEX	C1-C2-C3	2.95	120.31	113.64
51	N1	623	NEX	C27-C28-C29	-2.95	120.95	125.53
48	n	609	CHL	C3C-C4C-NC	-2.95	107.26	110.57
29	c1	503	CLA	C1-C2-C3	-2.95	120.94	126.04
29	b1	614	CLA	C2C-C1C-NC	2.95	112.74	109.97
48	G1	601	CHL	C1-C2-C3	-2.95	120.94	126.04
29	N1	612	CLA	CHD-C1D-ND	-2.95	121.74	124.45
36	b1	620	C7Z	C18-C5-C6	-2.95	121.21	124.53
48	r1	607	CHL	CMA-C3A-C4A	2.95	119.71	111.77
29	g1	610	CLA	C2D-C1D-ND	2.95	112.28	110.10
48	S	608	CHL	C4B-CHC-C1C	2.95	133.34	126.34
29	s1	605	CLA	O2A-CGA-CBA	2.95	121.17	111.91
29	y	614	CLA	C2C-C1C-NC	2.95	112.74	109.97
29	A	410	CLA	C2D-C1D-ND	2.95	112.28	110.10
29	n1	602	CLA	C3B-C4B-NB	-2.95	107.78	110.52
29	N1	604	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
29	S1	614	CLA	CHD-C1D-ND	-2.95	121.74	124.45
29	n1	611	CLA	CHD-C1D-ND	-2.95	121.74	124.45
49	Y1	621	LUT	C3-C4-C5	-2.95	105.98	111.85
29	G1	612	CLA	CMA-C3A-C4A	2.95	119.70	111.77
29	a1	406	CLA	O2A-CGA-CBA	2.95	121.16	111.91
29	S1	614	CLA	C1-C2-C3	-2.95	120.95	126.04
48	n1	601	CHL	C1-C2-C3	-2.95	120.95	126.04
37	c1	519	DGD	O1G-C1A-C2A	2.95	121.15	111.91
29	D	403	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
29	n	602	CLA	CHD-C1D-ND	-2.95	121.75	124.45
29	c	501	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
29	y1	603	CLA	C1-C2-C3	-2.95	120.95	126.04
48	Y	606	CHL	C1-O2A-CGA	2.95	124.17	116.44
48	N	606	CHL	C4D-CHA-C1A	2.94	124.83	121.25
51	y1	623	NEX	C12-C13-C14	2.94	123.46	118.94
29	C1	509	CLA	C1-C2-C3	-2.94	120.95	126.04
29	n	610	CLA	C1-O2A-CGA	2.94	124.17	116.44
29	b1	602	CLA	CMA-C3A-C4A	2.94	119.68	111.77
48	S1	608	CHL	CMA-C3A-C4A	2.94	119.68	111.77
49	G1	621	LUT	C18-C5-C6	-2.94	121.22	124.53
29	r	603	CLA	C2C-C1C-NC	2.94	112.73	109.97
29	S1	613	CLA	C2C-C1C-NC	2.94	112.73	109.97
48	n	608	CHL	CMA-C3A-C4A	2.94	119.68	111.77
48	N1	605	CHL	C3C-C4C-NC	-2.94	107.27	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	515	BCR	C1-C6-C5	-2.94	118.47	122.61
48	r	607	CHL	CMA-C3A-C4A	2.94	119.68	111.77
29	G	603	CLA	C1C-C2C-C3C	-2.94	103.86	106.96
29	b1	616	CLA	C1C-C2C-C3C	-2.94	103.86	106.96
29	s1	614	CLA	C2D-C1D-ND	2.94	112.27	110.10
29	G	610	CLA	C2C-C1C-NC	2.94	112.73	109.97
29	b	613	CLA	CMD-C2D-C3D	-2.94	120.85	127.61
29	B1	610	CLA	C2C-C1C-NC	2.94	112.73	109.97
29	B1	605	CLA	C1C-C2C-C3C	-2.94	103.86	106.96
48	g	601	CHL	C1-O2A-CGA	2.94	124.16	116.44
29	B	611	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
49	N	620	LUT	C22-C23-C24	-2.94	108.39	111.74
29	C1	508	CLA	C2C-C1C-NC	2.94	112.73	109.97
29	g1	610	CLA	CMC-C2C-C1C	2.94	129.51	125.04
29	S	617	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
29	s	613	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
29	N	610	CLA	C2C-C1C-NC	2.94	112.72	109.97
29	b	608	CLA	C2C-C1C-NC	2.94	112.72	109.97
29	g	604	CLA	C3B-C4B-NB	-2.94	107.79	110.52
48	s1	607	CHL	C2C-C3C-C4C	2.94	108.58	106.49
48	y	601	CHL	C4A-NA-C1A	2.94	108.03	106.71
29	g	612	CLA	C4B-CHC-C1C	2.94	133.30	126.34
36	b	620	C7Z	C28-C27-C26	-2.94	118.96	127.20
49	N	620	LUT	C38-C25-C24	-2.94	117.28	123.56
29	s	614	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
29	b	617	CLA	C2D-C1D-ND	2.94	112.27	110.10
29	d	402	CLA	CHD-C1D-ND	-2.93	121.76	124.45
29	R1	612	CLA	CHD-C1D-ND	-2.93	121.76	124.45
31	C	514	BCR	C35-C13-C12	2.93	122.70	118.08
48	s1	601	CHL	C3C-C4C-NC	-2.93	107.28	110.57
48	r	606	CHL	CMA-C3A-C4A	2.93	119.66	111.77
48	r1	607	CHL	C1-O2A-CGA	2.93	124.14	116.44
48	s	601	CHL	C2B-C1B-NB	-2.93	108.27	110.23
29	y1	614	CLA	C3B-C4B-NB	-2.93	107.79	110.52
31	b	618	BCR	C1-C6-C7	2.93	124.08	115.78
49	g1	620	LUT	C39-C29-C28	2.93	122.70	118.08
29	s	612	CLA	C2C-C1C-NC	2.93	112.72	109.97
29	c	504	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
29	s	602	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
29	B1	609	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
29	G1	614	CLA	CHD-C1D-ND	-2.93	121.76	124.45
29	y1	603	CLA	CHD-C1D-ND	-2.93	121.76	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a1	407	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
31	D1	404	BCR	C38-C26-C25	-2.93	121.24	124.53
29	B1	605	CLA	O2A-CGA-CBA	2.93	121.10	111.91
29	s	611	CLA	C1-C2-C3	-2.93	120.97	126.04
29	y	604	CLA	C2C-C1C-NC	2.93	112.72	109.97
29	c	512	CLA	C2D-C1D-ND	2.93	112.26	110.10
29	b	609	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
48	G	607	CHL	CHB-C4A-NA	2.93	128.56	124.51
29	C	513	CLA	C3B-C4B-NB	-2.93	107.80	110.52
29	s1	602	CLA	O2A-CGA-CBA	2.93	121.10	111.91
29	s1	603	CLA	C1-C2-C3	-2.93	120.98	126.04
48	S	608	CHL	C3B-C4B-NB	-2.93	107.80	110.52
29	n	604	CLA	CHD-C1D-ND	-2.93	121.76	124.45
49	R1	620	LUT	C18-C5-C4	2.93	119.78	114.36
29	S1	611	CLA	C3B-C4B-NB	-2.93	107.80	110.52
50	G	622	XAT	C38-C25-C26	-2.93	117.36	122.26
48	G	608	CHL	C2C-C3C-C4C	2.93	108.58	106.49
29	c	513	CLA	C2C-C1C-NC	2.93	112.71	109.97
29	G1	602	CLA	C2A-C1A-CHA	2.93	128.97	123.86
29	s	613	CLA	C1-O2A-CGA	2.93	124.12	116.44
29	G	613	CLA	C2D-C1D-ND	2.93	112.26	110.10
29	g	611	CLA	CMA-C3A-C4A	2.92	119.63	111.77
48	n	609	CHL	CHD-C4C-C3C	2.92	129.14	124.84
29	s1	602	CLA	C6-C5-C3	-2.92	105.79	113.45
29	Y1	613	CLA	O2A-CGA-CBA	2.92	121.08	111.91
29	b	607	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	C	517	BCR	C33-C5-C6	-2.92	121.25	124.53
29	b1	603	CLA	O2A-CGA-CBA	2.92	121.08	111.91
29	B1	605	CLA	C1-C2-C3	-2.92	120.99	126.04
29	S1	605	CLA	C1-C2-C3	-2.92	122.02	126.75
29	B1	613	CLA	C1C-C2C-C3C	-2.92	103.88	106.96
51	n1	623	NEX	C38-C25-C26	-2.92	117.36	122.26
43	D1	405	PL9	C8-C7-C3	2.92	120.24	111.98
40	D	409	LHG	O8-C23-C24	2.92	121.07	111.91
29	b1	603	CLA	C1-O2A-CGA	2.92	124.10	116.44
29	y1	610	CLA	CHD-C1D-ND	-2.92	121.77	124.45
29	y1	611	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
29	G	603	CLA	C2C-C1C-NC	2.92	112.71	109.97
48	Y1	607	CHL	CMA-C3A-C4A	2.92	119.62	111.77
29	Y1	613	CLA	C2D-C1D-ND	2.92	112.25	110.10
48	n1	609	CHL	C1-O2A-CGA	2.92	124.10	116.44
33	h1	102	LMG	O8-C28-C29	2.92	121.07	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	N1	624	LHG	O8-C23-C24	2.92	121.07	111.91
53	R	626	ERG	C19-C10-C1	-2.92	104.82	109.43
29	B	616	CLA	C4B-CHC-C1C	2.92	133.26	126.34
29	b1	609	CLA	C3B-C4B-NB	-2.92	107.81	110.52
29	C	505	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
29	y1	612	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
29	s	605	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	C1	515	BCR	C33-C5-C4	2.92	119.22	113.62
43	D1	405	PL9	C40-C39-C41	2.92	120.18	115.27
29	n	613	CLA	C1-C2-C3	-2.92	121.00	126.04
29	c	503	CLA	C2C-C1C-NC	2.92	112.70	109.97
40	C	525	LHG	O8-C23-C24	2.91	121.06	111.91
29	G	614	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
48	g	609	CHL	C3C-C4C-NC	-2.91	107.30	110.57
29	s1	604	CLA	C2C-C1C-NC	2.91	112.70	109.97
31	c	515	BCR	C34-C9-C10	-2.91	118.84	122.92
31	C	514	BCR	C23-C24-C25	-2.91	119.02	127.20
29	c1	507	CLA	CMA-C3A-C4A	2.91	119.60	111.77
29	b	607	CLA	C2C-C1C-NC	2.91	112.70	109.97
29	s1	611	CLA	C1C-C2C-C3C	-2.91	103.89	106.96
48	y1	605	CHL	C4B-CHC-C1C	2.91	133.24	126.34
29	a	407	CLA	CMA-C3A-C4A	2.91	119.60	111.77
29	b1	608	CLA	C2D-C1D-ND	2.91	112.25	110.10
47	i	101	4RF	O40-C41-C43	2.91	121.04	111.91
29	r	604	CLA	C2C-C1C-NC	2.91	112.70	109.97
29	C	513	CLA	CBA-CAA-C2A	2.91	122.45	113.86
29	g	603	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
51	g	623	NEX	C2-C1-C6	2.91	112.04	109.21
29	N	604	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
29	b	602	CLA	CMA-C3A-C4A	2.91	119.59	111.77
48	n1	605	CHL	C3B-C4B-NB	-2.91	107.82	110.52
48	g	606	CHL	C2C-C3C-C4C	2.91	108.56	106.49
49	Y	621	LUT	C38-C25-C24	-2.91	117.34	123.56
48	N	607	CHL	C3C-C4C-NC	-2.91	107.31	110.57
29	C	503	CLA	C2C-C1C-NC	2.91	112.70	109.97
51	r	622	NEX	C5-C6-C1	2.91	122.58	119.70
49	g	621	LUT	C38-C25-C24	-2.91	117.34	123.56
29	C1	513	CLA	CMA-C3A-C4A	2.91	119.58	111.77
48	n1	601	CHL	C3B-C4B-NB	-2.91	107.82	110.52
48	g1	608	CHL	CMA-C3A-C4A	2.91	119.58	111.77
29	B	610	CLA	CHD-C1D-ND	-2.91	121.78	124.45
29	S1	610	CLA	C4B-CHC-C1C	2.91	133.23	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y	614	CLA	C2C-C1C-NC	2.90	112.69	109.97
29	S	610	CLA	CHD-C1D-ND	-2.90	121.78	124.45
29	c1	511	CLA	C1C-C2C-C3C	-2.90	103.90	106.96
29	C1	505	CLA	C2D-C1D-ND	2.90	112.24	110.10
48	Y	609	CHL	CMA-C3A-C4A	2.90	119.58	111.77
29	a1	410	CLA	C1C-C2C-C3C	-2.90	103.90	106.96
29	B	609	CLA	CMA-C3A-C4A	2.90	119.58	111.77
29	y1	602	CLA	C3B-C4B-NB	-2.90	107.82	110.52
29	r1	603	CLA	C1-O2A-CGA	2.90	124.06	116.44
47	I1	102	4RF	O40-C41-C43	2.90	121.02	111.91
45	h	101	RRX	C36-C18-C19	2.90	122.65	118.08
49	Y	620	LUT	C31-C30-C29	-2.90	123.17	127.31
29	b	616	CLA	CHD-C1D-ND	-2.90	121.79	124.45
29	Y1	613	CLA	CHD-C1D-ND	-2.90	121.79	124.45
29	B	616	CLA	C6-C5-C3	-2.90	105.85	113.45
29	C1	509	CLA	CHD-C1D-ND	-2.90	121.79	124.45
48	n	605	CHL	C1-C2-C3	-2.90	121.03	126.04
29	S1	611	CLA	CHA-C4D-ND	2.90	138.57	132.50
48	Y1	607	CHL	C3C-C4C-NC	-2.90	107.32	110.57
48	R1	607	CHL	CMA-C3A-C4A	2.90	119.57	111.77
29	y	614	CLA	CMA-C3A-C4A	2.90	119.56	111.77
48	g1	608	CHL	C3B-C4B-NB	-2.90	107.83	110.52
53	r	626	ERG	C6-C7-C8	-2.90	116.36	122.07
29	B	610	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
29	r	610	CLA	C2D-C1D-ND	2.90	112.24	110.10
29	b1	609	CLA	CMA-C3A-C4A	2.90	119.56	111.77
29	c	504	CLA	C3B-C4B-NB	-2.90	107.83	110.52
48	y	607	CHL	C1-C2-C3	-2.90	121.03	126.04
29	s	617	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
48	G	607	CHL	CMA-C3A-C4A	2.90	119.56	111.77
30	A1	408	PHO	O2D-CGD-O1D	-2.90	118.17	123.84
48	G1	605	CHL	C4A-NA-C1A	2.90	108.01	106.71
29	b	605	CLA	CMA-C3A-C4A	2.90	119.56	111.77
29	C	509	CLA	CHD-C1D-ND	-2.90	121.79	124.45
29	C1	504	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
29	a1	410	CLA	O2A-CGA-CBA	2.90	120.99	111.91
50	G	622	XAT	O24-C25-C24	2.90	115.56	113.38
48	N1	607	CHL	CHB-C4A-NA	2.89	128.51	124.51
33	C	521	LMG	O8-C28-C29	2.89	120.99	111.91
37	c	519	DGD	O1G-C1A-C2A	2.89	120.99	111.91
29	C	502	CLA	C2D-C1D-ND	2.89	112.24	110.10
38	t	101	3PH	O31-C31-C32	2.89	120.98	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s	603	CLA	C2D-C1D-ND	2.89	112.23	110.10
29	b	604	CLA	O2A-CGA-CBA	2.89	120.98	111.91
29	g	603	CLA	CHD-C1D-ND	-2.89	121.80	124.45
48	g1	609	CHL	CHB-C4A-NA	2.89	128.51	124.51
29	s	617	CLA	O2A-CGA-CBA	2.89	120.98	111.91
29	c1	501	CLA	C1-C2-C3	-2.89	121.04	126.04
29	y	602	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
29	s1	611	CLA	OBD-CAD-C3D	-2.89	121.56	128.52
30	A1	408	PHO	C2D-C1D-ND	-2.89	107.53	109.53
29	y1	612	CLA	CMA-C3A-C4A	2.89	119.54	111.77
51	S	623	NEX	C19-C9-C10	-2.89	118.88	122.92
51	n	623	NEX	C5-C4-C3	2.89	115.17	111.75
29	B1	603	CLA	C2D-C1D-ND	2.89	112.23	110.10
29	b	616	CLA	C2C-C1C-NC	2.89	112.68	109.97
29	B1	613	CLA	CHD-C1D-ND	-2.89	121.80	124.45
48	S	606	CHL	C4D-CHA-C1A	2.89	124.76	121.25
31	c	515	BCR	C37-C22-C23	2.89	122.62	118.08
29	s1	609	CLA	C1-C2-C3	-2.89	121.05	126.04
29	b	614	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
51	R1	622	NEX	C40-C33-C34	-2.89	118.88	122.92
29	r1	608	CLA	CMA-C3A-C4A	2.89	119.53	111.77
29	r	603	CLA	CMA-C3A-C4A	2.88	119.53	111.77
29	b	609	CLA	C2D-C1D-ND	2.88	112.23	110.10
29	n	603	CLA	C1C-C2C-C3C	-2.88	103.92	106.96
48	y1	609	CHL	C1-C2-C3	-2.88	121.06	126.04
29	G1	602	CLA	O1D-CGD-CBD	-2.88	118.58	124.48
31	C	516	BCR	C27-C26-C25	-2.88	118.54	122.73
48	y	607	CHL	C4D-CHA-C1A	2.88	124.76	121.25
48	y1	601	CHL	CMA-C3A-C4A	2.88	119.52	111.77
48	y	609	CHL	C3B-C4B-NB	-2.88	107.84	110.52
30	a1	409	PHO	O2D-CGD-O1D	-2.88	118.20	123.84
29	b	603	CLA	O2A-CGA-CBA	2.88	120.95	111.91
29	C	511	CLA	C2C-C1C-NC	2.88	112.67	109.97
29	B1	617	CLA	C2C-C1C-NC	2.88	112.67	109.97
29	g	611	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
29	B1	607	CLA	C3B-C4B-NB	-2.88	107.84	110.52
29	c	504	CLA	C1D-ND-C4D	-2.88	104.29	106.33
29	g	610	CLA	O1D-CGD-CBD	-2.88	118.59	124.48
48	s	607	CHL	C2C-C3C-C4C	2.88	108.54	106.49
49	S	620	LUT	C40-C33-C32	2.88	122.61	118.08
29	S1	617	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
31	b1	618	BCR	C36-C18-C17	-2.88	118.89	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	N1	623	NEX	C40-C33-C34	-2.88	118.89	122.92
29	c	511	CLA	O2A-CGA-CBA	2.88	120.94	111.91
51	Y	623	NEX	C31-C30-C29	2.88	131.42	127.31
54	s1	625	LPX	O3-P1-O4	2.88	126.46	112.24
29	c1	501	CLA	O2A-CGA-CBA	2.88	120.94	111.91
48	S	601	CHL	C3C-C4C-NC	-2.88	107.34	110.57
29	b1	606	CLA	CHD-C1D-ND	-2.88	121.81	124.45
29	r1	608	CLA	C4B-CHC-C1C	2.88	133.16	126.34
29	b	614	CLA	C2D-C1D-ND	2.88	112.22	110.10
29	g1	611	CLA	C2D-C1D-ND	2.88	112.22	110.10
29	s1	610	CLA	CHD-C1D-ND	-2.87	121.81	124.45
48	N	606	CHL	C3C-C4C-NC	-2.87	107.35	110.57
29	n	614	CLA	CAA-C2A-C3A	-2.87	104.91	112.78
48	s1	608	CHL	C1-C2-C3	-2.87	121.07	126.04
29	R1	610	CLA	CMA-C3A-C4A	2.87	119.50	111.77
29	B	609	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
29	C	505	CLA	C3B-C4B-NB	-2.87	107.85	110.52
29	a	410	CLA	C1-C2-C3	-2.87	121.07	126.04
48	Y1	606	CHL	C2B-C1B-NB	-2.87	108.31	110.23
29	s1	614	CLA	CMA-C3A-C4A	2.87	119.49	111.77
29	b	609	CLA	C1-C2-C3	-2.87	121.08	126.04
29	N1	611	CLA	CMD-C2D-C3D	-2.87	121.01	127.61
29	g1	610	CLA	O1D-CGD-CBD	-2.87	118.61	124.48
45	H1	101	RRX	C36-C18-C19	2.87	122.60	118.08
29	G	612	CLA	C1D-ND-C4D	-2.87	104.30	106.33
29	B	607	CLA	CMA-C3A-C4A	2.87	119.49	111.77
48	Y1	606	CHL	C4B-CHC-C1C	2.87	133.15	126.34
44	F1	101	HEM	C4A-NA-C1A	2.87	108.16	105.35
29	B1	612	CLA	C2C-C1C-NC	2.87	112.66	109.97
29	C1	501	CLA	C2C-C1C-NC	2.87	112.66	109.97
29	N	611	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
29	n1	610	CLA	C1D-ND-C4D	-2.87	104.30	106.33
29	S	617	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	Y	608	CLA	C2D-C1D-ND	2.87	112.22	110.10
29	c1	504	CLA	C1-O2A-CGA	2.87	123.97	116.44
29	B	603	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
45	h1	101	RRX	C8-C9-C10	-2.87	114.54	118.94
29	B	604	CLA	CHD-C1D-ND	-2.87	121.82	124.45
29	b	605	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
29	a	405	CLA	CMC-C2C-C1C	2.87	129.41	125.04
51	g1	623	NEX	C27-C28-C29	-2.87	121.08	125.53
31	b	618	BCR	C23-C24-C25	-2.87	119.15	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c1	501	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
48	G1	607	CHL	C1-C2-C3	-2.87	121.09	126.04
29	R	602	CLA	O2A-CGA-CBA	2.87	120.90	111.91
29	s1	609	CLA	C1D-ND-C4D	-2.87	104.30	106.33
29	b1	612	CLA	OBD-CAD-C3D	-2.87	121.62	128.52
45	H	101	RRX	C30-C25-C26	-2.87	118.58	122.61
48	N	606	CHL	CMA-C3A-C4A	2.86	119.47	111.77
29	S1	605	CLA	C1-O2A-CGA	2.86	123.96	116.44
37	C	519	DGD	O1G-C1A-C2A	2.86	120.89	111.91
29	R	604	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
29	R	608	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
29	N	603	CLA	C2D-C1D-ND	2.86	112.21	110.10
48	y1	609	CHL	CMA-C3A-C4A	2.86	119.47	111.77
48	r	607	CHL	C3B-C4B-NB	-2.86	107.86	110.52
29	n	614	CLA	C2C-C1C-NC	2.86	112.65	109.97
29	g1	612	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
29	g1	603	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
38	S	626	3PH	O31-C31-C32	2.86	120.89	111.91
29	C	506	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
29	s	602	CLA	CHD-C1D-ND	-2.86	121.82	124.45
29	n1	603	CLA	C2D-C1D-ND	2.86	112.21	110.10
50	r1	621	XAT	C20-C13-C14	-2.86	118.92	122.92
29	s1	602	CLA	CMA-C3A-C4A	2.86	119.46	111.77
29	b1	605	CLA	C2C-C1C-NC	2.86	112.65	109.97
29	b1	607	CLA	C2C-C1C-NC	2.86	112.65	109.97
51	r1	622	NEX	C39-C29-C30	-2.86	118.92	122.92
29	b1	610	CLA	CHD-C1D-ND	-2.86	121.83	124.45
48	s	607	CHL	CHD-C1D-ND	-2.86	121.83	124.45
29	r	609	CLA	C2C-C1C-NC	2.86	112.65	109.97
49	s	620	LUT	C7-C8-C9	-2.86	121.91	126.23
50	R	621	XAT	C38-C25-C26	-2.86	117.47	122.26
29	Y1	610	CLA	C1-C2-C3	-2.86	121.10	126.04
29	B1	613	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
29	S1	602	CLA	C3B-C4B-NB	-2.86	107.86	110.52
29	R	602	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
31	C	514	BCR	C38-C26-C25	-2.86	121.32	124.53
48	y1	606	CHL	C2C-C3C-C4C	2.86	108.53	106.49
29	N1	611	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
51	r	622	NEX	C31-C30-C29	2.86	131.39	127.31
29	s1	613	CLA	C2D-C1D-ND	2.86	112.21	110.10
29	s	613	CLA	CMA-C3A-C4A	2.86	119.45	111.77
49	R	620	LUT	C8-C7-C6	-2.86	119.18	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	y1	604	CLA	C1-O2A-CGA	2.86	123.94	116.44
29	n1	614	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
29	a1	407	CLA	O1D-CGD-CBD	-2.86	118.64	124.48
29	Y	614	CLA	C1-C2-C3	-2.86	121.11	126.04
29	G	613	CLA	C1C-C2C-C3C	-2.85	103.95	106.96
29	s	603	CLA	C3B-C4B-NB	-2.85	107.87	110.52
29	b	617	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
30	A	408	PHO	O2D-CGD-O1D	-2.85	118.26	123.84
48	S1	607	CHL	CMA-C3A-C4A	2.85	119.44	111.77
29	r1	612	CLA	C2D-C1D-ND	2.85	112.21	110.10
29	S	609	CLA	CHD-C1D-ND	-2.85	121.83	124.45
37	C1	519	DGD	O1G-C1A-C2A	2.85	120.86	111.91
29	b	602	CLA	C2C-C1C-NC	2.85	112.64	109.97
31	a	411	BCR	C33-C5-C6	-2.85	121.33	124.53
29	N	613	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
29	r1	610	CLA	CMC-C2C-C1C	2.85	129.38	125.04
29	D	403	CLA	C2C-C1C-NC	2.85	112.64	109.97
51	R	622	NEX	C40-C33-C34	-2.85	118.93	122.92
53	r	626	ERG	C16-C17-C13	2.85	107.28	103.84
29	B1	605	CLA	C2D-C1D-ND	2.85	112.20	110.10
48	y	601	CHL	CHD-C4C-C3C	2.85	129.03	124.84
29	r1	603	CLA	C3B-C4B-NB	-2.85	107.87	110.52
48	R1	606	CHL	C3B-C4B-NB	-2.85	107.87	110.52
48	G	608	CHL	C3C-C4C-NC	-2.85	107.38	110.57
49	R	620	LUT	C1-C6-C5	-2.85	118.60	122.61
48	Y	605	CHL	CMA-C3A-C4A	2.85	119.43	111.77
29	G	604	CLA	CHD-C1D-ND	-2.85	121.84	124.45
29	b1	610	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
31	B	619	BCR	C23-C22-C21	-2.85	114.57	118.94
29	c	513	CLA	CBA-CAA-C2A	2.85	122.27	113.86
29	A1	407	CLA	CHD-C1D-ND	-2.85	121.84	124.45
29	Y1	612	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
29	B1	614	CLA	CHA-C4D-ND	2.85	138.45	132.50
29	N	603	CLA	C1-O2A-CGA	2.85	123.91	116.44
29	B	612	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
29	y	603	CLA	C1C-C2C-C3C	-2.85	103.97	106.96
29	c1	506	CLA	C2D-C1D-ND	2.84	112.20	110.10
29	c1	501	CLA	CMA-C3A-C4A	2.84	119.42	111.77
29	N	612	CLA	C2C-C1C-NC	2.84	112.64	109.97
48	Y	609	CHL	C2C-C3C-C4C	2.84	108.52	106.49
29	s1	617	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
30	a1	408	PHO	O2D-CGD-O1D	-2.84	118.28	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	R	609	CLA	C3B-C4B-NB	-2.84	107.88	110.52
29	Y1	602	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
48	g	608	CHL	C2C-C3C-C4C	2.84	108.52	106.49
51	Y1	623	NEX	C27-C28-C29	-2.84	121.12	125.53
48	S1	606	CHL	CHB-C4A-NA	2.84	128.44	124.51
29	S	614	CLA	C2C-C1C-NC	2.84	112.63	109.97
29	S1	609	CLA	C2C-C1C-NC	2.84	112.63	109.97
29	B	606	CLA	C2D-C1D-ND	2.84	112.20	110.10
29	c	502	CLA	C2D-C1D-ND	2.84	112.20	110.10
29	c1	506	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
29	y1	614	CLA	CHD-C1D-ND	-2.84	121.84	124.45
48	Y1	606	CHL	CMA-C3A-C4A	2.84	119.41	111.77
31	d	404	BCR	C35-C13-C12	2.84	122.55	118.08
29	g	614	CLA	CMA-C3A-C4A	2.84	119.41	111.77
29	g	610	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
29	S	611	CLA	C2D-C1D-ND	2.84	112.20	110.10
29	Y1	611	CLA	C1-C2-C3	-2.84	121.13	126.04
48	n	606	CHL	C2C-C3C-C4C	2.84	108.51	106.49
29	C	501	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
29	C	503	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
29	a	410	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
29	N	604	CLA	CHA-C4D-ND	2.84	138.44	132.50
48	Y1	605	CHL	C4A-NA-C1A	2.84	107.98	106.71
51	n1	623	NEX	C5-C4-C3	2.84	115.11	111.75
31	C1	517	BCR	C19-C18-C17	2.84	123.30	118.94
43	D1	405	PL9	C22-C23-C24	-2.84	120.83	127.66
48	G1	605	CHL	CMA-C3A-C4A	2.84	119.40	111.77
29	G1	610	CLA	C1-C2-C3	-2.84	121.14	126.04
31	a	411	BCR	C38-C26-C25	-2.84	121.34	124.53
31	B1	618	BCR	C37-C22-C21	-2.84	118.95	122.92
29	Y	612	CLA	C1-C2-C3	-2.84	121.14	126.04
29	c1	512	CLA	CMA-C3A-C4A	2.84	119.40	111.77
49	N1	621	LUT	C10-C11-C12	-2.84	114.36	123.22
50	r1	621	XAT	C40-C33-C34	-2.84	118.95	122.92
29	a	406	CLA	C6-C5-C3	-2.84	106.02	113.45
42	d1	401	BCT	O3-C-O1	-2.84	112.19	119.55
31	C	515	BCR	C34-C9-C10	-2.83	118.95	122.92
31	b	618	BCR	C36-C18-C17	-2.83	118.95	122.92
29	s	611	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
40	D	408	LHG	O8-C23-C24	2.83	120.80	111.91
40	S1	624	LHG	O8-C23-C24	2.83	120.80	111.91
29	S1	603	CLA	O2D-CGD-O1D	-2.83	118.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S1	604	CLA	CMA-C3A-C4A	2.83	119.39	111.77
48	g1	609	CHL	CMA-C3A-C4A	2.83	119.39	111.77
29	Y	614	CLA	CMD-C2D-C3D	-2.83	121.10	127.61
29	C	509	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
50	G1	622	XAT	C38-C25-C26	-2.83	117.52	122.26
36	b1	620	C7Z	C3-C4-C5	2.83	117.49	111.85
29	S	605	CLA	C1-O2A-CGA	2.83	123.87	116.44
29	b1	602	CLA	C4B-CHC-C1C	2.83	133.05	126.34
29	g1	613	CLA	CAC-C3C-C4C	2.83	128.48	124.81
29	B1	615	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
48	y	607	CHL	CMA-C3A-C4A	2.83	119.38	111.77
29	Y1	613	CLA	C2C-C1C-NC	2.83	112.62	109.97
29	N	614	CLA	CHD-C1D-ND	-2.83	121.85	124.45
33	A	413	LMG	O8-C28-C29	2.83	120.79	111.91
29	b	610	CLA	O2A-CGA-CBA	2.83	120.78	111.91
49	S	621	LUT	C16-C1-C6	-2.83	105.71	110.30
48	n	606	CHL	C4B-CHC-C1C	2.83	133.05	126.34
49	N1	620	LUT	C11-C10-C9	-2.83	123.27	127.31
51	s	623	NEX	C20-C13-C14	-2.83	118.96	122.92
29	N	610	CLA	CMA-C3A-C4A	2.83	119.37	111.77
29	s	605	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
51	y	623	NEX	C4-C3-C2	2.83	116.23	110.77
29	R	610	CLA	C1-O2A-CGA	2.83	123.86	116.44
29	R1	609	CLA	CHD-C1D-ND	-2.83	121.86	124.45
29	S	610	CLA	C1-O2A-CGA	2.83	123.86	116.44
29	C1	508	CLA	C2D-C1D-ND	2.83	112.19	110.10
39	j	101	DGA	OG1-CA1-CA2	2.82	120.77	111.91
29	y	612	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
48	S	607	CHL	C3B-C4B-NB	-2.82	107.89	110.52
29	n1	604	CLA	CHD-C1D-ND	-2.82	121.86	124.45
29	y1	602	CLA	CMA-C3A-C4A	2.82	119.36	111.77
29	R	612	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
29	Y	608	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
49	G	620	LUT	C18-C5-C6	-2.82	121.36	124.53
48	g	605	CHL	CMA-C3A-C4A	2.82	119.36	111.77
51	R	622	NEX	C19-C9-C10	-2.82	118.97	122.92
48	N	609	CHL	C1-O2A-CGA	2.82	123.85	116.44
48	N1	606	CHL	C3C-C4C-NC	-2.82	107.41	110.57
48	G	601	CHL	C4B-CHC-C1C	2.82	133.03	126.34
30	A	409	PHO	O1D-CGD-CBD	2.82	129.44	124.74
29	G1	603	CLA	CMA-C3A-C4A	2.82	119.35	111.77
36	B1	620	C7Z	C18-C5-C4	2.82	119.58	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	g	607	CHL	C4B-CHC-C1C	2.82	133.03	126.34
31	c	517	BCR	C36-C18-C17	-2.82	118.97	122.92
29	G1	602	CLA	CHA-C1A-NA	-2.82	119.94	126.40
29	a	410	CLA	CMA-C3A-C4A	2.82	119.35	111.77
29	b	611	CLA	C4B-CHC-C1C	2.82	133.02	126.34
29	d	402	CLA	C2D-C1D-ND	2.82	112.18	110.10
48	Y	601	CHL	C3C-C4C-NC	-2.82	107.41	110.57
29	s	603	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
29	C	511	CLA	CMA-C3A-C4A	2.82	119.34	111.77
29	r	612	CLA	CHD-C1D-ND	-2.82	121.86	124.45
29	R	602	CLA	C2C-C1C-NC	2.82	112.61	109.97
48	s1	607	CHL	CHD-C1D-ND	-2.82	121.87	124.45
29	d	402	CLA	C4B-CHC-C1C	2.82	133.02	126.34
29	b	602	CLA	O2A-CGA-CBA	2.82	120.74	111.91
29	S	610	CLA	C4B-CHC-C1C	2.82	133.01	126.34
29	s	605	CLA	O2A-CGA-CBA	2.82	120.74	111.91
45	H	101	RRX	C33-C5-C4	2.81	119.02	113.62
29	b1	605	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
29	s1	612	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
29	c1	507	CLA	C1-O2A-CGA	2.81	123.83	116.44
31	c1	516	BCR	C34-C9-C10	-2.81	118.98	122.92
51	y1	623	NEX	C39-C29-C30	-2.81	118.98	122.92
29	S	605	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
34	a	414	SPH	C3-C4-C5	-2.81	118.52	124.79
29	s1	605	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
48	g1	609	CHL	CHD-C4C-C3C	2.81	128.97	124.84
29	S1	613	CLA	CMA-C3A-C4A	2.81	119.33	111.77
49	N	620	LUT	C39-C29-C28	2.81	122.51	118.08
48	R	607	CHL	C4B-CHC-C1C	2.81	133.01	126.34
49	Y1	621	LUT	C38-C25-C24	-2.81	117.54	123.56
48	n	608	CHL	CHB-C4A-NA	2.81	128.40	124.51
50	n	622	XAT	C38-C25-C26	-2.81	117.55	122.26
51	Y	623	NEX	C39-C29-C30	-2.81	118.98	122.92
49	G	620	LUT	C22-C23-C24	-2.81	108.54	111.74
29	G1	613	CLA	C2C-C1C-NC	2.81	112.61	109.97
37	B1	623	DGD	C2G-O2G-C1B	-2.81	110.87	117.79
48	y	609	CHL	C1-O2A-CGA	2.81	123.82	116.44
37	B1	623	DGD	O1G-C1A-C2A	2.81	120.72	111.91
29	b	604	CLA	C2C-C1C-NC	2.81	112.60	109.97
48	N1	606	CHL	CMA-C3A-C4A	2.81	119.32	111.77
29	b	615	CLA	C1-O2A-CGA	2.81	123.81	116.44
36	B	620	C7Z	C28-C27-C26	-2.81	119.32	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	n1	608	CHL	C4B-CHC-C1C	2.81	133.00	126.34
29	N	602	CLA	CHD-C1D-ND	-2.81	121.88	124.45
29	b	616	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
29	B	613	CLA	CMD-C2D-C3D	-2.81	121.16	127.61
29	d	403	CLA	C1-C2-C3	-2.81	121.19	126.04
49	g	620	LUT	C35-C34-C33	-2.80	123.31	127.31
49	g1	621	LUT	C15-C14-C13	-2.80	123.31	127.31
29	n	610	CLA	C3B-C4B-NB	-2.80	107.91	110.52
29	C1	502	CLA	CMA-C3A-C4A	2.80	119.31	111.77
29	s	604	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
53	r1	626	ERG	C1-C10-C5	2.80	113.89	108.75
49	n1	621	LUT	C19-C9-C10	-2.80	119.00	122.92
49	Y	621	LUT	C7-C8-C9	-2.80	122.00	126.23
44	f1	101	HEM	C1C-CHC-C4B	-2.80	120.01	126.06
48	R	607	CHL	C3B-C4B-NB	-2.80	107.91	110.52
48	s	601	CHL	CHC-C4B-NB	-2.80	121.29	124.26
29	N1	603	CLA	C2D-C1D-ND	2.80	112.17	110.10
29	c1	511	CLA	C2D-C1D-ND	2.80	112.17	110.10
48	g1	609	CHL	C4A-NA-C1A	2.80	107.97	106.71
48	N	607	CHL	C4B-CHC-C1C	2.80	132.99	126.34
33	W	201	LMG	O8-C28-C29	2.80	120.70	111.91
33	b1	622	LMG	O8-C28-C29	2.80	120.70	111.91
29	Y	608	CLA	CMA-C3A-C4A	2.80	119.30	111.77
29	s	605	CLA	CMA-C3A-C4A	2.80	119.30	111.77
29	r	603	CLA	C1-C2-C3	-2.80	121.20	126.04
40	C1	525	LHG	O8-C23-C24	2.80	120.70	111.91
29	n	603	CLA	C3B-C4B-NB	-2.80	107.92	110.52
48	y	607	CHL	C4B-CHC-C1C	2.80	132.98	126.34
49	n	621	LUT	C15-C14-C13	-2.80	123.31	127.31
48	S1	607	CHL	C3B-C4B-NB	-2.80	107.92	110.52
29	R	610	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
48	n1	608	CHL	CHD-C1D-ND	-2.80	121.88	124.45
29	R	603	CLA	CHA-C4D-ND	2.80	138.36	132.50
29	b1	605	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
29	y	608	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
29	c1	505	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
31	b1	618	BCR	C38-C26-C27	2.80	118.99	113.62
48	G1	601	CHL	CHB-C4A-NA	2.80	128.38	124.51
29	s1	611	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
29	B	616	CLA	C2C-C1C-NC	2.80	112.59	109.97
29	G1	614	CLA	C2D-C1D-ND	2.80	112.17	110.10
29	B	607	CLA	C2C-C1C-NC	2.80	112.59	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	r	608	CLA	CMD-C2D-C3D	-2.80	121.18	127.61
40	n	624	LHG	O8-C23-C24	2.80	120.69	111.91
29	g1	610	CLA	C1D-ND-C4D	-2.80	104.35	106.33
51	Y	623	NEX	C20-C13-C14	-2.80	119.00	122.92
29	Y	613	CLA	C2D-C1D-ND	2.80	112.17	110.10
29	G	603	CLA	CHD-C1D-ND	-2.80	121.88	124.45
29	B1	604	CLA	O2A-CGA-CBA	2.80	120.68	111.91
29	b	610	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
29	B	610	CLA	C1-C2-C3	-2.80	121.21	126.04
29	b	612	CLA	O1D-CGD-CBD	-2.80	118.76	124.48
48	n1	601	CHL	CHB-C4A-NA	2.79	128.38	124.51
29	C1	510	CLA	C2C-C1C-NC	2.79	112.59	109.97
48	Y1	607	CHL	CHB-C4A-NA	2.79	128.38	124.51
31	d1	404	BCR	C37-C22-C21	-2.79	119.01	122.92
43	D1	405	PL9	C37-C38-C39	-2.79	120.94	127.66
29	B	617	CLA	C2D-C1D-ND	2.79	112.16	110.10
29	b1	610	CLA	C2C-C1C-NC	2.79	112.59	109.97
29	n1	610	CLA	CHD-C1D-ND	-2.79	121.89	124.45
29	S	614	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
50	r1	621	XAT	C7-C8-C9	-2.79	121.20	125.53
50	N1	622	XAT	C38-C25-C26	-2.79	117.58	122.26
48	y1	606	CHL	C3C-C4C-NC	-2.79	107.44	110.57
49	s1	621	LUT	C19-C9-C10	-2.79	119.01	122.92
48	s1	607	CHL	CMA-C3A-C4A	2.79	119.27	111.77
29	b1	611	CLA	CMA-C3A-C4A	2.79	119.27	111.77
29	C1	506	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
29	b1	609	CLA	C2D-C1D-ND	2.79	112.16	110.10
40	c	525	LHG	O8-C23-C24	2.79	120.66	111.91
30	a	409	PHO	C2D-C1D-ND	-2.79	107.60	109.53
29	B1	602	CLA	C4B-CHC-C1C	2.79	132.95	126.34
29	r1	602	CLA	C2C-C1C-NC	2.79	112.58	109.97
29	y	613	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
29	n1	602	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
29	G1	612	CLA	C4B-CHC-C1C	2.79	132.95	126.34
29	r	610	CLA	C2C-C1C-NC	2.79	112.58	109.97
51	Y	623	NEX	C26-C27-C28	-2.79	120.10	125.99
51	Y1	623	NEX	C19-C9-C10	-2.79	119.02	122.92
29	a	406	CLA	O2A-CGA-CBA	2.79	120.66	111.91
29	A1	407	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
29	s	614	CLA	C2C-C1C-NC	2.79	112.58	109.97
40	L	101	LHG	O8-C23-C24	2.79	120.65	111.91
48	N	607	CHL	CHD-C1D-ND	-2.79	121.89	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y	610	CLA	O1D-CGD-CBD	-2.79	118.78	124.48
29	Y1	612	CLA	O2A-CGA-CBA	2.79	120.65	111.91
29	c1	502	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
33	H1	102	LMG	O8-C9-C8	2.78	116.54	108.43
47	i1	101	4RF	O40-C41-C43	2.78	120.64	111.91
29	C1	506	CLA	CMA-C3A-C4A	2.78	119.25	111.77
29	B	614	CLA	C2C-C1C-NC	2.78	112.58	109.97
29	n	603	CLA	C2C-C1C-NC	2.78	112.58	109.97
29	g1	603	CLA	C4B-CHC-C1C	2.78	132.94	126.34
29	a1	406	CLA	CMD-C2D-C3D	-2.78	121.21	127.61
29	g	614	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
50	y1	622	XAT	C8-C9-C10	2.78	123.21	118.94
49	g	620	LUT	C18-C5-C6	-2.78	121.40	124.53
29	C	503	CLA	C2D-C1D-ND	2.78	112.15	110.10
29	B	608	CLA	CMA-C3A-C4A	2.78	119.25	111.77
29	Y	613	CLA	O2A-CGA-CBA	2.78	120.63	111.91
48	g	606	CHL	C1-O2A-CGA	2.78	123.74	116.44
29	Y1	603	CLA	C3B-C4B-NB	-2.78	107.94	110.52
29	N1	604	CLA	CMD-C2D-C3D	-2.78	121.22	127.61
29	g1	610	CLA	O2A-CGA-CBA	2.78	120.63	111.91
29	C	505	CLA	C1-C2-C3	-2.78	121.24	126.04
51	S1	623	NEX	C2-C1-C6	2.78	111.91	109.21
51	g1	623	NEX	C16-C1-C6	-2.78	107.98	110.47
29	Y1	612	CLA	C3B-C4B-NB	-2.78	107.94	110.52
48	g	608	CHL	C3B-C4B-NB	-2.78	107.94	110.52
29	Y	613	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
29	y1	613	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
29	D	403	CLA	CAA-C2A-C3A	-2.78	105.17	112.78
29	C1	508	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
49	g1	620	LUT	C35-C15-C14	-2.78	117.78	123.47
48	R	606	CHL	C3C-C4C-NC	-2.78	107.46	110.57
48	n	605	CHL	CHB-C4A-NA	2.78	128.35	124.51
29	g1	613	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
29	B	613	CLA	CHA-C4D-ND	2.78	138.31	132.50
29	B1	612	CLA	C2D-C1D-ND	2.78	112.15	110.10
48	Y	609	CHL	C1-O2A-CGA	2.78	123.73	116.44
29	g1	611	CLA	CMA-C3A-C4A	2.78	119.23	111.77
39	C	524	DGA	OG1-CA1-CA2	2.78	120.62	111.91
29	r1	608	CLA	CHD-C1D-ND	-2.78	121.90	124.45
29	y	611	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
29	c	506	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
55	Y	626	PTY	O4-C30-C31	2.77	120.61	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S1	614	CLA	C2C-C1C-NC	2.77	112.57	109.97
50	g1	622	XAT	C12-C13-C14	2.77	123.20	118.94
29	Y	603	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
48	S1	607	CHL	C4B-CHC-C1C	2.77	132.92	126.34
48	y1	606	CHL	C4A-NA-C1A	2.77	107.95	106.71
29	b	608	CLA	C2D-C1D-ND	2.77	112.15	110.10
31	C	514	BCR	C36-C18-C17	-2.77	119.04	122.92
29	y1	602	CLA	O2A-CGA-CBA	2.77	120.61	111.91
29	y1	612	CLA	C2C-C1C-NC	2.77	112.57	109.97
29	g1	604	CLA	C1D-ND-C4D	-2.77	104.36	106.33
29	Y1	614	CLA	C1-C2-C3	-2.77	121.25	126.04
48	G1	605	CHL	C2B-C1B-NB	-2.77	108.37	110.23
29	b	613	CLA	CHA-C4D-ND	2.77	138.30	132.50
29	s1	617	CLA	O2A-CGA-CBA	2.77	120.61	111.91
29	N1	611	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
29	r1	603	CLA	C2C-C1C-NC	2.77	112.57	109.97
29	B	604	CLA	O2A-CGA-CBA	2.77	120.61	111.91
29	g	603	CLA	C3B-C4B-NB	-2.77	107.94	110.52
43	d	405	PL9	C22-C23-C24	-2.77	120.99	127.66
29	N	603	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
29	B1	603	CLA	CMA-C3A-C4A	2.77	119.22	111.77
29	B	610	CLA	O2A-CGA-CBA	2.77	120.60	111.91
29	b1	617	CLA	CHD-C1D-ND	-2.77	121.91	124.45
48	r	606	CHL	CHB-C4A-NA	2.77	128.34	124.51
29	N1	604	CLA	CHA-C4D-ND	2.77	138.29	132.50
29	s	614	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
31	C	517	BCR	C36-C18-C17	-2.77	119.04	122.92
38	s1	626	3PH	O31-C31-C32	2.77	120.60	111.91
29	r1	603	CLA	C2D-C1D-ND	2.77	112.14	110.10
29	Y1	614	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
29	N1	614	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
48	n1	605	CHL	C1-O2A-CGA	2.77	123.71	116.44
29	S	605	CLA	O2A-CGA-CBA	2.77	120.60	111.91
29	B	607	CLA	O2A-CGA-CBA	2.77	120.60	111.91
29	S	611	CLA	CMA-C3A-C4A	2.77	119.21	111.77
29	S1	605	CLA	C2D-C1D-ND	2.77	112.14	110.10
29	R1	604	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
29	r	603	CLA	C3B-C4B-NB	-2.77	107.95	110.52
29	C	501	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
29	G1	614	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
48	g1	607	CHL	C4B-CHC-C1C	2.77	132.90	126.34
48	n1	608	CHL	C2C-C3C-C4C	2.77	108.46	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	r1	622	NEX	C16-C1-C6	-2.77	108.00	110.47
48	n	607	CHL	C4B-CHC-C1C	2.77	132.90	126.34
29	B	603	CLA	CHD-C1D-ND	-2.77	121.91	124.45
29	S1	614	CLA	C3B-C4B-NB	-2.77	107.95	110.52
29	n	612	CLA	C2D-C1D-ND	2.77	112.14	110.10
48	G1	607	CHL	C4B-CHC-C1C	2.77	132.90	126.34
51	G	623	NEX	C16-C1-C6	-2.77	108.00	110.47
29	C1	504	CLA	CAC-C3C-C4C	2.77	128.40	124.81
48	R1	606	CHL	CMA-C3A-C4A	2.77	119.21	111.77
29	y	603	CLA	C2D-C1D-ND	2.77	112.14	110.10
29	N1	604	CLA	OBD-CAD-C3D	-2.76	121.87	128.52
30	a	409	PHO	O1D-CGD-CBD	2.76	129.34	124.74
29	S	605	CLA	CMA-C3A-C4A	2.76	119.20	111.77
31	C	516	BCR	C35-C13-C12	2.76	122.43	118.08
55	y	626	PTY	O4-C30-C31	2.76	120.58	111.91
29	B1	607	CLA	CAA-C2A-C3A	-2.76	105.21	112.78
29	s	609	CLA	C1-C2-C3	-2.76	121.26	126.04
29	B	607	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
29	C	512	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
49	n	620	LUT	C31-C32-C33	-2.76	118.65	126.42
49	Y1	620	LUT	C18-C5-C6	-2.76	121.42	124.53
29	n1	603	CLA	C4B-CHC-C1C	2.76	132.89	126.34
29	N	602	CLA	C1-C2-C3	-2.76	121.26	126.04
29	Y1	604	CLA	C1-O2A-CGA	2.76	123.69	116.44
29	y1	612	CLA	CHD-C1D-ND	-2.76	121.92	124.45
29	G1	604	CLA	C2D-C1D-ND	2.76	112.14	110.10
30	A1	408	PHO	C1C-C2C-C3C	-2.76	106.31	108.61
29	s1	612	CLA	CMA-C3A-C4A	2.76	119.20	111.77
48	Y1	607	CHL	C2C-C3C-C4C	2.76	108.46	106.49
29	y	612	CLA	C3B-C4B-NB	-2.76	107.95	110.52
48	r1	607	CHL	C3B-C4B-NB	-2.76	107.95	110.52
29	G1	614	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
29	B	611	CLA	C2D-C1D-ND	2.76	112.14	110.10
29	y1	608	CLA	CMA-C3A-C4A	2.76	119.19	111.77
38	s	626	3PH	O31-C31-C32	2.76	120.57	111.91
29	s	602	CLA	C1-C2-C3	-2.76	121.27	126.04
29	N1	613	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
48	Y1	609	CHL	CMA-C3A-C4A	2.76	119.19	111.77
48	S	607	CHL	CHB-C4A-NA	2.76	128.33	124.51
48	G	609	CHL	C4B-CHC-C1C	2.76	132.88	126.34
29	c	506	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
29	Y1	608	CLA	C1C-C2C-C3C	-2.76	104.06	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b1	603	CLA	C3B-C4B-NB	-2.76	107.95	110.52
29	c	503	CLA	C1-C2-C3	-2.76	121.27	126.04
29	B	602	CLA	C4B-CHC-C1C	2.76	132.88	126.34
29	S	612	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
29	B1	603	CLA	CHD-C1D-ND	-2.76	121.92	124.45
48	R1	606	CHL	CHD-C1D-ND	-2.76	121.92	124.45
29	s1	604	CLA	CMD-C2D-C3D	-2.76	121.27	127.61
40	d1	409	LHG	O8-C23-C24	2.76	120.56	111.91
29	g	613	CLA	CMA-C3A-C4A	2.76	119.18	111.77
29	y	603	CLA	CMA-C3A-C4A	2.76	119.18	111.77
29	Y	610	CLA	C1D-ND-C4D	-2.76	104.38	106.33
48	n1	606	CHL	C4D-CHA-C1A	2.76	124.60	121.25
29	s1	604	CLA	CMA-C3A-C4A	2.76	119.18	111.77
29	B1	615	CLA	CMA-C3A-C4A	2.76	119.18	111.77
29	r	602	CLA	C2C-C1C-NC	2.76	112.55	109.97
48	g1	606	CHL	C4B-CHC-C1C	2.75	132.87	126.34
29	C1	512	CLA	C2D-C1D-ND	2.75	112.13	110.10
51	Y	623	NEX	C1-C2-C3	2.75	119.86	113.64
29	n	603	CLA	CHD-C1D-ND	-2.75	121.92	124.45
29	C1	506	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
31	d	404	BCR	C33-C5-C4	2.75	118.91	113.62
52	r1	625	LMT	C3'-C4'-C5'	-2.75	104.61	110.93
29	g	602	CLA	CMA-C3A-C4A	2.75	119.17	111.77
29	R1	608	CLA	C4B-CHC-C1C	2.75	132.87	126.34
29	C1	504	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
50	y	622	XAT	C26-C27-C28	-2.75	120.17	125.99
49	R	620	LUT	C7-C8-C9	-2.75	122.08	126.23
29	S1	611	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
29	N	604	CLA	OBD-CAD-C3D	-2.75	121.90	128.52
29	N	604	CLA	C2C-C1C-NC	2.75	112.55	109.97
48	R1	607	CHL	C1-O2A-CGA	2.75	123.66	116.44
48	G1	601	CHL	C3B-C4B-NB	-2.75	107.96	110.52
31	C	517	BCR	C31-C1-C6	-2.75	105.84	110.30
29	C	506	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
29	Y	602	CLA	O2A-CGA-CBA	2.75	120.53	111.91
29	D1	403	CLA	CMA-C3A-C4A	2.75	119.16	111.77
40	g1	624	LHG	C6-C5-C4	-2.75	105.29	111.79
49	n	621	LUT	C38-C25-C24	-2.75	117.68	123.56
49	r	620	LUT	C37-C21-C22	-2.75	104.23	109.44
49	S	621	LUT	C38-C25-C24	-2.75	117.68	123.56
48	G1	606	CHL	CMA-C3A-C4A	2.75	119.16	111.77
48	N	605	CHL	CMA-C3A-C4A	2.75	119.16	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	609	CLA	C3B-C4B-NB	-2.75	107.97	110.52
29	Y1	614	CLA	OBD-CAD-C3D	-2.75	121.91	128.52
29	y	602	CLA	C2C-C1C-NC	2.75	112.54	109.97
29	b1	615	CLA	CHA-C4D-ND	2.74	138.24	132.50
48	s	601	CHL	C4A-NA-C1A	2.74	107.94	106.71
29	R1	603	CLA	CMA-C3A-C4A	2.74	119.15	111.77
48	R	607	CHL	CHD-C1D-ND	-2.74	121.93	124.45
55	y1	627	PTY	C6-O7-C8	-2.74	112.78	117.90
29	n	611	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
29	R	609	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
29	C	502	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	c1	513	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	S1	603	CLA	CMA-C3A-C4A	2.74	119.14	111.77
53	R1	626	ERG	C13-C14-C8	2.74	118.80	113.48
29	B	617	CLA	C1-C2-C3	-2.74	121.30	126.04
40	d	409	LHG	C5-O7-C7	-2.74	111.04	117.79
54	s	625	LPX	O3-P1-O4	2.74	125.79	112.24
50	r	621	XAT	O24-C25-C38	-2.74	111.77	115.06
48	G	601	CHL	CMA-C3A-C4A	2.74	119.14	111.77
48	Y1	601	CHL	C3C-C4C-NC	-2.74	107.50	110.57
49	Y1	620	LUT	C35-C15-C14	-2.74	117.86	123.47
29	N1	614	CLA	C2D-C1D-ND	2.74	112.12	110.10
29	r1	603	CLA	O2A-CGA-CBA	2.74	120.50	111.91
29	S1	604	CLA	CAA-CBA-CGA	-2.74	105.25	113.25
48	N1	608	CHL	C1-O2A-CGA	2.74	123.63	116.44
29	D1	403	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	b1	605	CLA	CHA-C1A-NA	-2.74	120.13	126.40
29	D1	402	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
40	d	408	LHG	O8-C23-C24	2.74	120.50	111.91
29	n1	613	CLA	C1-O2A-CGA	2.74	123.62	116.44
29	C1	503	CLA	C2C-C1C-NC	2.74	112.54	109.97
29	Y	604	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
29	Y	604	CLA	O1D-CGD-CBD	-2.74	118.88	124.48
29	S	604	CLA	C1-O2A-CGA	2.74	123.62	116.44
29	y	614	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
29	y	602	CLA	O2A-CGA-CBA	2.74	120.49	111.91
48	G	601	CHL	C2B-C1B-NB	-2.74	108.40	110.23
48	r	606	CHL	C2B-C1B-NB	-2.74	108.40	110.23
48	S	601	CHL	C2C-C3C-C4C	2.74	108.44	106.49
29	C	510	CLA	CMD-C2D-C3D	-2.74	121.32	127.61
53	r1	626	ERG	C4-C5-C10	2.74	120.05	116.42
29	R1	612	CLA	C1C-C2C-C3C	-2.73	104.08	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	y	623	NEX	C39-C29-C30	-2.73	119.09	122.92
29	c1	503	CLA	C2D-C1D-ND	2.73	112.12	110.10
29	c1	513	CLA	CBA-CAA-C2A	2.73	121.93	113.86
29	G	610	CLA	CMA-C3A-C4A	2.73	119.12	111.77
29	S1	604	CLA	C1-C2-C3	-2.73	121.32	126.04
33	w1	201	LMG	O8-C28-C29	2.73	120.48	111.91
48	S	606	CHL	CMA-C3A-C4A	2.73	119.11	111.77
29	s	605	CLA	C1-O2A-CGA	2.73	123.61	116.44
29	y1	611	CLA	C2D-C1D-ND	2.73	112.12	110.10
48	g1	605	CHL	C4B-CHC-C1C	2.73	132.82	126.34
29	Y1	611	CLA	C3B-C4B-NB	-2.73	107.98	110.52
29	b1	616	CLA	C4B-CHC-C1C	2.73	132.81	126.34
48	S	608	CHL	C1-O2A-CGA	2.73	123.60	116.44
29	y	608	CLA	C2D-C1D-ND	2.73	112.11	110.10
29	n1	613	CLA	C2D-C1D-ND	2.73	112.11	110.10
29	b	605	CLA	CMD-C2D-C3D	-2.73	121.34	127.61
29	c	510	CLA	CMD-C2D-C3D	-2.73	121.34	127.61
29	C	511	CLA	C1-C2-C3	-2.73	121.33	126.04
48	S1	607	CHL	CHB-C4A-NA	2.73	128.28	124.51
29	n	612	CLA	CHD-C1D-ND	-2.73	121.95	124.45
29	S1	609	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
31	c1	514	BCR	C15-C14-C13	-2.73	123.42	127.31
51	R1	622	NEX	C15-C14-C13	2.73	131.20	127.31
29	B	615	CLA	C2C-C1C-NC	2.73	112.53	109.97
31	D	404	BCR	C33-C5-C6	-2.73	121.47	124.53
48	Y	606	CHL	C4B-CHC-C1C	2.73	132.80	126.34
29	B	605	CLA	CHA-C4D-ND	2.73	138.20	132.50
29	S1	602	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
29	N	611	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
29	c1	512	CLA	C1-C2-C3	-2.73	121.33	126.04
29	N	614	CLA	CMA-C3A-C4A	2.73	119.10	111.77
33	d1	411	LMG	O8-C28-C29	2.73	120.46	111.91
29	s	617	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
29	N1	603	CLA	C1-C2-C3	-2.73	121.33	126.04
48	g	609	CHL	C3B-C4B-NB	-2.72	107.99	110.52
48	g1	605	CHL	C3B-C4B-NB	-2.72	107.99	110.52
31	C	514	BCR	C33-C5-C6	-2.72	121.47	124.53
36	B1	620	C7Z	C18-C5-C6	-2.72	121.47	124.53
29	b	604	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
29	g	602	CLA	C1-C2-C3	-2.72	121.33	126.04
29	c1	505	CLA	C2C-C1C-NC	2.72	112.52	109.97
48	N1	601	CHL	C4D-CHA-C1A	2.72	124.56	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	Y1	624	LHG	C5-O7-C7	-2.72	111.08	117.79
29	A	410	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
48	g	601	CHL	CHB-C4A-NA	2.72	128.28	124.51
48	s	608	CHL	CMA-C3A-C4A	2.72	119.09	111.77
33	c1	523	LMG	O8-C28-C29	2.72	120.45	111.91
48	Y	601	CHL	CHB-C4A-NA	2.72	128.28	124.51
48	y1	606	CHL	C4B-CHC-C1C	2.72	132.79	126.34
31	b1	619	BCR	C1-C6-C5	-2.72	118.78	122.61
48	g	608	CHL	C4D-CHA-C1A	2.72	124.56	121.25
38	t1	101	3PH	O31-C31-C32	2.72	120.45	111.91
31	B	619	BCR	C12-C13-C14	-2.72	114.76	118.94
29	c1	506	CLA	CMA-C3A-C4A	2.72	119.09	111.77
29	s	603	CLA	C1-O2A-CGA	2.72	123.58	116.44
48	Y1	606	CHL	C1-C2-C3	-2.72	121.34	126.04
49	s	620	LUT	C40-C33-C32	2.72	122.36	118.08
29	S1	605	CLA	O2A-CGA-CBA	2.72	120.44	111.91
29	S	604	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
29	B1	603	CLA	O2A-CGA-CBA	2.72	120.44	111.91
29	a	410	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
29	b1	613	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
50	G	622	XAT	C11-C10-C9	-2.72	123.43	127.31
31	B1	618	BCR	C33-C5-C4	2.72	118.84	113.62
29	C1	512	CLA	CMA-C3A-C4A	2.72	119.08	111.77
48	r	606	CHL	C3B-C4B-NB	-2.72	107.99	110.52
29	n1	611	CLA	C4B-CHC-C1C	2.72	132.78	126.34
48	N	608	CHL	C4B-CHC-C1C	2.72	132.78	126.34
29	N	611	CLA	C2D-C1D-ND	2.72	112.11	110.10
29	c	503	CLA	C2D-C1D-ND	2.72	112.11	110.10
31	b	619	BCR	C33-C5-C6	-2.72	121.48	124.53
29	B	604	CLA	C3B-C4B-NB	-2.72	107.99	110.52
51	N1	623	NEX	C1-C2-C3	2.72	119.78	113.64
29	b1	609	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
29	s1	611	CLA	CMA-C3A-C4A	2.72	119.08	111.77
29	B1	604	CLA	C2C-C1C-NC	2.72	112.52	109.97
29	s1	611	CLA	C2D-C1D-ND	2.72	112.11	110.10
29	s1	614	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
31	B1	618	BCR	C8-C9-C10	2.71	123.11	118.94
49	y	620	LUT	C10-C11-C12	-2.71	114.75	123.22
29	r	610	CLA	O2A-CGA-CBA	2.71	120.42	111.91
29	R1	609	CLA	O2A-CGA-CBA	2.71	120.42	111.91
48	y1	609	CHL	CHC-C1C-NC	2.71	128.32	124.20
49	n1	620	LUT	C38-C25-C24	-2.71	117.76	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b1	617	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
29	a1	407	CLA	C3D-C2D-C1D	-2.71	102.13	105.83
29	Y	602	CLA	C4B-CHC-C1C	2.71	132.77	126.34
48	G	608	CHL	C4B-CHC-C1C	2.71	132.77	126.34
48	N1	609	CHL	C4D-CHA-C1A	2.71	124.55	121.25
29	N	603	CLA	C2C-C1C-NC	2.71	112.51	109.97
29	C1	507	CLA	C1-C2-C3	-2.71	121.35	126.04
40	G1	624	LHG	C6-C5-C4	-2.71	105.38	111.79
49	N	620	LUT	C15-C14-C13	-2.71	123.44	127.31
30	a1	408	PHO	C1C-C2C-C3C	-2.71	106.36	108.61
29	C	506	CLA	O2A-CGA-CBA	2.71	120.41	111.91
48	y	606	CHL	C4B-CHC-C1C	2.71	132.77	126.34
29	B1	613	CLA	CHA-C4D-ND	2.71	138.17	132.50
29	n	611	CLA	CAA-C2A-C3A	-2.71	105.36	112.78
31	b	618	BCR	C19-C18-C17	2.71	123.10	118.94
29	g1	613	CLA	CMC-C2C-C1C	2.71	129.17	125.04
29	B	616	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
29	s	604	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
29	s	610	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
29	Y	610	CLA	C2C-C1C-NC	2.71	112.51	109.97
29	G1	604	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
29	y	611	CLA	C2C-C1C-NC	2.71	112.51	109.97
29	R	608	CLA	CHA-C4D-ND	2.71	138.16	132.50
29	b1	612	CLA	CHA-C4D-ND	2.71	138.16	132.50
29	n1	614	CLA	CMA-C3A-C4A	2.71	119.05	111.77
48	y1	609	CHL	C4D-CHA-C1A	2.71	124.54	121.25
29	C	501	CLA	C2D-C1D-ND	2.71	112.10	110.10
29	s	611	CLA	C3B-C4B-NB	-2.71	108.00	110.52
29	C1	510	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
29	s	604	CLA	C1-C2-C3	-2.71	121.36	126.04
54	S	625	LPX	O3-P1-O4	2.71	125.61	112.24
29	s	611	CLA	CHD-C1D-ND	-2.71	121.97	124.45
29	C	513	CLA	C2C-C1C-NC	2.70	112.51	109.97
47	K1	101	4RF	O40-C41-C43	2.70	120.40	111.91
29	b1	605	CLA	CHA-C4D-ND	2.70	138.16	132.50
48	N	605	CHL	C1-O2A-CGA	2.70	123.54	116.44
29	G	604	CLA	CMA-C3A-C4A	2.70	119.04	111.77
48	G	606	CHL	C4D-CHA-C1A	2.70	124.54	121.25
29	b	604	CLA	CHA-C4D-ND	2.70	138.16	132.50
29	G	610	CLA	CAA-C2A-C3A	-2.70	105.37	112.78
29	B	609	CLA	CHD-C1D-ND	-2.70	121.97	124.45
29	C	506	CLA	CHD-C1D-ND	-2.70	121.97	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	509	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
29	d	403	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
29	g1	612	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
29	S	610	CLA	OBD-CAD-C3D	-2.70	122.01	128.52
48	y1	606	CHL	C3B-C4B-NB	-2.70	108.01	110.52
29	B	611	CLA	C1-O2A-CGA	2.70	123.54	116.44
29	b1	614	CLA	C2D-C1D-ND	2.70	112.10	110.10
29	G1	613	CLA	C1D-ND-C4D	-2.70	104.42	106.33
29	d	403	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
29	S	613	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
51	s	623	NEX	C19-C9-C10	-2.70	119.14	122.92
31	B	618	BCR	C19-C18-C17	2.70	123.09	118.94
48	S1	608	CHL	C1-O2A-CGA	2.70	123.53	116.44
29	n	612	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
47	i	101	4RF	O18-C16-C15	2.70	120.38	111.91
48	S	601	CHL	C4B-CHC-C1C	2.70	132.74	126.34
29	s1	610	CLA	O2A-CGA-CBA	2.70	120.38	111.91
29	B	613	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
31	c	515	BCR	C33-C5-C4	2.70	118.80	113.62
29	g	611	CLA	C4B-CHC-C1C	2.70	132.74	126.34
40	s	624	LHG	O8-C23-C24	2.70	120.38	111.91
29	C1	513	CLA	C3B-C4B-NB	-2.70	108.01	110.52
29	c1	507	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
48	y1	606	CHL	CHD-C1D-ND	-2.70	121.97	124.45
49	r1	620	LUT	C31-C32-C33	-2.70	118.83	126.42
29	B1	609	CLA	C1-O2A-CGA	2.70	123.53	116.44
31	d	404	BCR	C36-C18-C17	-2.70	119.14	122.92
49	S	620	LUT	C31-C30-C29	-2.70	123.46	127.31
29	A	407	CLA	CMA-C3A-C4A	2.70	119.03	111.77
29	S1	602	CLA	C1-C2-C3	-2.70	121.38	126.04
49	r1	620	LUT	C1-C6-C5	-2.70	118.81	122.61
29	G	603	CLA	C3B-C4B-NB	-2.70	108.01	110.52
29	r1	609	CLA	C1-C2-C3	-2.70	121.38	126.04
29	d1	403	CLA	C2C-C1C-NC	2.70	112.50	109.97
29	S	604	CLA	O2A-CGA-CBA	2.70	120.37	111.91
37	c	520	DGD	O1G-C1A-C2A	2.70	120.37	111.91
48	s	607	CHL	C3B-C4B-NB	-2.70	108.01	110.52
48	g	601	CHL	CMA-C3A-C4A	2.70	119.02	111.77
29	c	513	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
29	y	611	CLA	CHD-C1D-ND	-2.70	121.98	124.45
29	c	511	CLA	C2C-C1C-NC	2.70	112.50	109.97
29	s	610	CLA	C2C-C1C-NC	2.70	112.50	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	D1	405	PL9	C36-C34-C33	-2.70	115.66	121.12
29	N	612	CLA	CHA-C4D-ND	2.70	138.14	132.50
29	r1	610	CLA	CAA-C2A-C3A	-2.70	105.40	112.78
29	D	402	CLA	C4B-CHC-C1C	2.69	132.73	126.34
29	C1	504	CLA	C2D-C1D-ND	2.69	112.09	110.10
29	g1	602	CLA	C2D-C1D-ND	2.69	112.09	110.10
50	R	621	XAT	C40-C33-C34	-2.69	119.15	122.92
29	B1	603	CLA	C1-O2A-CGA	2.69	123.51	116.44
43	d1	405	PL9	C40-C39-C41	2.69	119.80	115.27
29	N	603	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
29	S	611	CLA	C1-C2-C3	-2.69	121.38	126.04
48	N	607	CHL	C1-C2-C3	-2.69	121.38	126.04
29	C	507	CLA	CHD-C1D-ND	-2.69	121.98	124.45
55	Y1	626	PTY	O4-C30-C31	2.69	120.36	111.91
29	b	612	CLA	C2D-C1D-ND	2.69	112.09	110.10
29	R1	602	CLA	CHD-C1D-ND	-2.69	121.98	124.45
29	b	614	CLA	CMD-C2D-C3D	-2.69	121.42	127.61
29	S1	609	CLA	C4B-CHC-C1C	2.69	132.72	126.34
29	D	402	CLA	O2A-CGA-CBA	2.69	120.36	111.91
49	r1	620	LUT	C18-C5-C4	2.69	119.34	114.36
48	S	601	CHL	CMA-C3A-C4A	2.69	119.01	111.77
29	B	603	CLA	C2D-C1D-ND	2.69	112.09	110.10
29	s	605	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
51	N1	623	NEX	C31-C30-C29	2.69	131.15	127.31
51	N	623	NEX	C38-C25-C26	-2.69	117.75	122.26
29	Y1	603	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
29	C	508	CLA	CMB-C2B-C3B	2.69	133.11	126.59
29	n1	612	CLA	CHD-C1D-ND	-2.69	121.98	124.45
29	S	610	CLA	C3B-C4B-NB	-2.69	108.02	110.52
29	A1	410	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
48	R	607	CHL	C1-O2A-CGA	2.69	123.50	116.44
48	n	608	CHL	C3B-C4B-NB	-2.69	108.02	110.52
49	Y	621	LUT	C18-C5-C6	-2.69	121.51	124.53
50	n1	622	XAT	C26-C27-C28	-2.69	120.31	125.99
29	G	603	CLA	C4B-CHC-C1C	2.69	132.72	126.34
29	y	610	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
30	A1	409	PHO	O2D-CGD-O1D	-2.69	118.58	123.84
29	B	604	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
29	S1	603	CLA	C1-O2A-CGA	2.69	123.50	116.44
31	C1	517	BCR	C23-C22-C21	2.69	123.07	118.94
29	s1	602	CLA	C2D-C1D-ND	2.69	112.08	110.10
48	R1	607	CHL	CHB-C4A-NA	2.69	128.23	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	410	CLA	O2A-CGA-CBA	2.69	120.34	111.91
29	c1	504	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
48	g	601	CHL	C1-C2-C3	-2.69	121.39	126.04
29	b1	604	CLA	C1D-ND-C4D	-2.69	104.43	106.33
48	Y	606	CHL	CHB-C4A-NA	2.69	128.23	124.51
31	C	516	BCR	C28-C27-C26	-2.69	109.28	114.08
29	c	501	CLA	CMA-C3A-C4A	2.69	119.00	111.77
29	G	611	CLA	C1-C2-C3	-2.69	121.40	126.04
29	S	603	CLA	C2D-C1D-ND	2.69	112.08	110.10
29	Y1	610	CLA	O1D-CGD-CBD	-2.69	118.99	124.48
29	n	604	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
29	s	613	CLA	C1D-ND-C4D	-2.69	104.43	106.33
30	a1	409	PHO	C1C-C2C-C3C	-2.69	106.38	108.61
48	s	608	CHL	CHB-C4A-NA	2.69	128.22	124.51
48	y1	609	CHL	CHB-C1B-NB	-2.68	121.42	124.26
48	y1	601	CHL	C3C-C4C-NC	-2.68	107.56	110.57
31	b1	619	BCR	C4-C5-C6	-2.68	118.83	122.73
48	n	608	CHL	C4B-CHC-C1C	2.68	132.70	126.34
48	g	607	CHL	C4A-NA-C1A	2.68	107.91	106.71
29	B	602	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
29	G	613	CLA	C3B-C4B-NB	-2.68	108.03	110.52
29	c1	504	CLA	CMD-C2D-C3D	-2.68	121.44	127.61
29	R	603	CLA	C2C-C1C-NC	2.68	112.48	109.97
29	Y1	602	CLA	CHA-C4D-ND	2.68	138.11	132.50
29	r	602	CLA	O2A-CGA-CBA	2.68	120.32	111.91
29	G1	610	CLA	O1D-CGD-CBD	-2.68	119.00	124.48
29	s1	611	CLA	CHA-C4D-ND	2.68	138.11	132.50
29	C	512	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
48	N	607	CHL	CMA-C3A-C4A	2.68	118.98	111.77
29	c	508	CLA	C2C-C1C-NC	2.68	112.48	109.97
31	B	619	BCR	C35-C13-C12	2.68	122.30	118.08
48	y	605	CHL	CHD-C4C-C3C	2.68	128.78	124.84
48	Y1	605	CHL	C4B-CHC-C1C	2.68	132.69	126.34
29	R	612	CLA	C3B-C4B-NB	-2.68	108.03	110.52
29	R1	609	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
31	c	517	BCR	C2-C1-C6	2.68	114.61	110.48
29	r	608	CLA	C2C-C1C-NC	2.68	112.48	109.97
50	g1	622	XAT	C39-C29-C30	-2.68	119.17	122.92
48	n	608	CHL	C3C-C4C-NC	-2.68	107.57	110.57
49	n1	621	LUT	C10-C11-C12	-2.68	114.86	123.22
29	n1	613	CLA	CMA-C3A-C4A	2.68	118.97	111.77
48	n	607	CHL	C2C-C3C-C4C	2.68	108.40	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	N	608	CHL	CHB-C4A-NA	2.68	128.22	124.51
50	y1	622	XAT	C40-C33-C34	-2.68	119.17	122.92
45	H	101	RRX	C32-C1-C6	-2.68	105.96	110.30
29	B	614	CLA	C1D-ND-C4D	-2.68	104.43	106.33
29	G	614	CLA	C1-O2A-CGA	2.68	123.47	116.44
48	R	607	CHL	CHB-C4A-NA	2.68	128.21	124.51
29	a1	406	CLA	CHA-C4D-ND	2.68	138.10	132.50
29	b1	614	CLA	CMA-C3A-C4A	2.68	118.97	111.77
38	T1	101	3PH	O31-C31-C32	2.68	120.31	111.91
48	y	609	CHL	CHD-C4C-C3C	2.68	128.77	124.84
29	n1	611	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
50	r1	621	XAT	C38-C25-C26	-2.68	117.78	122.26
29	c	501	CLA	C2C-C1C-NC	2.68	112.48	109.97
29	R1	608	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
29	y1	611	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
29	C1	511	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
29	B1	607	CLA	C2C-C1C-NC	2.67	112.48	109.97
29	s1	612	CLA	C2D-C1D-ND	2.67	112.07	110.10
29	a1	406	CLA	OBD-CAD-C3D	-2.67	122.09	128.52
37	b1	623	DGD	C4E-C3E-C2E	2.67	115.49	110.82
50	Y1	622	XAT	C19-C9-C10	-2.67	119.18	122.92
29	C1	502	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
29	y	613	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
51	r	622	NEX	C5-C4-C3	-2.67	108.58	111.75
29	g1	612	CLA	C4B-CHC-C1C	2.67	132.67	126.34
51	g	623	NEX	C15-C14-C13	2.67	131.12	127.31
29	A	405	CLA	CMD-C2D-C3D	-2.67	121.47	127.61
29	B1	614	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
48	s1	601	CHL	CHD-C4C-C3C	2.67	128.76	124.84
48	r1	606	CHL	C2B-C1B-NB	-2.67	108.44	110.23
30	A	409	PHO	C1-C2-C3	-2.67	121.43	126.04
29	S1	603	CLA	CHA-C4D-ND	2.67	138.08	132.50
29	G1	611	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
29	Y1	608	CLA	CHD-C1D-ND	-2.67	122.00	124.45
36	B	620	C7Z	C24-C25-C26	-2.67	114.90	120.85
48	G	601	CHL	CHD-C4C-C3C	2.67	128.76	124.84
29	r	603	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
29	S	605	CLA	CHA-C4D-ND	2.67	138.08	132.50
31	c1	514	BCR	C34-C9-C10	-2.67	119.19	122.92
48	G	601	CHL	C1-C2-C3	-2.67	121.43	126.04
29	B1	607	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
29	G1	613	CLA	C1C-C2C-C3C	-2.67	104.15	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	S	623	NEX	C31-C30-C29	2.67	131.12	127.31
29	y1	608	CLA	CMD-C2D-C3D	-2.67	121.48	127.61
29	n1	610	CLA	O2A-CGA-CBA	2.67	120.28	111.91
29	c	505	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
29	n	611	CLA	CMA-C3A-C4A	2.67	118.94	111.77
31	A1	411	BCR	C35-C13-C12	2.67	122.28	118.08
29	B	616	CLA	C1D-ND-C4D	-2.67	104.44	106.33
29	G1	614	CLA	CMA-C3A-C4A	2.67	118.94	111.77
29	y1	608	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
29	g1	602	CLA	C3B-C4B-NB	-2.67	108.04	110.52
29	r	603	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
29	s	614	CLA	O2A-CGA-CBA	2.67	120.28	111.91
36	B1	620	C7Z	C21-C26-C27	2.67	123.32	115.78
29	S	609	CLA	CAA-C2A-C3A	-2.67	105.48	112.78
29	A	410	CLA	C1-C2-C3	-2.67	121.43	126.04
29	b1	611	CLA	C1-C2-C3	-2.67	121.43	126.04
29	b1	612	CLA	C3D-C2D-C1D	-2.67	102.19	105.83
48	y1	601	CHL	C4D-CHA-C1A	2.67	124.49	121.25
48	G1	606	CHL	C3C-C4C-NC	-2.67	107.58	110.57
51	S1	623	NEX	C38-C25-C26	-2.67	117.79	122.26
50	r1	621	XAT	C15-C35-C34	2.66	128.93	123.47
49	r1	620	LUT	C20-C13-C14	-2.66	119.19	122.92
39	c	524	DGA	OG1-CA1-CA2	2.66	120.27	111.91
48	g1	606	CHL	CMA-C3A-C4A	2.66	118.93	111.77
29	C1	503	CLA	CHD-C1D-ND	-2.66	122.01	124.45
48	Y1	607	CHL	C4B-CHC-C1C	2.66	132.66	126.34
48	N1	607	CHL	C1-C2-C3	-2.66	121.44	126.04
47	K	101	4RF	O18-C16-C15	2.66	120.27	111.91
29	r1	608	CLA	C2D-C1D-ND	2.66	112.07	110.10
29	n	614	CLA	C1D-ND-C4D	-2.66	104.44	106.33
29	G1	610	CLA	C2C-C1C-NC	2.66	112.47	109.97
31	c1	517	BCR	C23-C22-C21	2.66	123.03	118.94
29	s1	605	CLA	CHD-C1D-ND	-2.66	122.01	124.45
29	y1	603	CLA	CHA-C4D-ND	2.66	138.07	132.50
29	c	512	CLA	O2A-CGA-CBA	2.66	120.26	111.91
31	b	619	BCR	C35-C13-C12	2.66	122.27	118.08
29	b1	616	CLA	CHD-C1D-ND	-2.66	122.01	124.45
29	g1	613	CLA	C1D-ND-C4D	-2.66	104.44	106.33
48	R1	606	CHL	C4A-NA-C1A	2.66	107.90	106.71
29	n1	604	CLA	CHA-C4D-ND	2.66	138.06	132.50
29	c1	503	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
48	y1	605	CHL	CHB-C4A-NA	2.66	128.19	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	n1	622	XAT	O4-C5-C4	-2.66	111.38	113.38
29	N	602	CLA	O2A-CGA-CBA	2.66	120.25	111.91
29	s1	611	CLA	O2A-CGA-CBA	2.66	120.25	111.91
29	R1	609	CLA	CMA-C3A-C4A	2.66	118.92	111.77
29	g1	603	CLA	CHD-C1D-ND	-2.66	122.01	124.45
29	y1	608	CLA	CHA-C4D-ND	2.66	138.06	132.50
29	y1	614	CLA	CHA-C4D-ND	2.66	138.06	132.50
45	h1	101	RRX	C1-C6-C5	-2.66	118.87	122.61
29	c1	511	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
29	y	614	CLA	C1-C2-C3	-2.66	121.44	126.04
29	Y	612	CLA	O2A-CGA-CBA	2.66	120.25	111.91
29	b	602	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
29	c1	513	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
29	r1	603	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
49	n1	621	LUT	C40-C33-C34	-2.66	119.20	122.92
29	b1	607	CLA	C3B-C4B-NB	-2.66	108.05	110.52
29	Y1	602	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
29	g1	613	CLA	O2A-CGA-CBA	2.66	120.25	111.91
29	y	614	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
29	R1	604	CLA	C2D-C1D-ND	2.66	112.06	110.10
41	C	527	LMK	O3-C4-C3	-2.66	113.87	122.98
29	G1	613	CLA	O2A-CGA-CBA	2.66	120.24	111.91
49	s1	621	LUT	C2-C3-C4	-2.66	106.67	110.30
29	A1	406	CLA	OBD-CAD-C3D	-2.66	122.13	128.52
29	r1	612	CLA	C2C-C1C-NC	2.66	112.46	109.97
29	s	614	CLA	CMD-C2D-C3D	-2.66	121.50	127.61
29	B	615	CLA	CHA-C4D-ND	2.66	138.05	132.50
37	C	520	DGD	O1G-C1A-C2A	2.66	120.24	111.91
53	r1	626	ERG	C6-C7-C8	-2.66	116.84	122.07
45	H1	101	RRX	C15-C16-C17	-2.66	118.03	123.47
29	B	611	CLA	C3B-C4B-NB	-2.65	108.05	110.52
49	S	621	LUT	C39-C29-C28	2.65	122.26	118.08
29	n1	604	CLA	C2D-C1D-ND	2.65	112.06	110.10
29	y	614	CLA	C3B-C4B-NB	-2.65	108.05	110.52
48	g1	601	CHL	C3B-C4B-NB	-2.65	108.05	110.52
51	s	623	NEX	C17-C1-C6	-2.65	108.10	110.47
29	n	612	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
29	R	610	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
29	c	513	CLA	CMA-C3A-C4A	2.65	118.90	111.77
29	g1	612	CLA	C1D-ND-C4D	-2.65	104.45	106.33
29	d1	402	CLA	C4B-CHC-C1C	2.65	132.63	126.34
50	R	621	XAT	C10-C11-C12	-2.65	114.94	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c1	504	CLA	C4B-CHC-C1C	2.65	132.63	126.34
29	s	614	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
45	h1	101	RRX	C2-C1-C6	2.65	114.56	110.48
48	S1	601	CHL	C3C-C4C-NC	-2.65	107.60	110.57
29	C1	511	CLA	CMD-C2D-C3D	-2.65	121.52	127.61
29	y	602	CLA	C4B-CHC-C1C	2.65	132.62	126.34
29	s	609	CLA	CMA-C3A-C4A	2.65	118.90	111.77
29	N1	602	CLA	C4B-CHC-C1C	2.65	132.62	126.34
49	n	620	LUT	C22-C23-C24	-2.65	108.72	111.74
29	Y1	614	CLA	C3B-C4B-NB	-2.65	108.06	110.52
29	Y	613	CLA	C1-O2A-CGA	2.65	123.39	116.44
29	B1	610	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
50	Y1	622	XAT	C20-C13-C14	-2.65	119.21	122.92
29	S	614	CLA	CMD-C2D-C3D	-2.65	121.52	127.61
48	n	606	CHL	CHB-C4A-NA	2.65	128.18	124.51
49	s	621	LUT	C7-C8-C9	-2.65	122.23	126.23
29	R1	609	CLA	C3B-C4B-NB	-2.65	108.06	110.52
48	S1	606	CHL	CMA-C3A-C4A	2.65	118.89	111.77
48	y1	601	CHL	CHB-C4A-NA	2.65	128.17	124.51
29	B	607	CLA	CHA-C4D-ND	2.65	138.04	132.50
51	g	623	NEX	C40-C33-C34	-2.65	119.21	122.92
48	Y	609	CHL	C1D-CHD-C4C	-2.65	120.35	126.06
29	A	405	CLA	C2D-C1D-ND	2.65	112.06	110.10
29	c	501	CLA	O2A-CGA-CBA	2.65	120.22	111.91
29	A	405	CLA	CMC-C2C-C1C	2.65	129.07	125.04
29	R1	610	CLA	C4B-CHC-C1C	2.65	132.62	126.34
29	s1	604	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
29	S	613	CLA	CHD-C1D-ND	-2.65	122.02	124.45
31	c1	514	BCR	C36-C18-C17	-2.65	119.22	122.92
29	C	509	CLA	CMD-C2D-C3D	-2.65	121.53	127.61
31	c	515	BCR	C23-C22-C21	-2.65	114.88	118.94
49	N1	621	LUT	C1-C6-C5	-2.65	118.89	122.61
29	c	512	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
29	b1	616	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
29	S	603	CLA	CHD-C1D-ND	-2.65	122.02	124.45
29	b	604	CLA	C3B-C4B-NB	-2.65	108.06	110.52
29	r	612	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
29	a	407	CLA	C1-O2A-CGA	2.64	123.38	116.44
29	b1	607	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
29	b1	617	CLA	OBD-CAD-C3D	-2.64	122.16	128.52
31	b	619	BCR	C33-C5-C4	2.64	118.70	113.62
29	r	602	CLA	CAA-C2A-C3A	-2.64	105.54	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c1	513	CLA	C2C-C1C-NC	2.64	112.45	109.97
51	y1	623	NEX	C27-C28-C29	-2.64	121.43	125.53
29	G	611	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
29	c	503	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
29	S	617	CLA	C2D-C1D-ND	2.64	112.05	110.10
48	Y1	605	CHL	C3B-C4B-NB	-2.64	108.06	110.52
29	c1	512	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
51	n	623	NEX	C17-C1-C6	-2.64	108.11	110.47
29	s	603	CLA	CHA-C4D-ND	2.64	138.03	132.50
51	g	623	NEX	C26-C27-C28	-2.64	120.41	125.99
29	g	610	CLA	C2C-C1C-NC	2.64	112.45	109.97
29	b	606	CLA	O2A-CGA-CBA	2.64	120.20	111.91
29	b	603	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
39	J	101	DGA	OG1-CA1-CA2	2.64	120.20	111.91
29	C1	504	CLA	C4B-CHC-C1C	2.64	132.60	126.34
49	Y1	620	LUT	C1-C2-C3	-2.64	107.68	113.64
29	d1	402	CLA	C2D-C1D-ND	2.64	112.05	110.10
29	Y1	603	CLA	CHA-C4D-ND	2.64	138.02	132.50
48	G1	609	CHL	CHB-C4A-NA	2.64	128.16	124.51
31	b1	619	BCR	C8-C7-C6	-2.64	119.79	127.20
29	C1	503	CLA	C4B-CHC-C1C	2.64	132.60	126.34
40	G	624	LHG	C6-C5-C4	-2.64	105.55	111.79
48	g	601	CHL	C4B-CHC-C1C	2.64	132.60	126.34
51	y	623	NEX	C38-C25-C26	-2.64	117.84	122.26
29	C1	511	CLA	CMA-C3A-C4A	2.64	118.86	111.77
29	b1	606	CLA	CAC-C3C-C4C	2.64	128.23	124.81
49	G	621	LUT	C31-C30-C29	-2.64	123.55	127.31
29	a1	405	CLA	CMD-C2D-C3D	-2.64	121.55	127.61
29	b	605	CLA	CHA-C4D-ND	2.64	138.02	132.50
29	C1	509	CLA	CMA-C3A-C4A	2.64	118.86	111.77
49	G	621	LUT	C20-C13-C12	2.64	122.23	118.08
48	g1	601	CHL	CHD-C4C-C3C	2.64	128.72	124.84
29	S	610	CLA	O2A-CGA-CBA	2.64	120.18	111.91
29	b1	605	CLA	C2A-C1A-CHA	2.64	128.47	123.86
31	B1	619	BCR	C36-C18-C17	-2.64	119.23	122.92
29	n1	602	CLA	O1D-CGD-CBD	-2.64	119.09	124.48
51	s1	623	NEX	C12-C13-C14	2.64	122.99	118.94
29	C1	501	CLA	C2A-C1A-CHA	2.64	128.47	123.86
37	C	518	DGD	O1G-C1A-C2A	2.64	120.18	111.91
29	C	502	CLA	CHD-C1D-ND	-2.64	122.03	124.45
29	B1	607	CLA	C1D-ND-C4D	-2.64	104.46	106.33
49	n	621	LUT	C16-C1-C6	-2.64	106.03	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D1	403	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
49	s	620	LUT	C30-C31-C32	-2.63	115.00	123.22
49	S1	620	LUT	C10-C11-C12	-2.63	115.00	123.22
48	N1	606	CHL	C2B-C1B-NB	-2.63	108.47	110.23
29	C1	501	CLA	O1D-CGD-CBD	-2.63	119.09	124.48
29	R	610	CLA	O2A-CGA-CBA	2.63	120.17	111.91
29	b	613	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	C	504	CLA	C2D-C1D-ND	2.63	112.05	110.10
29	N1	614	CLA	CMA-C3A-C4A	2.63	118.85	111.77
29	B1	610	CLA	O2A-CGA-CBA	2.63	120.17	111.91
29	G	604	CLA	CHA-C4D-ND	2.63	138.01	132.50
50	n	622	XAT	C18-C5-C6	-2.63	117.85	122.26
29	S	617	CLA	CMA-C3A-C4A	2.63	118.85	111.77
48	n1	609	CHL	CHB-C1B-NB	-2.63	121.47	124.26
29	Y	613	CLA	CHA-C4D-ND	2.63	138.01	132.50
29	Y1	610	CLA	O2A-CGA-CBA	2.63	120.17	111.91
29	s1	613	CLA	C2C-C1C-NC	2.63	112.44	109.97
38	T	101	3PH	O31-C31-C32	2.63	120.17	111.91
29	s1	605	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	c1	501	CLA	CHA-C4D-ND	2.63	138.00	132.50
29	r1	609	CLA	O2A-CGA-CBA	2.63	120.17	111.91
29	g	603	CLA	CHA-C4D-ND	2.63	138.00	132.50
29	S1	602	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
48	Y1	609	CHL	C4B-CHC-C1C	2.63	132.58	126.34
29	g	604	CLA	OBD-CAD-C3D	-2.63	122.19	128.52
29	S	614	CLA	CHA-C4D-ND	2.63	138.00	132.50
29	G	611	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
29	Y	611	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	r	610	CLA	CMA-C3A-C4A	2.63	118.84	111.77
50	G	622	XAT	C6-C7-C8	-2.63	120.43	125.99
29	Y1	604	CLA	O2A-CGA-CBA	2.63	120.16	111.91
48	s1	606	CHL	C4B-CHC-C1C	2.63	132.57	126.34
29	C	505	CLA	O2A-CGA-CBA	2.63	120.16	111.91
33	B	622	LMG	O8-C28-C29	2.63	120.16	111.91
29	y1	604	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
50	Y	622	XAT	C19-C9-C10	-2.63	119.24	122.92
29	C1	502	CLA	C4B-CHC-C1C	2.63	132.57	126.34
29	g1	611	CLA	C2C-C1C-NC	2.63	112.44	109.97
29	C1	503	CLA	CHA-C4D-ND	2.63	138.00	132.50
29	Y1	614	CLA	CHA-C4D-ND	2.63	138.00	132.50
29	y1	604	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
29	r	612	CLA	C1C-C2C-C3C	-2.63	104.19	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s1	613	CLA	C3B-C4B-NB	-2.63	108.08	110.52
29	C1	507	CLA	OBD-CAD-C3D	-2.63	122.20	128.52
29	c1	505	CLA	OBD-CAD-C3D	-2.63	122.20	128.52
29	b	604	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	c1	503	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	n1	614	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
29	b	613	CLA	C2C-C1C-NC	2.63	112.43	109.97
29	R1	603	CLA	C2D-C1D-ND	2.63	112.04	110.10
29	S	617	CLA	O2A-CGA-CBA	2.63	120.15	111.91
29	S1	603	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
29	G1	603	CLA	C4B-CHC-C1C	2.62	132.56	126.34
48	Y	607	CHL	C1-O2A-CGA	2.62	123.33	116.44
29	c1	502	CLA	CHA-C4D-ND	2.62	137.99	132.50
29	B	604	CLA	CHA-C4D-ND	2.62	137.99	132.50
48	n1	605	CHL	CMA-C3A-C4A	2.62	118.83	111.77
29	c1	510	CLA	CMD-C2D-C3D	-2.62	121.58	127.61
29	g1	602	CLA	CMC-C2C-C1C	2.62	129.03	125.04
29	B	612	CLA	O2A-CGA-CBA	2.62	120.14	111.91
29	y	612	CLA	O2A-CGA-CBA	2.62	120.14	111.91
29	s1	602	CLA	CAA-C2A-C3A	-2.62	105.59	112.78
29	C1	503	CLA	C2D-C1D-ND	2.62	112.04	110.10
29	S1	602	CLA	CHA-C4D-ND	2.62	137.99	132.50
29	s1	609	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
48	G1	606	CHL	C3B-C4B-NB	-2.62	108.08	110.52
29	y	612	CLA	C1D-ND-C4D	-2.62	104.47	106.33
50	n	622	XAT	C19-C9-C10	-2.62	119.25	122.92
49	y	621	LUT	C11-C10-C9	-2.62	123.57	127.31
36	b1	620	C7Z	C23-C24-C25	2.62	117.08	111.85
53	r	626	ERG	C13-C14-C8	2.62	118.56	113.48
29	B1	603	CLA	CHA-C4D-ND	2.62	137.98	132.50
29	c1	510	CLA	C3B-C4B-NB	-2.62	108.08	110.52
29	s	617	CLA	CAA-C2A-C3A	-2.62	105.60	112.78
45	h1	101	RRX	C35-C13-C12	2.62	122.21	118.08
29	c1	502	CLA	C4B-CHC-C1C	2.62	132.55	126.34
29	g	604	CLA	CMA-C3A-C4A	2.62	118.81	111.77
48	N1	601	CHL	CHD-C4C-C3C	2.62	128.69	124.84
48	n1	609	CHL	CHD-C4C-C3C	2.62	128.69	124.84
29	R	609	CLA	C2D-C1D-ND	2.62	112.03	110.10
48	n1	607	CHL	CHB-C4A-NA	2.62	128.13	124.51
29	n	604	CLA	C2C-C1C-NC	2.62	112.42	109.97
29	n	613	CLA	CHA-C4D-ND	2.62	137.98	132.50
29	g	614	CLA	C1C-C2C-C3C	-2.62	104.20	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	512	CLA	CMA-C3A-C4A	2.62	118.81	111.77
48	n	609	CHL	C1-O2A-CGA	2.62	123.31	116.44
30	a1	408	PHO	CMB-C2B-C3B	2.62	129.57	124.68
29	B	605	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
29	c	506	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
29	C	511	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
29	C1	501	CLA	CHA-C1A-NA	-2.62	120.41	126.40
29	B1	604	CLA	C1C-C2C-C3C	-2.62	104.21	106.96
29	g	614	CLA	O2A-CGA-CBA	2.62	120.12	111.91
29	S	604	CLA	C1D-ND-C4D	-2.62	104.48	106.33
29	b	610	CLA	C1D-ND-C4D	-2.62	104.48	106.33
31	C1	515	BCR	C38-C26-C25	-2.62	121.59	124.53
29	B1	602	CLA	C2D-C1D-ND	2.61	112.03	110.10
29	c1	510	CLA	CHA-C4D-ND	2.61	137.97	132.50
29	b1	607	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
29	C	509	CLA	CHA-C4D-ND	2.61	137.97	132.50
48	n	609	CHL	CHB-C1B-NB	-2.61	121.49	124.26
29	S	605	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
36	b	620	C7Z	C24-C25-C26	-2.61	115.02	120.85
29	r	609	CLA	C2D-C1D-ND	2.61	112.03	110.10
29	S1	610	CLA	C2D-C1D-ND	2.61	112.03	110.10
29	B1	617	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
44	f	101	HEM	C4D-ND-C1D	2.61	107.77	105.07
36	B	620	C7Z	C11-C12-C13	-2.61	119.08	126.42
29	b1	616	CLA	C6-C5-C3	-2.61	106.60	113.45
47	I	102	4RF	O18-C16-C15	2.61	120.11	111.91
29	b	610	CLA	C1-C2-C3	-2.61	121.53	126.04
29	s	603	CLA	CHA-C1A-NA	-2.61	120.42	126.40
29	Y	608	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
48	S1	608	CHL	CHB-C4A-NA	2.61	128.12	124.51
29	b1	616	CLA	CHA-C4D-ND	2.61	137.96	132.50
29	C1	501	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
49	g1	621	LUT	C38-C25-C24	-2.61	117.97	123.56
29	Y1	604	CLA	CMA-C3A-C4A	2.61	118.79	111.77
29	B1	616	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
49	s1	621	LUT	C31-C32-C33	-2.61	119.08	126.42
29	C1	509	CLA	CHA-C4D-ND	2.61	137.96	132.50
48	n	607	CHL	CMA-C3A-C4A	2.61	118.79	111.77
29	Y	612	CLA	CHD-C1D-ND	-2.61	122.06	124.45
29	r1	604	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
48	g1	605	CHL	C1-O2A-CGA	2.61	124.31	116.73
29	c1	506	CLA	O2A-CGA-CBA	2.61	120.10	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B1	619	BCR	C34-C9-C10	-2.61	119.27	122.92
51	Y1	623	NEX	C11-C10-C9	2.61	131.03	127.31
29	C	511	CLA	CAA-CBA-CGA	-2.61	105.63	113.25
29	n1	603	CLA	CHA-C4D-ND	2.61	137.96	132.50
29	r1	610	CLA	CHA-C4D-ND	2.61	137.96	132.50
29	y1	603	CLA	C3B-C4B-NB	-2.61	108.09	110.52
29	C1	510	CLA	C1D-ND-C4D	-2.61	104.48	106.33
29	c	501	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
33	C1	521	LMG	O8-C28-C29	2.61	120.09	111.91
29	n	613	CLA	C2D-C1D-ND	2.61	112.03	110.10
29	Y1	611	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
29	C1	509	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
29	r1	603	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
31	B	618	BCR	C23-C22-C21	-2.61	114.94	118.94
29	d1	403	CLA	O2A-CGA-CBA	2.61	120.09	111.91
29	S	602	CLA	CHA-C4D-ND	2.61	137.95	132.50
29	y1	603	CLA	C4B-CHC-C1C	2.61	132.52	126.34
29	B1	616	CLA	C2D-C1D-ND	2.61	112.03	110.10
29	b	617	CLA	C2C-C1C-NC	2.61	112.41	109.97
29	b1	602	CLA	C2C-C1C-NC	2.61	112.41	109.97
48	y1	605	CHL	CMA-C3A-C4A	2.61	118.78	111.77
45	H	101	RRX	C36-C18-C19	2.61	122.18	118.08
48	N1	609	CHL	CHB-C4A-NA	2.61	128.12	124.51
48	N	605	CHL	C4B-CHC-C1C	2.61	132.52	126.34
29	b1	607	CLA	CMA-C3A-C4A	2.61	118.78	111.77
29	C1	503	CLA	O2A-CGA-CBA	2.61	120.08	111.91
48	y1	609	CHL	CHD-C1D-ND	-2.61	122.06	124.45
31	a1	411	BCR	C29-C28-C27	2.60	117.20	111.38
29	Y1	608	CLA	CHA-C4D-ND	2.60	137.95	132.50
42	D1	401	BCT	O3-C-O1	-2.60	112.79	119.55
29	C	510	CLA	C2C-C1C-NC	2.60	112.41	109.97
29	b1	613	CLA	CHA-C4D-ND	2.60	137.95	132.50
48	G	605	CHL	C3B-C4B-NB	-2.60	108.10	110.52
29	R1	603	CLA	C1-C2-C3	-2.60	121.54	126.04
48	y	606	CHL	CHB-C4A-NA	2.60	128.11	124.51
29	B1	602	CLA	CHA-C4D-ND	2.60	137.94	132.50
29	g1	611	CLA	C3B-C4B-NB	-2.60	108.10	110.52
29	G1	612	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
29	b1	617	CLA	C2D-C1D-ND	2.60	112.02	110.10
48	y1	606	CHL	CHB-C4A-NA	2.60	128.11	124.51
29	B	609	CLA	OBD-CAD-C3D	-2.60	122.26	128.52
49	G	620	LUT	C18-C5-C4	2.60	119.17	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S1	609	CLA	C1D-ND-C4D	-2.60	104.49	106.33
29	Y1	613	CLA	C1-O2A-CGA	2.60	123.27	116.44
29	b1	609	CLA	CHD-C1D-ND	-2.60	122.06	124.45
29	S1	610	CLA	C1D-ND-C4D	-2.60	104.49	106.33
29	a	410	CLA	C2D-C1D-ND	2.60	112.02	110.10
29	y	604	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
29	R1	603	CLA	CAC-C3C-C4C	2.60	128.18	124.81
40	c	525	LHG	C6-C5-C4	-2.60	105.64	111.79
29	s	614	CLA	C4B-CHC-C1C	2.60	132.50	126.34
29	y	610	CLA	C4B-CHC-C1C	2.60	132.50	126.34
29	R	602	CLA	C3B-C4B-NB	-2.60	108.10	110.52
29	S1	617	CLA	C2D-C1D-ND	2.60	112.02	110.10
29	C	506	CLA	C6-C5-C3	-2.60	106.64	113.45
40	g	624	LHG	O8-C23-C24	2.60	120.06	111.91
29	S1	613	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
31	C1	514	BCR	C33-C5-C6	-2.60	121.61	124.53
36	b	620	C7Z	C15-C35-C34	-2.60	118.15	123.47
49	r	620	LUT	C30-C31-C32	-2.60	115.11	123.22
29	b1	607	CLA	CHD-C1D-ND	-2.60	122.07	124.45
50	N1	622	XAT	O4-C5-C18	-2.60	111.94	115.06
29	G1	610	CLA	C3B-C4B-NB	-2.60	108.11	110.52
49	n	620	LUT	C8-C7-C6	-2.60	119.91	127.20
48	y	601	CHL	CHB-C4A-NA	2.60	128.10	124.51
29	d	402	CLA	C1D-ND-C4D	-2.60	104.49	106.33
52	R1	625	LMT	C3'-C4'-C5'	-2.60	104.97	110.93
29	B1	616	CLA	CMD-C2D-C3D	-2.60	121.64	127.61
48	n1	609	CHL	C2C-C3C-C4C	2.60	108.34	106.49
29	c	503	CLA	CMA-C3A-C4A	2.60	118.75	111.77
37	b	623	DGD	O1G-C1A-C2A	2.59	120.05	111.91
29	C	506	CLA	CHA-C4D-ND	2.59	137.93	132.50
29	b1	617	CLA	C4B-CHC-C1C	2.59	132.49	126.34
29	c	512	CLA	C1-C2-C3	-2.59	121.56	126.04
29	G	612	CLA	C4B-CHC-C1C	2.59	132.49	126.34
29	b1	615	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
33	c	523	LMG	O8-C28-C29	2.59	120.05	111.91
29	N	603	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
48	G	609	CHL	C3C-C4C-NC	-2.59	107.66	110.57
29	g	604	CLA	CHA-C4D-ND	2.59	137.93	132.50
29	R	608	CLA	C4B-CHC-C1C	2.59	132.49	126.34
29	y	603	CLA	O1D-CGD-CBD	-2.59	119.18	124.48
29	Y	614	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
29	R	603	CLA	C1C-C2C-C3C	-2.59	104.23	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	617	CLA	OBD-CAD-C3D	-2.59	122.28	128.52
29	b1	610	CLA	C1-C2-C3	-2.59	121.56	126.04
29	c	510	CLA	CHA-C4D-ND	2.59	137.92	132.50
48	N	608	CHL	CMA-C3A-C4A	2.59	118.74	111.77
29	c1	512	CLA	CHA-C4D-ND	2.59	137.92	132.50
29	G	602	CLA	C2D-C1D-ND	2.59	112.01	110.10
29	c	513	CLA	C2D-C1D-ND	2.59	112.01	110.10
29	g	610	CLA	O2A-CGA-CBA	2.59	120.04	111.91
29	y	610	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
29	B	606	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
29	s1	610	CLA	CHA-C4D-ND	2.59	137.92	132.50
29	d1	402	CLA	C2C-C1C-NC	2.59	112.40	109.97
29	g	603	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
29	s	605	CLA	CHA-C4D-ND	2.59	137.92	132.50
29	a1	405	CLA	C1D-ND-C4D	-2.59	104.50	106.33
29	n1	602	CLA	CMA-C3A-C4A	2.59	118.73	111.77
29	c1	501	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
48	G	607	CHL	C1-C2-C3	-2.59	121.56	126.04
29	S	604	CLA	C2C-C1C-NC	2.59	112.40	109.97
29	C1	513	CLA	C4B-CHC-C1C	2.59	132.48	126.34
29	B	607	CLA	CMD-C2D-C3D	-2.59	121.66	127.61
29	y1	603	CLA	CMD-C2D-C3D	-2.59	121.66	127.61
29	G	602	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
49	s1	621	LUT	C1-C6-C7	2.59	123.10	115.78
29	C	509	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
29	B	617	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
29	Y	613	CLA	O1D-CGD-CBD	-2.59	119.19	124.48
48	G1	606	CHL	CHB-C4A-NA	2.59	128.09	124.51
29	c	505	CLA	CHA-C4D-ND	2.59	137.91	132.50
29	s1	613	CLA	C4B-CHC-C1C	2.59	132.48	126.34
29	c1	501	CLA	CHD-C1D-ND	-2.59	122.08	124.45
29	S	609	CLA	C1-O2A-CGA	2.59	123.23	116.44
29	s	612	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
29	y	603	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
29	C1	512	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
29	b1	603	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
29	C	501	CLA	C1-C2-C3	-2.59	121.57	126.04
40	s	624	LHG	C5-O7-C7	-2.59	111.42	117.79
29	Y	614	CLA	CHA-C4D-ND	2.59	137.91	132.50
29	n	604	CLA	C3B-C4B-NB	-2.59	108.11	110.52
29	C1	501	CLA	C3B-C4B-NB	-2.59	108.11	110.52
29	g1	604	CLA	O2D-CGD-O1D	-2.59	118.78	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	G	608	CHL	C4A-NA-C1A	2.59	107.87	106.71
48	r	607	CHL	C4D-CHA-C1A	2.59	124.40	121.25
49	R	620	LUT	C18-C5-C4	2.59	119.15	114.36
29	s1	604	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
29	c1	509	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
29	c	506	CLA	C1-O2A-CGA	2.59	123.23	116.44
29	c1	504	CLA	CHA-C4D-ND	2.59	137.91	132.50
31	b1	619	BCR	C33-C5-C6	-2.59	121.62	124.53
48	g	605	CHL	CHB-C4A-NA	2.59	128.09	124.51
29	g1	610	CLA	CMA-C3A-C4A	2.58	118.72	111.77
29	A1	406	CLA	C4B-CHC-C1C	2.58	132.47	126.34
31	A1	411	BCR	C36-C18-C17	-2.58	119.30	122.92
29	r1	602	CLA	O2A-CGA-CBA	2.58	120.02	111.91
29	b	607	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
29	N	603	CLA	C3B-C4B-NB	-2.58	108.12	110.52
29	B	606	CLA	CHA-C4D-ND	2.58	137.90	132.50
50	R1	621	XAT	C19-C9-C10	-2.58	119.30	122.92
29	c1	513	CLA	CHA-C4D-ND	2.58	137.90	132.50
29	R	612	CLA	CMA-C3A-C4A	2.58	118.72	111.77
47	K1	101	4RF	O18-C16-C15	2.58	120.01	111.91
31	C1	517	BCR	C23-C24-C25	-2.58	119.95	127.20
29	G	612	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
29	R1	610	CLA	CMC-C2C-C1C	2.58	128.97	125.04
48	s1	608	CHL	CMA-C3A-C4A	2.58	118.71	111.77
31	c	516	BCR	C19-C18-C17	2.58	122.90	118.94
29	y	604	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
29	R1	602	CLA	CMA-C3A-C4A	2.58	118.71	111.77
29	d1	402	CLA	O1D-CGD-CBD	-2.58	119.20	124.48
48	Y	606	CHL	C3C-C4C-NC	-2.58	107.68	110.57
29	d	402	CLA	C2C-C1C-NC	2.58	112.39	109.97
51	R	622	NEX	C26-C27-C28	-2.58	120.54	125.99
37	B	623	DGD	O1G-C1A-C2A	2.58	120.01	111.91
29	s1	609	CLA	CMA-C3A-C4A	2.58	118.71	111.77
29	b	603	CLA	C4B-CHC-C1C	2.58	132.46	126.34
29	g	614	CLA	CHD-C1D-ND	-2.58	122.08	124.45
29	G1	602	CLA	CHA-C4D-ND	2.58	137.90	132.50
29	G	610	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
29	C	504	CLA	C3B-C4B-NB	-2.58	108.12	110.52
29	C	510	CLA	CHA-C4D-ND	2.58	137.90	132.50
29	B	606	CLA	O2A-CGA-CBA	2.58	120.00	111.91
29	d1	403	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
29	D1	402	CLA	C1D-ND-C4D	-2.58	104.50	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	501	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
29	s1	612	CLA	C3B-C4B-NB	-2.58	108.12	110.52
29	s	611	CLA	C2D-C1D-ND	2.58	112.00	110.10
29	B1	606	CLA	CMD-C2D-C3D	-2.58	121.69	127.61
29	r1	612	CLA	CMD-C2D-C3D	-2.58	121.69	127.61
50	N1	622	XAT	C7-C8-C9	-2.58	121.53	125.53
53	r	626	ERG	C18-C13-C14	-2.58	106.07	110.24
29	C	509	CLA	C6-C5-C3	-2.58	106.70	113.45
29	d	402	CLA	CHA-C4D-ND	2.58	137.89	132.50
29	y1	610	CLA	CMA-C3A-C4A	2.58	118.70	111.77
29	b1	613	CLA	CHD-C1D-ND	-2.58	122.09	124.45
48	Y	601	CHL	C4B-CHC-C1C	2.58	132.45	126.34
29	c1	506	CLA	C1-C2-C3	-2.58	121.59	126.04
29	B	614	CLA	C3D-C2D-C1D	-2.58	102.31	105.83
29	N	610	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
29	d	402	CLA	C1-C2-C3	-2.58	121.59	126.04
48	n	607	CHL	C1-O2A-CGA	2.58	123.20	116.44
29	Y1	610	CLA	C2C-C1C-NC	2.58	112.39	109.97
29	C1	507	CLA	C3B-C4B-NB	-2.58	108.13	110.52
48	g	605	CHL	C4B-CHC-C1C	2.57	132.44	126.34
51	G	623	NEX	C31-C30-C29	2.57	130.98	127.31
51	R	622	NEX	C31-C30-C29	2.57	130.98	127.31
31	c	514	BCR	C36-C18-C17	-2.57	119.32	122.92
37	b1	623	DGD	O1G-C1A-C2A	2.57	119.99	111.91
29	Y	614	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
48	R1	607	CHL	C3B-C4B-NB	-2.57	108.13	110.52
29	B	614	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
48	Y	605	CHL	C4D-CHA-C1A	2.57	124.38	121.25
29	a1	410	CLA	CHD-C1D-ND	-2.57	122.09	124.45
30	A	408	PHO	O1D-CGD-CBD	2.57	129.03	124.74
29	B	607	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
29	C1	502	CLA	CHA-C4D-ND	2.57	137.88	132.50
29	y1	608	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
29	b1	608	CLA	CHA-C4D-ND	2.57	137.88	132.50
30	A1	408	PHO	CMB-C2B-C3B	2.57	129.49	124.68
48	n	606	CHL	CHD-C1D-ND	-2.57	122.09	124.45
29	s1	604	CLA	CHA-C4D-ND	2.57	137.88	132.50
29	b	603	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
29	s	609	CLA	C2D-C1D-ND	2.57	112.00	110.10
29	g1	610	CLA	CHA-C4D-ND	2.57	137.88	132.50
29	r1	602	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
49	S	620	LUT	C15-C35-C34	-2.57	118.21	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	y1	610	CLA	O2A-CGA-CBA	2.57	119.98	111.91
29	b1	613	CLA	CMD-C2D-C3D	-2.57	121.70	127.61
48	S	601	CHL	CHB-C4A-NA	2.57	128.07	124.51
29	r1	608	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
29	N1	602	CLA	CHD-C1D-ND	-2.57	122.09	124.45
50	g	622	XAT	C39-C29-C30	-2.57	119.32	122.92
29	B1	616	CLA	CHA-C4D-ND	2.57	137.88	132.50
29	d1	402	CLA	CHA-C4D-ND	2.57	137.88	132.50
29	C1	502	CLA	C1-C2-C3	-2.57	121.60	126.04
48	y	601	CHL	C4D-CHA-C1A	2.57	124.38	121.25
48	s1	608	CHL	C4D-CHA-C1A	2.57	124.38	121.25
29	R	608	CLA	CMD-C2D-C3D	-2.57	121.70	127.61
49	n1	621	LUT	C38-C25-C24	-2.57	118.06	123.56
48	S1	606	CHL	CHD-C4C-C3C	2.57	128.62	124.84
49	S1	621	LUT	C18-C5-C4	2.57	119.11	114.36
33	H1	102	LMG	O8-C28-C29	2.57	119.97	111.91
29	y1	613	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
48	S	606	CHL	CHB-C4A-NA	2.57	128.06	124.51
40	N	624	LHG	O8-C23-C24	2.57	119.97	111.91
29	Y	602	CLA	CMA-C3A-C4A	2.57	118.67	111.77
29	R1	608	CLA	C1D-ND-C4D	-2.57	104.51	106.33
29	r	602	CLA	CHA-C4D-ND	2.57	137.87	132.50
38	S1	626	3PH	O31-C31-C32	2.57	119.97	111.91
49	g1	620	LUT	C11-C10-C9	-2.57	123.65	127.31
45	H1	101	RRX	C11-C12-C13	-2.57	119.20	126.42
29	C	504	CLA	C1-C2-C3	-2.57	121.60	126.04
29	G	613	CLA	O2A-CGA-CBA	2.57	119.96	111.91
39	b1	625	DGA	OG1-CA1-CA2	2.57	119.96	111.91
29	R	609	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
49	n	621	LUT	C18-C5-C6	-2.57	121.65	124.53
29	A	407	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
48	g	605	CHL	C4D-CHA-C1A	2.57	124.37	121.25
29	S	612	CLA	CHA-C4D-ND	2.57	137.87	132.50
29	r	602	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
29	B1	603	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
29	B1	607	CLA	O2A-CGA-CBA	2.56	119.96	111.91
29	c1	504	CLA	C1-C2-C3	-2.56	121.61	126.04
29	Y	603	CLA	CMB-C2B-C1B	2.56	129.27	125.37
29	y	610	CLA	C2C-C1C-NC	2.56	112.37	109.97
29	d1	402	CLA	CHD-C1D-ND	-2.56	122.10	124.45
29	S	603	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
29	g	611	CLA	CAA-C2A-C3A	-2.56	105.76	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	y	621	LUT	C2-C3-C4	-2.56	106.80	110.30
29	G1	603	CLA	C3B-C4B-NB	-2.56	108.14	110.52
48	S	608	CHL	C2C-C3C-C4C	2.56	108.32	106.49
29	g1	613	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
29	y1	612	CLA	CHA-C4D-ND	2.56	137.86	132.50
29	B1	610	CLA	CHA-C4D-ND	2.56	137.86	132.50
29	Y	612	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
48	s1	606	CHL	CHD-C1D-ND	-2.56	122.10	124.45
48	G	606	CHL	C2B-C1B-NB	-2.56	108.52	110.23
29	R1	610	CLA	C3B-C4B-NB	-2.56	108.14	110.52
44	F	101	HEM	C4A-NA-C1A	2.56	107.86	105.35
29	D1	402	CLA	C4B-CHC-C1C	2.56	132.41	126.34
29	B1	605	CLA	CHA-C4D-ND	2.56	137.86	132.50
29	N1	612	CLA	CHA-C4D-ND	2.56	137.86	132.50
29	B	615	CLA	C2D-C1D-ND	2.56	111.99	110.10
29	r	612	CLA	C2D-C1D-ND	2.56	111.99	110.10
29	G	603	CLA	CMA-C3A-C4A	2.56	118.65	111.77
29	n1	614	CLA	C1-O2A-CGA	2.56	123.16	116.44
29	C1	507	CLA	O2A-CGA-CBA	2.56	119.94	111.91
29	B	611	CLA	C1-C2-C3	-2.56	121.62	126.04
29	b	605	CLA	CMB-C2B-C1B	2.56	129.27	125.37
29	b1	606	CLA	CHA-C4D-ND	2.56	137.85	132.50
29	A	405	CLA	C1D-ND-C4D	-2.56	104.52	106.33
29	s1	613	CLA	C1-C2-C3	-2.56	121.62	126.04
49	s	620	LUT	C20-C13-C12	2.56	122.11	118.08
29	b1	612	CLA	O2A-CGA-CBA	2.56	119.94	111.91
29	B	613	CLA	C1-C2-C3	-2.56	121.62	126.04
29	Y1	612	CLA	CHA-C4D-ND	2.56	137.85	132.50
48	n	606	CHL	CMA-C3A-C4A	2.56	118.65	111.77
29	N1	614	CLA	CHD-C1D-ND	-2.56	122.10	124.45
48	N	609	CHL	CHD-C4C-C3C	2.56	128.60	124.84
37	B	623	DGD	O2G-C1B-O1B	-2.56	117.52	123.70
29	C1	505	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
29	d1	402	CLA	O2A-CGA-CBA	2.56	119.94	111.91
48	G1	607	CHL	C3B-C4B-NB	-2.56	108.14	110.52
29	s	617	CLA	C2D-C1D-ND	2.56	111.99	110.10
48	n	609	CHL	C2C-C3C-C4C	2.56	108.31	106.49
29	s	609	CLA	CHA-C4D-ND	2.56	137.85	132.50
29	S1	609	CLA	CMD-C2D-C3D	-2.56	121.73	127.61
48	G	601	CHL	C3B-C4B-NB	-2.56	108.14	110.52
36	b	620	C7Z	C21-C26-C27	2.56	123.01	115.78
29	S1	605	CLA	CAA-C2A-C3A	-2.56	105.78	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c1	507	CLA	CMD-C2D-C3D	-2.56	121.73	127.61
36	B1	620	C7Z	C20-C13-C14	-2.56	119.34	122.92
29	N	602	CLA	C4B-CHC-C1C	2.56	132.40	126.34
29	Y1	614	CLA	C4B-CHC-C1C	2.56	132.40	126.34
29	c	511	CLA	C1-C2-C3	-2.56	121.62	126.04
34	A	414	SPH	C3-C4-C5	-2.56	119.09	124.79
29	A1	406	CLA	CHD-C1D-ND	-2.56	122.11	124.45
29	R1	608	CLA	CMA-C3A-C4A	2.56	118.64	111.77
29	B1	608	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
29	c1	507	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
48	y	601	CHL	CHB-C1B-NB	-2.56	121.55	124.26
29	c1	503	CLA	O2A-CGA-CBA	2.56	119.93	111.91
40	D1	408	LHG	O8-C23-C24	2.55	119.92	111.91
29	b1	602	CLA	CHA-C4D-ND	2.55	137.84	132.50
29	R	610	CLA	CHA-C4D-ND	2.55	137.84	132.50
29	C1	505	CLA	O1D-CGD-CBD	-2.55	119.26	124.48
29	y1	602	CLA	C16-C15-C13	-2.55	107.66	115.92
29	B	610	CLA	CAA-CBA-CGA	-2.55	105.79	113.25
29	b1	617	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
48	G1	609	CHL	C3C-C4C-NC	-2.55	107.71	110.57
29	B1	617	CLA	CHA-C4D-ND	2.55	137.84	132.50
29	G1	604	CLA	CHA-C4D-ND	2.55	137.84	132.50
29	D	403	CLA	C3B-C4B-NB	-2.55	108.15	110.52
48	N1	605	CHL	C3B-C4B-NB	-2.55	108.15	110.52
29	R	603	CLA	C6-C5-C3	-2.55	106.76	113.45
29	N1	602	CLA	O2A-CGA-CBA	2.55	119.92	111.91
29	y1	603	CLA	OBD-CAD-C3D	-2.55	122.38	128.52
29	n1	610	CLA	C3B-C4B-NB	-2.55	108.15	110.52
29	b	611	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
32	B1	621	SQD	O3-C3-C2	-2.55	104.45	110.35
29	Y1	613	CLA	CHA-C4D-ND	2.55	137.84	132.50
29	R	608	CLA	CHD-C1D-ND	-2.55	122.11	124.45
29	G1	604	CLA	CHD-C1D-ND	-2.55	122.11	124.45
29	b	609	CLA	O1D-CGD-CBD	-2.55	119.26	124.48
29	b1	602	CLA	C1-C2-C3	-2.55	121.63	126.04
29	y	603	CLA	CMB-C2B-C1B	2.55	129.25	125.37
29	r1	612	CLA	CHA-C1A-NA	-2.55	120.56	126.40
48	S1	607	CHL	C4D-CHA-C1A	2.55	124.35	121.25
48	s	608	CHL	C4B-CHC-C1C	2.55	132.39	126.34
29	c	511	CLA	C2D-C1D-ND	2.55	111.98	110.10
29	A1	406	CLA	C2D-C1D-ND	2.55	111.98	110.10
29	C1	511	CLA	C2D-C1D-ND	2.55	111.98	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	509	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
29	C	511	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
29	n	613	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
29	b	605	CLA	O2A-CGA-CBA	2.55	119.91	111.91
31	c	517	BCR	C34-C9-C10	-2.55	119.35	122.92
29	N1	614	CLA	CHA-C4D-ND	2.55	137.83	132.50
29	b	604	CLA	CHD-C1D-ND	-2.55	122.11	124.45
40	Y	624	LHG	C6-C5-C4	-2.55	105.76	111.79
29	b1	605	CLA	C3D-C2D-C1D	-2.55	102.35	105.83
31	c	514	BCR	C15-C14-C13	-2.55	123.67	127.31
29	c	503	CLA	CAA-C2A-C3A	-2.55	105.80	112.78
29	r	609	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
29	b1	608	CLA	C2C-C1C-NC	2.55	112.36	109.97
29	R1	612	CLA	C4B-CHC-C1C	2.55	132.38	126.34
48	Y1	601	CHL	CHD-C4C-C3C	2.55	128.59	124.84
48	G1	608	CHL	C2B-C1B-NB	-2.55	108.52	110.23
29	y1	613	CLA	C1-O2A-CGA	2.55	123.13	116.44
48	Y1	601	CHL	C4D-CHA-C1A	2.55	124.35	121.25
29	b1	606	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
29	S1	603	CLA	C4B-CHC-C1C	2.55	132.38	126.34
29	b1	615	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
29	d	403	CLA	CMD-C2D-C3D	-2.55	121.76	127.61
29	c	506	CLA	CMD-C2D-C3D	-2.55	121.76	127.61
29	c1	512	CLA	O2A-CGA-CBA	2.55	119.90	111.91
29	R1	602	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
29	S1	614	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
29	G	614	CLA	CHA-C4D-ND	2.55	137.82	132.50
54	S1	625	LPX	O3-P1-O4	2.55	124.82	112.24
29	A1	406	CLA	CHA-C4D-ND	2.55	137.82	132.50
29	c1	502	CLA	C3B-C4B-NB	-2.54	108.15	110.52
48	N1	605	CHL	C4D-CHA-C1A	2.54	124.35	121.25
48	g1	605	CHL	C2B-C1B-NB	-2.54	108.53	110.23
29	n1	604	CLA	O2A-CGA-CBA	2.54	119.89	111.91
49	y1	620	LUT	C31-C30-C29	-2.54	123.68	127.31
29	C1	507	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
29	B	614	CLA	O2A-CGA-CBA	2.54	119.89	111.91
29	g	612	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
37	C	520	DGD	O6D-C5D-C6D	2.54	111.80	106.67
31	c1	516	BCR	C19-C18-C17	2.54	122.84	118.94
49	N	620	LUT	C10-C11-C12	-2.54	115.28	123.22
29	S	602	CLA	CHD-C1D-ND	-2.54	122.12	124.45
29	a	407	CLA	C2D-C1D-ND	2.54	111.98	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	s	621	LUT	C20-C13-C12	2.54	122.08	118.08
48	Y1	609	CHL	C4A-NA-C1A	2.54	107.85	106.71
51	r	622	NEX	C16-C1-C6	-2.54	108.20	110.47
29	B	611	CLA	O2A-CGA-CBA	2.54	119.89	111.91
38	B	624	3PH	O31-C31-C32	2.54	119.89	111.91
29	C1	512	CLA	C4B-CHC-C1C	2.54	132.37	126.34
51	y1	623	NEX	C1-C2-C3	2.54	119.38	113.64
29	r	609	CLA	C4B-CHC-C1C	2.54	132.37	126.34
29	S1	611	CLA	O2A-CGA-CBA	2.54	119.88	111.91
29	y1	608	CLA	OBD-CAD-C3D	-2.54	122.41	128.52
40	c1	525	LHG	O8-C23-C24	2.54	119.88	111.91
29	s	614	CLA	CHA-C4D-ND	2.54	137.81	132.50
40	L	101	LHG	C5-O7-C7	-2.54	111.54	117.79
53	R	626	ERG	C13-C14-C8	2.54	118.41	113.48
29	C	505	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
48	N	607	CHL	C4D-CHA-C1A	2.54	124.34	121.25
29	y1	602	CLA	C4B-CHC-C1C	2.54	132.36	126.34
29	b	613	CLA	CHD-C1D-ND	-2.54	122.12	124.45
48	r1	607	CHL	CHB-C4A-NA	2.54	128.02	124.51
29	C	504	CLA	C2C-C1C-NC	2.54	112.35	109.97
31	A1	411	BCR	C12-C13-C14	-2.54	115.05	118.94
29	c1	507	CLA	CHA-C4D-ND	2.54	137.81	132.50
40	d	410	LHG	O8-C23-C24	2.54	119.88	111.91
29	s1	605	CLA	C1-O2A-CGA	2.54	123.11	116.44
29	S	611	CLA	CHD-C1D-ND	-2.54	122.12	124.45
29	S	603	CLA	CHA-C1A-NA	-2.54	120.58	126.40
29	B1	613	CLA	C1-C2-C3	-2.54	121.65	126.04
29	Y1	610	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
29	B1	607	CLA	CHA-C4D-ND	2.54	137.81	132.50
29	G	610	CLA	C2D-C1D-ND	2.54	111.97	110.10
29	C1	508	CLA	CMA-C3A-C4A	2.54	118.59	111.77
29	C	507	CLA	CHA-C4D-ND	2.54	137.81	132.50
29	n1	612	CLA	CHA-C4D-ND	2.54	137.81	132.50
48	S	607	CHL	C4B-CHC-C1C	2.54	132.36	126.34
29	y1	610	CLA	CHA-C4D-ND	2.54	137.81	132.50
33	d	411	LMG	C6-C5-C4	-2.54	107.06	113.00
48	G	609	CHL	C3B-C4B-NB	-2.54	108.16	110.52
29	Y1	611	CLA	C2C-C1C-NC	2.54	112.35	109.97
29	N1	612	CLA	C2D-C1D-ND	2.54	111.97	110.10
29	S1	610	CLA	OBD-CAD-C3D	-2.54	122.42	128.52
29	Y1	612	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
29	R	603	CLA	CHA-C1A-NA	-2.54	120.59	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s1	612	CLA	CHA-C4D-ND	2.54	137.80	132.50
29	Y	603	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
29	b	609	CLA	C2C-C1C-NC	2.54	112.35	109.97
29	b	607	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
48	r	607	CHL	CHD-C4C-C3C	2.53	128.57	124.84
29	G	611	CLA	C2D-C1D-ND	2.53	111.97	110.10
29	Y1	610	CLA	C2D-C1D-ND	2.53	111.97	110.10
33	W1	201	LMG	C4-C3-C2	2.53	115.25	110.82
29	b	607	CLA	CHA-C4D-ND	2.53	137.80	132.50
49	Y1	620	LUT	C31-C30-C29	-2.53	123.69	127.31
29	g	614	CLA	C3B-C4B-NB	-2.53	108.16	110.52
29	G	604	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
29	B	606	CLA	O1D-CGD-CBD	-2.53	119.30	124.48
29	C	510	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
48	S	606	CHL	C2C-C3C-C4C	2.53	108.30	106.49
29	B	602	CLA	CMA-C3A-C4A	2.53	118.58	111.77
29	B1	602	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
29	R	602	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
29	G	602	CLA	CMD-C2D-C3D	-2.53	121.79	127.61
29	s	617	CLA	CHA-C4D-ND	2.53	137.80	132.50
40	d1	408	LHG	O8-C23-C24	2.53	119.86	111.91
29	R	608	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
51	y1	623	NEX	C35-C34-C33	2.53	130.92	127.31
29	a1	410	CLA	CHA-C4D-ND	2.53	137.80	132.50
50	y	622	XAT	O4-C5-C4	-2.53	111.48	113.38
50	g1	622	XAT	C20-C13-C14	-2.53	119.38	122.92
31	c	517	BCR	C35-C13-C12	2.53	122.06	118.08
29	S1	612	CLA	CHD-C1D-ND	-2.53	122.13	124.45
29	n	612	CLA	OBD-CAD-C3D	-2.53	122.43	128.52
48	Y1	601	CHL	C3B-C4B-NB	-2.53	108.17	110.52
29	b1	608	CLA	CMA-C3A-C4A	2.53	118.58	111.77
29	c1	508	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
40	L1	101	LHG	O7-C7-O9	-2.53	117.59	123.70
29	c	512	CLA	C4B-CHC-C1C	2.53	132.34	126.34
31	C	514	BCR	C37-C22-C23	2.53	122.06	118.08
29	B	606	CLA	CMD-C2D-C3D	-2.53	121.79	127.61
29	A	406	CLA	O2A-CGA-CBA	2.53	119.85	111.91
29	Y	611	CLA	CMD-C2D-C3D	-2.53	121.80	127.61
48	y1	607	CHL	C4D-CHA-C1A	2.53	124.33	121.25
48	s	608	CHL	C4A-NA-C1A	2.53	107.84	106.71
29	s	613	CLA	C1-C2-C3	-2.53	121.67	126.04
29	D	403	CLA	O2A-CGA-CBA	2.53	119.84	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n	610	CLA	C4B-CHC-C1C	2.53	132.34	126.34
29	R1	603	CLA	C3B-C4B-NB	-2.53	108.17	110.52
50	G1	622	XAT	C19-C9-C10	-2.53	119.38	122.92
29	s	605	CLA	CMD-C2D-C3D	-2.53	121.80	127.61
29	b	609	CLA	CHA-C4D-ND	2.53	137.79	132.50
29	y	608	CLA	CHA-C4D-ND	2.53	137.79	132.50
29	c	501	CLA	CMD-C2D-C3D	-2.53	121.80	127.61
29	r	610	CLA	C2A-C1A-CHA	2.53	128.28	123.86
40	D	410	LHG	O8-C23-C24	2.53	119.84	111.91
31	D	404	BCR	C33-C5-C4	2.53	118.47	113.62
29	S1	614	CLA	CHA-C1A-NA	-2.53	120.61	126.40
29	N1	612	CLA	CMA-C3A-C4A	2.53	118.56	111.77
29	s	604	CLA	CHA-C4D-ND	2.53	137.78	132.50
29	y	614	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
49	G1	620	LUT	C2-C3-C4	-2.53	106.85	110.30
29	C1	513	CLA	CHA-C4D-ND	2.52	137.78	132.50
39	j1	101	DGA	OG1-CA1-CA2	2.52	119.83	111.91
29	n1	612	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
29	r1	609	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
48	G	605	CHL	CHD-C1D-ND	-2.52	122.13	124.45
29	b1	610	CLA	CHA-C4D-ND	2.52	137.78	132.50
29	Y1	614	CLA	CAA-C2A-C3A	-2.52	105.86	112.78
45	h	101	RRX	C30-C25-C26	-2.52	119.06	122.61
49	s	621	LUT	C15-C14-C13	-2.52	123.71	127.31
29	b1	613	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
49	N	621	LUT	C3-C4-C5	-2.52	106.83	111.85
53	R1	626	ERG	C20-C22-C23	-2.52	117.84	125.67
29	S1	610	CLA	C2C-C1C-NC	2.52	112.34	109.97
29	N1	610	CLA	C1D-ND-C4D	-2.52	104.54	106.33
29	n	613	CLA	C1-O2A-CGA	2.52	123.06	116.44
29	r	604	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
44	F1	101	HEM	CAD-C3D-C2D	-2.52	123.18	127.88
29	N	603	CLA	C1D-ND-C4D	-2.52	104.54	106.33
33	h	102	LMG	O8-C28-C29	2.52	119.82	111.91
49	G1	620	LUT	C38-C25-C24	-2.52	118.17	123.56
48	Y	607	CHL	C1-C2-C3	-2.52	121.68	126.04
29	n1	613	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
29	A	405	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
29	C1	512	CLA	CHA-C4D-ND	2.52	137.77	132.50
29	R1	602	CLA	C1-O2A-CGA	2.52	123.06	116.44
29	s	611	CLA	O2A-CGA-CBA	2.52	119.82	111.91
29	b1	610	CLA	C2D-C1D-ND	2.52	111.96	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	g	614	CLA	CHA-C4D-ND	2.52	137.77	132.50
29	G	604	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
50	G1	622	XAT	C18-C5-C6	-2.52	118.04	122.26
40	N1	624	LHG	C6-C5-C4	-2.52	105.83	111.79
48	Y	609	CHL	CHC-C1C-NC	2.52	128.03	124.20
33	h1	102	LMG	C8-O7-C10	-2.52	111.59	117.79
29	N	604	CLA	CMD-C2D-C3D	-2.52	121.82	127.61
39	C1	524	DGA	OG1-CA1-CA2	2.52	119.81	111.91
31	c1	514	BCR	C33-C5-C4	2.52	118.45	113.62
29	C	502	CLA	C1-O2A-CGA	2.52	123.05	116.44
29	b	615	CLA	C2D-C1D-ND	2.52	111.96	110.10
52	R	625	LMT	O5B-C1B-C2B	2.52	115.68	110.35
33	D	411	LMG	O8-C28-C29	2.52	119.81	111.91
29	Y	603	CLA	C3B-C4B-NB	-2.52	108.18	110.52
29	B	609	CLA	CHA-C4D-ND	2.52	137.77	132.50
29	r	612	CLA	CHA-C4D-ND	2.52	137.77	132.50
48	Y	606	CHL	CMA-C3A-C4A	2.52	118.54	111.77
29	N	602	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
49	S1	621	LUT	C7-C8-C9	-2.52	122.43	126.23
29	s1	612	CLA	C4B-CHC-C1C	2.52	132.31	126.34
51	y1	623	NEX	C17-C1-C6	-2.52	108.22	110.47
29	C1	507	CLA	CHA-C4D-ND	2.52	137.76	132.50
29	y	604	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
45	h1	101	RRX	C10-C11-C12	-2.52	115.36	123.22
48	S1	608	CHL	C4D-CHA-C1A	2.52	124.31	121.25
48	g	607	CHL	CHB-C4A-NA	2.52	127.99	124.51
29	G1	611	CLA	CHA-C4D-ND	2.52	137.76	132.50
29	Y1	603	CLA	O2A-CGA-CBA	2.52	119.80	111.91
29	c1	513	CLA	C1D-ND-C4D	-2.52	104.55	106.33
29	C1	506	CLA	CMD-C2D-C3D	-2.52	121.83	127.61
29	b1	602	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
48	N	605	CHL	C1-C2-C3	-2.52	121.69	126.04
29	c	509	CLA	CHA-C4D-ND	2.51	137.76	132.50
29	n	614	CLA	C3B-C4B-NB	-2.51	108.18	110.52
29	S	612	CLA	C4B-CHC-C1C	2.51	132.30	126.34
29	c	501	CLA	C2D-C1D-ND	2.51	111.96	110.10
48	S1	601	CHL	CHB-C4A-NA	2.51	127.99	124.51
29	G	604	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
29	s	612	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
29	B	611	CLA	CMA-C3A-C4A	2.51	118.53	111.77
29	R1	610	CLA	C2C-C1C-NC	2.51	112.33	109.97
48	r1	607	CHL	CHD-C4C-C3C	2.51	128.53	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C1	516	BCR	C34-C9-C10	-2.51	119.40	122.92
29	d1	402	CLA	CMA-C3A-C4A	2.51	118.53	111.77
29	c1	513	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
29	s	602	CLA	CHA-C4D-ND	2.51	137.76	132.50
29	b1	602	CLA	CMC-C2C-C1C	2.51	128.87	125.04
40	d1	410	LHG	C5-O7-C7	-2.51	111.61	117.79
29	g1	614	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	C1	505	CLA	C1-O2A-CGA	2.51	123.03	116.44
29	G	610	CLA	C4B-CHC-C1C	2.51	132.29	126.34
29	y1	608	CLA	O2A-CGA-CBA	2.51	119.79	111.91
29	b	602	CLA	C4B-CHC-C1C	2.51	132.29	126.34
29	b	608	CLA	CHA-C4D-ND	2.51	137.75	132.50
43	d	405	PL9	C27-C28-C29	-2.51	121.61	127.66
29	r1	609	CLA	C3B-C4B-NB	-2.51	108.19	110.52
29	g	613	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
43	d1	405	PL9	O2-C1-C6	2.51	124.94	120.59
29	C1	501	CLA	CHA-C4D-ND	2.51	137.75	132.50
30	A1	409	PHO	C1C-C2C-C3C	-2.51	106.52	108.61
29	r	610	CLA	C4B-CHC-C1C	2.51	132.29	126.34
29	Y	612	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	y	613	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	r1	603	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	R	608	CLA	O2A-CGA-CBA	2.51	119.78	111.91
29	d	403	CLA	O2A-CGA-CBA	2.51	119.78	111.91
29	C1	501	CLA	C4B-CHC-C1C	2.51	132.29	126.34
29	b1	614	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
48	g1	609	CHL	CHC-C1C-NC	2.51	128.01	124.20
29	S	603	CLA	CHA-C4D-ND	2.51	137.75	132.50
49	R	620	LUT	C35-C15-C14	-2.51	118.33	123.47
29	R	609	CLA	C1-C2-C3	-2.51	121.70	126.04
29	c	503	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	b	615	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	n	612	CLA	CHA-C4D-ND	2.51	137.75	132.50
51	y1	623	NEX	C26-C27-C28	-2.51	120.69	125.99
29	y1	612	CLA	O2A-CGA-CBA	2.51	119.78	111.91
50	Y	622	XAT	C39-C29-C30	-2.51	119.41	122.92
31	b	619	BCR	C23-C24-C25	-2.51	120.16	127.20
29	Y	604	CLA	CHA-C4D-ND	2.51	137.74	132.50
29	y1	611	CLA	CHA-C4D-ND	2.51	137.74	132.50
29	n	604	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
40	G1	624	LHG	O8-C23-C24	2.51	119.78	111.91
43	D1	405	PL9	C31-C32-C33	-2.51	103.64	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	y	602	CLA	CHA-C4D-ND	2.51	137.74	132.50
48	N	608	CHL	C1-O2A-CGA	2.51	123.02	116.44
29	y1	611	CLA	CHD-C1D-ND	-2.51	122.15	124.45
48	n	608	CHL	CHD-C1D-ND	-2.51	122.15	124.45
33	C	523	LMG	O8-C28-C29	2.51	119.77	111.91
47	k	101	4RF	O40-C41-C43	2.51	119.77	111.91
29	n1	610	CLA	C1-C2-C3	-2.51	121.71	126.04
29	b1	617	CLA	CHA-C4D-ND	2.51	137.74	132.50
51	Y	623	NEX	C4-C3-C2	2.51	115.61	110.77
29	c	511	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
29	A	410	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
29	s1	603	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
29	c1	510	CLA	CHA-C1A-NA	-2.51	120.66	126.40
29	b	603	CLA	CHA-C4D-ND	2.51	137.74	132.50
29	R1	602	CLA	CHA-C4D-ND	2.51	137.74	132.50
29	s1	602	CLA	C2C-C1C-NC	2.51	112.32	109.97
49	G	621	LUT	C38-C25-C24	-2.51	118.20	123.56
29	G1	610	CLA	CHA-C4D-ND	2.50	137.74	132.50
48	R1	607	CHL	C4A-NA-C1A	2.50	107.83	106.71
29	r	610	CLA	CMD-C2D-C3D	-2.50	121.85	127.61
39	J1	101	DGA	OG1-CA1-CA2	2.50	119.77	111.91
29	s	603	CLA	C2A-C1A-CHA	2.50	128.24	123.86
29	S	609	CLA	C2D-C1D-ND	2.50	111.95	110.10
29	C	513	CLA	CHA-C4D-ND	2.50	137.74	132.50
29	s1	609	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
29	g	602	CLA	C4B-CHC-C1C	2.50	132.28	126.34
29	G	614	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
51	Y1	623	NEX	C40-C33-C34	-2.50	119.42	122.92
50	n	622	XAT	O4-C5-C4	-2.50	111.50	113.38
29	r	603	CLA	CHA-C1A-NA	-2.50	120.67	126.40
29	b1	614	CLA	C1-C2-C3	-2.50	121.72	126.04
49	S	620	LUT	C8-C7-C6	-2.50	120.17	127.20
29	R1	608	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
50	y1	622	XAT	C20-C13-C14	-2.50	119.42	122.92
29	B	617	CLA	CHA-C4D-ND	2.50	137.73	132.50
49	G	620	LUT	C3-C4-C5	-2.50	106.87	111.85
29	R	609	CLA	C4B-CHC-C1C	2.50	132.27	126.34
48	G	606	CHL	C1-O2A-CGA	2.50	123.01	116.44
29	D	403	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
29	r	604	CLA	CHA-C4D-ND	2.50	137.73	132.50
29	y1	610	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
29	c1	511	CLA	CMD-C2D-C3D	-2.50	121.86	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	613	CLA	C3B-C4B-NB	-2.50	108.19	110.52
29	c	506	CLA	CHA-C4D-ND	2.50	137.73	132.50
29	S	605	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
29	A	410	CLA	CMB-C2B-C3B	2.50	132.64	126.59
29	g1	614	CLA	C4B-CHC-C1C	2.50	132.27	126.34
29	b	602	CLA	CHA-C4D-ND	2.50	137.73	132.50
31	c1	514	BCR	C40-C30-C25	-2.50	106.25	110.30
48	g	606	CHL	C2B-C1B-NB	-2.50	108.56	110.23
29	B	605	CLA	CMD-C2D-C3D	-2.50	121.87	127.61
49	N	620	LUT	C18-C5-C6	-2.50	121.72	124.53
29	B	603	CLA	CHA-C4D-ND	2.50	137.72	132.50
29	G	613	CLA	CHA-C4D-ND	2.50	137.72	132.50
29	r1	610	CLA	CMA-C3A-C4A	2.50	118.49	111.77
50	Y	622	XAT	C18-C5-C6	-2.50	118.08	122.26
29	C1	511	CLA	OBD-CAD-C3D	-2.50	122.51	128.52
29	C1	504	CLA	CHD-C1D-ND	-2.50	122.16	124.45
29	G1	602	CLA	C4D-CHA-C1A	2.50	124.29	121.25
29	B1	603	CLA	C6-C5-C3	-2.50	106.91	113.45
48	G	609	CHL	C1-O2A-CGA	2.50	123.00	116.44
29	R1	610	CLA	O2A-CGA-CBA	2.50	119.74	111.91
29	G1	602	CLA	C1-C2-C3	-2.50	121.72	126.04
29	S	602	CLA	CMA-C3A-C4A	2.50	118.48	111.77
29	n	614	CLA	C4B-CHC-C1C	2.50	132.26	126.34
48	S	608	CHL	CHB-C4A-NA	2.50	127.96	124.51
29	n1	614	CLA	CHA-C4D-ND	2.50	137.72	132.50
48	G	609	CHL	CHC-C1C-NC	2.50	127.99	124.20
29	g1	602	CLA	C1-O2A-CGA	2.50	122.99	116.44
29	c	506	CLA	O2A-CGA-CBA	2.50	119.74	111.91
49	s	621	LUT	C16-C1-C6	-2.50	106.25	110.30
29	n1	614	CLA	C2D-C1D-ND	2.50	111.94	110.10
29	A1	410	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
50	n1	622	XAT	C39-C29-C30	-2.50	119.43	122.92
29	c1	505	CLA	O1D-CGD-CBD	-2.49	119.38	124.48
29	G	611	CLA	CMA-C3A-C4A	2.49	118.48	111.77
48	G	606	CHL	C4B-CHC-C1C	2.49	132.25	126.34
32	m	101	SQD	O3-C3-C2	-2.49	104.58	110.35
29	R1	608	CLA	CHA-C4D-ND	2.49	137.71	132.50
48	S1	608	CHL	C2C-C3C-C4C	2.49	108.27	106.49
40	y1	624	LHG	O8-C23-C24	2.49	119.73	111.91
49	N	621	LUT	C7-C8-C9	-2.49	122.47	126.23
48	y1	609	CHL	C3C-C4C-NC	-2.49	107.78	110.57
29	y1	610	CLA	O1D-CGD-CBD	-2.49	119.39	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	S	624	LHG	C5-O7-C7	-2.49	111.66	117.79
48	G1	605	CHL	C1-O2A-CGA	2.49	123.97	116.73
29	b	605	CLA	C16-C15-C13	-2.49	107.86	115.92
31	b1	619	BCR	C36-C18-C17	-2.49	119.43	122.92
29	R	610	CLA	C3D-C2D-C1D	-2.49	102.43	105.83
29	b1	604	CLA	C2C-C1C-NC	2.49	112.31	109.97
29	r1	612	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
29	r1	602	CLA	C3B-C4B-NB	-2.49	108.20	110.52
29	g1	603	CLA	CHA-C4D-ND	2.49	137.71	132.50
49	g	620	LUT	C10-C11-C12	-2.49	115.44	123.22
53	R1	626	ERG	C14-C8-C7	-2.49	119.47	124.38
29	r	610	CLA	CHA-C4D-ND	2.49	137.71	132.50
29	C1	506	CLA	CHA-C4D-ND	2.49	137.71	132.50
29	R	602	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
29	C	511	CLA	O2A-CGA-CBA	2.49	119.72	111.91
29	n	603	CLA	CHA-C4D-ND	2.49	137.71	132.50
48	y1	601	CHL	C2C-C3C-C4C	2.49	108.26	106.49
29	s	603	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
29	r	612	CLA	C1-C2-C3	-2.49	121.74	126.04
29	s1	604	CLA	C4B-CHC-C1C	2.49	132.24	126.34
29	A	405	CLA	CHA-C4D-ND	2.49	137.71	132.50
29	B	607	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
29	C	512	CLA	O2A-CGA-CBA	2.49	119.72	111.91
32	a1	412	SQD	O3-C3-C2	-2.49	104.59	110.35
29	C1	511	CLA	O2A-CGA-CBA	2.49	119.72	111.91
29	B1	611	CLA	C1-O2A-CGA	2.49	122.97	116.44
29	S1	604	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
29	s1	605	CLA	CHA-C4D-ND	2.49	137.71	132.50
29	S	611	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
29	s1	610	CLA	C2C-C1C-NC	2.49	112.30	109.97
29	y1	614	CLA	C2C-C1C-NC	2.49	112.30	109.97
29	N1	611	CLA	CHA-C4D-ND	2.49	137.70	132.50
51	Y1	623	NEX	C26-C27-C28	-2.49	120.73	125.99
29	B1	607	CLA	C1-O2A-CGA	2.49	122.97	116.44
29	r	608	CLA	CHA-C4D-ND	2.49	137.70	132.50
43	D	405	PL9	C22-C23-C24	-2.49	121.67	127.66
29	b	615	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
29	B	602	CLA	C3B-C4B-NB	-2.49	108.21	110.52
29	G	602	CLA	CHA-C4D-ND	2.49	137.70	132.50
48	S	601	CHL	C2B-C1B-NB	-2.49	108.56	110.23
29	C	513	CLA	C1-O2A-CGA	2.49	122.97	116.44
29	C1	505	CLA	C2C-C1C-NC	2.49	112.30	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	607	CLA	C2D-C1D-ND	2.49	111.94	110.10
29	s	611	CLA	CHA-C4D-ND	2.49	137.70	132.50
29	S	611	CLA	CHA-C4D-ND	2.48	137.70	132.50
29	n	604	CLA	CHA-C4D-ND	2.48	137.70	132.50
29	B	603	CLA	C3B-C4B-NB	-2.48	108.21	110.52
29	b	608	CLA	C1-O2A-CGA	2.48	122.96	116.44
29	S	609	CLA	CHA-C4D-ND	2.48	137.69	132.50
29	Y	602	CLA	CHA-C4D-ND	2.48	137.69	132.50
29	B1	609	CLA	CHA-C4D-ND	2.48	137.69	132.50
29	b	608	CLA	O2A-CGA-CBA	2.48	119.70	111.91
29	y	614	CLA	C1D-ND-C4D	-2.48	104.57	106.33
29	C	503	CLA	O2A-CGA-CBA	2.48	119.70	111.91
29	c1	503	CLA	CMD-C2D-C3D	-2.48	121.90	127.61
48	y	605	CHL	C4D-CHA-C1A	2.48	124.27	121.25
48	N1	605	CHL	C4A-NA-C1A	2.48	107.82	106.71
29	c1	512	CLA	C4B-CHC-C1C	2.48	132.22	126.34
50	G1	622	XAT	O4-C5-C4	-2.48	111.52	113.38
29	n1	602	CLA	C4B-CHC-C1C	2.48	132.22	126.34
51	G	623	NEX	C40-C33-C34	-2.48	119.45	122.92
29	S1	609	CLA	CHA-C4D-ND	2.48	137.69	132.50
48	n	601	CHL	C1-C2-C3	-2.48	121.75	126.04
29	y	603	CLA	C3B-C4B-NB	-2.48	108.21	110.52
29	y1	614	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
51	g1	623	NEX	C28-C29-C30	2.48	122.75	118.94
41	C1	527	LMK	O3-C4-C3	-2.48	114.47	122.98
31	c	516	BCR	C36-C18-C17	-2.48	119.45	122.92
50	G	622	XAT	C8-C9-C10	2.48	122.75	118.94
29	b1	614	CLA	O2A-CGA-CBA	2.48	119.69	111.91
29	R	610	CLA	CHD-C1D-ND	-2.48	122.18	124.45
48	y	605	CHL	C3B-C4B-NB	-2.48	108.22	110.52
48	G1	607	CHL	C1-O2A-CGA	2.48	122.94	116.44
31	B	618	BCR	C37-C22-C23	2.48	121.98	118.08
51	R1	622	NEX	C19-C9-C10	-2.48	119.45	122.92
50	G1	622	XAT	C31-C30-C29	-2.48	123.78	127.31
29	N	611	CLA	CMA-C3A-C4A	2.48	118.43	111.77
29	S1	614	CLA	C4B-CHC-C1C	2.48	132.21	126.34
29	B	613	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
29	B1	604	CLA	C2D-C1D-ND	2.48	111.93	110.10
51	s	623	NEX	O24-C25-C38	-2.48	112.09	115.06
48	S1	601	CHL	C2B-C1B-NB	-2.48	108.57	110.23
29	n1	612	CLA	C3B-C4B-NB	-2.48	108.22	110.52
51	G1	623	NEX	C38-C25-C26	-2.48	118.11	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	501	CLA	CHA-C4D-ND	2.48	137.68	132.50
49	Y1	621	LUT	C18-C5-C6	-2.48	121.75	124.53
29	s	609	CLA	CHD-C1D-ND	-2.48	122.18	124.45
48	G	608	CHL	CHB-C4A-NA	2.48	127.94	124.51
29	B	610	CLA	CHA-C4D-ND	2.48	137.68	132.50
29	s1	610	CLA	C2D-C1D-ND	2.48	111.93	110.10
29	S1	604	CLA	O2A-CGA-CBA	2.47	119.67	111.91
29	g1	604	CLA	CHA-C4D-ND	2.47	137.68	132.50
29	Y	603	CLA	CHA-C4D-ND	2.47	137.68	132.50
29	y1	610	CLA	C4B-CHC-C1C	2.47	132.21	126.34
29	n	612	CLA	C3B-C4B-NB	-2.47	108.22	110.52
29	s	610	CLA	CHA-C4D-ND	2.47	137.67	132.50
29	B1	616	CLA	C4B-CHC-C1C	2.47	132.21	126.34
29	C	502	CLA	CMA-C3A-C4A	2.47	118.42	111.77
29	b1	609	CLA	CHA-C4D-ND	2.47	137.67	132.50
29	c1	512	CLA	CMA-C3A-C2A	2.47	123.80	113.83
33	A1	413	LMG	O1-C1-C2	2.47	112.16	108.30
29	c1	512	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
29	Y	612	CLA	C3B-C4B-NB	-2.47	108.22	110.52
48	S1	601	CHL	C4D-CHA-C1A	2.47	124.26	121.25
29	s1	603	CLA	CHA-C4D-ND	2.47	137.67	132.50
29	g1	614	CLA	C2D-C1D-ND	2.47	111.93	110.10
29	B1	615	CLA	CHA-C4D-ND	2.47	137.67	132.50
29	c1	509	CLA	CHA-C4D-ND	2.47	137.67	132.50
29	Y	603	CLA	C1D-ND-C4D	-2.47	104.58	106.33
48	y1	609	CHL	C2B-C1B-NB	-2.47	108.58	110.23
29	g	603	CLA	CMD-C2D-C3D	-2.47	121.93	127.61
29	N	604	CLA	C2D-C1D-ND	2.47	111.92	110.10
48	g1	608	CHL	C4B-CHC-C1C	2.47	132.20	126.34
29	B	605	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
29	a	406	CLA	CHA-C4D-ND	2.47	137.67	132.50
48	G1	606	CHL	CHD-C1D-ND	-2.47	122.18	124.45
29	r1	608	CLA	CHA-C4D-ND	2.47	137.67	132.50
29	n	602	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
49	g	621	LUT	C16-C1-C6	-2.47	106.29	110.30
29	S	610	CLA	CHA-C4D-ND	2.47	137.66	132.50
29	r	609	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
29	r	610	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
29	b1	606	CLA	O2A-CGA-CBA	2.47	119.66	111.91
29	D1	403	CLA	CHA-C4D-ND	2.47	137.66	132.50
29	a1	406	CLA	C4B-CHC-C1C	2.47	132.19	126.34
29	a	406	CLA	C2D-C1D-ND	2.47	111.92	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c1	508	CLA	C2C-C1C-NC	2.47	112.28	109.97
29	g	612	CLA	CHA-C4D-ND	2.47	137.66	132.50
29	s1	612	CLA	CHA-C1A-NA	-2.47	120.75	126.40
51	G	623	NEX	C20-C13-C14	-2.47	119.47	122.92
29	A1	405	CLA	C2D-C1D-ND	2.47	111.92	110.10
48	G	607	CHL	C4A-NA-C1A	2.47	107.81	106.71
48	n1	606	CHL	CHB-C4A-NA	2.47	127.92	124.51
48	G1	609	CHL	CHC-C1C-NC	2.47	127.94	124.20
48	s1	607	CHL	CHC-C4B-NB	-2.47	121.65	124.26
29	r1	609	CLA	CAC-C3C-C4C	2.47	128.01	124.81
29	C1	507	CLA	CHA-C1A-NA	-2.47	120.75	126.40
29	g	604	CLA	CMD-C2D-C3D	-2.47	121.94	127.61
29	C	513	CLA	CMA-C3A-C4A	2.47	118.40	111.77
29	c1	507	CLA	C1-C2-C3	-2.47	121.78	126.04
29	a	407	CLA	CHA-C4D-ND	2.47	137.66	132.50
29	g	602	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
29	B	612	CLA	C2D-C1D-ND	2.47	111.92	110.10
37	c	518	DGD	O1G-C1A-C2A	2.47	119.64	111.91
40	L1	101	LHG	O8-C23-C24	2.47	119.64	111.91
29	b1	613	CLA	CAC-C3C-C4C	2.47	128.01	124.81
29	N	610	CLA	CHA-C4D-ND	2.47	137.66	132.50
29	c	507	CLA	CHA-C4D-ND	2.47	137.66	132.50
29	Y1	608	CLA	C3D-C2D-C1D	-2.47	102.47	105.83
31	a	411	BCR	C34-C9-C10	-2.47	119.47	122.92
48	r1	606	CHL	CMA-C3A-C4A	2.46	118.40	111.77
29	s1	617	CLA	C1D-ND-C4D	-2.46	104.58	106.33
29	g1	611	CLA	C4B-CHC-C1C	2.46	132.18	126.34
29	b	614	CLA	CHA-C4D-ND	2.46	137.66	132.50
29	r1	612	CLA	CHA-C4D-ND	2.46	137.65	132.50
29	B1	613	CLA	C1-O2A-CGA	2.46	122.91	116.44
29	y	603	CLA	O2A-CGA-CBA	2.46	119.64	111.91
29	d1	403	CLA	C4B-CHC-C1C	2.46	132.18	126.34
29	G1	604	CLA	CMA-C3A-C4A	2.46	118.39	111.77
29	N	614	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
29	n1	603	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
37	c	518	DGD	C6E-C5E-C4E	-2.46	107.23	113.00
29	B1	602	CLA	O2A-CGA-CBA	2.46	119.64	111.91
29	y	611	CLA	C2D-C1D-ND	2.46	111.92	110.10
29	b1	615	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
48	y	606	CHL	C2B-C1B-NB	-2.46	108.58	110.23
33	b	622	LMG	O8-C28-C29	2.46	119.64	111.91
31	A	411	BCR	C38-C26-C25	-2.46	121.76	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B1	602	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
29	S1	609	CLA	CMA-C3A-C4A	2.46	118.39	111.77
29	r1	604	CLA	CMA-C3A-C4A	2.46	118.39	111.77
29	Y	610	CLA	CMC-C2C-C3C	2.46	132.80	126.12
29	r	608	CLA	CMA-C3A-C4A	2.46	118.39	111.77
29	n	612	CLA	CHA-C1A-NA	-2.46	120.76	126.40
43	D1	405	PL9	C11-C12-C13	-2.46	103.79	111.88
29	c1	509	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
29	R	603	CLA	CMA-C3A-C4A	2.46	118.39	111.77
49	S1	621	LUT	C20-C13-C14	-2.46	119.48	122.92
29	Y1	611	CLA	C4B-CHC-C1C	2.46	132.17	126.34
48	G	605	CHL	C4B-CHC-C1C	2.46	132.17	126.34
40	Y1	624	LHG	O8-C23-C24	2.46	119.63	111.91
29	C1	511	CLA	CHA-C4D-ND	2.46	137.65	132.50
29	B	603	CLA	O2A-CGA-CBA	2.46	119.63	111.91
29	B	615	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
29	d	403	CLA	CHA-C4D-ND	2.46	137.65	132.50
29	s1	610	CLA	C3B-C4B-NB	-2.46	108.23	110.52
29	c	503	CLA	O2A-CGA-CBA	2.46	119.63	111.91
29	n	611	CLA	C4B-CHC-C1C	2.46	132.17	126.34
29	G	613	CLA	CMD-C2D-C3D	-2.46	121.96	127.61
29	g	602	CLA	CHA-C4D-ND	2.46	137.64	132.50
29	s1	602	CLA	CHA-C4D-ND	2.46	137.64	132.50
29	S1	602	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
29	c1	512	CLA	CHD-C1D-ND	-2.46	122.19	124.45
29	N	613	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
29	d1	402	CLA	C3B-C4B-NB	-2.46	108.23	110.52
48	g1	606	CHL	CHD-C4C-C3C	2.46	128.45	124.84
29	Y1	611	CLA	CMD-C2D-C3D	-2.46	121.96	127.61
48	n1	606	CHL	CMA-C3A-C4A	2.46	118.38	111.77
50	r1	621	XAT	C4-C3-C2	-2.46	106.03	110.77
45	h	101	RRX	C16-C15-C14	-2.46	118.44	123.47
29	Y1	612	CLA	CHA-C1A-NA	-2.46	120.77	126.40
29	B1	612	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
48	n1	605	CHL	CHB-C4A-NA	2.46	127.91	124.51
29	n	602	CLA	CHA-C4D-ND	2.46	137.64	132.50
29	c	513	CLA	CHA-C4D-ND	2.46	137.64	132.50
48	s1	608	CHL	CHC-C1C-NC	2.46	127.93	124.20
31	b	619	BCR	C36-C18-C17	-2.46	119.48	122.92
29	b	606	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
29	S1	611	CLA	C2D-C1D-ND	2.46	111.91	110.10
29	N1	611	CLA	CAA-CBA-CGA	-2.46	106.08	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B1	605	CLA	CHA-C1A-NA	-2.46	120.78	126.40
29	C1	507	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
48	g	601	CHL	C2B-C1B-NB	-2.46	108.59	110.23
29	n1	612	CLA	C4B-CHC-C1C	2.46	132.16	126.34
48	n	605	CHL	C4B-CHC-C1C	2.46	132.16	126.34
29	c	509	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
29	B	616	CLA	C1-O2A-CGA	2.45	122.89	116.44
49	y	621	LUT	C35-C34-C33	-2.45	123.81	127.31
29	n1	604	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
29	R	602	CLA	CMC-C2C-C1C	2.45	128.78	125.04
29	b	617	CLA	C1-O2A-CGA	2.45	122.88	116.44
29	d1	403	CLA	C2D-C1D-ND	2.45	111.91	110.10
51	n	623	NEX	O24-C25-C24	-2.45	111.54	113.38
29	b	615	CLA	C3B-C4B-NB	-2.45	108.24	110.52
29	y1	614	CLA	CAA-C2A-C3A	-2.45	106.06	112.78
31	B	618	BCR	C1-C6-C7	2.45	122.72	115.78
29	B	612	CLA	C2C-C1C-NC	2.45	112.27	109.97
29	C1	504	CLA	CHA-C4D-ND	2.45	137.63	132.50
40	Y	624	LHG	O8-C23-C24	2.45	119.61	111.91
29	b1	612	CLA	CHD-C1D-ND	-2.45	122.20	124.45
29	s1	613	CLA	O2A-CGA-CBA	2.45	119.60	111.91
29	b1	610	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
29	N	611	CLA	CHA-C4D-ND	2.45	137.63	132.50
48	Y1	609	CHL	C3B-C4B-NB	-2.45	108.24	110.52
29	S1	602	CLA	C1D-ND-C4D	-2.45	104.59	106.33
29	n1	613	CLA	C1D-ND-C4D	-2.45	104.59	106.33
49	R1	620	LUT	C21-C26-C25	2.45	115.81	111.42
37	C1	520	DGD	O1G-C1A-C2A	2.45	119.60	111.91
40	S	624	LHG	O8-C23-C24	2.45	119.60	111.91
36	B1	620	C7Z	C40-C33-C34	-2.45	119.49	122.92
29	Y1	602	CLA	O2A-CGA-CBA	2.45	119.60	111.91
50	N	622	XAT	O4-C5-C18	-2.45	112.12	115.06
48	Y	609	CHL	CHA-C4D-ND	2.45	137.63	132.50
29	B1	612	CLA	O2A-CGA-CBA	2.45	119.60	111.91
29	g1	602	CLA	C2C-C1C-NC	2.45	112.27	109.97
29	g1	604	CLA	C2C-C1C-NC	2.45	112.27	109.97
29	b	603	CLA	C2D-C1D-ND	2.45	111.91	110.10
29	B1	606	CLA	C4B-CHC-C1C	2.45	132.15	126.34
29	S1	612	CLA	C4B-CHC-C1C	2.45	132.15	126.34
29	d1	403	CLA	CHA-C4D-ND	2.45	137.62	132.50
32	C	526	SQD	O3-C3-C2	-2.45	104.68	110.35
33	c	521	LMG	C8-O7-C10	-2.45	111.76	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A1	409	PHO	CMB-C2B-C3B	2.45	129.26	124.68
29	y	604	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
29	G1	602	CLA	O2A-CGA-CBA	2.45	119.59	111.91
29	c1	511	CLA	O2A-CGA-CBA	2.45	119.59	111.91
29	r	604	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
29	g1	602	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
48	g	607	CHL	C3C-C4C-NC	-2.45	107.82	110.57
51	s	623	NEX	C1-C2-C3	2.45	119.17	113.64
33	C1	523	LMG	O1-C1-C2	2.45	112.13	108.30
29	C	510	CLA	O2A-CGA-CBA	2.45	119.59	111.91
49	S	620	LUT	C8-C9-C10	-2.45	115.18	118.94
29	b	605	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
31	b	618	BCR	C34-C9-C10	-2.45	119.49	122.92
31	c1	517	BCR	C35-C13-C14	-2.45	119.49	122.92
51	y	623	NEX	C19-C9-C10	-2.45	119.49	122.92
51	G1	623	NEX	C4-C3-C2	2.45	115.50	110.77
49	Y	621	LUT	C35-C15-C14	-2.45	118.46	123.47
45	H1	101	RRX	C2-C1-C6	2.45	114.25	110.48
48	n1	608	CHL	C3C-C4C-NC	-2.45	107.83	110.57
29	S1	605	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
37	c1	518	DGD	C3G-C2G-C1G	-2.45	106.00	111.79
29	g1	613	CLA	CHA-C4D-ND	2.45	137.62	132.50
34	y1	625	SPH	C1-C2-C3	-2.45	107.76	113.03
29	B	604	CLA	C1-C2-C3	-2.45	121.81	126.04
29	y1	614	CLA	O2A-CGA-CBA	2.45	119.59	111.91
29	r1	602	CLA	C1D-ND-C4D	-2.45	104.60	106.33
48	y	605	CHL	CHC-C4B-NB	-2.45	121.67	124.26
29	G1	604	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
29	A	410	CLA	C4B-CHC-C1C	2.45	132.14	126.34
29	N	614	CLA	CHA-C4D-ND	2.45	137.62	132.50
48	N1	609	CHL	CHC-C1C-NC	2.45	127.91	124.20
29	r1	610	CLA	C4B-CHC-C1C	2.45	132.14	126.34
50	N1	622	XAT	C39-C29-C30	-2.45	119.50	122.92
49	y	621	LUT	C18-C5-C6	-2.45	121.78	124.53
29	G1	612	CLA	CHA-C4D-ND	2.45	137.61	132.50
49	r	620	LUT	C18-C5-C4	2.45	118.89	114.36
29	b1	605	CLA	CHD-C1D-ND	-2.45	122.21	124.45
29	D	402	CLA	CHA-C4D-ND	2.44	137.61	132.50
29	y1	613	CLA	CHA-C4D-ND	2.44	137.61	132.50
36	b	620	C7Z	C8-C7-C6	-2.44	120.34	127.20
29	C	502	CLA	CHA-C4D-ND	2.44	137.61	132.50
48	G1	608	CHL	C4B-CHC-C1C	2.44	132.13	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	G	607	CHL	C1-O2A-CGA	2.44	122.86	116.44
29	N	604	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
48	N	607	CHL	C2C-C3C-C4C	2.44	108.23	106.49
29	y	611	CLA	CHA-C4D-ND	2.44	137.61	132.50
29	Y1	602	CLA	C1-C2-C3	-2.44	121.82	126.04
52	R1	625	LMT	C1'-O5'-C5'	-2.44	108.89	113.69
29	R	608	CLA	CAC-C3C-C4C	2.44	127.98	124.81
29	s	603	CLA	O1D-CGD-CBD	-2.44	119.48	124.48
49	S	620	LUT	C32-C33-C34	-2.44	115.19	118.94
29	B1	615	CLA	CHA-C1A-NA	-2.44	120.80	126.40
50	n1	622	XAT	C19-C9-C10	-2.44	119.50	122.92
29	G	604	CLA	C2D-C1D-ND	2.44	111.90	110.10
29	y1	613	CLA	CMA-C3A-C4A	2.44	118.34	111.77
51	y	623	NEX	C40-C33-C34	-2.44	119.50	122.92
29	C1	512	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
48	G	609	CHL	C4D-CHA-C1A	2.44	124.22	121.25
29	s	609	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
52	r	625	LMT	C1B-C2B-C3B	2.44	115.08	110.00
29	Y1	603	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
31	C1	515	BCR	C8-C9-C10	2.44	122.69	118.94
48	Y	609	CHL	CHD-C4C-C3C	2.44	128.43	124.84
29	g1	604	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
29	g1	614	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
51	r1	622	NEX	C20-C13-C14	-2.44	119.50	122.92
29	C1	501	CLA	CMA-C3A-C4A	2.44	118.33	111.77
48	y1	601	CHL	C4B-CHC-C1C	2.44	132.13	126.34
29	G	603	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
29	C1	512	CLA	C2C-C1C-NC	2.44	112.26	109.97
29	a1	406	CLA	C2D-C1D-ND	2.44	111.90	110.10
29	N	603	CLA	CHA-C4D-ND	2.44	137.60	132.50
29	B	603	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
29	d	402	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
51	S1	623	NEX	C31-C30-C29	2.44	130.79	127.31
29	N1	602	CLA	C1-O2A-CGA	2.44	122.84	116.44
29	Y1	604	CLA	CHA-C4D-ND	2.44	137.60	132.50
49	G1	620	LUT	C30-C31-C32	-2.44	115.61	123.22
48	y	606	CHL	CMA-C3A-C4A	2.44	118.33	111.77
29	B	602	CLA	CHA-C4D-ND	2.44	137.60	132.50
48	G	605	CHL	CMA-C3A-C4A	2.44	118.33	111.77
29	b1	610	CLA	O2A-CGA-CBA	2.44	119.56	111.91
37	c1	520	DGD	O1G-C1A-C2A	2.44	119.56	111.91
29	S	611	CLA	C4B-CHC-C1C	2.44	132.12	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	508	CLA	CMA-C3A-C4A	2.44	118.33	111.77
29	g	610	CLA	CHA-C4D-ND	2.44	137.60	132.50
29	Y	608	CLA	C1-O2A-CGA	2.44	122.84	116.44
31	c1	514	BCR	C33-C5-C6	-2.44	121.79	124.53
29	Y1	604	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
29	N1	611	CLA	C4B-CHC-C1C	2.44	132.12	126.34
40	G	624	LHG	O8-C23-C24	2.44	119.55	111.91
29	S1	611	CLA	CHA-C1A-NA	-2.44	120.82	126.40
29	g	612	CLA	C3B-C4B-NB	-2.44	108.25	110.52
29	y	604	CLA	CHA-C4D-ND	2.44	137.59	132.50
29	C1	505	CLA	CHA-C4D-ND	2.44	137.59	132.50
48	G1	607	CHL	C4D-CHA-C1A	2.44	124.21	121.25
29	D1	402	CLA	CHA-C4D-ND	2.44	137.59	132.50
49	y	621	LUT	C35-C15-C14	-2.43	118.49	123.47
29	G	610	CLA	O1D-CGD-CBD	-2.43	119.50	124.48
29	R	609	CLA	CHA-C4D-ND	2.43	137.59	132.50
29	b1	603	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
48	r	607	CHL	CHB-C4A-NA	2.43	127.88	124.51
29	a1	406	CLA	C1-O2A-CGA	2.43	122.83	116.44
29	b1	612	CLA	C2C-C1C-NC	2.43	112.25	109.97
32	A1	412	SQD	O8-S-C6	-2.43	101.86	105.74
29	S1	604	CLA	C1-O2A-CGA	2.43	122.83	116.44
29	B1	612	CLA	CHA-C4D-ND	2.43	137.59	132.50
29	R1	602	CLA	C3B-C4B-NB	-2.43	108.26	110.52
29	b	606	CLA	C1D-ND-C4D	-2.43	104.61	106.33
29	c	511	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
49	y1	621	LUT	C38-C25-C24	-2.43	118.36	123.56
29	s	610	CLA	C2A-C1A-CHA	2.43	128.11	123.86
29	s	612	CLA	CHA-C4D-ND	2.43	137.59	132.50
29	n1	611	CLA	CHA-C4D-ND	2.43	137.58	132.50
29	S1	611	CLA	C1-C2-C3	-2.43	121.84	126.04
29	S1	611	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
29	R1	604	CLA	CHA-C4D-ND	2.43	137.58	132.50
29	G1	613	CLA	CHA-C4D-ND	2.43	137.58	132.50
48	y	607	CHL	C1-O2A-CGA	2.43	122.82	116.44
29	g1	612	CLA	C3B-C4B-NB	-2.43	108.26	110.52
29	C	502	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
29	y	610	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
29	Y1	613	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
49	S	621	LUT	C3-C4-C5	-2.43	107.02	111.85
29	y1	611	CLA	CHA-C1A-NA	-2.43	120.84	126.40
31	A	411	BCR	C36-C18-C17	-2.43	119.52	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s1	603	CLA	O1D-CGD-CBD	-2.43	119.52	124.48
29	B	617	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
29	D1	402	CLA	C2C-C1C-NC	2.43	112.25	109.97
29	c1	513	CLA	CMC-C2C-C1C	2.43	128.74	125.04
53	R	626	ERG	C11-C9-C8	-2.43	105.89	111.33
29	g1	602	CLA	CHA-C4D-ND	2.43	137.58	132.50
29	b1	611	CLA	C1-O2A-CGA	2.43	122.81	116.44
29	C	511	CLA	CHA-C4D-ND	2.43	137.58	132.50
48	N1	605	CHL	CMA-C3A-C4A	2.43	118.30	111.77
29	g	603	CLA	C4B-CHC-C1C	2.43	132.09	126.34
48	G1	609	CHL	C4A-NA-C1A	2.43	107.80	106.71
29	N1	614	CLA	CHA-C1A-NA	-2.43	120.84	126.40
29	r1	608	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
29	n1	611	CLA	O2A-CGA-CBA	2.43	119.52	111.91
29	R	604	CLA	C2D-C1D-ND	2.43	111.89	110.10
29	y1	614	CLA	C2D-C1D-ND	2.43	111.89	110.10
29	g	610	CLA	C3D-C2D-C1D	-2.43	102.52	105.83
29	B	616	CLA	C1-C2-C3	-2.43	121.85	126.04
29	s1	617	CLA	CHA-C4D-ND	2.43	137.57	132.50
48	G	609	CHL	CHD-C4C-C3C	2.43	128.41	124.84
29	B	615	CLA	C4B-CHC-C1C	2.43	132.09	126.34
49	Y1	621	LUT	C15-C14-C13	-2.43	123.85	127.31
29	a1	406	CLA	C1C-C2C-C3C	-2.43	104.41	106.96
48	N	609	CHL	C4D-CHA-C1A	2.43	124.20	121.25
29	s1	611	CLA	C4B-CHC-C1C	2.43	132.09	126.34
50	Y	622	XAT	C28-C29-C30	2.43	122.66	118.94
29	g1	604	CLA	O2A-CGA-CBA	2.43	119.52	111.91
29	y1	612	CLA	C1-O2A-CGA	2.43	122.81	116.44
29	N1	613	CLA	C1-O2A-CGA	2.42	122.81	116.44
29	N1	614	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
29	g	604	CLA	C4B-CHC-C1C	2.42	132.09	126.34
29	A	406	CLA	CMA-C3A-C4A	2.42	118.29	111.77
31	C1	516	BCR	C8-C9-C10	2.42	122.66	118.94
53	r	626	ERG	C13-C17-C20	-2.42	116.30	119.43
29	G1	603	CLA	C3D-C2D-C1D	-2.42	102.52	105.83
29	a1	410	CLA	CMA-C3A-C4A	2.42	118.29	111.77
29	n1	610	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
29	b1	610	CLA	C4B-CHC-C1C	2.42	132.09	126.34
29	Y1	610	CLA	CHA-C4D-ND	2.42	137.57	132.50
29	N	604	CLA	O2A-CGA-CBA	2.42	119.51	111.91
48	s	607	CHL	CHC-C4B-NB	-2.42	121.69	124.26
29	N	603	CLA	C1-C2-C3	-2.42	121.85	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	G1	610	CLA	C1D-ND-C4D	-2.42	104.61	106.33
29	g1	603	CLA	O2A-CGA-CBA	2.42	119.51	111.91
29	r1	604	CLA	CHA-C4D-ND	2.42	137.57	132.50
42	d	401	BCT	O3-C-O1	-2.42	113.26	119.55
49	Y	621	LUT	C10-C11-C12	-2.42	115.66	123.22
53	R1	626	ERG	C11-C9-C8	-2.42	105.90	111.33
29	G	610	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	N1	602	CLA	C3B-C4B-NB	-2.42	108.27	110.52
29	S	602	CLA	C2D-C1D-ND	2.42	111.89	110.10
29	a1	405	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	n	604	CLA	OBD-CAD-C3D	-2.42	122.69	128.52
31	b1	618	BCR	C28-C27-C26	-2.42	109.75	114.08
30	a1	408	PHO	CBA-CAA-C2A	-2.42	106.74	113.81
29	Y	611	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	b	609	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
29	y	611	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
29	S	609	CLA	CHA-C1A-NA	-2.42	120.86	126.40
29	b1	611	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	y	610	CLA	C1D-ND-C4D	-2.42	104.62	106.33
29	G1	612	CLA	C1D-ND-C4D	-2.42	104.62	106.33
29	s1	613	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	b	609	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
29	b1	607	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	Y	608	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
30	A1	409	PHO	O1D-CGD-CBD	2.42	128.77	124.74
29	r	610	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
29	S	614	CLA	C4B-CHC-C1C	2.42	132.07	126.34
49	G	621	LUT	C10-C11-C12	-2.42	115.67	123.22
36	b1	620	C7Z	C20-C13-C14	-2.42	119.54	122.92
50	R1	621	XAT	C24-C23-C22	-2.42	106.11	110.77
29	r1	610	CLA	C1D-ND-C4D	-2.42	104.62	106.33
51	N	623	NEX	C17-C1-C6	-2.42	108.31	110.47
29	g1	613	CLA	C1-O2A-CGA	2.42	122.78	116.44
48	n1	607	CHL	C4B-CHC-C1C	2.42	132.07	126.34
53	R	626	ERG	C12-C13-C17	-2.42	112.95	116.57
29	b	611	CLA	CHA-C4D-ND	2.42	137.55	132.50
29	G1	614	CLA	CHA-C4D-ND	2.42	137.55	132.50
29	S1	610	CLA	CHA-C4D-ND	2.42	137.55	132.50
50	Y1	622	XAT	O24-C25-C24	-2.42	111.57	113.38
29	S1	605	CLA	CHA-C1A-NA	-2.42	120.87	126.40
30	a	408	PHO	CMD-C2D-C3D	2.41	129.20	124.68
29	g	602	CLA	CMC-C2C-C1C	2.41	128.72	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	r1	612	CLA	C1D-ND-C4D	-2.41	104.62	106.33
29	n	602	CLA	CMA-C3A-C4A	2.41	118.26	111.77
29	A1	410	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
29	C1	505	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
29	c	511	CLA	CHA-C4D-ND	2.41	137.55	132.50
48	s1	601	CHL	C3A-C2A-C1A	2.41	104.95	101.34
49	Y1	620	LUT	C22-C23-C24	-2.41	108.99	111.74
29	C	506	CLA	CMD-C2D-C3D	-2.41	122.06	127.61
29	n	610	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
29	c1	501	CLA	C4B-CHC-C1C	2.41	132.06	126.34
29	C	503	CLA	CHA-C4D-ND	2.41	137.55	132.50
29	R	604	CLA	CHA-C4D-ND	2.41	137.55	132.50
29	D1	403	CLA	CMD-C2D-C3D	-2.41	122.06	127.61
31	D1	404	BCR	C30-C25-C24	2.41	122.60	115.78
29	C	501	CLA	CHA-C4D-ND	2.41	137.55	132.50
29	N1	602	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
29	N	610	CLA	C4B-CHC-C1C	2.41	132.06	126.34
49	y1	621	LUT	C15-C14-C13	-2.41	123.87	127.31
29	B1	613	CLA	C3B-C4B-NB	-2.41	108.28	110.52
48	N1	607	CHL	C3B-C4B-NB	-2.41	108.28	110.52
29	r1	609	CLA	C1-O2A-CGA	2.41	122.77	116.44
48	N	605	CHL	CHB-C4A-NA	2.41	127.85	124.51
29	n	611	CLA	CHA-C4D-ND	2.41	137.54	132.50
29	r1	603	CLA	C4B-CHC-C1C	2.41	132.06	126.34
29	c1	510	CLA	C6-C7-C8	-2.41	108.12	115.92
29	B1	606	CLA	CHA-C4D-ND	2.41	137.54	132.50
29	B1	608	CLA	CHA-C4D-ND	2.41	137.54	132.50
29	r	609	CLA	O2A-CGA-CBA	2.41	119.47	111.91
29	S1	602	CLA	CMA-C3A-C4A	2.41	118.25	111.77
48	N	606	CHL	C2B-C1B-NB	-2.41	108.62	110.23
29	B1	602	CLA	CAA-CBA-CGA	-2.41	106.21	113.25
51	g1	623	NEX	C1-C2-C3	2.41	119.09	113.64
29	A1	407	CLA	C4B-CHC-C1C	2.41	132.06	126.34
29	g	612	CLA	CHD-C1D-ND	-2.41	122.24	124.45
29	s1	614	CLA	CHA-C4D-ND	2.41	137.54	132.50
29	Y	612	CLA	CGD-CBD-CAD	-2.41	102.93	110.73
29	B	610	CLA	CMA-C3A-C4A	2.41	118.25	111.77
48	g1	606	CHL	C2C-C3C-C4C	2.41	108.21	106.49
29	S1	604	CLA	CHA-C4D-ND	2.41	137.54	132.50
49	N	621	LUT	C35-C34-C33	-2.41	123.87	127.31
29	b	603	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
29	B1	606	CLA	O2A-CGA-CBA	2.41	119.47	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y1	614	CLA	O2A-CGA-CBA	2.41	119.47	111.91
33	B1	622	LMG	O8-C28-C29	2.41	119.47	111.91
48	N	605	CHL	C2B-C1B-NB	-2.41	108.62	110.23
48	y	605	CHL	CHB-C4A-NA	2.41	127.84	124.51
48	R1	606	CHL	CHC-C4B-NB	-2.41	121.71	124.26
29	r	609	CLA	C1D-ND-C4D	-2.41	104.62	106.33
48	R1	606	CHL	C3C-C4C-NC	-2.41	107.87	110.57
49	y	620	LUT	C7-C8-C9	-2.41	122.60	126.23
29	c1	508	CLA	C4B-CHC-C1C	2.41	132.05	126.34
37	c1	518	DGD	O1G-C1A-C2A	2.41	119.47	111.91
48	n	609	CHL	C1-C2-C3	-2.41	121.88	126.04
29	Y1	613	CLA	CMD-C2D-C3D	-2.41	122.08	127.61
48	N1	601	CHL	CMA-C3A-C4A	2.41	118.24	111.77
29	b1	617	CLA	O2A-CGA-CBA	2.41	119.46	111.91
29	S1	613	CLA	CHA-C4D-ND	2.41	137.53	132.50
29	C1	510	CLA	O2A-CGA-CBA	2.41	119.46	111.91
29	C1	512	CLA	CHA-C1A-NA	-2.41	120.89	126.40
29	y1	604	CLA	O2A-CGA-CBA	2.41	119.46	111.91
29	Y1	612	CLA	CMA-C3A-C4A	2.41	118.24	111.77
44	F	101	HEM	C4D-ND-C1D	2.41	107.56	105.07
29	a1	410	CLA	C3B-C2B-C1B	-2.41	104.26	107.16
29	b1	610	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
29	C	508	CLA	CHA-C4D-ND	2.41	137.53	132.50
48	G1	601	CHL	C4A-NA-C1A	2.40	107.79	106.71
29	r1	602	CLA	C6-C5-C3	-2.40	107.15	113.45
29	R	610	CLA	OBD-CAD-C3D	-2.40	122.73	128.52
29	C1	513	CLA	CMD-C2D-C3D	-2.40	122.08	127.61
29	R	604	CLA	CMA-C3A-C4A	2.40	118.23	111.77
29	s1	610	CLA	CMA-C3A-C4A	2.40	118.23	111.77
29	N	611	CLA	CHA-C1A-NA	-2.40	120.89	126.40
29	c1	510	CLA	C4B-CHC-C1C	2.40	132.04	126.34
48	y1	605	CHL	C2C-C3C-C4C	2.40	108.20	106.49
33	A	413	LMG	C8-O7-C10	-2.40	111.88	117.79
29	R	612	CLA	CHA-C4D-ND	2.40	137.53	132.50
29	G	614	CLA	O2A-CGA-CBA	2.40	119.45	111.91
48	S	608	CHL	C4A-NA-C1A	2.40	107.79	106.71
40	N	624	LHG	C5-O7-C7	-2.40	111.88	117.79
29	b1	614	CLA	CHA-C1A-NA	-2.40	120.90	126.40
29	y1	608	CLA	C4B-CHC-C1C	2.40	132.03	126.34
29	g	602	CLA	C2C-C1C-NC	2.40	112.22	109.97
29	G1	611	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
29	c1	506	CLA	CHA-C4D-ND	2.40	137.52	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n	611	CLA	C3B-C4B-NB	-2.40	108.29	110.52
29	R	602	CLA	CHD-C1D-ND	-2.40	122.25	124.45
50	R	621	XAT	C11-C10-C9	2.40	130.74	127.31
29	S	613	CLA	CHA-C4D-ND	2.40	137.52	132.50
48	r1	606	CHL	C4B-CHC-C1C	2.40	132.03	126.34
29	N1	604	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
29	c1	505	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
29	Y1	611	CLA	O1D-CGD-CBD	-2.40	119.57	124.48
29	B	617	CLA	CHD-C1D-ND	-2.40	122.25	124.45
29	C	512	CLA	CHD-C1D-ND	-2.40	122.25	124.45
37	B	623	DGD	C4E-C3E-C2E	2.40	115.01	110.82
29	R1	603	CLA	C4B-CHC-C1C	2.40	132.03	126.34
29	G1	612	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
29	N1	612	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
32	b1	626	SQD	O3-C3-C2	-2.40	104.80	110.35
29	N	613	CLA	CHA-C4D-ND	2.40	137.52	132.50
29	R1	603	CLA	CHD-C1D-ND	-2.40	122.25	124.45
49	S	620	LUT	C18-C5-C6	-2.40	121.83	124.53
29	n	614	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
29	S1	610	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
29	y1	614	CLA	CMC-C2C-C1C	2.40	128.69	125.04
45	h1	101	RRX	C16-C15-C14	-2.40	118.56	123.47
29	c	507	CLA	CMA-C3A-C4A	2.40	118.22	111.77
29	y	603	CLA	CHA-C4D-ND	2.40	137.51	132.50
29	c1	501	CLA	OBD-CAD-C3D	-2.40	122.75	128.52
29	N	603	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
51	g1	623	NEX	C26-C27-C28	-2.40	120.92	125.99
51	S	623	NEX	C40-C33-C34	-2.40	119.57	122.92
29	G	614	CLA	C4B-CHC-C1C	2.40	132.02	126.34
29	C	504	CLA	CHA-C4D-ND	2.40	137.51	132.50
29	c1	508	CLA	CHA-C4D-ND	2.40	137.51	132.50
29	g	602	CLA	C2D-C1D-ND	2.40	111.87	110.10
29	S1	604	CLA	C2D-C1D-ND	2.40	111.87	110.10
29	C1	503	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
49	n	621	LUT	C10-C11-C12	-2.40	115.74	123.22
29	b	606	CLA	CHA-C4D-ND	2.40	137.51	132.50
48	N1	606	CHL	CHB-C4A-NA	2.40	127.83	124.51
29	c1	513	CLA	C4B-CHC-C1C	2.40	132.02	126.34
31	c	514	BCR	C33-C5-C6	-2.40	121.84	124.53
29	g1	610	CLA	CAC-C3C-C4C	2.40	127.92	124.81
48	N	601	CHL	C4B-CHC-C1C	2.40	132.02	126.34
31	a1	411	BCR	C1-C6-C5	-2.40	119.24	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b1	616	CLA	CHA-C1A-NA	-2.40	120.91	126.40
29	c	512	CLA	CHA-C4D-ND	2.39	137.51	132.50
29	B1	604	CLA	CHA-C4D-ND	2.39	137.51	132.50
48	n1	605	CHL	C1-C2-C3	-2.39	121.90	126.04
29	C1	504	CLA	CMA-C3A-C4A	2.39	118.21	111.77
29	A1	407	CLA	O2A-CGA-CBA	2.39	119.42	111.91
29	C1	503	CLA	CMC-C2C-C1C	2.39	128.69	125.04
36	b1	620	C7Z	C11-C12-C13	-2.39	119.69	126.42
31	a1	411	BCR	C38-C26-C25	-2.39	121.84	124.53
29	C	511	CLA	C2D-C1D-ND	2.39	111.87	110.10
29	N1	613	CLA	O2A-CGA-CBA	2.39	119.42	111.91
48	g	605	CHL	CMA-C3A-C2A	2.39	123.48	113.83
29	c	503	CLA	C7-C6-C5	-2.39	106.86	113.36
29	s1	610	CLA	CHA-C1A-NA	-2.39	120.92	126.40
29	n	614	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
29	B	608	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	b1	614	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	y	603	CLA	C1-C2-C3	-2.39	121.91	126.04
29	g	603	CLA	CHA-C1A-NA	-2.39	120.92	126.40
29	s	602	CLA	C1-O2A-CGA	2.39	122.72	116.44
29	b1	617	CLA	C1-O2A-CGA	2.39	122.72	116.44
29	r	608	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
29	c	508	CLA	C2D-C1D-ND	2.39	111.87	110.10
29	b1	611	CLA	C2D-C1D-ND	2.39	111.87	110.10
36	b	620	C7Z	C21-C26-C25	-2.39	119.24	122.61
29	b1	603	CLA	C4B-CHC-C1C	2.39	132.01	126.34
49	Y1	620	LUT	C15-C14-C13	-2.39	123.90	127.31
29	b	612	CLA	O2A-CGA-CBA	2.39	119.41	111.91
36	b1	620	C7Z	C1-C2-C3	2.39	119.04	113.64
29	b1	609	CLA	C1-O2A-CGA	2.39	122.72	116.44
29	G	603	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
29	B1	615	CLA	C3D-C2D-C1D	-2.39	102.57	105.83
49	s1	621	LUT	C32-C33-C34	2.39	122.61	118.94
55	y1	626	PTY	O4-C30-C31	2.39	119.41	111.91
29	r1	609	CLA	CMC-C2C-C1C	2.39	128.68	125.04
29	a1	405	CLA	C1-C2-C3	-2.39	121.91	126.04
38	B1	624	3PH	O31-C31-C32	2.39	119.41	111.91
29	A1	406	CLA	O2A-CGA-CBA	2.39	119.41	111.91
49	n1	621	LUT	C20-C13-C12	2.39	121.84	118.08
29	Y	610	CLA	C4B-CHC-C1C	2.39	132.01	126.34
29	N	602	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
48	G1	601	CHL	CHD-C4C-C3C	2.39	128.35	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	S1	606	CHL	C3B-C4B-NB	-2.39	108.30	110.52
29	G	603	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	N	612	CLA	C4B-CHC-C1C	2.39	132.01	126.34
29	g	604	CLA	C2D-C1D-ND	2.39	111.86	110.10
48	Y	607	CHL	CHD-C1D-ND	-2.39	122.26	124.45
29	S	611	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
29	b	615	CLA	CMC-C2C-C1C	2.39	128.68	125.04
29	R	608	CLA	CHA-C1A-NA	-2.39	120.93	126.40
31	D1	404	BCR	C37-C22-C21	-2.39	119.58	122.92
29	n	610	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	C1	513	CLA	C1D-ND-C4D	-2.39	104.64	106.33
29	R1	612	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	C1	503	CLA	C3B-C4B-NB	-2.39	108.30	110.52
44	f	101	HEM	C4C-NC-C1C	2.39	107.69	105.35
29	C	504	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
29	r	608	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
29	Y1	603	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
33	c1	523	LMG	C8-O7-C10	-2.39	111.91	117.79
48	y	607	CHL	CHB-C4A-NA	2.39	127.81	124.51
29	n1	612	CLA	CMD-C2D-C3D	-2.39	122.12	127.61
29	g1	612	CLA	CHA-C4D-ND	2.39	137.49	132.50
29	r	610	CLA	CHA-C1A-NA	-2.39	120.93	126.40
29	G	603	CLA	O2A-CGA-CBA	2.39	119.40	111.91
29	R	604	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
29	c	513	CLA	C1-C2-C3	-2.39	121.92	126.04
48	g	606	CHL	CHD-C4C-C3C	2.39	128.35	124.84
29	S1	605	CLA	CHA-C4D-ND	2.39	137.49	132.50
29	r	609	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
29	D1	402	CLA	OBD-CAD-C3D	-2.39	122.78	128.52
29	B	609	CLA	C1D-ND-C4D	-2.39	104.64	106.33
29	G1	610	CLA	C3D-C2D-C1D	-2.39	102.58	105.83
29	B	611	CLA	CHA-C4D-ND	2.39	137.49	132.50
29	a1	405	CLA	C1C-C2C-C3C	-2.39	104.45	106.96
29	b1	607	CLA	C2D-C1D-ND	2.39	111.86	110.10
29	y	610	CLA	CHA-C4D-ND	2.39	137.49	132.50
39	B	625	DGA	OG1-CA1-CA2	2.39	119.39	111.91
47	k1	101	4RF	O40-C41-C43	2.39	119.39	111.91
29	y1	614	CLA	CMD-C2D-C3D	-2.39	122.13	127.61
49	Y1	621	LUT	C20-C13-C12	2.39	121.83	118.08
29	D	403	CLA	C4B-CHC-C1C	2.39	132.00	126.34
31	c1	516	BCR	C37-C22-C21	-2.39	119.58	122.92
32	c1	526	SQD	O3-C3-C2	-2.39	104.83	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y1	608	CLA	CHA-C1A-NA	-2.39	120.94	126.40
29	s1	602	CLA	CAC-C3C-C4C	2.38	127.90	124.81
29	c1	509	CLA	C2D-C1D-ND	2.38	111.86	110.10
29	C	505	CLA	CHA-C4D-ND	2.38	137.49	132.50
29	Y1	602	CLA	CMD-C2D-C3D	-2.38	122.13	127.61
29	Y1	602	CLA	CHD-C1D-ND	-2.38	122.26	124.45
29	d	402	CLA	O2A-CGA-CBA	2.38	119.39	111.91
29	A1	405	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
29	c1	501	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
31	B1	619	BCR	C1-C6-C5	-2.38	119.26	122.61
49	N1	621	LUT	C35-C15-C14	-2.38	118.59	123.47
29	b1	605	CLA	C3B-C4B-NB	-2.38	108.31	110.52
29	A1	405	CLA	C1-O2A-CGA	2.38	122.69	116.44
29	A	405	CLA	C4B-CHC-C1C	2.38	131.99	126.34
29	C	502	CLA	C4B-CHC-C1C	2.38	131.99	126.34
29	B1	610	CLA	CHD-C1D-ND	-2.38	122.27	124.45
29	B1	605	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
29	n1	613	CLA	C4B-CHC-C1C	2.38	131.99	126.34
45	H1	101	RRX	C8-C7-C6	-2.38	120.51	127.20
29	G1	603	CLA	CHA-C4D-ND	2.38	137.48	132.50
29	S1	611	CLA	C2A-C1A-CHA	2.38	128.02	123.86
29	A1	407	CLA	C4D-CHA-C1A	2.38	124.15	121.25
29	b	613	CLA	O2A-CGA-CBA	2.38	119.38	111.91
29	a1	407	CLA	CHA-C4D-ND	2.38	137.48	132.50
29	Y	612	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
49	s	621	LUT	C35-C34-C33	-2.38	123.91	127.31
29	n	602	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
29	g1	611	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
40	y	624	LHG	O8-C23-C24	2.38	119.38	111.91
29	g1	603	CLA	CMA-C3A-C4A	2.38	118.17	111.77
29	n	610	CLA	CAA-CBA-CGA	2.38	120.21	113.25
29	d1	403	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
29	b	616	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
29	B1	603	CLA	CHA-C1A-NA	-2.38	120.95	126.40
29	G	611	CLA	CHA-C4D-ND	2.38	137.48	132.50
48	s1	608	CHL	CHC-C4B-NB	-2.38	121.74	124.26
29	S	617	CLA	CHA-C4D-ND	2.38	137.48	132.50
33	C	521	LMG	C8-O7-C10	-2.38	111.93	117.79
29	c	511	CLA	CHA-C1A-NA	-2.38	120.95	126.40
29	R	604	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
29	b	615	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
48	y1	607	CHL	CMA-C3A-C4A	2.38	118.17	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D	404	BCR	C35-C13-C12	2.38	121.82	118.08
31	c1	517	BCR	C33-C5-C4	2.38	118.18	113.62
49	r	620	LUT	C18-C5-C6	-2.38	121.86	124.53
29	c	512	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
29	B	612	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
29	b1	606	CLA	CMC-C2C-C1C	2.38	128.66	125.04
29	r	608	CLA	C4B-CHC-C1C	2.38	131.98	126.34
29	b	604	CLA	CMD-C2D-C3D	-2.38	122.15	127.61
49	s	621	LUT	C39-C29-C28	2.38	121.82	118.08
36	B1	620	C7Z	C11-C12-C13	-2.38	119.74	126.42
29	Y1	611	CLA	C2D-C1D-ND	2.38	111.86	110.10
29	Y	603	CLA	C4B-CHC-C1C	2.38	131.97	126.34
29	G1	613	CLA	CMC-C2C-C1C	2.38	128.66	125.04
29	S1	605	CLA	CHD-C1D-ND	-2.38	122.27	124.45
29	A1	407	CLA	CHA-C1A-NA	-2.38	120.96	126.40
29	C1	503	CLA	CHA-C1A-NA	-2.38	120.96	126.40
29	R1	603	CLA	CHA-C4D-ND	2.38	137.47	132.50
29	s1	609	CLA	CHA-C4D-ND	2.38	137.47	132.50
33	C1	523	LMG	O8-C28-C29	2.38	119.36	111.91
29	B	604	CLA	CMA-C3A-C4A	2.38	118.16	111.77
50	y	622	XAT	C18-C5-C6	-2.38	118.28	122.26
48	s1	601	CHL	C2C-C3C-C4C	2.38	108.18	106.49
48	g	607	CHL	CHC-C1C-NC	2.37	127.81	124.20
29	c	505	CLA	O1D-CGD-CBD	-2.37	119.62	124.48
29	C1	506	CLA	C2D-C1D-ND	2.37	111.85	110.10
29	c1	503	CLA	C3B-C4B-NB	-2.37	108.31	110.52
29	s1	603	CLA	C4B-CHC-C1C	2.37	131.97	126.34
40	d	409	LHG	O8-C23-C24	2.37	119.36	111.91
49	y	621	LUT	C10-C11-C12	-2.37	115.81	123.22
29	g1	614	CLA	CHA-C1A-NA	-2.37	120.96	126.40
29	s1	617	CLA	CHA-C1A-NA	-2.37	120.96	126.40
29	n	614	CLA	CMD-C2D-C3D	-2.37	122.15	127.61
49	R1	620	LUT	C35-C15-C14	-2.37	118.61	123.47
29	C	513	CLA	CHD-C1D-ND	-2.37	122.27	124.45
29	S	612	CLA	CHD-C1D-ND	-2.37	122.27	124.45
29	s	610	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
29	g	613	CLA	O2A-CGA-CBA	2.37	119.36	111.91
29	Y	604	CLA	C2C-C1C-NC	2.37	112.19	109.97
29	Y1	608	CLA	C4B-CHC-C1C	2.37	131.97	126.34
37	B1	623	DGD	O3G-C1D-C2D	2.37	112.01	108.30
33	w	201	LMG	O8-C28-C29	2.37	119.35	111.91
29	D1	403	CLA	C6-C5-C3	-2.37	107.23	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	N	611	CLA	C4B-CHC-C1C	2.37	131.96	126.34
29	a1	407	CLA	C4B-CHC-C1C	2.37	131.96	126.34
49	y1	621	LUT	C18-C5-C4	2.37	118.75	114.36
29	n	602	CLA	O2A-CGA-CBA	2.37	119.35	111.91
29	D1	402	CLA	O2A-CGA-CBA	2.37	119.35	111.91
29	B1	612	CLA	C4B-CHC-C1C	2.37	131.96	126.34
49	r1	620	LUT	C11-C12-C13	-2.37	119.75	126.42
29	g	604	CLA	C2C-C1C-NC	2.37	112.19	109.97
29	N	613	CLA	C2D-C1D-ND	2.37	111.85	110.10
29	C	506	CLA	CMC-C2C-C3C	2.37	132.55	126.12
53	R	626	ERG	C11-C9-C10	2.37	119.46	113.58
29	b1	609	CLA	C4B-CHC-C1C	2.37	131.96	126.34
29	A	406	CLA	CHA-C4D-ND	2.37	137.46	132.50
29	d	402	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
32	M1	101	SQD	O3-C3-C2	-2.37	104.87	110.35
48	G1	605	CHL	C3B-C4B-NB	-2.37	108.32	110.52
29	C	505	CLA	C2D-C1D-ND	2.37	111.85	110.10
29	B1	603	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
44	F1	101	HEM	C4D-ND-C1D	2.37	107.52	105.07
48	Y1	609	CHL	C2B-C1B-NB	-2.37	108.64	110.23
29	c1	503	CLA	CHA-C4D-ND	2.37	137.45	132.50
29	C	503	CLA	C1C-C2C-C3C	-2.37	104.47	106.96
29	y	602	CLA	CAC-C3C-C4C	2.37	127.88	124.81
48	g1	609	CHL	C3B-C4B-NB	-2.37	108.32	110.52
48	Y	607	CHL	C4B-CHC-C1C	2.37	131.95	126.34
29	G	613	CLA	C4B-CHC-C1C	2.37	131.95	126.34
50	g1	622	XAT	C26-C27-C28	-2.37	120.99	125.99
29	n	614	CLA	CHA-C4D-ND	2.37	137.45	132.50
50	g1	622	XAT	C38-C25-C26	-2.37	118.30	122.26
29	S	610	CLA	C1-C2-C3	-2.37	121.95	126.04
29	a1	410	CLA	C4B-CHC-C1C	2.37	131.95	126.34
29	C1	513	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
29	n	604	CLA	O2A-CGA-CBA	2.37	119.33	111.91
29	r1	604	CLA	O2A-CGA-CBA	2.37	119.33	111.91
48	y	607	CHL	CHD-C4C-C3C	2.37	128.32	124.84
50	N1	622	XAT	C40-C33-C32	2.37	121.80	118.08
29	y1	613	CLA	C1-C2-C3	-2.37	121.95	126.04
40	n1	624	LHG	O8-C23-C24	2.37	119.33	111.91
29	B1	604	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
29	N	610	CLA	C3B-C4B-NB	-2.36	108.32	110.52
29	S	609	CLA	CMA-C3A-C4A	2.36	118.13	111.77
48	s1	606	CHL	CMA-C3A-C4A	2.36	118.13	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B1	612	CLA	CMC-C2C-C1C	2.36	128.64	125.04
30	A	409	PHO	O2A-CGA-O1A	-2.36	117.62	123.59
36	B	620	C7Z	C21-C26-C27	2.36	122.47	115.78
29	C1	510	CLA	CHA-C4D-ND	2.36	137.44	132.50
49	S1	620	LUT	C30-C31-C32	-2.36	115.84	123.22
29	R	608	CLA	C1-C2-C3	-2.36	121.95	126.04
29	c	508	CLA	O2A-CGA-CBA	2.36	119.33	111.91
29	G1	603	CLA	C1D-ND-C4D	-2.36	104.66	106.33
29	y1	604	CLA	CHA-C4D-ND	2.36	137.44	132.50
51	G1	623	NEX	C16-C1-C6	-2.36	108.36	110.47
29	N1	602	CLA	CHA-C4D-ND	2.36	137.44	132.50
48	s	607	CHL	C2B-C1B-NB	-2.36	108.65	110.23
29	n1	613	CLA	CHA-C4D-ND	2.36	137.44	132.50
29	b	605	CLA	CHD-C1D-ND	-2.36	122.28	124.45
29	A1	406	CLA	CHA-C1A-NA	-2.36	120.99	126.40
29	Y1	614	CLA	CMA-C3A-C4A	2.36	118.12	111.77
29	b	616	CLA	CHA-C4D-ND	2.36	137.44	132.50
29	n	613	CLA	C4B-CHC-C1C	2.36	131.94	126.34
29	C	508	CLA	C6-C5-C3	-2.36	107.26	113.45
29	B	613	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
29	S1	604	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
31	A	411	BCR	C37-C22-C23	2.36	121.80	118.08
45	h	101	RRX	C35-C13-C12	2.36	121.80	118.08
29	C1	509	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
51	g1	623	NEX	C40-C33-C34	-2.36	119.62	122.92
29	G	612	CLA	C3B-C4B-NB	-2.36	108.33	110.52
29	Y	604	CLA	C4B-CHC-C1C	2.36	131.94	126.34
29	G1	614	CLA	C4B-CHC-C1C	2.36	131.94	126.34
29	B1	616	CLA	CHA-C1A-NA	-2.36	120.99	126.40
48	G1	608	CHL	CHB-C4A-NA	2.36	127.78	124.51
48	g1	605	CHL	CHB-C4A-NA	2.36	127.78	124.51
49	R	620	LUT	C30-C31-C32	-2.36	115.85	123.22
31	B	618	BCR	C36-C18-C17	-2.36	119.62	122.92
48	g	607	CHL	C1-O2A-CGA	2.36	122.63	116.44
29	c1	504	CLA	O2A-CGA-CBA	2.36	119.31	111.91
29	c	504	CLA	C4B-CHC-C1C	2.36	131.93	126.34
51	s1	623	NEX	O24-C25-C24	-2.36	111.61	113.38
29	c1	508	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
31	c	516	BCR	C34-C9-C10	-2.36	119.62	122.92
34	y	625	SPH	C1-C2-C3	-2.36	107.95	113.03
29	G	613	CLA	C1-O2A-CGA	2.36	122.63	116.44
50	r	621	XAT	C38-C25-C26	-2.36	118.31	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n1	610	CLA	C4B-CHC-C1C	2.36	131.93	126.34
29	N	604	CLA	C3B-C4B-NB	-2.36	108.33	110.52
29	b1	603	CLA	CHA-C4D-ND	2.36	137.43	132.50
29	S	614	CLA	C2D-C1D-ND	2.36	111.84	110.10
29	C1	512	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
29	S	614	CLA	C6-C5-C3	-2.36	107.28	113.45
29	A1	405	CLA	CHA-C4D-ND	2.36	137.43	132.50
29	s1	603	CLA	CHA-C1A-NA	-2.36	121.00	126.40
29	s	612	CLA	C1D-ND-C4D	-2.36	104.66	106.33
29	B1	606	CLA	C1-O2A-CGA	2.36	122.62	116.44
29	Y1	602	CLA	C4B-CHC-C1C	2.36	131.93	126.34
43	D1	405	PL9	O2-C1-C6	2.36	124.67	120.59
29	S1	613	CLA	C1C-C2C-C3C	-2.36	104.48	106.96
29	s	610	CLA	O2A-CGA-CBA	2.36	119.30	111.91
29	N1	603	CLA	CHA-C4D-ND	2.36	137.43	132.50
29	b	616	CLA	C1D-ND-C4D	-2.36	104.66	106.33
51	R1	622	NEX	O24-C25-C24	-2.35	111.61	113.38
29	y1	602	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
29	G	602	CLA	C4B-CHC-C1C	2.35	131.92	126.34
53	R1	626	ERG	C16-C17-C13	2.35	106.68	103.84
29	B1	604	CLA	C3B-C4B-NB	-2.35	108.33	110.52
29	r	612	CLA	CHA-C1A-NA	-2.35	121.01	126.40
29	B	608	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
29	Y	602	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
29	s	613	CLA	O2A-CGA-CBA	2.35	119.29	111.91
48	s1	607	CHL	C3B-C4B-NB	-2.35	108.33	110.52
29	n1	602	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
50	g	622	XAT	C40-C33-C34	-2.35	119.63	122.92
29	y	614	CLA	C4B-CHC-C1C	2.35	131.92	126.34
31	c1	516	BCR	C33-C5-C4	2.35	118.14	113.62
48	R1	606	CHL	C2B-C1B-NB	-2.35	108.66	110.23
43	d1	405	PL9	C27-C28-C29	-2.35	122.00	127.66
29	R	612	CLA	C4B-CHC-C1C	2.35	131.92	126.34
29	b	611	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
29	B1	604	CLA	C1-C2-C3	-2.35	121.97	126.04
29	R	612	CLA	CHA-C1A-NA	-2.35	121.01	126.40
48	R1	607	CHL	CHD-C1D-ND	-2.35	122.29	124.45
29	C1	511	CLA	C4B-CHC-C1C	2.35	131.91	126.34
29	y	612	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
50	g	622	XAT	C27-C28-C29	2.35	129.18	125.53
31	b	618	BCR	C8-C7-C6	-2.35	120.60	127.20
51	S	623	NEX	O24-C25-C38	-2.35	112.24	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b1	611	CLA	CHA-C1A-NA	-2.35	121.01	126.40
29	y1	602	CLA	C3D-C2D-C1D	-2.35	102.62	105.83
29	B1	607	CLA	C4B-CHC-C1C	2.35	131.91	126.34
29	b	607	CLA	CMA-C3A-C4A	2.35	118.09	111.77
43	d	405	PL9	C20-C19-C21	2.35	119.22	115.27
29	R1	612	CLA	C3B-C4B-NB	-2.35	108.33	110.52
29	c	512	CLA	CHA-C1A-NA	-2.35	121.02	126.40
29	r	609	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
49	n	620	LUT	C18-C5-C4	2.35	118.71	114.36
29	B1	611	CLA	O2A-CGA-CBA	2.35	119.28	111.91
48	s	608	CHL	C2B-C1B-NB	-2.35	108.66	110.23
37	c	520	DGD	C2G-O2G-C1B	-2.35	112.01	117.79
51	Y1	623	NEX	C12-C13-C14	2.35	122.55	118.94
29	n	611	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
29	b1	611	CLA	CAC-C3C-C4C	2.35	127.86	124.81
29	r	609	CLA	CHA-C4D-ND	2.35	137.41	132.50
29	D	403	CLA	CMA-C3A-C4A	2.35	118.09	111.77
29	C1	503	CLA	C1C-C2C-C3C	-2.35	104.49	106.96
29	G1	602	CLA	C1C-C2C-C3C	-2.35	104.49	106.96
29	b1	609	CLA	C1-C2-C3	-2.35	121.98	126.04
29	g	604	CLA	O2A-CGA-CBA	2.35	119.28	111.91
29	b	605	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
29	C	511	CLA	CHA-C1A-NA	-2.35	121.02	126.40
29	B1	611	CLA	CHA-C4D-ND	2.35	137.41	132.50
29	n	612	CLA	C4B-CHC-C1C	2.35	131.91	126.34
29	n1	614	CLA	C4B-CHC-C1C	2.35	131.91	126.34
29	N	602	CLA	C3B-C4B-NB	-2.35	108.34	110.52
29	b	602	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
29	s	609	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
29	y	614	CLA	CHA-C4D-ND	2.35	137.41	132.50
29	B1	602	CLA	CHD-C1D-ND	-2.35	122.30	124.45
48	n	607	CHL	CHD-C4C-C3C	2.35	128.29	124.84
49	n1	620	LUT	C10-C11-C12	-2.35	115.89	123.22
31	b	619	BCR	C12-C13-C14	-2.35	115.34	118.94
29	s1	614	CLA	C3B-C4B-NB	-2.35	108.34	110.52
36	B1	620	C7Z	C8-C7-C6	-2.35	120.61	127.20
29	b	607	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
38	b	624	3PH	O31-C31-C32	2.35	119.27	111.91
29	S1	603	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
48	R	606	CHL	C2B-C1B-NB	-2.34	108.66	110.23
29	b	610	CLA	C4B-CHC-C1C	2.34	131.90	126.34
29	s1	604	CLA	O2A-CGA-CBA	2.34	119.26	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	y	621	LUT	C7-C8-C9	-2.34	122.69	126.23
29	S1	617	CLA	CHA-C1A-NA	-2.34	121.03	126.40
29	S1	617	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
48	s	606	CHL	CHA-C1A-NA	-2.34	121.03	126.40
49	s	621	LUT	C19-C9-C8	2.34	121.77	118.08
29	b1	608	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
29	b1	607	CLA	C1C-C2C-C3C	-2.34	104.49	106.96
29	G1	611	CLA	CHD-C1D-ND	-2.34	122.30	124.45
49	g	620	LUT	C2-C3-C4	-2.34	107.10	110.30
29	S1	609	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
29	C	509	CLA	C1-C2-C3	-2.34	121.99	126.04
29	Y1	604	CLA	C2D-C1D-ND	2.34	111.83	110.10
29	a	410	CLA	CHA-C4D-ND	2.34	137.40	132.50
48	Y	606	CHL	C2B-C1B-NB	-2.34	108.66	110.23
29	c	505	CLA	C1-O2A-CGA	2.34	122.59	116.44
29	g1	611	CLA	CHA-C4D-ND	2.34	137.40	132.50
29	S1	614	CLA	CMA-C3A-C4A	2.34	118.07	111.77
29	C	501	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
48	G	607	CHL	C3B-C4B-NB	-2.34	108.34	110.52
29	r1	610	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
29	R1	602	CLA	C4B-CHC-C1C	2.34	131.89	126.34
48	N1	607	CHL	C4B-CHC-C1C	2.34	131.89	126.34
48	G1	609	CHL	C1-O2A-CGA	2.34	122.58	116.44
29	a1	405	CLA	C1-O2A-CGA	2.34	122.58	116.44
29	C	507	CLA	C2A-C1A-CHA	2.34	127.95	123.86
29	r	610	CLA	C3B-C4B-NB	-2.34	108.34	110.52
29	b1	602	CLA	CHA-C1A-NA	-2.34	121.04	126.40
48	G	609	CHL	C4A-NA-C1A	2.34	107.76	106.71
29	D1	402	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
50	R1	621	XAT	C39-C29-C30	-2.34	119.65	122.92
29	g1	604	CLA	C4B-CHC-C1C	2.34	131.89	126.34
29	s1	605	CLA	C3B-C4B-NB	-2.34	108.34	110.52
29	B	614	CLA	CHA-C4D-ND	2.34	137.39	132.50
29	Y	614	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
31	B1	619	BCR	C19-C18-C17	2.34	122.53	118.94
48	Y1	601	CHL	CHC-C1C-NC	2.34	127.75	124.20
29	n1	603	CLA	CHD-C1D-ND	-2.34	122.31	124.45
29	y1	608	CLA	C1-O2A-CGA	2.34	122.58	116.44
32	a	412	SQD	O3-C3-C2	-2.34	104.94	110.35
29	B	617	CLA	C1-O2A-CGA	2.34	122.58	116.44
29	d1	403	CLA	CMB-C2B-C3B	2.34	132.25	126.59
29	A1	407	CLA	CHA-C4D-ND	2.34	137.39	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y	603	CLA	CMA-C3A-C4A	2.34	118.05	111.77
29	c1	508	CLA	CHA-C1A-NA	-2.34	121.05	126.40
49	G	620	LUT	C35-C15-C14	-2.34	118.69	123.47
48	G1	606	CHL	C4D-CHA-C1A	2.34	124.09	121.25
50	g	622	XAT	O4-C5-C18	-2.34	112.26	115.06
48	n	606	CHL	C4D-CHA-C1A	2.33	124.09	121.25
44	f1	101	HEM	C4A-NA-C1A	2.33	107.63	105.35
31	b1	618	BCR	C37-C22-C21	-2.33	119.65	122.92
48	n	609	CHL	CHC-C1C-NC	2.33	127.74	124.20
29	c1	512	CLA	C2D-C1D-ND	2.33	111.82	110.10
29	Y1	602	CLA	CAC-C3C-C4C	2.33	127.84	124.81
48	g	609	CHL	C4B-CHC-C1C	2.33	131.87	126.34
48	N	608	CHL	C2C-C3C-C4C	2.33	108.15	106.49
29	b1	603	CLA	OBD-CAD-C3D	-2.33	122.91	128.52
29	R1	603	CLA	CHA-C1A-NA	-2.33	121.06	126.40
50	R1	621	XAT	C20-C13-C14	-2.33	119.66	122.92
29	b1	603	CLA	CMA-C3A-C4A	2.33	118.04	111.77
49	s	621	LUT	C15-C35-C34	-2.33	118.70	123.47
29	b1	606	CLA	CMA-C3A-C4A	2.33	118.04	111.77
29	G	602	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
29	B1	615	CLA	C4B-CHC-C1C	2.33	131.87	126.34
29	S1	610	CLA	O2A-CGA-CBA	2.33	119.22	111.91
40	y	624	LHG	C6-C5-C4	-2.33	106.27	111.79
29	Y	612	CLA	C1D-ND-C4D	-2.33	104.68	106.33
29	B1	610	CLA	C1D-ND-C4D	-2.33	104.68	106.33
49	s	620	LUT	C35-C15-C14	-2.33	118.70	123.47
49	g1	621	LUT	C18-C5-C6	-2.33	121.91	124.53
29	R	602	CLA	CHA-C4D-ND	2.33	137.37	132.50
29	G	611	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
29	A	405	CLA	C6-C5-C3	-2.33	107.34	113.45
29	a	407	CLA	O2A-CGA-CBA	2.33	119.22	111.91
29	R1	612	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
29	Y1	613	CLA	C1D-ND-C4D	-2.33	104.68	106.33
29	n	603	CLA	CMA-C3A-C4A	2.33	118.03	111.77
29	c	510	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
29	r	604	CLA	C2D-C1D-ND	2.33	111.82	110.10
29	y	613	CLA	O2A-CGA-CBA	2.33	119.22	111.91
29	Y1	604	CLA	C3B-C4B-NB	-2.33	108.36	110.52
29	N1	602	CLA	C1D-ND-C4D	-2.33	104.68	106.33
29	g	614	CLA	CHA-C1A-NA	-2.33	121.07	126.40
29	A1	407	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
52	R1	625	LMT	O5'-C1'-O1'	-2.33	104.46	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S	612	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
29	y	603	CLA	C4B-CHC-C1C	2.33	131.86	126.34
43	d1	405	PL9	C35-C34-C36	2.33	119.19	115.27
29	g	602	CLA	C3B-C4B-NB	-2.33	108.36	110.52
29	R1	608	CLA	C3B-C4B-NB	-2.33	108.36	110.52
48	S1	608	CHL	C1-C2-C3	-2.33	122.02	126.04
29	A	407	CLA	CHA-C4D-ND	2.33	137.37	132.50
48	N	601	CHL	C2B-C1B-NB	-2.33	108.67	110.23
29	C1	504	CLA	C3B-C4B-NB	-2.33	108.36	110.52
29	g1	610	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
29	n1	613	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
29	s1	604	CLA	C2D-C1D-ND	2.33	111.82	110.10
29	g	613	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
29	r1	612	CLA	C4B-CHC-C1C	2.33	131.85	126.34
29	s1	605	CLA	C4B-CHC-C1C	2.33	131.85	126.34
31	B1	618	BCR	C31-C1-C6	-2.33	106.53	110.30
29	D	403	CLA	CHA-C4D-ND	2.33	137.36	132.50
49	S1	621	LUT	C39-C29-C30	-2.33	119.67	122.92
29	B	608	CLA	O2A-CGA-CBA	2.32	119.20	111.91
29	Y1	611	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
29	s1	605	CLA	C2D-C1D-ND	2.32	111.82	110.10
29	b	615	CLA	C4B-CHC-C1C	2.32	131.85	126.34
29	B1	606	CLA	CHA-C1A-NA	-2.32	121.08	126.40
48	G1	601	CHL	C2B-C1B-NB	-2.32	108.67	110.23
29	b	612	CLA	C1C-C2C-C3C	-2.32	104.51	106.96
29	b1	608	CLA	C1C-C2C-C3C	-2.32	104.51	106.96
29	N1	610	CLA	C2C-C1C-NC	2.32	112.15	109.97
29	S	604	CLA	CHA-C4D-ND	2.32	137.36	132.50
43	d1	405	PL9	C32-C33-C34	-2.32	122.06	127.66
29	S1	611	CLA	CBB-CAB-C3B	-2.32	116.06	127.62
29	s	613	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
47	k1	101	4RF	O18-C16-C15	2.32	119.20	111.91
29	g	604	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
29	r	602	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
29	B1	616	CLA	C3B-C4B-NB	-2.32	108.36	110.52
29	c1	511	CLA	CHA-C4D-ND	2.32	137.36	132.50
29	r1	609	CLA	CHA-C4D-ND	2.32	137.36	132.50
29	b1	608	CLA	O2A-CGA-CBA	2.32	119.20	111.91
36	b1	620	C7Z	C21-C26-C25	-2.32	119.34	122.61
50	G1	622	XAT	C6-C7-C8	-2.32	121.08	125.99
29	b	606	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
29	Y1	613	CLA	O2D-CGD-O1D	-2.32	119.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	Y	609	CHL	C2B-C1B-NB	-2.32	108.67	110.23
49	Y1	620	LUT	C38-C25-C24	-2.32	118.59	123.56
48	N	607	CHL	C1-O2A-CGA	2.32	122.54	116.44
29	S1	613	CLA	C3B-C4B-NB	-2.32	108.36	110.52
29	G1	614	CLA	O2A-CGA-CBA	2.32	119.19	111.91
29	B1	609	CLA	C2D-C1D-ND	2.32	111.81	110.10
29	Y	613	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
29	g	602	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
33	B1	622	LMG	C8-O7-C10	-2.32	112.08	117.79
49	g	621	LUT	C19-C9-C8	2.32	121.73	118.08
29	C	512	CLA	CHA-C4D-ND	2.32	137.35	132.50
29	R	610	CLA	C1D-ND-C4D	-2.32	104.69	106.33
29	b1	602	CLA	C1D-ND-C4D	-2.32	104.69	106.33
29	S1	609	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
49	N	620	LUT	C37-C21-C26	2.32	113.06	109.55
29	N	604	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
48	g	605	CHL	C3B-C4B-NB	-2.32	108.36	110.52
29	G	602	CLA	O2A-CGA-CBA	2.32	119.19	111.91
48	S	601	CHL	C4D-CHA-C1A	2.32	124.07	121.25
53	r1	626	ERG	C12-C13-C17	-2.32	113.10	116.57
29	S	604	CLA	C4B-CHC-C1C	2.32	131.84	126.34
49	Y1	620	LUT	C11-C10-C9	-2.32	124.00	127.31
29	B	616	CLA	C3D-C2D-C1D	-2.32	102.67	105.83
29	g1	603	CLA	CHA-C1A-NA	-2.32	121.08	126.40
29	b	602	CLA	C1-C2-C3	-2.32	122.03	126.04
29	c	511	CLA	C4B-CHC-C1C	2.32	131.84	126.34
29	N	610	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
29	b	611	CLA	C3D-C2D-C1D	-2.32	102.67	105.83
29	s1	610	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
48	G1	606	CHL	C2C-C3C-C4C	2.32	108.14	106.49
50	g1	622	XAT	C6-C7-C8	-2.32	121.09	125.99
48	r	606	CHL	C4B-CHC-C1C	2.32	131.84	126.34
51	n1	623	NEX	C28-C29-C30	2.32	122.50	118.94
29	C1	506	CLA	C3B-C4B-NB	-2.32	108.36	110.52
29	B	616	CLA	CHA-C4D-ND	2.32	137.35	132.50
49	Y	620	LUT	C16-C1-C6	-2.32	106.54	110.30
48	n	605	CHL	CMA-C3A-C4A	2.32	118.00	111.77
29	S	609	CLA	C3B-C4B-NB	-2.32	108.36	110.52
29	C1	508	CLA	C3B-C4B-NB	-2.32	108.36	110.52
29	D1	403	CLA	C3B-C4B-NB	-2.32	108.36	110.52
29	r1	612	CLA	C3B-C4B-NB	-2.32	108.36	110.52
29	b	615	CLA	C2C-C1C-NC	2.32	112.14	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	G	610	CLA	O2A-CGA-CBA	2.32	119.18	111.91
53	R1	626	ERG	C11-C12-C13	2.32	116.75	112.78
48	s	606	CHL	CMA-C3A-C4A	2.32	118.00	111.77
48	N	601	CHL	CHD-C4C-C3C	2.32	128.25	124.84
29	y	612	CLA	CHA-C4D-ND	2.32	137.35	132.50
29	N	614	CLA	C4B-CHC-C1C	2.32	131.83	126.34
49	G1	620	LUT	C10-C11-C12	-2.32	115.99	123.22
29	y	608	CLA	C4B-CHC-C1C	2.32	131.83	126.34
29	S	604	CLA	CMD-C2D-C3D	-2.32	122.29	127.61
29	c1	509	CLA	CMD-C2D-C3D	-2.32	122.29	127.61
40	g1	624	LHG	O8-C23-C24	2.32	119.17	111.91
31	c1	517	BCR	C12-C13-C14	2.32	122.49	118.94
29	b	610	CLA	C2C-C1C-NC	2.32	112.14	109.97
29	A	410	CLA	CHA-C4D-ND	2.32	137.34	132.50
29	G1	603	CLA	CHA-C1A-NA	-2.32	121.10	126.40
29	n	610	CLA	C3D-C2D-C1D	-2.31	102.67	105.83
48	G1	606	CHL	CHD-C4C-C3C	2.31	128.24	124.84
29	B1	606	CLA	C1C-C2C-C3C	-2.31	104.52	106.96
29	b	617	CLA	C3B-C4B-NB	-2.31	108.37	110.52
29	g	613	CLA	C4B-CHC-C1C	2.31	131.83	126.34
29	G	603	CLA	C1D-ND-C4D	-2.31	104.69	106.33
29	r	603	CLA	CHA-C4D-ND	2.31	137.34	132.50
48	g	608	CHL	CHB-C4A-NA	2.31	127.71	124.51
29	n	603	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
49	n1	621	LUT	C18-C5-C6	-2.31	121.93	124.53
29	g	611	CLA	CHA-C4D-ND	2.31	137.34	132.50
48	N1	605	CHL	CHD-C4C-C3C	2.31	128.24	124.84
48	g1	605	CHL	CHD-C4C-C3C	2.31	128.24	124.84
29	s	609	CLA	C4B-CHC-C1C	2.31	131.82	126.34
29	N1	613	CLA	C1D-ND-C4D	-2.31	104.69	106.33
48	n	601	CHL	C1-O2A-CGA	2.31	122.51	116.44
29	R	603	CLA	O2A-CGA-CBA	2.31	119.17	111.91
49	Y	621	LUT	C16-C1-C6	-2.31	106.55	110.30
29	B1	610	CLA	C4B-CHC-C1C	2.31	131.82	126.34
29	G	611	CLA	O2A-CGA-CBA	2.31	119.16	111.91
29	s1	611	CLA	C2A-C1A-CHA	2.31	127.90	123.86
29	N	612	CLA	CHA-C1A-NA	-2.31	121.10	126.40
29	N1	614	CLA	C1-O2A-CGA	2.31	122.51	116.44
29	g	603	CLA	CMA-C3A-C4A	2.31	117.99	111.77
29	B	604	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
29	Y1	610	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
49	G	620	LUT	C31-C32-C33	-2.31	119.92	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	N	604	CLA	C4B-CHC-C1C	2.31	131.82	126.34
29	y	610	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
29	b1	611	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
48	s1	606	CHL	C3B-C4B-NB	-2.31	108.37	110.52
29	C	509	CLA	C11-C12-C13	-2.31	108.45	115.92
49	g	620	LUT	C38-C25-C24	-2.31	118.61	123.56
29	C1	506	CLA	O2A-CGA-CBA	2.31	119.16	111.91
53	R	626	ERG	C1-C10-C9	-2.31	103.50	108.28
29	c1	509	CLA	C4B-CHC-C1C	2.31	131.82	126.34
29	S	604	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
29	G1	604	CLA	C4B-CHC-C1C	2.31	131.82	126.34
29	Y1	603	CLA	CHA-C1A-NA	-2.31	121.11	126.40
43	d	405	PL9	C31-C32-C33	-2.31	104.29	111.88
49	y	620	LUT	C18-C5-C6	-2.31	121.93	124.53
29	b	614	CLA	C1D-ND-C4D	-2.31	104.69	106.33
49	N	620	LUT	C37-C21-C22	-2.31	105.06	109.44
29	N	610	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
29	y1	614	CLA	CHA-C1A-NA	-2.31	121.11	126.40
29	b1	604	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
29	S1	604	CLA	CAC-C3C-C4C	2.31	127.81	124.81
29	n	603	CLA	C4B-CHC-C1C	2.31	131.81	126.34
29	C1	505	CLA	O2A-CGA-CBA	2.31	119.15	111.91
43	D	405	PL9	C37-C38-C39	-2.31	122.10	127.66
29	s1	609	CLA	O2A-CGA-CBA	2.31	119.15	111.91
29	n	614	CLA	CMC-C2C-C1C	2.31	128.55	125.04
29	r	603	CLA	CHD-C1D-ND	-2.31	122.33	124.45
29	b1	608	CLA	CHD-C1D-ND	-2.31	122.33	124.45
29	s	605	CLA	C4B-CHC-C1C	2.31	131.81	126.34
29	b1	604	CLA	C3B-C4B-NB	-2.31	108.37	110.52
29	c1	509	CLA	C3B-C4B-NB	-2.31	108.37	110.52
29	B1	609	CLA	CHA-C1A-NA	-2.31	121.11	126.40
31	A	411	BCR	C33-C5-C4	2.31	118.05	113.62
29	s1	602	CLA	C4B-CHC-C1C	2.31	131.81	126.34
29	R1	602	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
29	B	608	CLA	C4B-CHC-C1C	2.31	131.81	126.34
29	b	606	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
29	s	617	CLA	CHA-C1A-NA	-2.31	121.12	126.40
49	G	620	LUT	C10-C11-C12	-2.31	116.02	123.22
29	N1	611	CLA	CAC-C3C-C4C	2.31	127.80	124.81
33	b1	622	LMG	C7-O1-C1	-2.31	109.23	113.74
29	c1	513	CLA	CHA-C1A-NA	-2.31	121.12	126.40
29	Y	611	CLA	O2D-CGD-O1D	-2.31	119.33	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b1	606	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
50	R	621	XAT	C26-C27-C28	-2.31	121.12	125.99
29	C1	501	CLA	O2A-CGA-CBA	2.31	119.14	111.91
29	S1	604	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
29	S	614	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
37	C1	518	DGD	O1G-C1A-C2A	2.30	119.14	111.91
48	N	609	CHL	CHB-C4A-NA	2.30	127.70	124.51
29	b1	606	CLA	CHA-C1A-NA	-2.30	121.12	126.40
29	C	503	CLA	C4B-CHC-C1C	2.30	131.80	126.34
29	b1	608	CLA	CHA-C1A-NA	-2.30	121.12	126.40
29	c1	507	CLA	C2D-C1D-ND	2.30	111.80	110.10
29	N	613	CLA	C4B-CHC-C1C	2.30	131.80	126.34
29	R1	602	CLA	O2A-CGA-CBA	2.30	119.14	111.91
39	B1	625	DGA	OG1-CA1-CA2	2.30	119.14	111.91
29	r1	603	CLA	CMD-C2D-C3D	-2.30	122.31	127.61
29	S	614	CLA	CHA-C1A-NA	-2.30	121.12	126.40
29	c	507	CLA	CHA-C1A-NA	-2.30	121.12	126.40
29	c	511	CLA	C6-C5-C3	-2.30	107.41	113.45
36	b1	620	C7Z	C18-C5-C4	2.30	118.62	114.36
29	C	506	CLA	CHD-C4C-C3C	2.30	128.23	124.84
29	r	610	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
32	M	101	SQD	O3-C3-C2	-2.30	105.02	110.35
29	b	616	CLA	C4B-CHC-C1C	2.30	131.80	126.34
29	c	511	CLA	CAA-CBA-CGA	-2.30	106.52	113.25
29	N	612	CLA	CHD-C1D-ND	-2.30	122.34	124.45
29	s	610	CLA	CHA-C1A-NA	-2.30	121.12	126.40
29	Y1	604	CLA	C4B-CHC-C1C	2.30	131.80	126.34
29	b	616	CLA	C1-C2-C3	-2.30	122.06	126.04
51	y1	623	NEX	C38-C25-C26	-2.30	118.40	122.26
29	s1	614	CLA	CHA-C1A-NA	-2.30	121.13	126.40
29	Y1	603	CLA	C4B-CHC-C1C	2.30	131.80	126.34
29	Y	608	CLA	CHA-C4D-ND	2.30	137.31	132.50
29	r1	604	CLA	C4B-CHC-C1C	2.30	131.79	126.34
51	S	623	NEX	C5-C6-C1	2.30	121.98	119.70
48	Y1	605	CHL	CHB-C4A-NA	2.30	127.69	124.51
29	r1	602	CLA	C4B-CHC-C1C	2.30	131.79	126.34
29	y	614	CLA	O2A-CGA-CBA	2.30	119.13	111.91
50	N	622	XAT	C4-C3-C2	-2.30	106.33	110.77
29	n	610	CLA	CMA-C3A-C4A	2.30	117.95	111.77
49	y	621	LUT	C19-C9-C8	2.30	121.70	118.08
29	C1	506	CLA	C6-C5-C3	-2.30	107.42	113.45
31	B	618	BCR	C15-C14-C13	-2.30	124.03	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	G1	620	LUT	C16-C1-C6	-2.30	106.57	110.30
29	B1	617	CLA	CAA-CBA-CGA	-2.30	106.53	113.25
29	b	609	CLA	O2A-CGA-CBA	2.30	119.12	111.91
29	a	406	CLA	C1-O2A-CGA	2.30	122.48	116.44
36	b1	620	C7Z	C40-C33-C34	-2.30	119.70	122.92
31	d1	404	BCR	C38-C26-C25	-2.30	121.95	124.53
51	R1	622	NEX	C4-C3-C2	2.30	115.21	110.77
29	A1	407	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
29	Y1	612	CLA	C1D-ND-C4D	-2.30	104.70	106.33
29	c	507	CLA	C2D-C1D-ND	2.30	111.80	110.10
29	c	513	CLA	C4B-CHC-C1C	2.30	131.79	126.34
51	R1	622	NEX	C24-C23-C22	-2.30	106.33	110.77
29	s	602	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
29	Y1	612	CLA	CHD-C1D-ND	-2.30	122.34	124.45
29	N1	611	CLA	C3B-C4B-NB	-2.30	108.38	110.52
29	C1	502	CLA	CHA-C1A-NA	-2.30	121.14	126.40
29	D1	402	CLA	CHA-C1A-NA	-2.30	121.14	126.40
31	c	516	BCR	C37-C22-C23	2.30	121.70	118.08
48	n1	608	CHL	C4D-CHA-C1A	2.30	124.05	121.25
31	C1	516	BCR	C37-C22-C21	-2.30	119.70	122.92
29	G	604	CLA	OBD-CAD-C3D	-2.30	122.99	128.52
34	A	414	SPH	O3-C3-C2	2.30	110.96	107.31
29	R	604	CLA	C4B-CHC-C1C	2.30	131.78	126.34
48	y	605	CHL	CHC-C1C-NC	2.30	127.69	124.20
29	S1	612	CLA	CHA-C1A-NA	-2.30	121.14	126.40
29	G	602	CLA	C1C-C2C-C3C	-2.30	104.54	106.96
31	C	517	BCR	C23-C24-C25	-2.30	120.75	127.20
29	Y1	611	CLA	CHA-C4D-ND	2.30	137.30	132.50
29	A1	410	CLA	C1-O2A-CGA	2.30	122.47	116.44
29	S1	603	CLA	CHD-C1D-ND	-2.30	122.34	124.45
50	g	622	XAT	C20-C13-C14	-2.30	119.71	122.92
29	R1	610	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
51	S1	623	NEX	C1-C2-C3	2.30	118.83	113.64
48	n	601	CHL	C2B-C1B-NB	-2.30	108.69	110.23
29	b1	605	CLA	C4B-CHC-C1C	2.30	131.78	126.34
29	B	615	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
32	A	412	SQD	O3-C3-C2	-2.30	105.04	110.35
29	Y	602	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
29	B	616	CLA	CHA-C1A-NA	-2.30	121.14	126.40
49	s1	620	LUT	C40-C33-C32	2.29	121.69	118.08
48	G1	609	CHL	CHD-C4C-C3C	2.29	128.21	124.84
29	g1	611	CLA	O1D-CGD-CBD	-2.29	119.79	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	505	CLA	C1C-C2C-C3C	-2.29	104.54	106.96
32	C1	526	SQD	O3-C3-C2	-2.29	105.05	110.35
29	c1	512	CLA	CHA-C1A-NA	-2.29	121.14	126.40
29	g1	602	CLA	C4B-CHC-C1C	2.29	131.78	126.34
29	y	608	CLA	CHA-C1A-NA	-2.29	121.14	126.40
29	y1	608	CLA	CHA-C1A-NA	-2.29	121.15	126.40
29	B	614	CLA	C4B-CHC-C1C	2.29	131.78	126.34
29	c	510	CLA	C4B-CHC-C1C	2.29	131.78	126.34
30	a1	409	PHO	C2D-C1D-ND	-2.29	107.94	109.53
31	C	515	BCR	C1-C6-C7	2.29	122.26	115.78
29	G	604	CLA	CHA-C1A-NA	-2.29	121.15	126.40
29	R1	604	CLA	O2A-CGA-CBA	2.29	119.10	111.91
29	R1	604	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
29	s1	613	CLA	C1-O2A-CGA	2.29	122.46	116.44
29	b1	607	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
29	N	613	CLA	CHD-C1D-ND	-2.29	122.35	124.45
29	Y	613	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
29	c	508	CLA	CHA-C4D-ND	2.29	137.29	132.50
29	g1	603	CLA	C1-C2-C3	-2.29	122.08	126.04
36	b	620	C7Z	C31-C32-C33	-2.29	119.98	126.42
29	G1	604	CLA	CHA-C1A-NA	-2.29	121.15	126.40
29	r	604	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
29	c	504	CLA	C2C-C1C-NC	2.29	112.12	109.97
29	c	504	CLA	C1-O2A-CGA	2.29	122.45	116.44
29	C	512	CLA	CMA-C3A-C4A	2.29	117.92	111.77
29	N1	613	CLA	CHA-C4D-ND	2.29	137.29	132.50
49	N	621	LUT	C38-C25-C24	-2.29	118.66	123.56
51	g1	623	NEX	C31-C32-C33	2.29	132.84	126.42
29	B1	610	CLA	C1-O2A-CGA	2.29	122.45	116.44
29	g	603	CLA	O2A-CGA-CBA	2.29	119.09	111.91
50	y1	622	XAT	O24-C25-C24	2.29	115.10	113.38
29	c	502	CLA	CHA-C4D-ND	2.29	137.28	132.50
41	C	527	LMK	C9-O8-C28	-2.29	109.39	113.80
51	G	623	NEX	C4-C3-C2	2.29	115.19	110.77
29	c	501	CLA	C4B-CHC-C1C	2.29	131.76	126.34
29	C	508	CLA	C2C-C1C-NC	2.29	112.11	109.97
48	G	605	CHL	C1-O2A-CGA	2.29	123.38	116.73
29	G1	604	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
29	A1	406	CLA	C6-C5-C3	-2.29	107.46	113.45
29	c1	503	CLA	C4B-CHC-C1C	2.29	131.76	126.34
29	R	604	CLA	O2A-CGA-CBA	2.29	119.08	111.91
48	G	607	CHL	C4D-CHA-C1A	2.29	124.03	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	411	BCR	C35-C13-C12	2.29	121.68	118.08
29	r	604	CLA	C4B-CHC-C1C	2.29	131.76	126.34
29	R1	602	CLA	CHA-C1A-NA	-2.29	121.16	126.40
31	B	619	BCR	C8-C7-C6	-2.29	120.78	127.20
29	b	617	CLA	CHA-C4D-ND	2.29	137.28	132.50
29	n	604	CLA	C4B-CHC-C1C	2.29	131.76	126.34
29	b	605	CLA	CHA-C1A-NA	-2.29	121.16	126.40
29	s1	603	CLA	C3D-C2D-C1D	-2.29	102.71	105.83
29	S	603	CLA	C1-O2A-CGA	2.29	122.44	116.44
29	y	614	CLA	OBD-CAD-C3D	-2.29	123.02	128.52
29	B1	614	CLA	CMC-C2C-C3C	2.29	132.32	126.12
29	S	602	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
29	S1	614	CLA	CHA-C4D-ND	2.28	137.28	132.50
29	b	604	CLA	CAA-C2A-C3A	-2.28	106.52	112.78
48	G	609	CHL	CHB-C4A-NA	2.28	127.67	124.51
48	n	608	CHL	C2C-C3C-C4C	2.28	108.12	106.49
29	s	602	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
29	B1	617	CLA	C2D-C1D-ND	2.28	111.79	110.10
50	G	622	XAT	C39-C29-C30	-2.28	119.72	122.92
31	B1	619	BCR	C35-C13-C12	2.28	121.67	118.08
29	a	407	CLA	CHA-C1A-NA	-2.28	121.17	126.40
31	C	517	BCR	C27-C26-C25	-2.28	119.42	122.73
29	B	616	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
51	N	623	NEX	C31-C32-C33	2.28	132.83	126.42
29	n1	602	CLA	O2A-CGA-CBA	2.28	119.07	111.91
48	Y1	601	CHL	CHB-C4A-NA	2.28	127.67	124.51
29	y1	612	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
48	n1	605	CHL	C3A-C2A-C1A	2.28	104.76	101.34
29	b	607	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
29	S1	612	CLA	CMA-C3A-C4A	2.28	117.91	111.77
29	N	611	CLA	OBD-CAD-C3D	-2.28	123.03	128.52
29	r1	608	CLA	O2A-CGA-CBA	2.28	119.07	111.91
43	d1	405	PL9	C22-C23-C24	-2.28	122.17	127.66
51	G1	623	NEX	C40-C33-C34	-2.28	119.73	122.92
48	G1	606	CHL	CHA-C1A-NA	-2.28	121.17	126.40
49	G1	620	LUT	C18-C5-C6	-2.28	121.97	124.53
29	C1	511	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
33	A1	413	LMG	O6-C5-C4	2.28	113.84	109.69
29	A	407	CLA	C4B-CHC-C1C	2.28	131.75	126.34
29	C	508	CLA	C4B-CHC-C1C	2.28	131.75	126.34
53	R1	626	ERG	C11-C9-C10	2.28	119.24	113.58
29	B	605	CLA	C1C-C2C-C3C	-2.28	104.56	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	507	CLA	CHA-C1A-NA	-2.28	121.17	126.40
29	g1	610	CLA	C4B-CHC-C1C	2.28	131.75	126.34
29	s	604	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
29	Y1	602	CLA	CMA-C3A-C4A	2.28	117.90	111.77
49	N	620	LUT	C20-C13-C12	2.28	121.67	118.08
51	g	623	NEX	O24-C25-C24	-2.28	111.67	113.38
29	B1	614	CLA	CHA-C1A-NA	-2.28	121.18	126.40
29	N	612	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
49	r	620	LUT	C38-C25-C24	-2.28	118.68	123.56
29	R1	609	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
29	C1	503	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
29	C	507	CLA	C4B-CHC-C1C	2.28	131.74	126.34
29	b	609	CLA	CHD-C1D-ND	-2.28	122.36	124.45
29	B	608	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
29	y1	613	CLA	C1D-ND-C4D	-2.28	104.72	106.33
29	A1	410	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
29	d	403	CLA	C4B-CHC-C1C	2.28	131.74	126.34
29	G1	602	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
29	c1	508	CLA	C3B-C4B-NB	-2.28	108.40	110.52
29	G	614	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
48	g	605	CHL	C1-O2A-CGA	2.28	123.34	116.73
29	B1	604	CLA	CHA-C1A-NA	-2.28	121.19	126.40
32	b	621	SQD	O3-C3-C2	-2.28	105.09	110.35
29	r	602	CLA	OBD-CAD-C3D	-2.28	123.04	128.52
29	S1	617	CLA	C4B-CHC-C1C	2.28	131.74	126.34
29	g1	604	CLA	CMA-C3A-C4A	2.28	117.89	111.77
29	C	503	CLA	C3B-C4B-NB	-2.28	108.40	110.52
29	a	407	CLA	C2A-C1A-CHA	2.27	127.84	123.86
29	B1	616	CLA	OBD-CAD-C3D	-2.27	123.05	128.52
29	Y	604	CLA	C1-C2-C3	-2.27	122.11	126.04
29	g1	613	CLA	C4B-CHC-C1C	2.27	131.73	126.34
29	B1	612	CLA	C1C-C2C-C3C	-2.27	104.56	106.96
29	Y1	611	CLA	C1C-C2C-C3C	-2.27	104.56	106.96
45	H1	101	RRX	C23-C22-C21	-2.27	115.45	118.94
29	g1	611	CLA	CHD-C1D-ND	-2.27	122.36	124.45
51	r1	622	NEX	O24-C25-C38	-2.27	112.33	115.06
29	s1	613	CLA	CHA-C1A-NA	-2.27	121.19	126.40
29	N	612	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
29	b1	616	CLA	CMA-C3A-C4A	2.27	117.88	111.77
29	g1	611	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
29	S1	610	CLA	CHA-C1A-NA	-2.27	121.19	126.40
29	b	610	CLA	CHA-C4D-ND	2.27	137.25	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C1	507	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
29	n1	612	CLA	CHA-C1A-NA	-2.27	121.19	126.40
29	c	508	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
29	G	610	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
29	c	504	CLA	CHA-C4D-ND	2.27	137.25	132.50
29	c1	511	CLA	C1D-ND-C4D	-2.27	104.72	106.33
29	b	609	CLA	CHA-C1A-NA	-2.27	121.19	126.40
29	N	604	CLA	CMA-C3A-C4A	2.27	117.88	111.77
29	B	617	CLA	C4B-CHC-C1C	2.27	131.73	126.34
29	c	503	CLA	CHA-C1A-NA	-2.27	121.20	126.40
29	n1	602	CLA	CMC-C2C-C1C	2.27	128.50	125.04
29	s	602	CLA	C4B-CHC-C1C	2.27	131.72	126.34
48	n1	608	CHL	C4A-NA-C1A	2.27	107.73	106.71
29	R1	612	CLA	C6-C5-C3	-2.27	107.50	113.45
39	b	625	DGA	OG1-CA1-CA2	2.27	119.03	111.91
29	C1	511	CLA	CAC-C3C-C4C	2.27	127.76	124.81
29	r	603	CLA	OBD-CAD-C3D	-2.27	123.06	128.52
29	y	613	CLA	C6-C5-C3	-2.27	107.50	113.45
29	G1	602	CLA	C2D-C1D-ND	2.27	111.78	110.10
48	s	606	CHL	C3B-C4B-NB	-2.27	108.41	110.52
29	r1	612	CLA	C1-O2A-CGA	2.27	122.40	116.44
29	r	608	CLA	C1-C2-C3	-2.27	122.12	126.04
43	D	405	PL9	O1-C4-C3	-2.27	118.22	120.72
29	S1	604	CLA	C4B-CHC-C1C	2.27	131.72	126.34
29	R1	609	CLA	CHA-C4D-ND	2.27	137.25	132.50
29	S1	612	CLA	CHA-C4D-ND	2.27	137.25	132.50
29	B	602	CLA	C1D-ND-C4D	-2.27	104.72	106.33
45	h	101	RRX	C19-C18-C17	-2.27	115.46	118.94
29	s1	617	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
29	r1	602	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
29	n1	610	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
51	G	623	NEX	C19-C9-C10	-2.27	119.75	122.92
49	S1	621	LUT	C38-C25-C24	-2.27	118.71	123.56
29	s1	614	CLA	O2A-CGA-CBA	2.27	119.03	111.91
29	s1	611	CLA	CHA-C1A-NA	-2.27	121.20	126.40
48	y	606	CHL	C4D-CHA-C1A	2.27	124.01	121.25
29	b1	606	CLA	C4B-CHC-C1C	2.27	131.72	126.34
29	a	407	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
29	G1	613	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
51	y	623	NEX	C40-C33-C32	2.27	121.65	118.08
29	b1	616	CLA	C2D-C1D-ND	2.27	111.78	110.10
32	B	621	SQD	O3-C3-C2	-2.27	105.11	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	606	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
29	S	613	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
29	b1	611	CLA	O2A-CGA-CBA	2.27	119.02	111.91
29	b1	604	CLA	C4B-CHC-C1C	2.27	131.72	126.34
29	A	410	CLA	C3B-C4B-NB	-2.27	108.41	110.52
29	n1	612	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
49	y1	621	LUT	C40-C33-C34	-2.27	119.75	122.92
43	d	405	PL9	C36-C34-C33	-2.27	116.53	121.12
29	r1	602	CLA	CHA-C4D-ND	2.26	137.24	132.50
29	G	604	CLA	C4B-CHC-C1C	2.26	131.71	126.34
29	b	606	CLA	C4B-CHC-C1C	2.26	131.71	126.34
29	s	610	CLA	C4B-CHC-C1C	2.26	131.71	126.34
29	s1	614	CLA	C4B-CHC-C1C	2.26	131.71	126.34
37	c	518	DGD	C1E-C2E-C3E	-2.26	105.28	110.00
29	S	610	CLA	C2C-C1C-NC	2.26	112.09	109.97
43	D1	405	PL9	O2-C1-C2	-2.26	116.59	121.78
29	B	609	CLA	O2A-CGA-CBA	2.26	119.01	111.91
29	B	605	CLA	C3B-C4B-NB	-2.26	108.42	110.52
29	r1	610	CLA	O2A-CGA-CBA	2.26	119.01	111.91
29	C	508	CLA	CHB-C1B-NB	2.26	126.65	124.26
29	N1	610	CLA	CMA-C3A-C4A	2.26	117.86	111.77
29	R1	608	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
29	n1	611	CLA	C3B-C4B-NB	-2.26	108.42	110.52
29	c	507	CLA	C1-C2-C3	-2.26	122.13	126.04
29	r1	609	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
29	C1	505	CLA	C1D-ND-C4D	-2.26	104.73	106.33
48	n	608	CHL	C4A-NA-C1A	2.26	107.72	106.71
29	C	506	CLA	C4B-CHC-C1C	2.26	131.70	126.34
29	R	603	CLA	OBD-CAD-C3D	-2.26	123.08	128.52
49	g	621	LUT	C1-C6-C5	-2.26	119.43	122.61
31	a1	411	BCR	C36-C18-C17	-2.26	119.75	122.92
29	Y	610	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
29	n	602	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
48	G1	609	CHL	C4D-CHA-C1A	2.26	124.00	121.25
40	Y1	624	LHG	C6-C5-C4	-2.26	106.44	111.79
29	S1	611	CLA	C4B-CHC-C1C	2.26	131.70	126.34
29	Y	608	CLA	CHA-C1A-NA	-2.26	121.22	126.40
29	n1	603	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
29	B1	609	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
29	g	604	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
49	g1	620	LUT	C7-C8-C9	-2.26	122.82	126.23
31	B	619	BCR	C19-C18-C17	2.26	122.41	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	505	CLA	OBD-CAD-C3D	-2.26	123.08	128.52
29	B1	608	CLA	CAC-C3C-C4C	2.26	127.74	124.81
29	N	613	CLA	C3B-C4B-NB	-2.26	108.42	110.52
29	N	602	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
29	c1	508	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
40	D1	409	LHG	O8-C23-C24	2.26	119.00	111.91
45	H	101	RRX	C19-C18-C17	-2.26	115.47	118.94
44	f	101	HEM	C4A-NA-C1A	2.26	107.56	105.35
37	C1	518	DGD	O6D-C5D-C6D	2.26	111.23	106.67
29	N1	610	CLA	CHA-C4D-ND	2.26	137.23	132.50
29	c1	512	CLA	C1-O2A-CGA	2.26	122.37	116.44
29	b	611	CLA	C3B-C4B-NB	-2.26	108.42	110.52
29	D	403	CLA	C1D-ND-C4D	-2.26	104.73	106.33
48	y	606	CHL	C1-C2-C3	-2.26	122.14	126.04
29	G1	610	CLA	C4B-CHC-C1C	2.26	131.70	126.34
29	S	617	CLA	C4B-CHC-C1C	2.26	131.69	126.34
49	r1	620	LUT	C35-C15-C14	-2.26	118.85	123.47
29	c	503	CLA	C4B-CHC-C1C	2.26	131.69	126.34
29	s1	609	CLA	C4B-CHC-C1C	2.26	131.69	126.34
29	y1	610	CLA	C6-C5-C3	-2.26	107.53	113.45
29	A1	406	CLA	C2A-C1A-CHA	2.26	127.81	123.86
29	c1	510	CLA	O2A-CGA-CBA	2.26	118.99	111.91
48	Y	609	CHL	CHD-C1D-C2D	2.26	130.22	125.48
29	S	602	CLA	CHA-C1A-NA	-2.26	121.23	126.40
49	S1	620	LUT	C1-C6-C5	-2.26	119.43	122.61
48	G1	608	CHL	CHA-C1A-NA	-2.26	121.23	126.40
29	r1	608	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
29	c1	511	CLA	CHA-C1A-NA	-2.26	121.23	126.40
32	B1	626	SQD	O3-C3-C2	-2.26	105.13	110.35
29	C	511	CLA	C4B-CHC-C1C	2.26	131.69	126.34
29	C	505	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
48	R	607	CHL	C2B-C1B-NB	-2.26	108.72	110.23
29	C	507	CLA	C2D-C1D-ND	2.26	111.77	110.10
29	y	613	CLA	C4B-CHC-C1C	2.26	131.69	126.34
29	G1	602	CLA	C4B-CHC-C1C	2.26	131.69	126.34
29	S1	613	CLA	C1D-ND-C4D	-2.26	104.73	106.33
29	n1	614	CLA	C3B-C4B-NB	-2.26	108.42	110.52
29	R1	608	CLA	CHA-C1A-NA	-2.25	121.23	126.40
29	b1	604	CLA	C3D-C2D-C1D	-2.25	102.75	105.83
29	S	611	CLA	O2A-CGA-CBA	2.25	118.98	111.91
29	R	610	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
29	b	608	CLA	C1C-C2C-C3C	-2.25	104.59	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S1	613	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
29	G	614	CLA	CHA-C1A-NA	-2.25	121.24	126.40
29	b1	608	CLA	C4B-CHC-C1C	2.25	131.68	126.34
48	N1	609	CHL	C1D-CHD-C4C	-2.25	121.20	126.06
29	S	609	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
29	N1	610	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
29	C1	505	CLA	C3B-C4B-NB	-2.25	108.42	110.52
29	b	608	CLA	CMA-C3A-C4A	2.25	117.83	111.77
49	Y	621	LUT	C11-C10-C9	-2.25	124.09	127.31
29	A	406	CLA	C6-C5-C3	-2.25	107.55	113.45
29	B	612	CLA	CHA-C4D-ND	2.25	137.21	132.50
29	s1	603	CLA	C3B-C4B-NB	-2.25	108.43	110.52
48	y	607	CHL	C3B-C4B-NB	-2.25	108.43	110.52
29	S1	617	CLA	CHA-C4D-ND	2.25	137.21	132.50
50	y1	622	XAT	C39-C29-C30	-2.25	119.77	122.92
48	n	601	CHL	C4B-CHC-C1C	2.25	131.68	126.34
29	Y	604	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
48	G	609	CHL	C2B-C1B-NB	-2.25	108.72	110.23
29	b	602	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
29	s1	610	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
29	a	405	CLA	CHA-C4D-ND	2.25	137.21	132.50
49	G1	620	LUT	C15-C35-C34	-2.25	118.86	123.47
29	s	614	CLA	C6-C5-C3	-2.25	107.55	113.45
29	G1	602	CLA	C16-C15-C13	-2.25	108.64	115.92
29	A1	410	CLA	CHA-C4D-ND	2.25	137.21	132.50
29	A1	405	CLA	C6-C7-C8	-2.25	108.65	115.92
49	S1	621	LUT	C11-C10-C9	-2.25	124.10	127.31
29	s	610	CLA	C2D-C1D-ND	2.25	111.76	110.10
29	Y1	603	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
29	C1	512	CLA	CMB-C2B-C3B	2.25	132.04	126.59
53	r1	626	ERG	C1-C2-C3	2.25	113.35	110.47
29	B	611	CLA	CHA-C1A-NA	-2.25	121.25	126.40
29	g	604	CLA	CHA-C1A-NA	-2.25	121.25	126.40
48	N	608	CHL	C3B-C4B-NB	-2.25	108.43	110.52
43	d1	405	PL9	O2-C1-C2	-2.25	116.63	121.78
49	Y	620	LUT	C38-C25-C24	-2.25	118.75	123.56
29	S1	605	CLA	C2A-C1A-CHA	2.25	127.79	123.86
31	c1	514	BCR	C23-C24-C25	-2.25	120.89	127.20
51	y	623	NEX	O24-C25-C38	-2.25	112.36	115.06
49	G1	621	LUT	C31-C32-C33	-2.25	120.10	126.42
49	n	621	LUT	C2-C3-C4	-2.25	107.23	110.30
48	G1	601	CHL	CMA-C3A-C4A	2.25	117.82	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	R	622	NEX	O24-C25-C24	-2.25	111.69	113.38
49	g1	621	LUT	C11-C12-C13	-2.25	120.10	126.42
29	C	508	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
29	S1	614	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
29	B1	609	CLA	CHD-C1D-ND	-2.25	122.39	124.45
29	n1	611	CLA	C1D-ND-C4D	-2.25	104.74	106.33
50	g	622	XAT	C40-C33-C32	2.25	121.62	118.08
29	b1	602	CLA	O2A-CGA-CBA	2.25	118.96	111.91
30	a	408	PHO	C1C-C2C-C3C	-2.25	106.74	108.61
48	G1	607	CHL	CHB-C4A-NA	2.25	127.62	124.51
53	R1	626	ERG	C19-C10-C1	-2.25	105.88	109.43
29	B	603	CLA	CHA-C1A-NA	-2.25	121.25	126.40
29	b	610	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
29	n1	602	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
29	n	611	CLA	O2A-CGA-CBA	2.25	118.96	111.91
29	s	604	CLA	C2D-C1D-ND	2.25	111.76	110.10
33	H	102	LMG	O8-C28-C29	2.25	118.96	111.91
29	c	506	CLA	C1-C2-C3	-2.25	122.16	126.04
29	b1	614	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
29	r	604	CLA	O2A-CGA-CBA	2.25	118.96	111.91
29	d1	402	CLA	CAC-C3C-C4C	2.25	127.72	124.81
49	N1	621	LUT	C18-C5-C4	2.25	118.52	114.36
29	r	602	CLA	C3B-C4B-NB	-2.25	108.43	110.52
48	n1	601	CHL	CHC-C4B-NB	-2.25	121.88	124.26
29	y1	614	CLA	CMA-C3A-C4A	2.25	117.81	111.77
50	n	622	XAT	O24-C25-C38	-2.25	112.36	115.06
33	c1	521	LMG	C8-O7-C10	-2.25	112.26	117.79
29	B	602	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
29	B1	612	CLA	C1D-ND-C4D	-2.25	104.74	106.33
29	c1	501	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
48	y1	606	CHL	C2B-C1B-NB	-2.24	108.73	110.23
29	c	505	CLA	CHD-C1D-ND	-2.24	122.39	124.45
29	g1	611	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
48	y	609	CHL	CHB-C4A-NA	2.24	127.62	124.51
40	s1	624	LHG	C5-O7-C7	-2.24	112.27	117.79
32	A1	412	SQD	O3-C3-C2	-2.24	105.16	110.35
31	c	517	BCR	C4-C5-C6	-2.24	119.47	122.73
29	C1	501	CLA	C1D-ND-C4D	-2.24	104.74	106.33
29	B1	607	CLA	CGD-CBD-CAD	-2.24	103.47	110.73
29	A1	405	CLA	CHA-C1A-NA	-2.24	121.26	126.40
29	G	614	CLA	C2D-C1D-ND	2.24	111.76	110.10
31	c1	517	BCR	C29-C30-C25	2.24	113.93	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B1	608	CLA	C2A-C1A-CHA	2.24	127.78	123.86
29	N1	611	CLA	CMA-C3A-C4A	2.24	117.80	111.77
37	c1	518	DGD	C6E-C5E-C4E	-2.24	107.75	113.00
29	c1	513	CLA	CHD-C1D-ND	-2.24	122.39	124.45
33	A1	413	LMG	O8-C28-C29	2.24	118.94	111.91
29	g1	610	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
29	C1	511	CLA	CMB-C2B-C1B	2.24	128.78	125.37
29	S1	609	CLA	CHA-C1A-NA	-2.24	121.26	126.40
29	N1	603	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
29	a	405	CLA	C3B-C4B-NB	-2.24	108.44	110.52
29	G1	604	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
29	A	406	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
29	C	506	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
29	b1	607	CLA	C4B-CHC-C1C	2.24	131.65	126.34
37	b	623	DGD	O2G-C1B-O1B	-2.24	118.29	123.70
29	b1	604	CLA	O2A-CGA-CBA	2.24	118.94	111.91
48	g1	607	CHL	CHD-C1D-ND	-2.24	122.39	124.45
50	R1	621	XAT	C18-C5-C6	-2.24	118.51	122.26
29	s1	613	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
29	g	613	CLA	CHA-C4D-ND	2.24	137.19	132.50
29	n1	611	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
29	S	610	CLA	CHA-C1A-NA	-2.24	121.27	126.40
48	n1	608	CHL	C1-O2A-CGA	2.24	122.32	116.44
40	S1	624	LHG	O7-C7-O9	-2.24	118.29	123.70
29	B1	606	CLA	CAC-C3C-C4C	2.24	127.72	124.81
29	R1	612	CLA	CHA-C1A-NA	-2.24	121.27	126.40
29	c1	506	CLA	C1-O2A-CGA	2.24	122.32	116.44
29	R1	602	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
29	Y	610	CLA	CMC-C2C-C1C	-2.24	121.63	125.04
29	s	613	CLA	CHA-C4D-ND	2.24	137.18	132.50
29	A	405	CLA	C1-O2A-CGA	2.24	122.32	116.44
29	Y	614	CLA	C4B-CHC-C1C	2.24	131.65	126.34
29	A1	410	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
29	d1	402	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
48	N	606	CHL	CHB-C4A-NA	2.24	127.61	124.51
29	C1	513	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
29	R	612	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
29	y	602	CLA	C3B-C4B-NB	-2.24	108.44	110.52
29	b	612	CLA	CHA-C4D-ND	2.24	137.18	132.50
37	C1	518	DGD	C6E-C5E-C4E	-2.24	107.76	113.00
48	Y1	606	CHL	CHD-C4C-C3C	2.24	128.13	124.84
48	Y	605	CHL	C2B-C1B-NB	-2.24	108.73	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	g1	608	CHL	C2B-C1B-NB	-2.24	108.73	110.23
29	s	612	CLA	C4B-CHC-C1C	2.24	131.65	126.34
32	B	626	SQD	O3-C3-C2	-2.24	105.18	110.35
29	C	513	CLA	C1D-ND-C4D	-2.24	104.75	106.33
29	n	604	CLA	C1D-ND-C4D	-2.24	104.75	106.33
29	g1	611	CLA	C1D-ND-C4D	-2.24	104.75	106.33
50	R	621	XAT	C20-C13-C12	2.24	121.60	118.08
29	y1	602	CLA	C11-C12-C13	-2.24	108.69	115.92
29	G	614	CLA	C1C-C2C-C3C	-2.24	104.61	106.96
29	y1	608	CLA	C2D-C1D-ND	2.24	111.75	110.10
29	C1	509	CLA	C4B-CHC-C1C	2.24	131.64	126.34
48	Y1	607	CHL	CHD-C1D-ND	-2.24	122.40	124.45
49	R	620	LUT	C1-C6-C7	2.24	122.10	115.78
30	a	409	PHO	O2A-CGA-O1A	-2.24	117.95	123.59
29	S1	603	CLA	O2A-CGA-CBA	2.24	118.92	111.91
29	D	402	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
29	C1	502	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
48	r	606	CHL	C3C-C4C-NC	-2.24	108.06	110.57
29	s	611	CLA	C4B-CHC-C1C	2.23	131.64	126.34
29	S	617	CLA	C3B-C4B-NB	-2.23	108.44	110.52
44	f	101	HEM	C1B-NB-C4B	2.23	107.38	105.07
29	c	505	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
29	c1	501	CLA	CHA-C1A-NA	-2.23	121.28	126.40
29	B1	612	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
29	b1	602	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
29	C1	508	CLA	CHA-C4D-ND	2.23	137.17	132.50
29	R1	603	CLA	O2A-CGA-CBA	2.23	118.92	111.91
30	A1	408	PHO	O1D-CGD-CBD	2.23	128.46	124.74
29	Y	614	CLA	C11-C12-C13	-2.23	108.70	115.92
29	d1	402	CLA	CHA-C1A-NA	-2.23	121.28	126.40
30	a	409	PHO	CMA-C3A-C4A	-2.23	109.49	114.38
29	y	611	CLA	CHA-C1A-NA	-2.23	121.28	126.40
29	r1	602	CLA	CMC-C2C-C1C	2.23	128.44	125.04
29	g	611	CLA	C1D-ND-C4D	-2.23	104.75	106.33
29	y1	613	CLA	C4B-CHC-C1C	2.23	131.63	126.34
37	B	623	DGD	O5D-C6D-C5D	2.23	113.18	109.05
29	C	508	CLA	C3B-C4B-NB	-2.23	108.44	110.52
29	s1	611	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
29	c1	501	CLA	C2D-C1D-ND	2.23	111.75	110.10
29	S	609	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
29	S	613	CLA	C4B-CHC-C1C	2.23	131.63	126.34
51	s1	623	NEX	C27-C28-C29	-2.23	122.07	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S1	602	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
48	r	607	CHL	C2B-C1B-NB	-2.23	108.74	110.23
29	c1	505	CLA	CHA-C4D-ND	2.23	137.17	132.50
29	y1	613	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
29	n1	604	CLA	C4B-CHC-C1C	2.23	131.63	126.34
32	m1	101	SQD	O3-C3-C2	-2.23	105.19	110.35
29	s	602	CLA	C2C-C1C-NC	2.23	112.06	109.97
50	g	622	XAT	C20-C13-C12	2.23	121.59	118.08
29	n1	603	CLA	CHA-C1A-NA	-2.23	121.29	126.40
48	y1	606	CHL	C1-O2A-CGA	2.23	122.30	116.44
29	C1	510	CLA	C4B-CHC-C1C	2.23	131.63	126.34
49	s1	620	LUT	C37-C21-C26	2.23	112.92	109.55
29	R	610	CLA	CHC-C1C-NC	-2.23	120.82	124.20
49	S1	621	LUT	C1-C6-C7	2.23	122.09	115.78
48	y1	607	CHL	C2B-C1B-NB	-2.23	108.74	110.23
29	C	512	CLA	C4B-CHC-C1C	2.23	131.63	126.34
29	S1	617	CLA	C1D-ND-C4D	-2.23	104.75	106.33
29	b	616	CLA	CHA-C1A-NA	-2.23	121.29	126.40
49	r1	620	LUT	C19-C9-C10	-2.23	119.80	122.92
29	C1	503	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
29	c	512	CLA	C3B-C4B-NB	-2.23	108.45	110.52
29	y1	612	CLA	C3B-C4B-NB	-2.23	108.45	110.52
29	B	602	CLA	O2A-CGA-CBA	2.23	118.90	111.91
29	B	615	CLA	O2A-CGA-CBA	2.23	118.90	111.91
29	B1	611	CLA	CHA-C1A-NA	-2.23	121.29	126.40
29	C1	510	CLA	CHA-C1A-NA	-2.23	121.29	126.40
29	c	505	CLA	C4B-CHC-C1C	2.23	131.62	126.34
29	Y1	604	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
29	s1	604	CLA	CHA-C1A-NA	-2.23	121.29	126.40
48	G1	601	CHL	C1-O2A-CGA	2.23	122.29	116.44
48	g1	601	CHL	C1-O2A-CGA	2.23	122.29	116.44
48	Y	605	CHL	CHB-C4A-NA	2.23	127.59	124.51
50	N	622	XAT	C40-C33-C34	-2.23	119.80	122.92
29	G	612	CLA	CHA-C1A-NA	-2.23	121.30	126.40
29	B1	611	CLA	CMA-C3A-C4A	2.23	117.76	111.77
29	c	513	CLA	CHD-C1D-ND	-2.23	122.41	124.45
29	B1	604	CLA	C4B-CHC-C1C	2.23	131.62	126.34
29	B1	608	CLA	CHA-C1A-NA	-2.23	121.30	126.40
29	s1	602	CLA	CHA-C1A-NA	-2.23	121.30	126.40
29	N	610	CLA	O2A-CGA-CBA	2.23	118.90	111.91
29	R1	609	CLA	C4B-CHC-C1C	2.23	131.62	126.34
29	r	602	CLA	C4B-CHC-C1C	2.23	131.62	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S	604	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
50	g1	622	XAT	C35-C34-C33	2.23	130.49	127.31
29	b1	615	CLA	CHA-C1A-NA	-2.23	121.30	126.40
29	C1	506	CLA	C1-C2-C3	-2.23	122.19	126.04
29	y1	611	CLA	OBD-CAD-C3D	-2.23	123.16	128.52
31	c	515	BCR	C28-C29-C30	-2.23	106.64	114.60
48	n1	601	CHL	CHA-C1A-NA	-2.23	121.30	126.40
33	W1	201	LMG	C38-C37-C36	2.23	125.72	114.42
49	n	620	LUT	C20-C13-C12	2.23	121.58	118.08
29	C1	503	CLA	CAC-C3C-C4C	2.23	127.70	124.81
29	y	602	CLA	C1C-C2C-C3C	-2.23	104.62	106.96
29	R1	603	CLA	C1C-C2C-C3C	-2.23	104.62	106.96
29	a1	407	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
29	N1	603	CLA	C4B-CHC-C1C	2.22	131.62	126.34
29	s1	617	CLA	C4B-CHC-C1C	2.22	131.62	126.34
29	S1	603	CLA	CHA-C1A-NA	-2.22	121.30	126.40
49	y1	620	LUT	C15-C14-C13	-2.22	124.14	127.31
29	B1	605	CLA	C2A-C1A-CHA	2.22	127.75	123.86
29	B	612	CLA	C4B-CHC-C1C	2.22	131.61	126.34
29	Y	614	CLA	O2A-CGA-CBA	2.22	118.89	111.91
29	y1	602	CLA	CHA-C4D-ND	2.22	137.15	132.50
29	B1	615	CLA	C2A-C1A-CHA	2.22	127.75	123.86
31	b	619	BCR	C34-C9-C10	-2.22	119.81	122.92
29	g	602	CLA	O1D-CGD-CBD	-2.22	119.93	124.48
31	c1	517	BCR	C8-C7-C6	-2.22	120.96	127.20
29	A1	410	CLA	C4B-CHC-C1C	2.22	131.61	126.34
29	C1	512	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
29	N	610	CLA	C1D-ND-C4D	-2.22	104.76	106.33
29	c1	509	CLA	CMA-C3A-C4A	2.22	117.75	111.77
30	a	409	PHO	C1C-C2C-C3C	-2.22	106.76	108.61
31	b	619	BCR	C39-C30-C25	-2.22	106.69	110.30
49	N	621	LUT	C10-C11-C12	-2.22	116.28	123.22
29	C	505	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
29	d	402	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
29	C1	502	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
49	R1	620	LUT	C8-C7-C6	-2.22	120.96	127.20
48	n	606	CHL	CHD-C4C-C3C	2.22	128.11	124.84
29	S1	605	CLA	C4B-CHC-C1C	2.22	131.61	126.34
31	c	515	BCR	C34-C9-C8	2.22	121.58	118.08
29	y	608	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
29	C	501	CLA	C1D-ND-C4D	-2.22	104.76	106.33
29	B1	616	CLA	C1D-ND-C4D	-2.22	104.76	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	n	621	LUT	C1-C6-C5	-2.22	119.48	122.61
29	N1	610	CLA	C4B-CHC-C1C	2.22	131.61	126.34
48	N1	607	CHL	C4D-CHA-C1A	2.22	123.95	121.25
29	G	604	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
29	Y	612	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
29	s	617	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
29	D1	402	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
29	g	610	CLA	C4B-CHC-C1C	2.22	131.60	126.34
48	n	605	CHL	CHC-C4B-NB	-2.22	121.91	124.26
48	g	607	CHL	C4D-CHA-C1A	2.22	123.95	121.25
29	B1	609	CLA	C2A-C1A-CHA	2.22	127.74	123.86
40	s1	624	LHG	O8-C23-O10	-2.22	117.99	123.59
29	s	603	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
29	G1	613	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
29	a	410	CLA	CMC-C2C-C1C	2.22	128.42	125.04
48	y1	607	CHL	CHD-C4C-C3C	2.22	128.10	124.84
29	b1	603	CLA	C1D-ND-C4D	-2.22	104.76	106.33
50	r1	621	XAT	C35-C34-C33	-2.22	124.14	127.31
29	B1	603	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
48	y	601	CHL	C1-O2A-CGA	2.22	122.26	116.44
49	N1	620	LUT	C10-C11-C12	-2.22	116.30	123.22
29	y1	612	CLA	C4B-CHC-C1C	2.22	131.60	126.34
29	b1	605	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
29	S	613	CLA	C2D-C1D-ND	2.22	111.74	110.10
48	n1	605	CHL	CHD-C4C-C3C	2.22	128.10	124.84
29	g	603	CLA	OBD-CAD-C3D	-2.22	123.19	128.52
43	D	405	PL9	C40-C39-C41	2.22	119.00	115.27
51	n	623	NEX	C19-C9-C10	-2.22	119.82	122.92
49	n	620	LUT	C38-C25-C24	-2.22	118.82	123.56
29	s	603	CLA	C4B-CHC-C1C	2.22	131.59	126.34
29	A	410	CLA	CMA-C3A-C4A	2.22	117.73	111.77
48	g	607	CHL	C3B-C4B-NB	-2.22	108.46	110.52
48	y1	607	CHL	CHB-C1B-NB	-2.22	121.91	124.26
48	R1	607	CHL	CHA-C1A-NA	-2.22	121.32	126.40
29	N	603	CLA	C4B-CHC-C1C	2.22	131.59	126.34
29	C1	505	CLA	C4B-CHC-C1C	2.22	131.59	126.34
29	B	611	CLA	C3D-C2D-C1D	-2.22	102.81	105.83
31	d1	404	BCR	C30-C25-C24	2.22	122.05	115.78
29	A1	410	CLA	CAC-C3C-C4C	2.22	127.69	124.81
37	B	623	DGD	O6D-C5D-C6D	2.22	111.14	106.67
29	b1	610	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
48	Y1	607	CHL	C3A-C2A-C1A	2.22	104.66	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	G	622	XAT	C20-C13-C14	-2.22	119.82	122.92
29	N	614	CLA	CHA-C1A-NA	-2.22	121.33	126.40
44	f	101	HEM	CMB-C2B-C1B	-2.21	121.67	125.04
29	y1	603	CLA	O2A-CGA-CBA	2.21	118.86	111.91
29	Y	613	CLA	C4B-CHC-C1C	2.21	131.59	126.34
48	y1	605	CHL	CHD-C4C-C3C	2.21	128.09	124.84
50	r	621	XAT	C40-C33-C34	-2.21	119.82	122.92
29	G1	611	CLA	C4B-CHC-C1C	2.21	131.59	126.34
29	b1	613	CLA	C4B-CHC-C1C	2.21	131.59	126.34
48	n1	608	CHL	CHB-C4A-NA	2.21	127.57	124.51
29	R	612	CLA	C1D-ND-C4D	-2.21	104.76	106.33
29	g1	614	CLA	C1D-ND-C4D	-2.21	104.76	106.33
50	r	621	XAT	C11-C10-C9	2.21	130.47	127.31
29	C1	512	CLA	O2A-CGA-CBA	2.21	118.86	111.91
29	G	611	CLA	C4B-CHC-C1C	2.21	131.59	126.34
29	n	611	CLA	CHA-C1A-NA	-2.21	121.33	126.40
29	r	610	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
48	N1	606	CHL	C1-O2A-CGA	2.21	122.25	116.44
51	y1	623	NEX	C16-C1-C6	-2.21	108.49	110.47
31	C1	517	BCR	C28-C27-C26	-2.21	110.12	114.08
29	c	512	CLA	C2A-C1A-CHA	2.21	127.73	123.86
48	Y1	607	CHL	C3B-C4B-NB	-2.21	108.46	110.52
29	C	513	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
49	Y	621	LUT	C18-C5-C4	2.21	118.45	114.36
48	N	607	CHL	CHD-C4C-C3C	2.21	128.09	124.84
29	S	603	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
29	c1	508	CLA	O2A-CGA-CBA	2.21	118.85	111.91
29	N1	603	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
48	g1	609	CHL	C2B-C1B-NB	-2.21	108.75	110.23
29	N1	614	CLA	C2A-C1A-CHA	2.21	127.73	123.86
29	R1	604	CLA	CHA-C1A-NA	-2.21	121.33	126.40
29	s	612	CLA	CMA-C3A-C4A	2.21	117.72	111.77
29	Y1	603	CLA	CMA-C3A-C4A	2.21	117.72	111.77
29	a	405	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
29	g	612	CLA	CHA-C1A-NA	-2.21	121.33	126.40
29	n1	611	CLA	CHA-C1A-NA	-2.21	121.33	126.40
29	r1	609	CLA	C4B-CHC-C1C	2.21	131.58	126.34
29	a	410	CLA	C3B-C4B-NB	-2.21	108.46	110.52
29	r	609	CLA	C3B-C4B-NB	-2.21	108.46	110.52
49	G	620	LUT	C20-C13-C12	2.21	121.56	118.08
29	C	508	CLA	C2D-C1D-ND	2.21	111.73	110.10
29	C	505	CLA	CMA-C3A-C4A	2.21	117.71	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n1	612	CLA	CMA-C3A-C4A	2.21	117.71	111.77
48	s	607	CHL	CHA-C1A-NA	-2.21	121.34	126.40
29	R1	604	CLA	C4B-CHC-C1C	2.21	131.58	126.34
32	b1	621	SQD	O3-C3-C2	-2.21	105.24	110.35
49	s	621	LUT	C2-C3-C4	-2.21	107.28	110.30
29	A1	410	CLA	O2A-CGA-CBA	2.21	118.84	111.91
29	S	609	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
29	r1	604	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
51	S	623	NEX	C38-C25-C26	-2.21	118.56	122.26
29	C	509	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
29	S	609	CLA	C4B-CHC-C1C	2.21	131.58	126.34
29	C	501	CLA	C1-O2A-CGA	2.21	122.24	116.44
50	y	622	XAT	C11-C10-C9	-2.21	124.16	127.31
31	A1	411	BCR	C34-C9-C10	-2.21	119.83	122.92
29	R	612	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
48	N	601	CHL	C1-O2A-CGA	2.21	122.24	116.44
40	D	409	LHG	O8-C23-O10	-2.21	118.02	123.59
29	N	602	CLA	CHA-C4D-ND	2.21	137.12	132.50
29	y1	614	CLA	C4B-CHC-C1C	2.21	131.57	126.34
29	C1	506	CLA	C4B-CHC-C1C	2.21	131.57	126.34
29	G1	612	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
29	y1	612	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
31	C1	517	BCR	C8-C7-C6	-2.21	121.00	127.20
29	y	613	CLA	CHD-C1D-ND	-2.21	122.43	124.45
29	C	508	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
48	g1	606	CHL	C1-O2A-CGA	2.21	122.23	116.44
29	C1	513	CLA	CHA-C1A-NA	-2.21	121.34	126.40
29	n	610	CLA	C2C-C1C-NC	2.21	112.04	109.97
29	s1	613	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
29	Y	611	CLA	CHA-C1A-NA	-2.21	121.35	126.40
29	d1	403	CLA	CHA-C1A-NA	-2.21	121.35	126.40
31	d1	404	BCR	C23-C22-C21	2.21	122.33	118.94
29	y	613	CLA	C1-O2A-CGA	2.21	122.23	116.44
31	B1	618	BCR	C35-C13-C12	2.21	121.55	118.08
29	N1	613	CLA	C4B-CHC-C1C	2.21	131.57	126.34
33	a	413	LMG	O8-C28-C29	2.20	118.83	111.91
29	G	611	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
29	c	510	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
53	R	626	ERG	C6-C7-C8	-2.20	117.73	122.07
48	g1	608	CHL	CHB-C4A-NA	2.20	127.56	124.51
29	r1	612	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
29	Y1	611	CLA	CHA-C1A-NA	-2.20	121.35	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	g	620	LUT	C37-C21-C26	2.20	112.88	109.55
29	d1	402	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
29	s1	610	CLA	C3D-C2D-C1D	-2.20	102.82	105.83
29	C	510	CLA	C4B-CHC-C1C	2.20	131.56	126.34
29	y1	608	CLA	C3B-C4B-NB	-2.20	108.47	110.52
29	C1	513	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
31	B	618	BCR	C34-C9-C10	-2.20	119.84	122.92
29	g1	603	CLA	C1D-ND-C4D	-2.20	104.77	106.33
29	C1	501	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
29	N1	603	CLA	CHA-C1A-NA	-2.20	121.35	126.40
29	G1	604	CLA	C3B-C4B-NB	-2.20	108.47	110.52
48	g1	605	CHL	C4D-CHA-C1A	2.20	123.93	121.25
51	s	623	NEX	C26-C27-C28	-2.20	121.34	125.99
29	S	611	CLA	CHA-C1A-NA	-2.20	121.36	126.40
29	G1	614	CLA	C1-O2A-CGA	2.20	122.22	116.44
29	A1	406	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
30	a	408	PHO	O2D-CGD-O1D	-2.20	119.53	123.84
29	G1	613	CLA	C4B-CHC-C1C	2.20	131.56	126.34
48	n	607	CHL	C1-C2-C3	-2.20	122.24	126.04
29	y	603	CLA	CAC-C3C-C4C	2.20	127.67	124.81
29	c	509	CLA	CHA-C1A-NA	-2.20	121.36	126.40
29	A	407	CLA	O2A-CGA-CBA	2.20	118.81	111.91
50	g1	622	XAT	C18-C5-C6	-2.20	118.57	122.26
29	r1	604	CLA	CHA-C1A-NA	-2.20	121.36	126.40
29	R	609	CLA	O2A-CGA-CBA	2.20	118.81	111.91
29	Y1	610	CLA	CHA-C1A-NA	-2.20	121.36	126.40
48	n	609	CHL	C2B-C1B-NB	-2.20	108.76	110.23
29	c	510	CLA	C1D-ND-C4D	-2.20	104.77	106.33
29	s1	602	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
29	y1	612	CLA	CHA-C1A-NA	-2.20	121.36	126.40
48	Y	601	CHL	C4A-NA-C1A	2.20	107.69	106.71
29	a	407	CLA	C4B-CHC-C1C	2.20	131.56	126.34
48	G	606	CHL	CHC-C1C-NC	2.20	127.54	124.20
30	a1	409	PHO	O2A-CGA-O1A	-2.20	118.04	123.59
31	c1	514	BCR	C37-C22-C21	-2.20	119.84	122.92
29	Y	612	CLA	CHA-C1A-NA	-2.20	121.36	126.40
48	r1	606	CHL	CHA-C1A-NA	-2.20	121.36	126.40
48	N	607	CHL	C3B-C4B-NB	-2.20	108.47	110.52
29	c	510	CLA	O2A-CGA-CBA	2.20	118.81	111.91
31	D1	404	BCR	C12-C13-C14	-2.20	115.57	118.94
29	N	611	CLA	C3B-C4B-NB	-2.20	108.48	110.52
29	g1	612	CLA	CMD-C2D-C3D	-2.20	122.56	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s1	610	CLA	C2A-C1A-CHA	2.20	127.70	123.86
48	R	607	CHL	C4A-NA-C1A	2.20	107.69	106.71
29	y1	610	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
29	S	609	CLA	C1C-C2C-C3C	-2.20	104.65	106.96
48	N	606	CHL	C1-O2A-CGA	2.20	122.21	116.44
48	G1	605	CHL	CHC-C4B-NB	-2.20	121.93	124.26
29	R	612	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
29	S1	604	CLA	C3B-C4B-NB	-2.20	108.48	110.52
29	A	407	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
51	g1	623	NEX	O24-C25-C38	-2.20	112.42	115.06
50	r	621	XAT	C19-C9-C8	2.20	121.54	118.08
29	C1	512	CLA	C6-C5-C3	-2.20	107.69	113.45
29	B	604	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
29	N1	604	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
29	Y	612	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
45	h1	101	RRX	C33-C5-C4	2.20	117.83	113.62
29	C	505	CLA	C1-O2A-CGA	2.20	122.21	116.44
29	N	604	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
29	b	605	CLA	C2A-C1A-CHA	2.20	127.70	123.86
29	y1	603	CLA	CMA-C3A-C4A	2.20	117.67	111.77
29	N1	612	CLA	CHA-C1A-NA	-2.20	121.37	126.40
29	b1	617	CLA	CHA-C1A-NA	-2.20	121.37	126.40
29	B1	617	CLA	C3B-C4B-NB	-2.20	108.48	110.52
30	a1	409	PHO	CMB-C2B-C3B	2.20	128.79	124.68
29	b	605	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
29	n	602	CLA	CHC-C1C-NC	-2.19	120.87	124.20
29	B1	606	CLA	OBD-CAD-C3D	-2.19	123.24	128.52
29	Y	603	CLA	O2A-CGA-CBA	2.19	118.80	111.91
29	c	511	CLA	C3B-C4B-NB	-2.19	108.48	110.52
29	b1	608	CLA	C3B-C4B-NB	-2.19	108.48	110.52
31	c	517	BCR	C33-C5-C4	2.19	117.83	113.62
29	c	508	CLA	CAA-C2A-C3A	-2.19	106.77	112.78
29	C1	507	CLA	C4B-CHC-C1C	2.19	131.54	126.34
29	N	611	CLA	O2A-CGA-CBA	2.19	118.79	111.91
29	C1	504	CLA	CHA-C1A-NA	-2.19	121.37	126.40
29	c1	509	CLA	CHA-C1A-NA	-2.19	121.37	126.40
29	b1	611	CLA	C3B-C4B-NB	-2.19	108.48	110.52
29	S	613	CLA	CHA-C1A-NA	-2.19	121.38	126.40
29	c	508	CLA	C4B-CHC-C1C	2.19	131.54	126.34
29	y	612	CLA	C4B-CHC-C1C	2.19	131.54	126.34
29	B1	603	CLA	C4B-CHC-C1C	2.19	131.54	126.34
29	c1	503	CLA	CHA-C1A-NA	-2.19	121.38	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y	610	CLA	CHA-C4D-ND	2.19	137.09	132.50
29	d1	403	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
29	y	614	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
40	D1	410	LHG	C5-O7-C7	-2.19	112.39	117.79
29	C	510	CLA	CHA-C1A-NA	-2.19	121.38	126.40
48	S	608	CHL	C4D-CHA-C1A	2.19	123.92	121.25
29	r	604	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
48	s	608	CHL	CHC-C4B-NB	-2.19	121.94	124.26
29	R	610	CLA	C2C-C1C-NC	2.19	112.02	109.97
45	h	101	RRX	C30-C29-C28	-2.19	108.70	113.64
36	B	620	C7Z	C39-C29-C28	2.19	121.53	118.08
51	r1	622	NEX	C5-C4-C3	-2.19	109.15	111.75
29	G	603	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
29	R	604	CLA	CHA-C1A-NA	-2.19	121.38	126.40
29	b1	612	CLA	CHA-C1A-NA	-2.19	121.38	126.40
29	g	602	CLA	C6-C7-C8	-2.19	108.84	115.92
29	c1	507	CLA	C4B-CHC-C1C	2.19	131.53	126.34
48	y1	605	CHL	C2B-C1B-NB	-2.19	108.76	110.23
48	Y	601	CHL	C1-O2A-CGA	2.19	122.19	116.44
29	C	507	CLA	O2A-CGA-CBA	2.19	118.78	111.91
29	b1	602	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
48	s1	607	CHL	C4B-CHC-C1C	2.19	131.53	126.34
29	r	604	CLA	C3B-C4B-NB	-2.19	108.48	110.52
29	B1	609	CLA	C3B-C4B-NB	-2.19	108.48	110.52
29	y	602	CLA	C2D-C1D-ND	2.19	111.72	110.10
29	y	611	CLA	C4B-CHC-C1C	2.19	131.53	126.34
29	y	612	CLA	C1-C2-C3	-2.19	122.26	126.04
48	N	606	CHL	C1-C2-C3	-2.19	122.26	126.04
50	R1	621	XAT	C15-C35-C34	2.19	127.96	123.47
49	g	620	LUT	C8-C7-C6	-2.19	121.06	127.20
29	y1	613	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
29	G1	602	CLA	CHD-C1D-ND	-2.19	122.44	124.45
29	s1	611	CLA	CHD-C1D-ND	-2.19	122.44	124.45
29	G	610	CLA	CHA-C1A-NA	-2.19	121.39	126.40
29	b	611	CLA	CHA-C1A-NA	-2.19	121.39	126.40
29	r1	602	CLA	CHA-C1A-NA	-2.19	121.39	126.40
31	C1	515	BCR	C1-C6-C7	2.19	121.97	115.78
53	r1	626	ERG	C16-C17-C13	2.19	106.48	103.84
29	Y1	611	CLA	C1D-ND-C4D	-2.19	104.78	106.33
29	s	603	CLA	OBD-CAD-C3D	-2.19	123.26	128.52
29	s	610	CLA	CMA-C3A-C4A	2.19	117.65	111.77
29	C1	506	CLA	CAA-C2A-C3A	-2.19	106.79	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	403	CLA	C3B-C4B-NB	-2.19	108.49	110.52
29	Y1	614	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
49	Y	620	LUT	C15-C35-C34	-2.19	119.00	123.47
48	s	607	CHL	C4B-CHC-C1C	2.19	131.52	126.34
50	G1	622	XAT	C26-C27-C28	-2.19	121.37	125.99
29	g	613	CLA	C1D-ND-C4D	-2.19	104.78	106.33
29	C1	510	CLA	C3B-C4B-NB	-2.19	108.49	110.52
29	g	604	CLA	C1C-C2C-C3C	-2.19	104.66	106.96
29	N1	610	CLA	C1C-C2C-C3C	-2.19	104.66	106.96
48	G1	605	CHL	CMA-C3A-C2A	2.19	122.65	113.83
48	S	606	CHL	CHD-C4C-C3C	2.19	128.05	124.84
29	n	611	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
29	B1	611	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
29	C	506	CLA	CHA-C1A-NA	-2.19	121.39	126.40
29	b	609	CLA	CMB-C2B-C3B	2.19	131.88	126.59
29	Y1	612	CLA	C2A-C1A-CHA	2.19	127.68	123.86
29	C1	502	CLA	C2D-C1D-ND	2.18	111.71	110.10
29	S	610	CLA	C2A-C1A-CHA	2.18	127.68	123.86
49	n	620	LUT	C15-C35-C34	-2.18	119.00	123.47
29	C	509	CLA	C4B-CHC-C1C	2.18	131.52	126.34
29	S1	609	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
31	c1	515	BCR	C23-C24-C25	-2.18	121.07	127.20
29	C	513	CLA	CHA-C1A-NA	-2.18	121.40	126.40
51	s1	623	NEX	C38-C25-C26	-2.18	118.60	122.26
29	s	602	CLA	C1D-ND-C4D	-2.18	104.78	106.33
29	r1	604	CLA	C1D-ND-C4D	-2.18	104.78	106.33
29	r1	609	CLA	C1D-ND-C4D	-2.18	104.78	106.33
49	R	620	LUT	C39-C29-C28	2.18	121.52	118.08
36	B	620	C7Z	C4-C5-C6	-2.18	115.98	120.85
29	g1	603	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
40	d	410	LHG	C5-O7-C7	-2.18	112.42	117.79
29	a1	406	CLA	CHA-C1A-NA	-2.18	121.40	126.40
29	r	612	CLA	C4B-CHC-C1C	2.18	131.51	126.34
29	A	407	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
49	n	620	LUT	C10-C11-C12	-2.18	116.41	123.22
49	N	620	LUT	C36-C21-C26	-2.18	106.24	109.55
29	a1	405	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
29	Y	614	CLA	C2D-C1D-ND	2.18	111.71	110.10
29	a1	407	CLA	CHA-C1A-NA	-2.18	121.40	126.40
29	Y	604	CLA	C1D-ND-C4D	-2.18	104.78	106.33
29	n1	603	CLA	C1D-ND-C4D	-2.18	104.78	106.33
29	S1	605	CLA	C3B-C4B-NB	-2.18	108.49	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	613	CLA	C4B-CHC-C1C	2.18	131.51	126.34
45	h1	101	RRX	C16-C17-C18	-2.18	124.20	127.31
29	n	604	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
50	r1	621	XAT	C8-C9-C10	2.18	122.29	118.94
29	c	508	CLA	CAC-C3C-C4C	2.18	127.64	124.81
29	Y	613	CLA	C3B-C4B-NB	-2.18	108.49	110.52
48	g	608	CHL	C3A-C2A-C1A	2.18	104.61	101.34
51	G1	623	NEX	C1-C2-C3	2.18	118.57	113.64
49	Y	621	LUT	C3-C4-C5	-2.18	107.51	111.85
51	s1	623	NEX	C20-C13-C14	-2.18	119.87	122.92
29	C	510	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
29	A	406	CLA	CMC-C2C-C3C	2.18	132.03	126.12
29	g1	602	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
29	R	602	CLA	C1-C2-C3	-2.18	122.27	126.04
29	a1	410	CLA	C1-O2A-CGA	2.18	122.16	116.44
29	y1	603	CLA	CHA-C1A-NA	-2.18	121.41	126.40
29	N1	610	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
29	b	605	CLA	CAC-C3C-C4C	2.18	127.64	124.81
32	c	526	SQD	O3-C3-C2	-2.18	105.31	110.35
29	B	607	CLA	C4B-CHC-C1C	2.18	131.50	126.34
29	D1	403	CLA	CHA-C1A-NA	-2.18	121.41	126.40
29	c	511	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
29	C1	509	CLA	C2D-C1D-ND	2.18	111.71	110.10
29	s	613	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
29	C1	512	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
29	c	510	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
29	c1	502	CLA	CHA-C1A-NA	-2.18	121.41	126.40
31	c1	517	BCR	C39-C30-C25	-2.18	106.77	110.30
29	c	505	CLA	O2A-CGA-CBA	2.18	118.74	111.91
29	a1	410	CLA	CAA-CBA-CGA	-2.18	106.89	113.25
29	S	614	CLA	C3B-C4B-NB	-2.18	108.50	110.52
29	Y	602	CLA	C16-C15-C13	-2.18	108.88	115.92
31	B1	618	BCR	C23-C22-C21	2.18	122.28	118.94
31	c1	514	BCR	C1-C6-C5	-2.18	119.55	122.61
31	c1	515	BCR	C29-C28-C27	2.18	116.24	111.38
48	S1	607	CHL	CHD-C4C-C3C	2.18	128.04	124.84
29	C1	505	CLA	CMB-C2B-C3B	2.18	131.86	126.59
37	b	623	DGD	O5D-C1E-C2E	2.18	111.70	108.30
29	G	612	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
48	G1	609	CHL	C3B-C4B-NB	-2.18	108.50	110.52
29	C1	505	CLA	CHD-C1D-ND	-2.18	122.45	124.45
29	y1	610	CLA	CHA-C1A-NA	-2.18	121.41	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	r	608	CLA	C1D-ND-C4D	-2.18	104.79	106.33
29	C1	507	CLA	CMA-C3A-C4A	2.18	117.62	111.77
50	R	621	XAT	C6-C7-C8	-2.18	121.39	125.99
49	n1	621	LUT	C2-C3-C4	-2.18	107.33	110.30
29	B	617	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
29	y1	614	CLA	C1-O2A-CGA	2.18	122.15	116.44
29	b1	604	CLA	CHA-C4D-ND	2.18	137.05	132.50
50	y1	622	XAT	C11-C10-C9	-2.17	124.21	127.31
33	d	411	LMG	O8-C28-O10	-2.17	118.10	123.59
29	s	610	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
50	n1	622	XAT	C6-C7-C8	-2.17	121.39	125.99
33	a1	413	LMG	C7-O1-C1	-2.17	109.49	113.74
29	c1	505	CLA	C4B-CHC-C1C	2.17	131.50	126.34
49	g	621	LUT	C10-C11-C12	-2.17	116.43	123.22
29	s1	614	CLA	C3D-C2D-C1D	-2.17	102.86	105.83
49	y1	621	LUT	C37-C21-C36	2.17	111.10	107.89
49	S	620	LUT	C17-C1-C6	2.17	113.83	110.30
29	B1	615	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
29	y	604	CLA	O2A-CGA-CBA	2.17	118.73	111.91
29	c1	512	CLA	C2A-C1A-CHA	2.17	127.66	123.86
29	b1	605	CLA	CMA-C3A-C4A	2.17	117.61	111.77
55	y	626	PTY	C12-C11-C8	-2.17	105.72	113.62
49	G	620	LUT	C1-C2-C3	2.17	118.55	113.64
48	n	606	CHL	C2B-C1B-NB	-2.17	108.78	110.23
29	n1	604	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
29	A1	405	CLA	C4B-CHC-C1C	2.17	131.49	126.34
29	A	407	CLA	C2D-C1D-ND	2.17	111.70	110.10
48	Y	606	CHL	C1-C2-C3	-2.17	122.29	126.04
36	B1	620	C7Z	C17-C1-C6	-2.17	106.78	110.30
48	s	608	CHL	C1-O2A-CGA	2.17	122.14	116.44
29	G1	603	CLA	O2A-CGA-CBA	2.17	118.72	111.91
29	R1	604	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
29	B	605	CLA	CHA-C1A-NA	-2.17	121.43	126.40
29	B1	602	CLA	CHA-C1A-NA	-2.17	121.43	126.40
29	N1	612	CLA	C4B-CHC-C1C	2.17	131.48	126.34
29	S	612	CLA	C1D-ND-C4D	-2.17	104.79	106.33
29	c1	505	CLA	C1D-ND-C4D	-2.17	104.79	106.33
29	s	609	CLA	CHA-C1A-NA	-2.17	121.43	126.40
29	r	612	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
44	f1	101	HEM	C4D-ND-C1D	2.17	107.31	105.07
48	N1	606	CHL	CHA-C1A-NA	-2.17	121.43	126.40
29	C1	511	CLA	C3D-C2D-C1D	-2.17	102.87	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	G1	613	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
29	c	513	CLA	C3B-C4B-NB	-2.17	108.50	110.52
48	n1	606	CHL	C1-C2-C3	-2.17	122.29	126.04
29	A	405	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
29	R	609	CLA	C1-O2A-CGA	2.17	122.13	116.44
29	B1	604	CLA	C1-O2A-CGA	2.17	122.13	116.44
29	Y1	608	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
29	C	511	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
48	g	608	CHL	C2B-C1B-NB	-2.17	108.78	110.23
48	s1	607	CHL	C2B-C1B-NB	-2.17	108.78	110.23
51	N1	623	NEX	C26-C27-C28	-2.17	121.41	125.99
29	d	402	CLA	C1C-C2C-C3C	-2.17	104.68	106.96
29	C1	513	CLA	C11-C12-C13	-2.17	108.92	115.92
29	n	603	CLA	C1D-ND-C4D	-2.17	104.80	106.33
29	b1	608	CLA	C2A-C1A-CHA	2.17	127.65	123.86
29	S	604	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
29	y	614	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
29	S	610	CLA	C1C-C2C-C3C	-2.17	104.68	106.96
29	C	502	CLA	CHA-C1A-NA	-2.17	121.44	126.40
29	N1	604	CLA	CHA-C1A-NA	-2.17	121.44	126.40
29	c	510	CLA	C3B-C4B-NB	-2.17	108.51	110.52
29	b	612	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
31	c	517	BCR	C12-C13-C14	-2.16	115.62	118.94
29	a	406	CLA	CMA-C3A-C4A	2.16	117.59	111.77
29	a1	406	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
48	Y	601	CHL	CHC-C1C-NC	2.16	127.49	124.20
29	S	613	CLA	CMC-C2C-C3C	2.16	131.99	126.12
29	g1	611	CLA	CHA-C1A-NA	-2.16	121.44	126.40
48	Y1	605	CHL	C2B-C1B-NB	-2.16	108.78	110.23
29	b	606	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
29	a1	405	CLA	CMA-C3A-C4A	2.16	117.59	111.77
29	Y	610	CLA	OBD-CAD-C3D	-2.16	123.31	128.52
29	B1	607	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
29	Y	603	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
50	R	621	XAT	C24-C23-C22	-2.16	106.59	110.77
29	s	605	CLA	C3B-C4B-NB	-2.16	108.51	110.52
29	y1	613	CLA	C3B-C4B-NB	-2.16	108.51	110.52
29	Y1	610	CLA	C1C-C2C-C3C	-2.16	104.68	106.96
29	n1	602	CLA	CHA-C4D-ND	2.16	137.02	132.50
31	C	516	BCR	C37-C22-C23	2.16	121.48	118.08
48	g	605	CHL	C2B-C1B-NB	-2.16	108.78	110.23
29	n	614	CLA	O2A-CGA-CBA	2.16	118.69	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B1	612	CLA	CMA-C3A-C4A	2.16	117.59	111.77
29	C	512	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
29	n	614	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
49	Y1	620	LUT	C31-C32-C33	-2.16	120.34	126.42
29	S1	617	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
31	b1	619	BCR	C29-C28-C27	2.16	116.21	111.38
31	c1	517	BCR	C27-C26-C25	-2.16	119.59	122.73
29	c	503	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
29	b1	605	CLA	CMA-C3A-C2A	2.16	122.55	113.83
29	C	510	CLA	C2D-C1D-ND	2.16	111.70	110.10
29	R	604	CLA	OBD-CAD-C3D	-2.16	123.32	128.52
31	C	516	BCR	C38-C26-C27	2.16	117.77	113.62
48	g	609	CHL	C1C-C2C-C3C	-2.16	105.40	107.11
33	W	201	LMG	O8-C28-O10	-2.16	118.14	123.59
31	a	411	BCR	C23-C22-C21	-2.16	115.62	118.94
29	S1	614	CLA	O2A-CGA-CBA	2.16	118.69	111.91
29	Y	602	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
50	g1	622	XAT	C19-C9-C10	-2.16	119.90	122.92
48	g1	607	CHL	CHC-C1C-NC	2.16	127.48	124.20
36	B1	620	C7Z	C28-C27-C26	-2.16	121.13	127.20
29	y	608	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
29	b	611	CLA	C1D-ND-C4D	-2.16	104.80	106.33
52	r1	625	LMT	C1'-O5'-C5'	-2.16	109.45	113.69
29	C1	502	CLA	C3B-C4B-NB	-2.16	108.51	110.52
29	r1	608	CLA	C3B-C4B-NB	-2.16	108.51	110.52
51	n	623	NEX	O24-C25-C38	-2.16	112.47	115.06
29	n1	612	CLA	C2D-C1D-ND	2.16	111.69	110.10
29	B	616	CLA	C2A-C1A-CHA	2.16	127.63	123.86
29	n	611	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
29	Y	612	CLA	C4B-CHC-C1C	2.16	131.46	126.34
31	C1	516	BCR	C30-C25-C26	-2.16	119.57	122.61
29	G1	602	CLA	CMA-C3A-C4A	2.16	117.57	111.77
29	c1	503	CLA	C1D-ND-C4D	-2.16	104.80	106.33
29	G	613	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
43	d	405	PL9	C40-C39-C41	2.16	118.90	115.27
29	g1	614	CLA	O2A-CGA-CBA	2.16	118.68	111.91
29	N	612	CLA	C2D-C1D-ND	2.16	111.69	110.10
52	r1	625	LMT	O5B-C1B-C2B	2.16	114.92	110.35
29	r	602	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
29	b1	602	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
29	B1	603	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
29	b	610	CLA	C3B-C4B-NB	-2.16	108.51	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c1	501	CLA	C3B-C4B-NB	-2.16	108.51	110.52
29	G1	604	CLA	O2A-CGA-CBA	2.16	118.68	111.91
43	d	405	PL9	C37-C38-C39	-2.16	122.47	127.66
29	C	507	CLA	OBD-CAD-C3D	-2.16	123.33	128.52
53	r1	626	ERG	C24-C23-C22	-2.16	118.98	125.67
29	g	612	CLA	C1D-ND-C4D	-2.16	104.80	106.33
49	y1	621	LUT	C2-C3-C4	-2.16	107.35	110.30
29	s	604	CLA	CMA-C3A-C4A	2.16	117.57	111.77
29	a	410	CLA	C4B-CHC-C1C	2.16	131.45	126.34
31	c1	514	BCR	C31-C1-C6	-2.16	106.80	110.30
29	n1	614	CLA	CHA-C1A-NA	-2.16	121.46	126.40
29	c	509	CLA	C4B-CHC-C1C	2.16	131.45	126.34
29	Y	608	CLA	C1D-ND-C4D	-2.16	104.80	106.33
29	S	610	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
29	b	602	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
29	b1	617	CLA	C1-C2-C3	-2.15	122.32	126.04
29	C1	510	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
31	C1	517	BCR	C33-C5-C4	2.15	117.75	113.62
29	a	405	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
29	a1	405	CLA	CHA-C1A-NA	-2.15	121.47	126.40
29	G1	611	CLA	O2A-CGA-CBA	2.15	118.67	111.91
29	G	603	CLA	CMC-C2C-C1C	2.15	128.32	125.04
36	B1	620	C7Z	C19-C9-C10	-2.15	119.91	122.92
29	r1	603	CLA	C1D-ND-C4D	-2.15	104.81	106.33
29	b	617	CLA	CMA-C3A-C4A	2.15	117.56	111.77
29	b1	608	CLA	C1-C2-C3	-2.15	122.32	126.04
29	R	608	CLA	CMA-C3A-C4A	2.15	117.56	111.77
29	B1	613	CLA	CHA-C1A-NA	-2.15	121.47	126.40
49	s	621	LUT	C19-C9-C10	-2.15	119.91	122.92
29	N	602	CLA	C2C-C1C-NC	2.15	111.99	109.97
29	G1	611	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
49	N1	621	LUT	C15-C14-C13	-2.15	124.24	127.31
49	n1	620	LUT	C18-C5-C6	-2.15	122.11	124.53
51	N	623	NEX	C19-C9-C10	-2.15	119.91	122.92
29	G	603	CLA	CHA-C1A-NA	-2.15	121.47	126.40
33	C1	523	LMG	C9-C8-C7	-2.15	106.70	111.79
29	A1	410	CLA	CGD-CBD-CAD	-2.15	103.76	110.73
29	R1	612	CLA	CAC-C3C-C4C	2.15	127.60	124.81
29	n1	604	CLA	CHA-C1A-NA	-2.15	121.47	126.40
29	c	512	CLA	C1-O2A-CGA	2.15	122.09	116.44
29	R	603	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
29	c1	503	CLA	O1D-CGD-CBD	-2.15	120.08	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	R1	606	CHL	C4B-CHC-C1C	2.15	131.44	126.34
29	G	613	CLA	C1D-ND-C4D	-2.15	104.81	106.33
29	y1	614	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
29	c1	513	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
31	b1	618	BCR	C33-C5-C6	-2.15	122.11	124.53
48	N	606	CHL	C2C-C3C-C4C	2.15	108.02	106.49
29	G1	602	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
49	S	621	LUT	C30-C31-C32	-2.15	116.51	123.22
29	B	614	CLA	CHA-C1A-NA	-2.15	121.47	126.40
29	g1	602	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
29	C	507	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
29	S1	609	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
29	c	507	CLA	C4B-CHC-C1C	2.15	131.44	126.34
29	s	611	CLA	CHA-C1A-NA	-2.15	121.47	126.40
29	B	608	CLA	C1D-ND-C4D	-2.15	104.81	106.33
29	C	510	CLA	C3B-C4B-NB	-2.15	108.52	110.52
29	S1	610	CLA	C1-O2A-CGA	2.15	122.08	116.44
48	s	608	CHL	C2C-C3C-C4C	2.15	108.02	106.49
29	s1	603	CLA	O2A-CGA-CBA	2.15	118.65	111.91
49	N	621	LUT	C18-C5-C6	-2.15	122.11	124.53
29	C	509	CLA	CHA-C1A-NA	-2.15	121.48	126.40
29	n1	604	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
48	G	601	CHL	C4A-NA-C1A	2.15	107.67	106.71
29	B	603	CLA	C4B-CHC-C1C	2.15	131.43	126.34
49	S	621	LUT	C19-C9-C8	2.15	121.46	118.08
29	n	602	CLA	C3B-C4B-NB	-2.15	108.52	110.52
29	N1	603	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
29	A1	410	CLA	C1D-ND-C4D	-2.15	104.81	106.33
33	w	201	LMG	C4-C3-C2	2.15	114.57	110.82
49	g1	621	LUT	C39-C29-C30	-2.15	119.91	122.92
47	i1	101	4RF	O18-C16-C15	2.15	118.65	111.91
29	b	608	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
29	N1	602	CLA	CMC-C2C-C1C	2.15	128.31	125.04
29	b1	617	CLA	CMA-C3A-C4A	2.15	117.54	111.77
48	S1	608	CHL	CHD-C4C-C3C	2.15	128.00	124.84
29	s	612	CLA	CHA-C1A-NA	-2.15	121.48	126.40
48	s1	601	CHL	CHC-C1C-NC	2.15	127.46	124.20
29	N1	604	CLA	C2D-C1D-ND	2.15	111.69	110.10
36	B	620	C7Z	C1-C6-C7	2.15	121.85	115.78
29	b1	617	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
29	D	403	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
29	S	602	CLA	C4B-CHC-C1C	2.15	131.43	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	504	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
29	N	612	CLA	CMA-C3A-C4A	2.15	117.54	111.77
31	b	619	BCR	C37-C22-C23	2.15	121.46	118.08
29	B	605	CLA	CHD-C1D-ND	-2.15	122.48	124.45
29	s	612	CLA	CMB-C2B-C3B	2.15	131.78	126.59
29	r1	603	CLA	CHA-C1A-NA	-2.15	121.48	126.40
29	c1	513	CLA	CMA-C3A-C4A	2.15	117.54	111.77
44	f1	101	HEM	C1B-NB-C4B	2.15	107.29	105.07
31	D	404	BCR	C23-C24-C25	-2.15	121.18	127.20
30	A	409	PHO	C2D-C1D-ND	-2.14	108.05	109.53
29	b	611	CLA	CMA-C3A-C4A	2.14	117.54	111.77
49	N1	620	LUT	C35-C34-C33	-2.14	124.25	127.31
29	g	611	CLA	C1-O2A-CGA	2.14	122.07	116.44
29	G	612	CLA	O2D-CGD-O1D	-2.14	119.64	123.84
29	c	512	CLA	CMB-C2B-C3B	2.14	131.78	126.59
29	B	610	CLA	C3B-C4B-NB	-2.14	108.53	110.52
29	b	609	CLA	CMA-C3A-C4A	2.14	117.53	111.77
29	S1	617	CLA	CMD-C2D-C3D	-2.14	122.68	127.61
29	g1	610	CLA	CHA-C1A-NA	-2.14	121.49	126.40
48	s	601	CHL	CMA-C3A-C4A	2.14	117.53	111.77
49	S1	621	LUT	C31-C30-C29	-2.14	124.25	127.31
29	y	608	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
31	C	514	BCR	C8-C9-C10	2.14	122.23	118.94
29	R1	610	CLA	C1C-C2C-C3C	-2.14	104.70	106.96
29	s1	605	CLA	CMD-C2D-C3D	-2.14	122.68	127.61
29	n	603	CLA	CHA-C1A-NA	-2.14	121.49	126.40
31	B	619	BCR	C34-C9-C10	-2.14	119.92	122.92
29	N	610	CLA	C2A-C1A-CHA	2.14	127.61	123.86
29	S	602	CLA	C6-C7-C8	-2.14	108.99	115.92
48	g	609	CHL	CHB-C4A-NA	2.14	127.47	124.51
29	B	605	CLA	C4B-CHC-C1C	2.14	131.42	126.34
29	B	610	CLA	C1D-ND-C4D	-2.14	104.81	106.33
29	C	512	CLA	C1D-ND-C4D	-2.14	104.81	106.33
29	B	603	CLA	C1-O2A-CGA	2.14	122.06	116.44
48	R1	606	CHL	CHC-C1C-NC	2.14	127.45	124.20
29	n	614	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
29	b1	603	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
29	y1	611	CLA	C3B-C4B-NB	-2.14	108.53	110.52
29	c	513	CLA	CHA-C1A-NA	-2.14	121.49	126.40
29	s	613	CLA	C4B-CHC-C1C	2.14	131.42	126.34
29	G	612	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
51	g	623	NEX	C16-C1-C6	-2.14	108.56	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	R	620	LUT	C31-C30-C29	-2.14	124.25	127.31
48	n1	606	CHL	C1-O2A-CGA	2.14	122.06	116.44
29	S1	610	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
29	N1	614	CLA	C4B-CHC-C1C	2.14	131.41	126.34
29	b	602	CLA	C1D-ND-C4D	-2.14	104.81	106.33
50	N1	622	XAT	C19-C9-C10	-2.14	119.93	122.92
29	B	604	CLA	C4B-CHC-C1C	2.14	131.41	126.34
29	B1	605	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
29	N1	610	CLA	C2A-C1A-CHA	2.14	127.60	123.86
49	N1	620	LUT	C39-C29-C30	-2.14	119.93	122.92
29	B	615	CLA	CMC-C2C-C1C	2.14	128.30	125.04
29	A	410	CLA	C3B-C2B-C1B	-2.14	104.58	107.16
29	N	614	CLA	C3B-C4B-NB	-2.14	108.53	110.52
37	b	623	DGD	O5D-C6D-C5D	2.14	113.00	109.05
29	C1	509	CLA	CHA-C1A-NA	-2.14	121.50	126.40
29	C1	511	CLA	CHA-C1A-NA	-2.14	121.50	126.40
29	b	607	CLA	C4B-CHC-C1C	2.14	131.41	126.34
44	F1	101	HEM	C3D-C4D-ND	-2.14	107.79	110.17
29	c1	501	CLA	C2A-C1A-CHA	2.14	127.60	123.86
29	n1	603	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
29	b	611	CLA	O2A-CGA-CBA	2.14	118.62	111.91
29	N1	602	CLA	CHA-C1A-NA	-2.14	121.50	126.40
29	n1	613	CLA	CHA-C1A-NA	-2.14	121.50	126.40
29	r	610	CLA	C1D-ND-C4D	-2.14	104.82	106.33
29	R1	609	CLA	C1D-ND-C4D	-2.14	104.82	106.33
29	g	612	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
29	y	612	CLA	CHA-C1A-NA	-2.14	121.50	126.40
31	C1	517	BCR	C33-C5-C6	-2.14	122.13	124.53
48	r1	607	CHL	CHC-C1C-NC	2.14	127.44	124.20
29	s1	609	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
44	F	101	HEM	CMC-C2C-C1C	-2.14	120.95	124.71
29	C1	513	CLA	CBA-CAA-C2A	2.14	120.17	113.86
29	Y	613	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
49	s1	620	LUT	C18-C5-C4	2.14	118.31	114.36
33	W1	201	LMG	O8-C28-O10	-2.14	118.20	123.59
50	R1	621	XAT	C40-C33-C34	-2.14	119.93	122.92
30	a1	409	PHO	O1D-CGD-CBD	2.14	128.29	124.74
29	s1	612	CLA	O2D-CGD-O1D	-2.13	119.66	123.84
29	b1	608	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
31	d1	404	BCR	C28-C27-C26	-2.13	110.27	114.08
29	y1	610	CLA	C3B-C4B-NB	-2.13	108.53	110.52
48	S	607	CHL	CHC-C4B-NB	-2.13	122.00	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	608	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
29	S	612	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
34	Y1	625	SPH	C3-C4-C5	-2.13	120.03	124.79
29	c	510	CLA	C2D-C1D-ND	2.13	111.68	110.10
29	C	504	CLA	C4B-CHC-C1C	2.13	131.40	126.34
29	G	613	CLA	CMC-C2C-C1C	2.13	128.29	125.04
48	G1	601	CHL	C4D-CHA-C1A	2.13	123.84	121.25
29	D	403	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
29	g	613	CLA	C3B-C4B-NB	-2.13	108.54	110.52
31	b1	618	BCR	C8-C7-C6	-2.13	121.21	127.20
29	c	510	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
48	n1	609	CHL	CHC-C1C-NC	2.13	127.44	124.20
53	r	626	ERG	C11-C12-C13	2.13	116.44	112.78
29	g	614	CLA	C4B-CHC-C1C	2.13	131.39	126.34
43	d1	405	PL9	C20-C19-C21	2.13	118.86	115.27
48	g	605	CHL	CHC-C1C-NC	2.13	127.44	124.20
29	N	602	CLA	C1C-C2C-C3C	-2.13	104.72	106.96
29	N	614	CLA	O2A-CGA-CBA	2.13	118.59	111.91
29	s	604	CLA	CHA-C1A-NA	-2.13	121.52	126.40
29	B1	617	CLA	C1-O2A-CGA	2.13	122.03	116.44
49	S1	621	LUT	C19-C9-C10	-2.13	119.94	122.92
50	R	621	XAT	C39-C29-C30	-2.13	119.94	122.92
31	A1	411	BCR	C38-C26-C25	-2.13	122.14	124.53
49	S	620	LUT	C16-C1-C6	-2.13	106.84	110.30
29	b	617	CLA	C4B-CHC-C1C	2.13	131.39	126.34
29	g	602	CLA	CHA-C1A-NA	-2.13	121.52	126.40
29	c1	506	CLA	C6-C5-C3	-2.13	107.87	113.45
31	d	404	BCR	C23-C24-C25	-2.13	121.22	127.20
50	n1	622	XAT	C40-C33-C34	-2.13	119.94	122.92
48	n	601	CHL	CHD-C4C-C3C	2.13	127.97	124.84
29	s	602	CLA	CMA-C3A-C4A	2.13	117.50	111.77
29	R	603	CLA	C4B-CHC-C1C	2.13	131.39	126.34
29	c	502	CLA	C4B-CHC-C1C	2.13	131.39	126.34
50	R	621	XAT	C19-C9-C8	2.13	121.43	118.08
29	y1	602	CLA	CHA-C1A-NA	-2.13	121.52	126.40
43	d1	405	PL9	C50-C49-C48	-2.13	116.50	122.65
29	D	402	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
49	Y	621	LUT	C30-C31-C32	-2.13	116.58	123.22
31	C1	515	BCR	C35-C13-C12	2.13	121.43	118.08
29	G	603	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
32	b	626	SQD	O8-S-C6	-2.13	102.35	105.74
29	a1	405	CLA	O1D-CGD-CBD	-2.13	120.13	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d1	403	CLA	C6-C7-C8	-2.13	109.04	115.92
50	Y1	622	XAT	C32-C33-C34	2.13	122.21	118.94
29	n	614	CLA	CHA-C1A-NA	-2.13	121.53	126.40
29	y1	603	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
29	G1	614	CLA	C1D-ND-C4D	-2.13	104.82	106.33
29	n1	610	CLA	CBA-CAA-C2A	2.13	120.14	113.86
29	R	602	CLA	CHA-C1A-NA	-2.13	121.53	126.40
29	c	513	CLA	C1-O2A-CGA	2.13	122.02	116.44
29	Y	611	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
29	y1	602	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
29	b1	605	CLA	C11-C10-C8	-2.13	109.05	115.92
29	b1	615	CLA	O2A-CGA-CBA	2.13	118.58	111.91
53	R	626	ERG	C4-C5-C10	2.13	119.24	116.42
43	D1	405	PL9	C20-C19-C21	2.13	118.85	115.27
49	g	621	LUT	C37-C21-C26	2.13	112.77	109.55
29	C	512	CLA	CHA-C1A-NA	-2.13	121.53	126.40
29	C	501	CLA	O2A-CGA-CBA	2.12	118.58	111.91
29	N1	611	CLA	O2A-CGA-CBA	2.12	118.58	111.91
29	D1	403	CLA	O2A-CGA-CBA	2.12	118.57	111.91
48	n1	607	CHL	CHD-C4C-C3C	2.12	127.96	124.84
29	G1	602	CLA	CAA-C2A-C1A	-2.12	105.02	111.97
29	C1	505	CLA	C1-C2-C3	-2.12	122.37	126.04
29	B	611	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
29	C	501	CLA	C4B-CHC-C1C	2.12	131.37	126.34
31	C	517	BCR	C8-C9-C10	2.12	122.20	118.94
29	C1	510	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
29	n	610	CLA	C1D-ND-C4D	-2.12	104.83	106.33
29	S1	612	CLA	C1D-ND-C4D	-2.12	104.83	106.33
29	g1	614	CLA	CAC-C3C-C4C	2.12	127.56	124.81
48	G	609	CHL	C1-C2-C3	-2.12	122.37	126.04
29	A1	410	CLA	C3B-C4B-NB	-2.12	108.55	110.52
48	g	608	CHL	C4A-NA-C1A	2.12	107.66	106.71
48	N	609	CHL	CHC-C1C-NC	2.12	127.42	124.20
44	f	101	HEM	C3B-C2B-C1B	2.12	108.06	106.49
29	Y1	614	CLA	CHA-C1A-NA	-2.12	121.54	126.40
51	R	622	NEX	C38-C25-C26	-2.12	118.70	122.26
29	A	406	CLA	C4B-CHC-C1C	2.12	131.37	126.34
29	N	602	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
29	g	610	CLA	OBD-CAD-C3D	-2.12	123.42	128.52
29	s1	605	CLA	CHA-C1A-NA	-2.12	121.54	126.40
33	C1	523	LMG	O6-C1-C2	-2.12	105.86	110.35
29	D1	403	CLA	C4B-CHC-C1C	2.12	131.37	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S	613	CLA	C1-O2A-CGA	2.12	122.01	116.44
29	C1	511	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
33	h1	102	LMG	C6-C5-C4	-2.12	108.04	113.00
29	B1	607	CLA	C2D-C1D-ND	2.12	111.67	110.10
29	B1	603	CLA	CMC-C2C-C1C	2.12	128.27	125.04
29	n1	603	CLA	C3B-C4B-NB	-2.12	108.55	110.52
29	G	614	CLA	CAC-C3C-C4C	2.12	127.56	124.81
44	F	101	HEM	C1B-NB-C4B	2.12	107.26	105.07
29	B1	611	CLA	CHD-C1D-ND	-2.12	122.51	124.45
31	c1	516	BCR	C31-C1-C6	-2.12	106.86	110.30
29	n	602	CLA	C2D-C1D-ND	2.12	111.67	110.10
29	r	609	CLA	C1-O2A-CGA	2.12	122.00	116.44
29	g1	604	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
48	R	606	CHL	C4D-CHA-C1A	2.12	123.83	121.25
49	S	621	LUT	C1-C6-C5	-2.12	119.63	122.61
29	B1	616	CLA	CMB-C2B-C1B	2.12	128.60	125.37
29	R	610	CLA	CHA-C1A-NA	-2.12	121.55	126.40
29	a	405	CLA	C4B-CHC-C1C	2.12	131.36	126.34
29	G	602	CLA	CHA-C1A-NA	-2.12	121.55	126.40
29	Y	603	CLA	CHA-C1A-NA	-2.12	121.55	126.40
43	D1	405	PL9	C35-C34-C36	2.12	118.83	115.27
29	y	610	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
29	r1	610	CLA	C2C-C1C-NC	2.12	111.96	109.97
48	N1	601	CHL	CHC-C1C-NC	2.12	127.42	124.20
29	b	603	CLA	CHA-C1A-NA	-2.12	121.55	126.40
51	S	623	NEX	C17-C1-C6	-2.12	108.58	110.47
29	N	604	CLA	CHA-C1A-NA	-2.12	121.55	126.40
29	R1	610	CLA	CHA-C4D-ND	2.12	136.93	132.50
48	S1	608	CHL	CHC-C1C-NC	2.12	127.42	124.20
48	S1	601	CHL	C3A-C2A-C1A	2.12	104.51	101.34
29	s	602	CLA	CHA-C1A-NA	-2.12	121.55	126.40
51	n1	623	NEX	C24-C23-C22	-2.12	106.69	110.77
51	r	622	NEX	C32-C33-C34	2.12	122.19	118.94
29	c	507	CLA	CMD-C2D-C3D	-2.12	122.75	127.61
29	S	614	CLA	O2A-CGA-CBA	2.12	118.55	111.91
29	G1	610	CLA	C1C-C2C-C3C	-2.12	104.73	106.96
30	A	408	PHO	C1C-C2C-C3C	-2.12	106.85	108.61
29	G	613	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
29	n	604	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
29	C1	504	CLA	O2A-CGA-CBA	2.12	118.55	111.91
49	n	620	LUT	C35-C15-C14	-2.12	119.14	123.47
49	R	620	LUT	C11-C12-C13	-2.12	120.47	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C1	508	CLA	CHA-C1A-NA	-2.12	121.55	126.40
29	A1	406	CLA	C3D-C2D-C1D	-2.11	102.94	105.83
48	n	606	CHL	CHC-C1C-NC	2.11	127.41	124.20
30	a	409	PHO	C1-C2-C3	-2.11	122.39	126.04
29	B1	606	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
29	r	602	CLA	CHA-C1A-NA	-2.11	121.56	126.40
29	Y1	602	CLA	C2D-C1D-ND	2.11	111.66	110.10
29	c1	505	CLA	O2A-CGA-CBA	2.11	118.54	111.91
29	a	406	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
29	c	502	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
44	f1	101	HEM	C4C-NC-C1C	2.11	107.42	105.35
29	b1	607	CLA	CBB-CAB-C3B	-2.11	117.10	127.62
29	C	509	CLA	O2A-CGA-CBA	2.11	118.54	111.91
29	S	610	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
36	b1	620	C7Z	C28-C27-C26	-2.11	121.27	127.20
29	B	610	CLA	C4B-CHC-C1C	2.11	131.35	126.34
29	C1	509	CLA	O2A-CGA-CBA	2.11	118.54	111.91
29	G	612	CLA	CHA-C4D-ND	2.11	136.92	132.50
29	B1	617	CLA	CHA-C1A-NA	-2.11	121.56	126.40
29	y	604	CLA	CMA-C3A-C4A	2.11	117.45	111.77
29	b	609	CLA	OBD-CAD-C3D	-2.11	123.44	128.52
29	C	510	CLA	C1D-ND-C4D	-2.11	104.83	106.33
45	h1	101	RRX	C28-C27-C26	2.11	116.06	111.85
31	C1	514	BCR	C37-C22-C23	2.11	121.41	118.08
29	y	610	CLA	C3B-C4B-NB	-2.11	108.56	110.52
29	b	614	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
51	g	623	NEX	C19-C9-C10	-2.11	119.96	122.92
29	n1	611	CLA	CMA-C3A-C4A	2.11	117.45	111.77
29	S	605	CLA	C4B-CHC-C1C	2.11	131.35	126.34
29	g1	612	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
29	D1	403	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
50	y	622	XAT	C6-C7-C8	-2.11	121.53	125.99
29	b1	610	CLA	C3B-C4B-NB	-2.11	108.56	110.52
50	Y	622	XAT	C40-C33-C34	-2.11	119.97	122.92
29	C1	513	CLA	C2C-C1C-NC	2.11	111.95	109.97
29	S	604	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
29	n1	610	CLA	CHA-C4D-ND	2.11	136.91	132.50
29	B	610	CLA	C1C-C2C-C3C	-2.11	104.74	106.96
29	g	613	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
29	n1	612	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
29	c1	502	CLA	CMA-C3A-C4A	2.11	117.45	111.77
31	C	515	BCR	C38-C26-C25	-2.11	122.16	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A1	408	PHO	CMA-C3A-C4A	-2.11	109.75	114.38
51	s1	623	NEX	C28-C29-C30	2.11	122.18	118.94
29	C1	502	CLA	CHD-C1D-ND	-2.11	122.52	124.45
29	R	610	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
29	S1	602	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
50	G1	622	XAT	C32-C33-C34	2.11	122.18	118.94
29	A1	407	CLA	C1-O2A-CGA	2.11	121.98	116.44
29	a	405	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
29	N1	613	CLA	C6-C5-C3	-2.11	107.92	113.45
29	S1	614	CLA	C4D-CHA-C1A	2.11	123.81	121.25
29	G1	610	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
29	B	613	CLA	CHA-C1A-NA	-2.11	121.57	126.40
29	n1	603	CLA	O2A-CGA-CBA	2.11	118.52	111.91
29	Y	604	CLA	C1C-C2C-C3C	-2.11	104.74	106.96
29	b	607	CLA	C3B-C4B-NB	-2.11	108.56	110.52
37	C1	519	DGD	O1G-C1A-O1A	-2.11	118.27	123.59
39	C1	524	DGA	OG2-CB1-OB1	-2.11	118.61	123.70
44	f	101	HEM	CAA-CBA-CGA	-2.11	109.07	113.60
29	G1	604	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
31	d1	404	BCR	C1-C6-C7	2.11	121.74	115.78
51	n	623	NEX	C40-C33-C34	-2.11	119.97	122.92
29	y	611	CLA	O2A-CGA-CBA	2.11	118.52	111.91
29	b1	604	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
48	y	609	CHL	C4D-CHA-C1A	2.11	123.81	121.25
44	F1	101	HEM	CAD-C3D-C4D	2.11	128.34	124.66
49	Y	620	LUT	C7-C8-C9	-2.11	123.05	126.23
29	c	502	CLA	O2A-CGA-CBA	2.11	118.52	111.91
29	c1	511	CLA	C4B-CHC-C1C	2.11	131.33	126.34
29	B	605	CLA	OBD-CAD-C3D	-2.11	123.45	128.52
49	y1	620	LUT	C19-C9-C10	-2.11	119.97	122.92
29	s1	612	CLA	C2A-C1A-CHA	2.11	127.54	123.86
42	D	401	BCT	O3-C-O1	-2.10	114.09	119.55
29	N1	613	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
31	D1	404	BCR	C24-C25-C26	-2.10	116.36	121.46
29	b1	612	CLA	CAA-CBA-CGA	-2.10	107.10	113.25
52	R1	625	LMT	O1'-C1'-C2'	2.10	111.59	108.30
29	g	610	CLA	C2A-C1A-CHA	2.10	127.54	123.86
29	g	613	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
29	s1	602	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
32	M	101	SQD	O8-S-C6	-2.10	102.39	105.74
48	G	607	CHL	C3C-C4C-NC	-2.10	108.21	110.57
29	S	617	CLA	CHA-C1A-NA	-2.10	121.58	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	Y	620	LUT	C19-C9-C8	2.10	121.39	118.08
48	r	606	CHL	CHC-C1C-NC	2.10	127.39	124.20
29	G	604	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
29	Y	614	CLA	CMC-C2C-C1C	2.10	128.24	125.04
29	b	602	CLA	CMC-C2C-C1C	2.10	128.24	125.04
29	C1	503	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
29	S	610	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
49	n1	620	LUT	C11-C10-C9	-2.10	124.31	127.31
48	N1	608	CHL	CHA-C1A-NA	-2.10	121.58	126.40
48	n	607	CHL	C4A-NA-C1A	2.10	107.65	106.71
49	S1	621	LUT	C40-C33-C34	-2.10	119.98	122.92
29	Y1	612	CLA	C1-O2A-CGA	2.10	121.96	116.44
29	c	506	CLA	CHA-C1A-NA	-2.10	121.58	126.40
48	R1	606	CHL	CHA-C1A-NA	-2.10	121.58	126.40
29	C	504	CLA	C1C-C2C-C3C	-2.10	104.75	106.96
29	S1	612	CLA	C1C-C2C-C3C	-2.10	104.75	106.96
48	G1	601	CHL	CHC-C1C-NC	2.10	127.39	124.20
31	C	516	BCR	C12-C13-C14	-2.10	115.72	118.94
29	n	612	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
29	B	609	CLA	C3B-C4B-NB	-2.10	108.57	110.52
29	B	610	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
29	C1	504	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
48	Y	605	CHL	CHD-C4C-C3C	2.10	127.93	124.84
29	B	612	CLA	CMA-C3A-C4A	2.10	117.42	111.77
29	G	602	CLA	C1-O2A-CGA	2.10	121.95	116.44
37	B1	623	DGD	O2G-C1B-O1B	-2.10	118.63	123.70
48	s	608	CHL	CHC-C1C-NC	2.10	127.39	124.20
29	b	608	CLA	C2A-C1A-CHA	2.10	127.53	123.86
29	b	602	CLA	CHA-C1A-NA	-2.10	121.59	126.40
50	R	621	XAT	O4-C5-C18	-2.10	112.54	115.06
29	Y	613	CLA	CHA-C1A-NA	-2.10	121.59	126.40
29	B1	613	CLA	C4B-CHC-C1C	2.10	131.32	126.34
29	s	613	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
32	m1	101	SQD	O5-C1-O6	-2.10	105.00	109.97
49	y1	621	LUT	C20-C13-C12	2.10	121.38	118.08
29	B1	605	CLA	C1D-ND-C4D	-2.10	104.84	106.33
29	g1	602	CLA	C3B-C2B-C1B	-2.10	104.63	107.16
29	B	608	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
29	C	506	CLA	C1-C2-C3	-2.10	122.42	126.04
29	b	615	CLA	C1D-ND-C4D	-2.10	104.84	106.33
29	S1	612	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
29	r1	609	CLA	CHA-C1A-NA	-2.10	121.59	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	410	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
31	C1	515	BCR	C8-C7-C6	-2.10	121.31	127.20
48	N	605	CHL	CHD-C4C-C3C	2.10	127.92	124.84
49	y	620	LUT	C15-C35-C34	-2.10	119.18	123.47
49	G1	621	LUT	C39-C29-C30	-2.10	119.99	122.92
44	F1	101	HEM	C1B-NB-C4B	2.10	107.24	105.07
29	a1	406	CLA	C11-C10-C8	-2.10	109.14	115.92
29	G1	611	CLA	CHA-C1A-NA	-2.10	121.60	126.40
29	N1	610	CLA	CHA-C1A-NA	-2.10	121.60	126.40
51	r1	622	NEX	C38-C25-C26	-2.10	118.75	122.26
48	G	605	CHL	C4A-NA-C1A	2.10	107.65	106.71
50	R1	621	XAT	C6-C7-C8	-2.10	121.56	125.99
37	C1	518	DGD	O5D-C6D-C5D	-2.09	105.17	109.05
29	y	604	CLA	C1D-ND-C4D	-2.09	104.85	106.33
49	G	621	LUT	C18-C5-C6	-2.09	122.18	124.53
29	y	611	CLA	C3B-C4B-NB	-2.09	108.57	110.52
29	g1	613	CLA	C3B-C4B-NB	-2.09	108.57	110.52
29	c1	507	CLA	OBD-CAD-C3D	-2.09	123.48	128.52
31	B1	618	BCR	C1-C6-C7	2.09	121.70	115.78
29	g1	602	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
33	D1	411	LMG	O8-C28-O10	-2.09	118.31	123.59
29	y1	602	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
29	S	603	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
31	a	411	BCR	C37-C22-C23	2.09	121.38	118.08
31	C	516	BCR	C34-C9-C10	-2.09	119.99	122.92
29	S1	602	CLA	C4B-CHC-C1C	2.09	131.30	126.34
29	b	617	CLA	C1D-ND-C4D	-2.09	104.85	106.33
31	c	514	BCR	C37-C22-C21	-2.09	119.99	122.92
49	n1	621	LUT	C15-C14-C13	-2.09	124.32	127.31
48	n	607	CHL	C4D-CHA-C1A	2.09	123.80	121.25
29	g1	614	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
37	c1	519	DGD	O6D-C5D-C6D	2.09	110.89	106.67
33	c	521	LMG	O8-C28-O10	-2.09	118.31	123.59
29	b1	614	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
29	b	611	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
29	Y1	602	CLA	CHA-C1A-NA	-2.09	121.61	126.40
29	C1	502	CLA	O2A-CGA-CBA	2.09	118.47	111.91
29	S1	617	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
29	C	508	CLA	O2A-CGA-CBA	2.09	118.47	111.91
48	g1	601	CHL	CHC-C1C-NC	2.09	127.38	124.20
48	G	606	CHL	CHD-C4C-C3C	2.09	127.91	124.84
29	N	602	CLA	CMC-C2C-C1C	2.09	128.22	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	502	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
29	A	410	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
29	G	610	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
29	G1	602	CLA	C1-O2A-CGA	2.09	121.93	116.44
29	b1	611	CLA	C4D-CHA-C1A	2.09	123.79	121.25
29	a	405	CLA	O2A-CGA-CBA	2.09	118.47	111.91
29	c	503	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
29	n	613	CLA	CHD-C1D-ND	-2.09	122.53	124.45
29	C1	501	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
29	s	612	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
29	G1	613	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
29	R1	612	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
29	S1	613	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
29	c1	502	CLA	CHD-C1D-ND	-2.09	122.53	124.45
48	s1	607	CHL	CHA-C1A-NA	-2.09	121.62	126.40
29	b1	609	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
29	b1	604	CLA	CHA-C1A-NA	-2.09	121.62	126.40
29	n	603	CLA	C2A-C1A-CHA	2.09	127.51	123.86
29	n1	602	CLA	CHA-C1A-NA	-2.09	121.62	126.40
29	c1	504	CLA	CAC-C3C-C4C	2.09	127.52	124.81
29	n1	602	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
48	n1	606	CHL	CHD-C4C-C3C	2.09	127.91	124.84
48	G	601	CHL	C1-O2A-CGA	2.09	121.92	116.44
29	b1	603	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
29	b1	603	CLA	CHA-C1A-NA	-2.09	121.62	126.40
31	A1	411	BCR	C37-C22-C23	2.09	121.36	118.08
29	y1	612	CLA	C1D-ND-C4D	-2.09	104.85	106.33
29	b1	607	CLA	O2A-CGA-CBA	2.09	118.45	111.91
29	G1	614	CLA	CHA-C1A-NA	-2.09	121.62	126.40
29	b1	613	CLA	O2A-CGA-CBA	2.09	118.45	111.91
29	N	610	CLA	CMD-C2D-C3D	-2.09	122.82	127.61
48	s	601	CHL	C4B-CHC-C1C	2.09	131.28	126.34
29	c	502	CLA	CHA-C1A-NA	-2.08	121.62	126.40
29	g	614	CLA	C1-O2A-CGA	2.08	121.91	116.44
29	y	612	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
29	s	609	CLA	C3B-C4B-NB	-2.08	108.58	110.52
36	b1	620	C7Z	C39-C29-C30	-2.08	120.00	122.92
29	c	504	CLA	O2A-CGA-CBA	2.08	118.45	111.91
34	a1	414	SPH	C3-C4-C5	-2.08	120.14	124.79
29	y1	610	CLA	C1C-C2C-C3C	-2.08	104.77	106.96
29	b1	607	CLA	C1-O2A-CGA	2.08	121.91	116.44
29	c1	503	CLA	C3D-C2D-C1D	-2.08	102.99	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n1	604	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
29	c	505	CLA	C3B-C4B-NB	-2.08	108.58	110.52
31	c1	517	BCR	C1-C6-C5	-2.08	119.68	122.61
29	C1	504	CLA	C16-C15-C13	-2.08	109.19	115.92
48	s1	608	CHL	C2C-C3C-C4C	2.08	107.97	106.49
44	F	101	HEM	CAA-CBA-CGA	-2.08	109.12	113.60
48	N	606	CHL	CHD-C4C-C3C	2.08	127.90	124.84
29	B1	607	CLA	C7-C6-C5	-2.08	107.70	113.36
29	c1	507	CLA	CHA-C1A-NA	-2.08	121.63	126.40
29	A1	405	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
29	g	612	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
29	S	610	CLA	C1D-ND-C4D	-2.08	104.86	106.33
29	Y1	603	CLA	C2D-C1D-ND	2.08	111.64	110.10
29	b	612	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
29	N1	603	CLA	O2A-CGA-CBA	2.08	118.44	111.91
31	d1	404	BCR	C33-C5-C6	-2.08	122.19	124.53
29	C	502	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
29	y1	614	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
29	S	603	CLA	C4B-CHC-C1C	2.08	131.27	126.34
29	R	612	CLA	O2A-CGA-CBA	2.08	118.44	111.91
29	s	617	CLA	C1D-ND-C4D	-2.08	104.86	106.33
29	B1	617	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
32	B	621	SQD	O5-C5-C4	-2.08	105.92	109.69
29	s	617	CLA	C4B-CHC-C1C	2.08	131.27	126.34
29	r	608	CLA	C2D-C1D-ND	2.08	111.64	110.10
51	N1	623	NEX	C12-C13-C14	2.08	122.13	118.94
29	R1	609	CLA	CHA-C1A-NA	-2.08	121.64	126.40
29	b	610	CLA	C1C-C2C-C3C	-2.08	104.77	106.96
48	g1	607	CHL	C3B-C4B-NB	-2.08	108.59	110.52
29	c	503	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
29	y1	608	CLA	C1D-ND-C4D	-2.08	104.86	106.33
29	b	614	CLA	C4B-CHC-C1C	2.08	131.27	126.34
29	C	503	CLA	CHA-C1A-NA	-2.08	121.64	126.40
29	C	513	CLA	C4B-CHC-C1C	2.08	131.27	126.34
29	a	410	CLA	C1-O2A-CGA	2.08	121.90	116.44
29	C1	506	CLA	CHA-C1A-NA	-2.08	121.64	126.40
29	Y	613	CLA	C11-C10-C8	-2.08	109.20	115.92
30	a	409	PHO	C1A-C2A-C3A	-2.08	100.86	102.84
48	N	609	CHL	C1-C2-C3	-2.08	122.45	126.04
31	C	517	BCR	C2-C3-C4	-2.08	106.73	111.38
29	B1	608	CLA	C11-C12-C13	-2.08	109.21	115.92
29	Y1	610	CLA	C1-O2A-CGA	2.08	121.89	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	r1	608	CLA	C1D-ND-C4D	-2.08	104.86	106.33
44	f1	101	HEM	CMB-C2B-C1B	-2.08	121.88	125.04
29	g	613	CLA	CHA-C1A-NA	-2.08	121.64	126.40
29	N	603	CLA	O2A-CGA-CBA	2.08	118.42	111.91
29	c1	502	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
29	c	509	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
29	b	604	CLA	C4B-CHC-C1C	2.08	131.26	126.34
29	y1	602	CLA	CMC-C2C-C1C	2.08	128.20	125.04
29	A	410	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
48	y1	605	CHL	CHC-C1C-NC	2.08	127.35	124.20
49	g1	620	LUT	C18-C5-C4	2.08	118.20	114.36
29	s1	604	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
31	B	619	BCR	C1-C6-C5	-2.07	119.69	122.61
31	c1	515	BCR	C38-C26-C25	-2.07	122.20	124.53
29	y	613	CLA	C2D-C1D-ND	2.07	111.63	110.10
31	a	411	BCR	C36-C18-C17	-2.07	120.02	122.92
50	y	622	XAT	C39-C29-C30	-2.07	120.02	122.92
29	C	503	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
29	N1	603	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
30	A	408	PHO	C2D-C1D-ND	-2.07	108.09	109.53
29	B1	614	CLA	O2A-CGA-CBA	2.07	118.42	111.91
29	s1	602	CLA	C3B-C4B-NB	-2.07	108.59	110.52
40	D1	410	LHG	O8-C23-C24	2.07	118.42	111.91
29	N1	603	CLA	C1D-ND-C4D	-2.07	104.86	106.33
29	s1	603	CLA	C1D-ND-C4D	-2.07	104.86	106.33
31	B	619	BCR	C31-C1-C6	-2.07	106.94	110.30
49	S1	621	LUT	C8-C7-C6	-2.07	121.38	127.20
29	b	612	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
29	n1	611	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
29	B1	608	CLA	C3B-C4B-NB	-2.07	108.59	110.52
29	B	613	CLA	C4B-CHC-C1C	2.07	131.25	126.34
29	n	602	CLA	CAC-C3C-C4C	2.07	127.50	124.81
29	Y	611	CLA	C4B-CHC-C1C	2.07	131.25	126.34
51	s	623	NEX	C38-C25-C26	-2.07	118.79	122.26
29	S	603	CLA	O2A-CGA-CBA	2.07	118.41	111.91
29	s1	609	CLA	C3B-C4B-NB	-2.07	108.59	110.52
36	b	620	C7Z	C20-C13-C14	-2.07	120.02	122.92
29	S	617	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
29	y1	604	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
29	r	603	CLA	C4B-CHC-C1C	2.07	131.25	126.34
49	y1	621	LUT	C19-C9-C10	-2.07	120.02	122.92
33	W1	201	LMG	C37-C36-C35	2.07	124.94	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	y1	611	CLA	C4B-CHC-C1C	2.07	131.25	126.34
48	S	608	CHL	C1-C2-C3	-2.07	122.46	126.04
29	R	612	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
29	c	512	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
29	g1	604	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
29	n	603	CLA	C1-O2A-CGA	2.07	121.88	116.44
29	s	602	CLA	C1C-C2C-C3C	-2.07	104.78	106.96
29	c	507	CLA	C3B-C2B-C1B	-2.07	104.66	107.16
29	C	508	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
53	r1	626	ERG	C20-C22-C23	-2.07	119.25	125.67
29	n	610	CLA	CHA-C1A-NA	-2.07	121.66	126.40
29	N1	612	CLA	C3B-C4B-NB	-2.07	108.59	110.52
33	w1	201	LMG	O8-C28-O10	-2.07	118.37	123.59
29	s	613	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
48	N	605	CHL	C4D-CHA-C1A	2.07	123.77	121.25
30	a1	408	PHO	O1D-CGD-CBD	2.07	128.19	124.74
32	A	412	SQD	O8-S-C6	-2.07	102.44	105.74
29	g	602	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
29	B1	615	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
31	D1	404	BCR	C34-C9-C10	-2.07	120.03	122.92
29	N1	602	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
48	n	605	CHL	CHA-C1A-NA	-2.07	121.66	126.40
49	s	620	LUT	C15-C35-C34	-2.07	119.24	123.47
29	y1	610	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
29	b	603	CLA	OBD-CAD-C3D	-2.07	123.54	128.52
31	c1	515	BCR	C37-C22-C21	-2.07	120.03	122.92
29	D1	403	CLA	C2D-C1D-ND	2.07	111.63	110.10
29	b	610	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
29	Y	610	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
29	b1	617	CLA	C1D-ND-C4D	-2.07	104.87	106.33
29	c1	503	CLA	OBD-CAD-C3D	-2.07	123.54	128.52
29	s	614	CLA	C3B-C4B-NB	-2.07	108.60	110.52
48	S	608	CHL	C2B-C1B-NB	-2.07	108.85	110.23
29	R1	602	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
33	A	413	LMG	O7-C10-O9	-2.07	118.71	123.70
29	D	403	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
29	R1	608	CLA	C11-C10-C8	-2.07	109.24	115.92
29	y	604	CLA	C4B-CHC-C1C	2.07	131.24	126.34
29	C	508	CLA	CHA-C1A-NA	-2.07	121.67	126.40
29	b1	613	CLA	C11-C12-C13	-2.07	109.24	115.92
29	s	604	CLA	C4B-CHC-C1C	2.07	131.24	126.34
29	N1	604	CLA	C4B-CHC-C1C	2.07	131.24	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	607	CLA	CHA-C1A-NA	-2.07	121.67	126.40
29	A1	405	CLA	C1C-C2C-C3C	-2.07	104.78	106.96
49	S	621	LUT	C1-C2-C3	-2.07	108.98	113.64
29	n	603	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
43	d	405	PL9	O1-C4-C3	-2.06	118.45	120.72
49	r	620	LUT	C11-C12-C13	-2.06	120.62	126.42
29	Y1	604	CLA	CHA-C1A-NA	-2.06	121.67	126.40
29	c	501	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
29	d	402	CLA	OBD-CAD-C3D	-2.06	123.55	128.52
29	y1	604	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
29	c	512	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
29	Y1	610	CLA	C4B-CHC-C1C	2.06	131.23	126.34
29	C1	502	CLA	OBD-CAD-C3D	-2.06	123.55	128.52
29	y	602	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
29	s1	617	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
29	r	612	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
49	N	621	LUT	C8-C7-C6	-2.06	121.41	127.20
29	N1	612	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
29	B1	615	CLA	O2A-CGA-CBA	2.06	118.38	111.91
29	d1	402	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
29	C	501	CLA	CHA-C1A-NA	-2.06	121.67	126.40
33	h	102	LMG	O7-C10-O9	-2.06	118.72	123.70
29	b	605	CLA	C4B-CHC-C1C	2.06	131.23	126.34
29	g	603	CLA	CMC-C2C-C1C	2.06	128.18	125.04
29	Y	604	CLA	O2A-CGA-CBA	2.06	118.38	111.91
29	Y	603	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
33	A1	413	LMG	C3-C4-C5	2.06	113.92	110.24
29	d	403	CLA	CHA-C1A-NA	-2.06	121.68	126.40
29	B	616	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
29	s1	611	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
29	c	509	CLA	C6-C5-C3	-2.06	108.05	113.45
51	Y1	623	NEX	C28-C29-C30	2.06	122.10	118.94
31	c	517	BCR	C37-C22-C21	-2.06	120.04	122.92
50	R1	621	XAT	C26-C27-C28	-2.06	121.64	125.99
29	N	611	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
29	a	410	CLA	C3B-C2B-C1B	-2.06	104.67	107.16
41	C	527	LMK	C9-C8-C7	-2.06	106.92	111.79
29	S1	603	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
29	a	406	CLA	C5-C3-C2	2.06	125.28	121.12
29	n1	614	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
32	b	621	SQD	O8-S-C6	-2.06	102.46	105.74
29	N1	610	CLA	O2A-CGA-CBA	2.06	118.37	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	y1	601	CHL	C3B-C4B-NB	-2.06	108.61	110.52
51	S1	623	NEX	C40-C33-C34	-2.06	120.04	122.92
48	G	606	CHL	CHB-C4A-NA	2.06	127.36	124.51
29	s	610	CLA	C6-C5-C3	-2.06	108.06	113.45
30	a1	408	PHO	C1-C2-C3	-2.06	122.48	126.04
50	Y1	622	XAT	C38-C25-C26	-2.06	118.81	122.26
48	N1	606	CHL	C4B-CHC-C1C	2.06	131.22	126.34
33	w	201	LMG	O1-C1-C2	2.06	111.52	108.30
29	b1	612	CLA	C4B-CHC-C1C	2.06	131.22	126.34
29	g	614	CLA	CAC-C3C-C4C	2.06	127.48	124.81
48	n	609	CHL	C4A-NA-C1A	2.06	107.63	106.71
31	D	404	BCR	C8-C9-C10	2.06	122.10	118.94
33	a	413	LMG	C8-O7-C10	-2.06	112.73	117.79
29	S	605	CLA	C2D-C1D-ND	2.06	111.62	110.10
29	N1	613	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	b	618	BCR	C35-C13-C14	-2.06	120.04	122.92
29	G1	611	CLA	C3B-C4B-NB	-2.06	108.61	110.52
29	c1	510	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
37	b1	623	DGD	C1E-C2E-C3E	2.06	114.28	110.00
29	a	405	CLA	CMB-C2B-C3B	2.06	131.57	126.59
55	Y	627	PTY	O4-C30-C31	2.06	121.35	112.38
29	r1	612	CLA	C2A-C1A-CHA	2.06	127.45	123.86
29	B	617	CLA	CHA-C1A-NA	-2.06	121.69	126.40
29	N	603	CLA	CHA-C1A-NA	-2.06	121.69	126.40
29	g1	602	CLA	CHA-C1A-NA	-2.06	121.69	126.40
48	N1	607	CHL	CHA-C1A-NA	-2.06	121.69	126.40
29	B	603	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
29	s1	613	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
29	B	614	CLA	C2A-C1A-CHA	2.06	127.45	123.86
48	y1	606	CHL	CHA-C1A-NA	-2.05	121.69	126.40
29	S	611	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
29	c	507	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
29	G	603	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
29	c1	508	CLA	C2D-C1D-ND	2.05	111.62	110.10
29	a1	406	CLA	C6-C5-C3	-2.05	108.07	113.45
31	b1	619	BCR	C23-C24-C25	-2.05	121.43	127.20
33	C1	523	LMG	C3-C4-C5	2.05	113.90	110.24
29	b1	613	CLA	C6-C5-C3	-2.05	108.07	113.45
29	y	608	CLA	O2A-CGA-CBA	2.05	118.35	111.91
29	a1	410	CLA	CHA-C1A-NA	-2.05	121.69	126.40
29	B	617	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
29	c1	511	CLA	C3D-C2D-C1D	-2.05	103.03	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	g1	622	XAT	C28-C29-C30	2.05	122.09	118.94
29	s	602	CLA	CMC-C2C-C1C	2.05	128.16	125.04
29	a	406	CLA	CHA-C1A-NA	-2.05	121.70	126.40
29	Y	602	CLA	C6-C5-C3	-2.05	108.07	113.45
51	g	623	NEX	C31-C32-C33	2.05	132.18	126.42
29	n	611	CLA	C2A-C1A-CHA	2.05	127.45	123.86
29	a1	407	CLA	C2A-C1A-CHA	2.05	127.45	123.86
29	Y	614	CLA	CBB-CAB-C3B	-2.05	117.41	127.62
29	Y	613	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
31	c	516	BCR	C35-C13-C12	2.05	121.31	118.08
29	S1	610	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
33	a	413	LMG	C6-C5-C4	-2.05	108.20	113.00
31	c1	514	BCR	C4-C5-C6	-2.05	119.75	122.73
33	W	201	LMG	O7-C10-O9	-2.05	118.75	123.70
29	c	509	CLA	C11-C10-C8	-2.05	109.29	115.92
29	c1	510	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
29	B	606	CLA	CHA-C1A-NA	-2.05	121.70	126.40
29	Y1	612	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
43	d1	405	PL9	C31-C32-C33	-2.05	105.14	111.88
29	n	613	CLA	C11-C12-C13	-2.05	109.29	115.92
29	S1	614	CLA	C1D-ND-C4D	-2.05	104.88	106.33
40	D	410	LHG	C5-O7-C7	-2.05	112.75	117.79
29	r1	604	CLA	C3B-C4B-NB	-2.05	108.61	110.52
29	B	613	CLA	O2A-CGA-CBA	2.05	118.34	111.91
43	D	405	PL9	C32-C33-C34	-2.05	122.73	127.66
40	D	410	LHG	C6-C5-C4	-2.05	106.94	111.79
29	Y1	612	CLA	C4B-CHC-C1C	2.05	131.20	126.34
29	G	602	CLA	C1D-ND-C4D	-2.05	104.88	106.33
49	g	621	LUT	C11-C10-C9	-2.05	124.39	127.31
29	b	614	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
29	b	616	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
31	B1	619	BCR	C35-C13-C14	-2.05	120.06	122.92
29	a1	406	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
51	y	623	NEX	C26-C27-C28	-2.05	121.67	125.99
48	S	607	CHL	CHD-C4C-C3C	2.05	127.85	124.84
29	B1	605	CLA	CMA-C3A-C2A	2.05	122.08	113.83
29	c1	506	CLA	CHA-C1A-NA	-2.05	121.71	126.40
29	c1	505	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
48	N	607	CHL	CMA-C3A-C2A	2.05	122.08	113.83
49	N1	620	LUT	C39-C29-C28	2.05	121.30	118.08
29	G1	603	CLA	CMD-C2D-C3D	-2.05	122.91	127.61
29	b1	610	CLA	CHA-C1A-NA	-2.05	121.71	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	s1	606	CHL	CHD-C4C-C3C	2.05	127.85	124.84
29	s	609	CLA	C1-O2A-CGA	2.04	121.81	116.44
51	N	623	NEX	O24-C25-C24	2.04	114.92	113.38
36	B1	620	C7Z	C31-C30-C29	-2.04	124.39	127.31
29	N1	604	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
29	B1	608	CLA	C4B-CHC-C1C	2.04	131.19	126.34
29	g1	602	CLA	C1C-C2C-C3C	-2.04	104.81	106.96
29	N1	611	CLA	OBD-CAD-C3D	-2.04	123.60	128.52
29	b1	614	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
48	R	606	CHL	CHC-C1C-NC	2.04	127.30	124.20
48	g1	606	CHL	CHC-C1C-NC	2.04	127.30	124.20
48	N1	605	CHL	C2C-C3C-C4C	2.04	107.95	106.49
29	C1	512	CLA	C1D-ND-C4D	-2.04	104.88	106.33
29	R1	612	CLA	C1D-ND-C4D	-2.04	104.88	106.33
29	y1	603	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
29	Y1	612	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
37	c1	520	DGD	C3B-C2B-C1B	-2.04	106.19	113.62
29	G	611	CLA	CHA-C1A-NA	-2.04	121.72	126.40
29	c	507	CLA	C2A-C1A-CHA	2.04	127.43	123.86
29	R1	610	CLA	C6-C5-C3	-2.04	108.10	113.45
48	s	601	CHL	CHC-C1C-NC	2.04	127.30	124.20
31	C1	514	BCR	C37-C22-C21	-2.04	120.06	122.92
29	D1	403	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
29	n	613	CLA	C2A-C1A-CHA	2.04	127.43	123.86
29	Y	608	CLA	C4B-CHC-C1C	2.04	131.18	126.34
29	C	503	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
29	A1	405	CLA	CAC-C3C-C4C	2.04	127.46	124.81
29	g	610	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
29	R1	602	CLA	C2D-C1D-ND	2.04	111.61	110.10
48	N1	608	CHL	CHC-C4B-NB	-2.04	122.09	124.26
29	N	602	CLA	C6-C7-C8	-2.04	109.32	115.92
29	G1	613	CLA	C1-O2A-CGA	2.04	121.80	116.44
31	C1	517	BCR	C35-C13-C12	2.04	121.29	118.08
29	C	506	CLA	CAC-C3C-C4C	2.04	127.46	124.81
29	B	603	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
29	c1	507	CLA	O2A-CGA-CBA	2.04	118.31	111.91
51	y	623	NEX	C16-C1-C6	-2.04	108.64	110.47
29	c1	508	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
31	B1	619	BCR	C4-C5-C6	-2.04	119.77	122.73
36	B	620	C7Z	C31-C32-C33	-2.04	120.68	126.42
29	G	614	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
53	R1	626	ERG	C6-C7-C8	-2.04	118.05	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	D1	405	PL9	C20-C19-C18	-2.04	118.44	123.68
48	N1	601	CHL	C2B-C1B-NB	-2.04	108.86	110.23
37	C1	518	DGD	C3G-C2G-C1G	-2.04	106.96	111.79
49	n	621	LUT	C37-C21-C22	-2.04	105.57	109.44
48	n	608	CHL	C1-O2A-CGA	2.04	121.80	116.44
49	n	621	LUT	C19-C9-C8	2.04	121.29	118.08
29	B1	617	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
29	b1	613	CLA	C2D-C1D-ND	2.04	111.61	110.10
49	G	620	LUT	C8-C7-C6	-2.04	121.47	127.20
29	C1	512	CLA	C3B-C4B-NB	-2.04	108.62	110.52
29	C1	508	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
29	s1	610	CLA	C4B-CHC-C1C	2.04	131.17	126.34
36	b1	620	C7Z	C8-C7-C6	-2.04	121.48	127.20
29	B	602	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	c	514	BCR	C19-C18-C17	2.04	122.07	118.94
49	s	620	LUT	C31-C30-C29	-2.04	124.40	127.31
29	N	610	CLA	CHA-C1A-NA	-2.04	121.73	126.40
29	B1	617	CLA	CHD-C1D-ND	-2.04	122.58	124.45
49	R	620	LUT	C31-C32-C33	-2.04	120.69	126.42
40	C1	525	LHG	C6-C5-C4	-2.04	106.97	111.79
29	Y	604	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
51	y1	623	NEX	C28-C29-C30	2.04	122.07	118.94
49	s1	620	LUT	C31-C30-C29	-2.04	124.40	127.31
29	Y1	608	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
29	n1	613	CLA	C3B-C4B-NB	-2.04	108.62	110.52
29	s1	617	CLA	C3B-C4B-NB	-2.04	108.62	110.52
49	G	620	LUT	C38-C25-C24	-2.04	119.20	123.56
50	R1	621	XAT	C5-C4-C3	-2.04	108.72	112.75
29	B	616	CLA	CMA-C3A-C2A	2.04	122.05	113.83
43	D	405	PL9	O2-C1-C2	-2.04	117.11	121.78
48	y	607	CHL	CHA-C1A-NA	-2.04	121.73	126.40
50	R	621	XAT	C20-C13-C14	-2.04	120.07	122.92
29	b1	605	CLA	C11-C12-C13	-2.04	109.34	115.92
29	C	501	CLA	C3B-C4B-NB	-2.04	108.63	110.52
49	g	620	LUT	C3-C4-C5	-2.04	107.80	111.85
29	b1	611	CLA	CHD-C1D-ND	-2.04	122.58	124.45
31	D	404	BCR	C3-C4-C5	-2.04	110.44	114.08
29	N1	603	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
43	D	405	PL9	C50-C49-C48	-2.04	116.76	122.65
31	b	618	BCR	C30-C25-C26	-2.04	119.75	122.61
29	n	603	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
40	d	408	LHG	O8-C23-O10	-2.04	118.46	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s	602	CLA	C3D-C2D-C1D	-2.03	103.05	105.83
43	D	405	PL9	C11-C12-C13	-2.03	105.19	111.88
29	r	602	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
49	S	621	LUT	C28-C29-C30	-2.03	115.82	118.94
29	g	610	CLA	CHA-C1A-NA	-2.03	121.74	126.40
29	B	605	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
29	g1	614	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
29	S1	613	CLA	C4B-CHC-C1C	2.03	131.16	126.34
29	r	612	CLA	CMA-C3A-C4A	2.03	117.24	111.77
29	g1	604	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
51	N	623	NEX	C26-C27-C28	-2.03	121.69	125.99
48	g1	601	CHL	C1-C2-C3	-2.03	122.53	126.04
48	N1	605	CHL	CHC-C1C-NC	2.03	127.29	124.20
29	g	611	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
29	C1	508	CLA	CMB-C2B-C3B	2.03	131.51	126.59
49	s	620	LUT	C36-C21-C26	-2.03	106.47	109.55
29	Y	602	CLA	CAC-C3C-C4C	2.03	127.45	124.81
29	D1	402	CLA	CMC-C2C-C1C	2.03	128.13	125.04
29	Y	608	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
29	N1	614	CLA	C3B-C4B-NB	-2.03	108.63	110.52
29	b	604	CLA	CMA-C3A-C4A	2.03	117.23	111.77
29	B1	602	CLA	C1-C2-C3	-2.03	122.53	126.04
29	B1	606	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
49	S1	621	LUT	C16-C1-C6	-2.03	107.00	110.30
29	b	609	CLA	C2A-C1A-CHA	2.03	127.41	123.86
48	n1	609	CHL	CHB-C4A-NA	2.03	127.32	124.51
48	s1	601	CHL	C1D-CHD-C4C	-2.03	121.68	126.06
29	B1	612	CLA	CHA-C1A-NA	-2.03	121.75	126.40
29	G1	612	CLA	CHA-C1A-NA	-2.03	121.75	126.40
29	b	615	CLA	O2A-CGA-CBA	2.03	118.28	111.91
29	y1	613	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
29	b	612	CLA	C4B-CHC-C1C	2.03	131.15	126.34
29	R	603	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
29	G1	614	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
29	G1	610	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
29	b1	606	CLA	CAC-C3C-C2C	-2.03	124.06	127.53
29	r1	612	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
50	R1	621	XAT	O4-C5-C18	-2.03	112.62	115.06
50	g1	622	XAT	O24-C25-C38	-2.03	112.62	115.06
44	F1	101	HEM	C2A-C1A-NA	-2.03	107.88	110.15
29	B1	617	CLA	C4B-CHC-C1C	2.03	131.15	126.34
29	B	605	CLA	C16-C15-C13	-2.03	109.36	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	s	601	CHL	C3B-C2B-C1B	2.03	109.61	107.16
31	c1	516	BCR	C23-C24-C25	-2.03	121.50	127.20
51	y1	623	NEX	C40-C33-C32	2.03	121.27	118.08
31	d1	404	BCR	C31-C1-C6	-2.03	107.01	110.30
29	N1	603	CLA	C6-C5-C3	-2.03	108.14	113.45
29	N1	610	CLA	C3B-C4B-NB	-2.03	108.63	110.52
29	c	506	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
53	R1	626	ERG	C4-C5-C10	2.03	119.11	116.42
48	n	608	CHL	C3A-C2A-C1A	2.03	104.38	101.34
29	c	504	CLA	C1C-C2C-C3C	-2.03	104.82	106.96
29	N1	604	CLA	O2A-CGA-CBA	2.03	118.27	111.91
48	y1	606	CHL	CHD-C4C-C3C	2.03	127.82	124.84
29	y1	614	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
43	d1	405	PL9	C37-C38-C39	-2.03	122.78	127.66
29	y1	612	CLA	CMA-C3A-C2A	2.03	122.01	113.83
49	Y	620	LUT	C30-C31-C32	-2.03	116.89	123.22
29	b	603	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
29	b	616	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
48	s1	601	CHL	CHB-C4A-NA	2.03	127.32	124.51
29	B	613	CLA	C6-C5-C3	-2.03	108.14	113.45
29	R	602	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
29	s1	605	CLA	C2A-C1A-CHA	2.03	127.40	123.86
29	r1	608	CLA	CHA-C1A-NA	-2.03	121.75	126.40
29	g	603	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
33	c	523	LMG	C1-C2-C3	-2.03	105.77	110.00
29	S1	604	CLA	C1D-ND-C4D	-2.03	104.89	106.33
29	B1	612	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
29	a	405	CLA	CAC-C3C-C4C	2.03	127.44	124.81
49	y	620	LUT	C30-C31-C32	-2.03	116.89	123.22
29	C	503	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
29	S1	605	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
29	G1	610	CLA	CHA-C1A-NA	-2.03	121.76	126.40
29	C1	507	CLA	C2D-C1D-ND	2.03	111.60	110.10
29	d1	402	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
48	N1	601	CHL	C1-O2A-CGA	2.03	121.76	116.44
29	C1	502	CLA	C11-C12-C13	-2.03	109.37	115.92
52	r1	625	LMT	C3B-C4B-C5B	-2.03	106.63	110.24
29	d1	403	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
50	y1	622	XAT	C12-C13-C14	2.03	122.05	118.94
51	g1	623	NEX	C19-C9-C10	-2.03	120.09	122.92
51	S1	623	NEX	C4-C3-C2	2.03	114.68	110.77
29	a	406	CLA	C4B-CHC-C1C	2.03	131.14	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	y1	620	LUT	C2-C3-C4	-2.02	107.53	110.30
29	N	603	CLA	CAA-C2A-C3A	-2.02	107.23	112.78
29	g	613	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
29	r	608	CLA	CHA-C1A-NA	-2.02	121.76	126.40
29	b1	607	CLA	CHA-C1A-NA	-2.02	121.76	126.40
31	C	515	BCR	C35-C13-C12	2.02	121.27	118.08
29	C	505	CLA	C4B-CHC-C1C	2.02	131.14	126.34
29	D1	403	CLA	C6-C7-C8	-2.02	109.38	115.92
48	n1	609	CHL	C4A-NA-C1A	2.02	107.62	106.71
29	c	504	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
29	B	610	CLA	CHA-C1A-NA	-2.02	121.76	126.40
48	s1	608	CHL	CHB-C4A-NA	2.02	127.31	124.51
31	c	514	BCR	C38-C26-C27	2.02	117.50	113.62
29	N1	603	CLA	CBC-CAC-C3C	-2.02	106.85	112.43
29	B	614	CLA	C3B-C4B-NB	-2.02	108.64	110.52
31	b1	618	BCR	C1-C6-C7	2.02	121.50	115.78
29	b	604	CLA	C2D-C1D-ND	2.02	111.59	110.10
29	y	604	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
29	c1	506	CLA	CAA-CBA-CGA	-2.02	107.34	113.25
48	N	606	CHL	C3A-C2A-C1A	2.02	104.37	101.34
49	s1	620	LUT	C30-C31-C32	-2.02	116.90	123.22
29	g	611	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
43	D1	405	PL9	C7-C8-C9	-2.02	123.42	126.79
43	D	405	PL9	C20-C19-C21	2.02	118.67	115.27
29	b1	604	CLA	C4D-CHA-C1A	2.02	123.71	121.25
48	N	608	CHL	C4D-CHA-C1A	2.02	123.71	121.25
29	C	509	CLA	C2D-C1D-ND	2.02	111.59	110.10
29	y1	604	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
29	B1	606	CLA	C2A-C1A-CHA	2.02	127.39	123.86
49	N	621	LUT	C31-C30-C29	-2.02	124.42	127.31
29	b1	609	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
29	Y1	613	CLA	C4B-CHC-C1C	2.02	131.13	126.34
48	N1	608	CHL	C4B-CHC-C1C	2.02	131.13	126.34
29	S1	613	CLA	CMB-C2B-C1B	2.02	128.45	125.37
31	C1	516	BCR	C23-C24-C25	-2.02	121.53	127.20
29	n	614	CLA	CAC-C3C-C4C	2.02	127.43	124.81
29	b1	612	CLA	C1C-C2C-C3C	-2.02	104.83	106.96
48	n	606	CHL	C3A-C2A-C1A	2.02	104.36	101.34
31	d	404	BCR	C12-C13-C14	-2.02	115.84	118.94
44	f1	101	HEM	CAC-C3C-C4C	-2.02	120.02	124.90
29	s1	613	CLA	C1D-ND-C4D	-2.02	104.90	106.33
29	s1	614	CLA	C1D-ND-C4D	-2.02	104.90	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	407	CLA	CHA-C1A-NA	-2.02	121.77	126.40
38	b	624	3PH	O21-C21-O22	-2.02	118.82	123.70
48	N1	605	CHL	C3A-C2A-C1A	2.02	104.36	101.34
29	Y	603	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
48	n1	601	CHL	C1-O2A-CGA	2.02	121.74	116.44
29	a1	410	CLA	CMB-C2B-C3B	2.02	131.48	126.59
29	g1	610	CLA	C3B-C4B-NB	-2.02	108.64	110.52
48	N	606	CHL	CHC-C1C-NC	2.02	127.27	124.20
29	y1	612	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
29	C1	501	CLA	CMA-C3A-C2A	2.02	121.97	113.83
29	b	617	CLA	O2A-CGA-CBA	2.02	118.24	111.91
29	D	402	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
29	b	605	CLA	C11-C10-C8	-2.02	109.39	115.92
29	y1	604	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
55	y	627	PTY	C6-O7-C8	-2.02	114.14	117.90
51	S	623	NEX	O24-C25-C24	-2.02	111.87	113.38
51	Y	623	NEX	C11-C10-C9	2.02	130.19	127.31
29	B	615	CLA	CHA-C1A-NA	-2.02	121.78	126.40
29	r	603	CLA	O2A-CGA-CBA	2.02	118.24	111.91
29	s1	605	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
49	s	620	LUT	C37-C21-C26	2.02	112.60	109.55
29	g	602	CLA	C1-O2A-CGA	2.02	121.74	116.44
29	G	613	CLA	CHA-C1A-NA	-2.02	121.78	126.40
29	c1	507	CLA	C1D-ND-C4D	-2.02	104.90	106.33
32	b	626	SQD	O3-C3-C2	-2.02	105.69	110.35
29	g	610	CLA	C3B-C4B-NB	-2.02	108.64	110.52
29	c1	502	CLA	C1C-C2C-C3C	-2.02	104.84	106.96
29	B1	613	CLA	O2A-CGA-CBA	2.02	118.24	111.91
29	N1	611	CLA	CHA-C1A-NA	-2.02	121.78	126.40
29	y	612	CLA	CBB-CAB-C3B	-2.02	117.59	127.62
29	G1	603	CLA	C2A-C1A-CHA	2.02	127.38	123.86
48	g	608	CHL	CHD-C4C-C3C	2.02	127.80	124.84
37	B1	623	DGD	O1G-C1A-O1A	-2.02	118.50	123.59
49	N1	620	LUT	C2-C3-C4	-2.02	107.55	110.30
29	n	603	CLA	O2A-CGA-CBA	2.02	118.23	111.91
48	S1	607	CHL	C2B-C1B-NB	-2.02	108.88	110.23
29	b1	610	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
29	S	617	CLA	C1D-ND-C4D	-2.01	104.90	106.33
29	B1	615	CLA	C1D-ND-C4D	-2.01	104.90	106.33
29	C	508	CLA	C6-C7-C8	-2.01	109.41	115.92
29	c	508	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
29	a1	410	CLA	CMD-C2D-C3D	-2.01	122.98	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	y1	611	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
29	S	611	CLA	C2A-C1A-CHA	2.01	127.38	123.86
29	a1	407	CLA	O2A-CGA-CBA	2.01	118.23	111.91
49	s1	620	LUT	C15-C35-C34	-2.01	119.35	123.47
29	y1	610	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
32	b1	621	SQD	O8-S-C6	-2.01	102.53	105.74
29	C1	509	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
33	B1	622	LMG	O7-C10-O9	-2.01	118.84	123.70
49	n1	621	LUT	C12-C13-C14	-2.01	115.85	118.94
31	B1	619	BCR	C1-C6-C7	2.01	121.47	115.78
48	S	606	CHL	C4A-NA-C1A	2.01	107.61	106.71
29	C	513	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
32	A1	412	SQD	C1-C2-C3	-2.01	105.80	110.00
47	k	101	4RF	O18-C16-C15	2.01	118.22	111.91
31	b	618	BCR	C37-C22-C23	2.01	121.25	118.08
50	N	622	XAT	C19-C9-C10	-2.01	120.10	122.92
29	N	614	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
29	D	402	CLA	C2C-C1C-NC	2.01	111.86	109.97
29	c1	508	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
29	c1	509	CLA	C11-C10-C8	-2.01	109.42	115.92
32	C	526	SQD	O8-S-C6	-2.01	102.53	105.74
49	y	621	LUT	C16-C1-C6	-2.01	107.04	110.30
50	n	622	XAT	C39-C29-C30	-2.01	120.11	122.92
50	y	622	XAT	C40-C33-C34	-2.01	120.11	122.92
29	G	611	CLA	C1-O2A-CGA	2.01	121.72	116.44
29	n	602	CLA	CHA-C1A-NA	-2.01	121.79	126.40
29	S	604	CLA	C3B-C4B-NB	-2.01	108.65	110.52
29	c	506	CLA	CMA-C3A-C4A	2.01	117.18	111.77
31	B1	618	BCR	C30-C25-C26	-2.01	119.78	122.61
48	R1	607	CHL	CHC-C4B-NB	-2.01	122.13	124.26
29	Y	602	CLA	C2D-C1D-ND	2.01	111.59	110.10
48	g	608	CHL	CHC-C1C-NC	2.01	127.25	124.20
31	B1	619	BCR	C37-C22-C21	-2.01	120.11	122.92
29	c	503	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
30	a1	409	PHO	C1-C2-C3	-2.01	122.57	126.04
29	Y	614	CLA	C11-C10-C8	-2.01	109.42	115.92
29	y	613	CLA	C6-C7-C8	-2.01	109.42	115.92
49	y	620	LUT	C35-C15-C14	-2.01	119.36	123.47
49	N1	620	LUT	C19-C9-C10	-2.01	120.11	122.92
29	R	602	CLA	C1D-ND-C4D	-2.01	104.91	106.33
29	B	615	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
29	n	612	CLA	C3D-C2D-C1D	-2.01	103.09	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S	612	CLA	CHA-C1A-NA	-2.01	121.80	126.40
29	Y	613	CLA	C16-C15-C13	-2.01	109.42	115.92
50	Y1	622	XAT	C4-C3-C2	-2.01	106.89	110.77
29	Y1	602	CLA	C3B-C2B-C1B	-2.01	104.74	107.16
29	y	603	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	B1	618	BCR	C2-C1-C6	2.01	113.57	110.48
29	g	611	CLA	C3B-C4B-NB	-2.01	108.65	110.52
31	B	619	BCR	C39-C30-C25	-2.01	107.04	110.30
51	y	623	NEX	C5-C4-C3	2.01	114.12	111.75
29	b	607	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
29	c1	506	CLA	C4B-CHC-C1C	2.01	131.10	126.34
50	G1	622	XAT	C25-C24-C23	2.01	116.72	112.75
29	c1	511	CLA	C3B-C4B-NB	-2.01	108.65	110.52
29	b1	608	CLA	CMB-C2B-C3B	2.01	131.45	126.59
29	g	602	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
49	n1	621	LUT	C31-C30-C29	-2.01	124.45	127.31
29	g1	602	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
33	a1	413	LMG	O7-C10-O9	-2.01	118.85	123.70
49	r	620	LUT	C35-C15-C14	-2.01	119.36	123.47
29	C	512	CLA	C1-C2-C3	-2.01	122.57	126.04
29	G	602	CLA	C16-C15-C13	-2.01	109.43	115.92
29	B1	602	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
29	G1	604	CLA	C2A-C1A-CHA	2.01	127.37	123.86
29	B1	608	CLA	O2A-CGA-CBA	2.01	118.20	111.91
29	C	509	CLA	C11-C10-C8	-2.01	109.44	115.92
49	y	620	LUT	C8-C7-C6	-2.01	121.57	127.20
29	N1	614	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
29	c1	506	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
29	Y1	614	CLA	O2D-CGD-O1D	-2.01	119.92	123.84
54	s1	625	LPX	C3-C4-C5	-2.01	106.89	112.79
29	b1	617	CLA	C3B-C4B-NB	-2.00	108.66	110.52
31	c	517	BCR	C31-C1-C6	-2.00	107.05	110.30
29	N	614	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
37	b	623	DGD	O6D-C5D-C6D	2.00	110.71	106.67
53	r1	626	ERG	C13-C14-C8	2.00	117.37	113.48
33	d1	411	LMG	C1-O6-C5	2.00	117.62	113.69
29	G	613	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
29	B	606	CLA	C4B-CHC-C1C	2.00	131.09	126.34
29	C	502	CLA	C3B-C4B-NB	-2.00	108.66	110.52
29	Y1	613	CLA	C3B-C4B-NB	-2.00	108.66	110.52
29	a	410	CLA	CMB-C2B-C3B	2.00	131.44	126.59
29	b	607	CLA	CHA-C1A-NA	-2.00	121.81	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s	605	CLA	CHA-C1A-NA	-2.00	121.81	126.40
32	m	101	SQD	O8-S-C6	-2.00	102.55	105.74
31	b	619	BCR	C4-C5-C6	-2.00	119.82	122.73
29	B1	607	CLA	CMC-C2C-C1C	2.00	128.09	125.04
48	g	601	CHL	C4D-CHA-C1A	2.00	123.69	121.25
29	B	607	CLA	OBD-CAD-C3D	-2.00	123.70	128.52
29	r	608	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
29	r1	610	CLA	CHD-C1D-ND	-2.00	122.61	124.45
29	B	612	CLA	CHA-C1A-NA	-2.00	121.81	126.40
48	Y	605	CHL	CHD-C1D-C2D	2.00	129.68	125.48
29	b	607	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
31	b1	619	BCR	C1-C6-C7	2.00	121.44	115.78
29	S	603	CLA	C2A-C1A-CHA	2.00	127.36	123.86
31	D	404	BCR	C34-C9-C10	-2.00	120.12	122.92
29	s1	617	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
29	a	405	CLA	OBD-CAD-C3D	-2.00	123.70	128.52
29	D1	403	CLA	CAC-C3C-C4C	2.00	127.41	124.81
29	r	612	CLA	C3B-C4B-NB	-2.00	108.66	110.52
31	c	514	BCR	C40-C30-C25	-2.00	107.05	110.30
33	h	102	LMG	C8-O7-C10	-2.00	112.87	117.79
29	B1	608	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
29	r	612	CLA	O2A-CGA-CBA	2.00	118.19	111.91
48	S	606	CHL	C2B-C1B-NB	-2.00	108.89	110.23
29	y1	610	CLA	C1D-ND-C4D	-2.00	104.91	106.33
29	D1	402	CLA	CAC-C3C-C4C	2.00	127.41	124.81

All (109) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	B	620	C7Z	C3
36	b	620	C7Z	C3
36	B1	620	C7Z	C3
36	b1	620	C7Z	C3
41	C	527	LMK	C8
41	C	527	LMK	C3
41	c	527	LMK	C8
41	c	527	LMK	C3
41	C1	527	LMK	C8
41	C1	527	LMK	C3
41	c1	527	LMK	C8
41	c1	527	LMK	C3
45	H	101	RRX	C28

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Mol	Chain	Res	Type	Atom
45	h	101	RRX	C28
45	H1	101	RRX	C28
45	h1	101	RRX	C28
48	N	601	CHL	C8
48	N	605	CHL	C8
48	N	606	CHL	C8
48	N	607	CHL	C8
48	N	609	CHL	C8
48	G	601	CHL	C8
48	G	605	CHL	C3A
48	G	607	CHL	C8
48	G	609	CHL	C8
48	S	608	CHL	C8
48	Y	601	CHL	C8
48	Y	606	CHL	C8
48	Y	607	CHL	C8
48	Y	609	CHL	C8
48	n	601	CHL	C8
48	n	605	CHL	C8
48	n	606	CHL	C8
48	n	607	CHL	C8
48	n	609	CHL	C8
48	g	601	CHL	C8
48	g	605	CHL	C3A
48	g	607	CHL	C8
48	g	609	CHL	C8
48	s	608	CHL	C8
48	y	601	CHL	C8
48	y	606	CHL	C8
48	y	607	CHL	C8
48	y	609	CHL	C8
48	N1	601	CHL	C8
48	N1	605	CHL	C8
48	N1	606	CHL	C8
48	N1	607	CHL	C8
48	N1	609	CHL	C8
48	G1	601	CHL	C8
48	G1	605	CHL	C3A
48	G1	607	CHL	C8
48	G1	609	CHL	C8
48	S1	608	CHL	C8
48	Y1	601	CHL	C8

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Mol	Chain	Res	Type	Atom
48	Y1	606	CHL	C8
48	Y1	607	CHL	C8
48	Y1	609	CHL	C8
48	n1	601	CHL	C8
48	n1	605	CHL	C8
48	n1	606	CHL	C8
48	n1	607	CHL	C8
48	n1	609	CHL	C8
48	g1	601	CHL	C8
48	g1	605	CHL	C3A
48	g1	607	CHL	C8
48	g1	609	CHL	C8
48	s1	608	CHL	C8
48	y1	601	CHL	C8
48	y1	606	CHL	C8
48	y1	607	CHL	C8
48	y1	609	CHL	C8
49	G	621	LUT	C26
49	R	620	LUT	C26
49	n1	621	LUT	C26
50	N	622	XAT	C6
50	G	622	XAT	C26
50	n	622	XAT	C6
50	g	622	XAT	C6
50	g	622	XAT	C26
50	r	621	XAT	C6
50	r	621	XAT	C26
50	N1	622	XAT	C6
50	G1	622	XAT	C26
50	Y1	622	XAT	C26
50	g1	622	XAT	C26
50	r1	621	XAT	C26
51	g	623	NEX	C26
51	g1	623	NEX	C26
53	R	626	ERG	C9
53	R	626	ERG	C10
53	R	626	ERG	C24
53	R	626	ERG	C14
53	R	626	ERG	C20
53	r	626	ERG	C9
53	r	626	ERG	C10
53	r	626	ERG	C24

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Mol	Chain	Res	Type	Atom
53	r	626	ERG	C14
53	r	626	ERG	C20
53	R1	626	ERG	C9
53	R1	626	ERG	C10
53	R1	626	ERG	C24
53	R1	626	ERG	C14
53	R1	626	ERG	C20
53	r1	626	ERG	C9
53	r1	626	ERG	C10
53	r1	626	ERG	C24
53	r1	626	ERG	C14
53	r1	626	ERG	C20

All (9888) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A	405	CLA	O2A-C1-C2-C3
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	A	406	CLA	C2-C1-O2A-CGA
29	A	407	CLA	C2-C1-O2A-CGA
29	A	407	CLA	CHA-CBD-CGD-O1D
29	A	407	CLA	CHA-CBD-CGD-O2D
29	A	410	CLA	C2-C3-C5-C6
29	A	410	CLA	C4-C3-C5-C6
29	B	602	CLA	C3A-C2A-CAA-CBA
29	B	602	CLA	CHA-CBD-CGD-O1D
29	B	602	CLA	CHA-CBD-CGD-O2D
29	B	602	CLA	CAD-CBD-CGD-O1D
29	B	602	CLA	CAD-CBD-CGD-O2D
29	B	603	CLA	CHA-CBD-CGD-O1D
29	B	603	CLA	CHA-CBD-CGD-O2D
29	B	603	CLA	CBD-CGD-O2D-CED
29	B	604	CLA	CBD-CGD-O2D-CED
29	B	604	CLA	C14-C13-C15-C16
29	B	606	CLA	CHA-CBD-CGD-O1D
29	B	606	CLA	CHA-CBD-CGD-O2D
29	B	606	CLA	CAD-CBD-CGD-O1D
29	B	607	CLA	C1A-C2A-CAA-CBA
29	B	607	CLA	CHA-CBD-CGD-O1D
29	B	607	CLA	CHA-CBD-CGD-O2D
29	B	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	B	607	CLA	C4-C3-C5-C6
29	B	608	CLA	C1A-C2A-CAA-CBA
29	B	608	CLA	C3A-C2A-CAA-CBA
29	B	608	CLA	CBD-CGD-O2D-CED
29	B	608	CLA	C2-C3-C5-C6
29	B	608	CLA	C4-C3-C5-C6
29	B	609	CLA	C1A-C2A-CAA-CBA
29	B	610	CLA	C3A-C2A-CAA-CBA
29	B	610	CLA	CHA-CBD-CGD-O1D
29	B	610	CLA	CHA-CBD-CGD-O2D
29	B	610	CLA	CAD-CBD-CGD-O1D
29	B	610	CLA	CAD-CBD-CGD-O2D
29	B	610	CLA	CBD-CGD-O2D-CED
29	B	611	CLA	C1A-C2A-CAA-CBA
29	B	611	CLA	C3A-C2A-CAA-CBA
29	B	612	CLA	CHA-CBD-CGD-O1D
29	B	612	CLA	CHA-CBD-CGD-O2D
29	B	612	CLA	CBD-CGD-O2D-CED
29	B	613	CLA	C1A-C2A-CAA-CBA
29	B	613	CLA	C3A-C2A-CAA-CBA
29	B	614	CLA	CBD-CGD-O2D-CED
29	C	501	CLA	C1A-C2A-CAA-CBA
29	C	502	CLA	CHA-CBD-CGD-O1D
29	C	502	CLA	CHA-CBD-CGD-O2D
29	C	502	CLA	CAD-CBD-CGD-O1D
29	C	503	CLA	CHA-CBD-CGD-O1D
29	C	503	CLA	CHA-CBD-CGD-O2D
29	C	503	CLA	CAD-CBD-CGD-O1D
29	C	503	CLA	CBD-CGD-O2D-CED
29	C	503	CLA	C2-C3-C5-C6
29	C	503	CLA	C4-C3-C5-C6
29	C	504	CLA	C2B-C3B-CAB-CBB
29	C	504	CLA	C4B-C3B-CAB-CBB
29	C	504	CLA	CHA-CBD-CGD-O1D
29	C	504	CLA	CHA-CBD-CGD-O2D
29	C	504	CLA	CAD-CBD-CGD-O1D
29	C	505	CLA	C2B-C3B-CAB-CBB
29	C	505	CLA	C4B-C3B-CAB-CBB
29	C	505	CLA	CHA-CBD-CGD-O1D
29	C	506	CLA	C2-C1-O2A-CGA
29	C	508	CLA	CHA-CBD-CGD-O1D
29	C	508	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	C	509	CLA	C2-C1-O2A-CGA
29	C	509	CLA	C6-C7-C8-C9
29	C	513	CLA	C1A-C2A-CAA-CBA
29	D	403	CLA	C2-C3-C5-C6
29	D	403	CLA	C4-C3-C5-C6
29	N	602	CLA	CBD-CGD-O2D-CED
29	N	603	CLA	C2-C1-O2A-CGA
29	N	604	CLA	C1A-C2A-CAA-CBA
29	N	604	CLA	C3A-C2A-CAA-CBA
29	N	610	CLA	C1A-C2A-CAA-CBA
29	N	610	CLA	C3A-C2A-CAA-CBA
29	N	610	CLA	C2B-C3B-CAB-CBB
29	N	610	CLA	C4B-C3B-CAB-CBB
29	N	612	CLA	C2B-C3B-CAB-CBB
29	N	612	CLA	C4B-C3B-CAB-CBB
29	N	612	CLA	CHA-CBD-CGD-O2D
29	N	613	CLA	CHA-CBD-CGD-O1D
29	N	613	CLA	CHA-CBD-CGD-O2D
29	N	614	CLA	C1A-C2A-CAA-CBA
29	G	602	CLA	C1A-C2A-CAA-CBA
29	G	602	CLA	C3A-C2A-CAA-CBA
29	G	603	CLA	CBD-CGD-O2D-CED
29	G	603	CLA	C11-C10-C8-C9
29	G	610	CLA	CBD-CGD-O2D-CED
29	G	611	CLA	CHA-CBD-CGD-O1D
29	G	611	CLA	CHA-CBD-CGD-O2D
29	G	611	CLA	CBD-CGD-O2D-CED
29	G	613	CLA	C2B-C3B-CAB-CBB
29	G	613	CLA	C4B-C3B-CAB-CBB
29	G	613	CLA	CHA-CBD-CGD-O1D
29	G	613	CLA	CHA-CBD-CGD-O2D
29	G	613	CLA	CBD-CGD-O2D-CED
29	R	603	CLA	C3A-C2A-CAA-CBA
29	R	603	CLA	C4B-C3B-CAB-CBB
29	R	608	CLA	C1A-C2A-CAA-CBA
29	R	608	CLA	C3A-C2A-CAA-CBA
29	R	608	CLA	CHA-CBD-CGD-O1D
29	R	608	CLA	CBD-CGD-O2D-CED
29	R	609	CLA	C2B-C3B-CAB-CBB
29	R	609	CLA	C4B-C3B-CAB-CBB
29	R	610	CLA	C2B-C3B-CAB-CBB
29	R	610	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	R	610	CLA	CHA-CBD-CGD-O1D
29	R	610	CLA	CHA-CBD-CGD-O2D
29	R	610	CLA	CBD-CGD-O2D-CED
29	R	612	CLA	C2-C1-O2A-CGA
29	R	612	CLA	C4B-C3B-CAB-CBB
29	S	602	CLA	C2-C1-O2A-CGA
29	S	602	CLA	CHA-CBD-CGD-O2D
29	S	603	CLA	C1A-C2A-CAA-CBA
29	S	603	CLA	C3A-C2A-CAA-CBA
29	S	603	CLA	C2B-C3B-CAB-CBB
29	S	603	CLA	C4B-C3B-CAB-CBB
29	S	603	CLA	CHA-CBD-CGD-O1D
29	S	603	CLA	CHA-CBD-CGD-O2D
29	S	603	CLA	CBD-CGD-O2D-CED
29	S	605	CLA	C1A-C2A-CAA-CBA
29	S	609	CLA	C2B-C3B-CAB-CBB
29	S	609	CLA	C4B-C3B-CAB-CBB
29	S	609	CLA	CBD-CGD-O2D-CED
29	S	610	CLA	C3A-C2A-CAA-CBA
29	S	610	CLA	CBD-CGD-O2D-CED
29	S	611	CLA	C1A-C2A-CAA-CBA
29	S	611	CLA	C3A-C2A-CAA-CBA
29	S	611	CLA	CHA-CBD-CGD-O1D
29	S	611	CLA	CHA-CBD-CGD-O2D
29	S	617	CLA	CHA-CBD-CGD-O1D
29	S	617	CLA	CHA-CBD-CGD-O2D
29	S	617	CLA	CBD-CGD-O2D-CED
29	Y	603	CLA	C4B-C3B-CAB-CBB
29	Y	604	CLA	CHA-CBD-CGD-O1D
29	Y	604	CLA	CHA-CBD-CGD-O2D
29	Y	608	CLA	C1A-C2A-CAA-CBA
29	Y	610	CLA	CBD-CGD-O2D-CED
29	Y	611	CLA	C2-C3-C5-C6
29	Y	611	CLA	C4-C3-C5-C6
29	Y	613	CLA	CHA-CBD-CGD-O1D
29	Y	613	CLA	CHA-CBD-CGD-O2D
29	Y	614	CLA	C2B-C3B-CAB-CBB
29	Y	614	CLA	C4B-C3B-CAB-CBB
29	a	405	CLA	C2-C1-O2A-CGA
29	a	405	CLA	CHA-CBD-CGD-O1D
29	a	405	CLA	CHA-CBD-CGD-O2D
29	a	405	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	a	405	CLA	O2A-C1-C2-C3
29	a	406	CLA	C1A-C2A-CAA-CBA
29	a	406	CLA	C3A-C2A-CAA-CBA
29	a	406	CLA	C2-C1-O2A-CGA
29	a	407	CLA	C1A-C2A-CAA-CBA
29	a	407	CLA	C2-C1-O2A-CGA
29	a	410	CLA	C2-C3-C5-C6
29	a	410	CLA	C4-C3-C5-C6
29	b	602	CLA	CHA-CBD-CGD-O1D
29	b	602	CLA	CHA-CBD-CGD-O2D
29	b	603	CLA	CHA-CBD-CGD-O1D
29	b	603	CLA	CHA-CBD-CGD-O2D
29	b	604	CLA	CBD-CGD-O2D-CED
29	b	605	CLA	C1A-C2A-CAA-CBA
29	b	605	CLA	C2B-C3B-CAB-CBB
29	b	605	CLA	CHA-CBD-CGD-O1D
29	b	605	CLA	CHA-CBD-CGD-O2D
29	b	605	CLA	CAD-CBD-CGD-O1D
29	b	608	CLA	C1A-C2A-CAA-CBA
29	b	608	CLA	C3A-C2A-CAA-CBA
29	b	608	CLA	CHA-CBD-CGD-O1D
29	b	608	CLA	CHA-CBD-CGD-O2D
29	b	608	CLA	CAD-CBD-CGD-O1D
29	b	608	CLA	CAD-CBD-CGD-O2D
29	b	608	CLA	C2-C3-C5-C6
29	b	608	CLA	C4-C3-C5-C6
29	b	608	CLA	C11-C10-C8-C9
29	b	609	CLA	C2-C3-C5-C6
29	b	609	CLA	C4-C3-C5-C6
29	b	610	CLA	CBD-CGD-O2D-CED
29	b	611	CLA	CBD-CGD-O2D-CED
29	b	612	CLA	CHA-CBD-CGD-O1D
29	b	612	CLA	CHA-CBD-CGD-O2D
29	b	613	CLA	C1A-C2A-CAA-CBA
29	b	613	CLA	C3A-C2A-CAA-CBA
29	b	613	CLA	CHA-CBD-CGD-O1D
29	b	613	CLA	CHA-CBD-CGD-O2D
29	b	613	CLA	CAD-CBD-CGD-O1D
29	b	613	CLA	CAD-CBD-CGD-O2D
29	b	616	CLA	CHA-CBD-CGD-O1D
29	b	616	CLA	CHA-CBD-CGD-O2D
29	b	617	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	c	501	CLA	CHA-CBD-CGD-O1D
29	c	501	CLA	CHA-CBD-CGD-O2D
29	c	502	CLA	CHA-CBD-CGD-O1D
29	c	502	CLA	CHA-CBD-CGD-O2D
29	c	502	CLA	CAD-CBD-CGD-O1D
29	c	504	CLA	CHA-CBD-CGD-O1D
29	c	504	CLA	CHA-CBD-CGD-O2D
29	c	504	CLA	CAD-CBD-CGD-O1D
29	c	504	CLA	CAD-CBD-CGD-O2D
29	c	505	CLA	CHA-CBD-CGD-O1D
29	c	505	CLA	CHA-CBD-CGD-O2D
29	c	506	CLA	C2-C1-O2A-CGA
29	c	508	CLA	CHA-CBD-CGD-O1D
29	c	508	CLA	CHA-CBD-CGD-O2D
29	c	509	CLA	C2-C1-O2A-CGA
29	c	511	CLA	CBD-CGD-O2D-CED
29	c	512	CLA	C1A-C2A-CAA-CBA
29	c	512	CLA	CBA-CGA-O2A-C1
29	c	512	CLA	O1A-CGA-O2A-C1
29	c	513	CLA	C1A-C2A-CAA-CBA
29	d	402	CLA	CBD-CGD-O2D-CED
29	d	403	CLA	CBD-CGD-O2D-CED
29	d	403	CLA	C4-C3-C5-C6
29	n	602	CLA	C2B-C3B-CAB-CBB
29	n	602	CLA	C4B-C3B-CAB-CBB
29	n	610	CLA	C1A-C2A-CAA-CBA
29	n	610	CLA	CBD-CGD-O2D-CED
29	n	611	CLA	CBD-CGD-O2D-CED
29	n	612	CLA	CBD-CGD-O2D-CED
29	n	613	CLA	C1A-C2A-CAA-CBA
29	n	613	CLA	CBD-CGD-O2D-CED
29	n	614	CLA	C1A-C2A-CAA-CBA
29	n	614	CLA	CBD-CGD-O2D-CED
29	g	602	CLA	C3A-C2A-CAA-CBA
29	g	604	CLA	C2-C1-O2A-CGA
29	g	610	CLA	CHA-CBD-CGD-O1D
29	g	610	CLA	CHA-CBD-CGD-O2D
29	g	610	CLA	CBD-CGD-O2D-CED
29	g	611	CLA	CBD-CGD-O2D-CED
29	r	602	CLA	C6-C7-C8-C9
29	r	603	CLA	C1A-C2A-CAA-CBA
29	r	603	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	r	603	CLA	C4B-C3B-CAB-CBB
29	r	603	CLA	CBD-CGD-O2D-CED
29	r	604	CLA	C1A-C2A-CAA-CBA
29	r	604	CLA	CHA-CBD-CGD-O1D
29	r	604	CLA	CHA-CBD-CGD-O2D
29	r	604	CLA	CBD-CGD-O2D-CED
29	r	608	CLA	C1A-C2A-CAA-CBA
29	r	608	CLA	C3A-C2A-CAA-CBA
29	r	608	CLA	CHA-CBD-CGD-O1D
29	r	608	CLA	CHA-CBD-CGD-O2D
29	r	609	CLA	O1A-CGA-O2A-C1
29	r	609	CLA	CHA-CBD-CGD-O1D
29	r	609	CLA	CHA-CBD-CGD-O2D
29	r	609	CLA	CBD-CGD-O2D-CED
29	s	602	CLA	C2-C1-O2A-CGA
29	s	603	CLA	C1A-C2A-CAA-CBA
29	s	603	CLA	C3A-C2A-CAA-CBA
29	s	605	CLA	C1A-C2A-CAA-CBA
29	s	605	CLA	CBA-CGA-O2A-C1
29	s	605	CLA	O1A-CGA-O2A-C1
29	s	605	CLA	C4B-C3B-CAB-CBB
29	s	605	CLA	CHA-CBD-CGD-O2D
29	s	609	CLA	C1A-C2A-CAA-CBA
29	s	609	CLA	C3A-C2A-CAA-CBA
29	s	609	CLA	C2A-CAA-CBA-CGA
29	s	609	CLA	CHA-CBD-CGD-O1D
29	s	609	CLA	CHA-CBD-CGD-O2D
29	s	610	CLA	C1A-C2A-CAA-CBA
29	s	610	CLA	C3A-C2A-CAA-CBA
29	s	610	CLA	C2B-C3B-CAB-CBB
29	s	610	CLA	C4B-C3B-CAB-CBB
29	s	611	CLA	C1A-C2A-CAA-CBA
29	s	611	CLA	C3A-C2A-CAA-CBA
29	s	611	CLA	CHA-CBD-CGD-O1D
29	s	611	CLA	CHA-CBD-CGD-O2D
29	s	613	CLA	C2B-C3B-CAB-CBB
29	s	613	CLA	C4B-C3B-CAB-CBB
29	s	613	CLA	CHA-CBD-CGD-O1D
29	s	613	CLA	CHA-CBD-CGD-O2D
29	s	613	CLA	CBD-CGD-O2D-CED
29	s	614	CLA	CBD-CGD-O2D-CED
29	s	617	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	s	617	CLA	C2A-CAA-CBA-CGA
29	s	617	CLA	C2-C1-O2A-CGA
29	s	617	CLA	CBD-CGD-O2D-CED
29	y	603	CLA	C2-C1-O2A-CGA
29	y	603	CLA	C4B-C3B-CAB-CBB
29	y	603	CLA	CBD-CGD-O2D-CED
29	y	608	CLA	C1A-C2A-CAA-CBA
29	y	608	CLA	CHA-CBD-CGD-O1D
29	y	608	CLA	CHA-CBD-CGD-O2D
29	y	608	CLA	CBD-CGD-O2D-CED
29	y	610	CLA	CHA-CBD-CGD-O1D
29	y	610	CLA	CHA-CBD-CGD-O2D
29	y	610	CLA	CBD-CGD-O2D-CED
29	y	612	CLA	C2B-C3B-CAB-CBB
29	y	612	CLA	C4B-C3B-CAB-CBB
29	y	613	CLA	CHA-CBD-CGD-O1D
29	y	613	CLA	CHA-CBD-CGD-O2D
29	y	613	CLA	CBD-CGD-O2D-CED
29	A1	405	CLA	C1A-C2A-CAA-CBA
29	A1	405	CLA	C3A-C2A-CAA-CBA
29	A1	405	CLA	C2A-CAA-CBA-CGA
29	A1	405	CLA	CBD-CGD-O2D-CED
29	A1	406	CLA	C1A-C2A-CAA-CBA
29	A1	406	CLA	C3A-C2A-CAA-CBA
29	A1	406	CLA	C2-C1-O2A-CGA
29	A1	407	CLA	C2-C1-O2A-CGA
29	A1	407	CLA	CHA-CBD-CGD-O1D
29	A1	407	CLA	CHA-CBD-CGD-O2D
29	B1	602	CLA	C3A-C2A-CAA-CBA
29	B1	603	CLA	CHA-CBD-CGD-O1D
29	B1	603	CLA	CHA-CBD-CGD-O2D
29	B1	603	CLA	CBD-CGD-O2D-CED
29	B1	604	CLA	CBD-CGD-O2D-CED
29	B1	604	CLA	C2-C3-C5-C6
29	B1	604	CLA	C4-C3-C5-C6
29	B1	605	CLA	C2B-C3B-CAB-CBB
29	B1	605	CLA	C4B-C3B-CAB-CBB
29	B1	606	CLA	C2B-C3B-CAB-CBB
29	B1	606	CLA	C4B-C3B-CAB-CBB
29	B1	607	CLA	C1A-C2A-CAA-CBA
29	B1	608	CLA	C1A-C2A-CAA-CBA
29	B1	608	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	B1	608	CLA	C2B-C3B-CAB-CBB
29	B1	608	CLA	C4B-C3B-CAB-CBB
29	B1	608	CLA	CHA-CBD-CGD-O1D
29	B1	608	CLA	CHA-CBD-CGD-O2D
29	B1	608	CLA	CAD-CBD-CGD-O1D
29	B1	608	CLA	C4-C3-C5-C6
29	B1	609	CLA	C1A-C2A-CAA-CBA
29	B1	609	CLA	C2B-C3B-CAB-CBB
29	B1	609	CLA	C4B-C3B-CAB-CBB
29	B1	609	CLA	CHA-CBD-CGD-O2D
29	B1	610	CLA	C3A-C2A-CAA-CBA
29	B1	610	CLA	CAD-CBD-CGD-O1D
29	B1	610	CLA	CAD-CBD-CGD-O2D
29	B1	612	CLA	CHA-CBD-CGD-O1D
29	B1	612	CLA	CHA-CBD-CGD-O2D
29	B1	613	CLA	C2-C1-O2A-CGA
29	B1	613	CLA	CHA-CBD-CGD-O1D
29	B1	613	CLA	CHA-CBD-CGD-O2D
29	B1	613	CLA	CAD-CBD-CGD-O1D
29	B1	613	CLA	CAD-CBD-CGD-O2D
29	B1	613	CLA	CBD-CGD-O2D-CED
29	B1	614	CLA	C2-C1-O2A-CGA
29	B1	614	CLA	CHA-CBD-CGD-O1D
29	B1	614	CLA	CHA-CBD-CGD-O2D
29	B1	614	CLA	CBD-CGD-O2D-CED
29	B1	616	CLA	CHA-CBD-CGD-O1D
29	B1	616	CLA	CBD-CGD-O2D-CED
29	B1	617	CLA	CBD-CGD-O2D-CED
29	C1	501	CLA	C1A-C2A-CAA-CBA
29	C1	501	CLA	CBD-CGD-O2D-CED
29	C1	502	CLA	CBD-CGD-O2D-CED
29	C1	503	CLA	C2-C3-C5-C6
29	C1	503	CLA	C4-C3-C5-C6
29	C1	504	CLA	CHA-CBD-CGD-O1D
29	C1	504	CLA	CHA-CBD-CGD-O2D
29	C1	504	CLA	CAD-CBD-CGD-O1D
29	C1	504	CLA	CAD-CBD-CGD-O2D
29	C1	504	CLA	CBD-CGD-O2D-CED
29	C1	504	CLA	C4-C3-C5-C6
29	C1	506	CLA	C2-C1-O2A-CGA
29	C1	506	CLA	C2B-C3B-CAB-CBB
29	C1	506	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	C1	506	CLA	CHA-CBD-CGD-O1D
29	C1	506	CLA	CHA-CBD-CGD-O2D
29	C1	506	CLA	CAD-CBD-CGD-O1D
29	C1	507	CLA	CHA-CBD-CGD-O1D
29	C1	507	CLA	CHA-CBD-CGD-O2D
29	C1	508	CLA	CHA-CBD-CGD-O1D
29	C1	508	CLA	CHA-CBD-CGD-O2D
29	C1	510	CLA	CBD-CGD-O2D-CED
29	C1	513	CLA	C1A-C2A-CAA-CBA
29	C1	513	CLA	CBD-CGD-O2D-CED
29	D1	402	CLA	C3A-C2A-CAA-CBA
29	D1	402	CLA	CHA-CBD-CGD-O1D
29	D1	402	CLA	CHA-CBD-CGD-O2D
29	N1	602	CLA	C2-C3-C5-C6
29	N1	602	CLA	C4-C3-C5-C6
29	N1	603	CLA	C2-C1-O2A-CGA
29	N1	603	CLA	C2B-C3B-CAB-CBB
29	N1	603	CLA	C4B-C3B-CAB-CBB
29	N1	603	CLA	CBD-CGD-O2D-CED
29	N1	604	CLA	C1A-C2A-CAA-CBA
29	N1	604	CLA	C3A-C2A-CAA-CBA
29	N1	604	CLA	C2B-C3B-CAB-CBB
29	N1	604	CLA	C4B-C3B-CAB-CBB
29	N1	610	CLA	C1A-C2A-CAA-CBA
29	N1	610	CLA	C3A-C2A-CAA-CBA
29	N1	612	CLA	C4B-C3B-CAB-CBB
29	N1	612	CLA	CBD-CGD-O2D-CED
29	N1	613	CLA	CHA-CBD-CGD-O1D
29	N1	613	CLA	CHA-CBD-CGD-O2D
29	N1	614	CLA	C1A-C2A-CAA-CBA
29	G1	602	CLA	C1A-C2A-CAA-CBA
29	G1	602	CLA	C3A-C2A-CAA-CBA
29	G1	603	CLA	CBD-CGD-O2D-CED
29	G1	610	CLA	CHA-CBD-CGD-O1D
29	G1	610	CLA	CHA-CBD-CGD-O2D
29	G1	613	CLA	CBD-CGD-O2D-CED
29	R1	602	CLA	CBD-CGD-O2D-CED
29	R1	603	CLA	C3A-C2A-CAA-CBA
29	R1	603	CLA	C4B-C3B-CAB-CBB
29	R1	603	CLA	CHA-CBD-CGD-O1D
29	R1	603	CLA	CHA-CBD-CGD-O2D
29	R1	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	R1	604	CLA	CHA-CBD-CGD-O1D
29	R1	604	CLA	CHA-CBD-CGD-O2D
29	R1	608	CLA	C3A-C2A-CAA-CBA
29	R1	610	CLA	CHA-CBD-CGD-O1D
29	R1	610	CLA	CHA-CBD-CGD-O2D
29	R1	610	CLA	CBD-CGD-O2D-CED
29	R1	612	CLA	C3A-C2A-CAA-CBA
29	S1	602	CLA	C2-C1-O2A-CGA
29	S1	602	CLA	C4-C3-C5-C6
29	S1	602	CLA	C11-C10-C8-C9
29	S1	603	CLA	C1A-C2A-CAA-CBA
29	S1	603	CLA	CHA-CBD-CGD-O1D
29	S1	603	CLA	CHA-CBD-CGD-O2D
29	S1	605	CLA	C1A-C2A-CAA-CBA
29	S1	605	CLA	CHA-CBD-CGD-O1D
29	S1	605	CLA	CHA-CBD-CGD-O2D
29	S1	609	CLA	CBD-CGD-O2D-CED
29	S1	610	CLA	C3A-C2A-CAA-CBA
29	S1	610	CLA	CHA-CBD-CGD-O1D
29	S1	610	CLA	CHA-CBD-CGD-O2D
29	S1	610	CLA	CBD-CGD-O2D-CED
29	S1	610	CLA	O1D-CGD-O2D-CED
29	S1	611	CLA	C1A-C2A-CAA-CBA
29	S1	611	CLA	C3A-C2A-CAA-CBA
29	S1	611	CLA	C2B-C3B-CAB-CBB
29	S1	611	CLA	C4B-C3B-CAB-CBB
29	S1	611	CLA	CBD-CGD-O2D-CED
29	S1	611	CLA	C2-C3-C5-C6
29	S1	611	CLA	C4-C3-C5-C6
29	S1	612	CLA	CBD-CGD-O2D-CED
29	S1	613	CLA	C2B-C3B-CAB-CBB
29	S1	613	CLA	C4B-C3B-CAB-CBB
29	S1	614	CLA	C2-C1-O2A-CGA
29	S1	614	CLA	C2B-C3B-CAB-CBB
29	S1	614	CLA	C4B-C3B-CAB-CBB
29	S1	614	CLA	CBD-CGD-O2D-CED
29	Y1	603	CLA	CBD-CGD-O2D-CED
29	Y1	604	CLA	C2-C1-O2A-CGA
29	Y1	604	CLA	CHA-CBD-CGD-O2D
29	Y1	608	CLA	C2B-C3B-CAB-CBB
29	Y1	608	CLA	C4B-C3B-CAB-CBB
29	Y1	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	Y1	611	CLA	C4-C3-C5-C6
29	Y1	613	CLA	CBD-CGD-O2D-CED
29	Y1	614	CLA	CBD-CGD-O2D-CED
29	a1	405	CLA	CHA-CBD-CGD-O1D
29	a1	405	CLA	CHA-CBD-CGD-O2D
29	a1	405	CLA	CBD-CGD-O2D-CED
29	a1	406	CLA	CBA-CGA-O2A-C1
29	a1	406	CLA	O1A-CGA-O2A-C1
29	a1	406	CLA	CHA-CBD-CGD-O1D
29	a1	406	CLA	CHA-CBD-CGD-O2D
29	a1	407	CLA	C2A-CAA-CBA-CGA
29	a1	410	CLA	CBA-CGA-O2A-C1
29	a1	410	CLA	C4-C3-C5-C6
29	b1	602	CLA	CBD-CGD-O2D-CED
29	b1	603	CLA	CBA-CGA-O2A-C1
29	b1	603	CLA	O1A-CGA-O2A-C1
29	b1	603	CLA	CHA-CBD-CGD-O1D
29	b1	603	CLA	CHA-CBD-CGD-O2D
29	b1	604	CLA	CBD-CGD-O2D-CED
29	b1	604	CLA	C2-C3-C5-C6
29	b1	604	CLA	C4-C3-C5-C6
29	b1	605	CLA	C1A-C2A-CAA-CBA
29	b1	605	CLA	C2-C1-O2A-CGA
29	b1	606	CLA	CBD-CGD-O2D-CED
29	b1	606	CLA	C4-C3-C5-C6
29	b1	607	CLA	C1A-C2A-CAA-CBA
29	b1	607	CLA	C2B-C3B-CAB-CBB
29	b1	607	CLA	C4B-C3B-CAB-CBB
29	b1	607	CLA	CHA-CBD-CGD-O1D
29	b1	607	CLA	CHA-CBD-CGD-O2D
29	b1	607	CLA	CBD-CGD-O2D-CED
29	b1	608	CLA	C1A-C2A-CAA-CBA
29	b1	608	CLA	C3A-C2A-CAA-CBA
29	b1	608	CLA	CHA-CBD-CGD-O1D
29	b1	608	CLA	CAD-CBD-CGD-O1D
29	b1	608	CLA	CAD-CBD-CGD-O2D
29	b1	609	CLA	C1A-C2A-CAA-CBA
29	b1	609	CLA	C3A-C2A-CAA-CBA
29	b1	609	CLA	CHA-CBD-CGD-O1D
29	b1	609	CLA	CHA-CBD-CGD-O2D
29	b1	609	CLA	CBD-CGD-O2D-CED
29	b1	609	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	b1	612	CLA	CHA-CBD-CGD-O2D
29	b1	613	CLA	C2-C1-O2A-CGA
29	b1	614	CLA	C4B-C3B-CAB-CBB
29	b1	615	CLA	C1A-C2A-CAA-CBA
29	b1	615	CLA	C2-C3-C5-C6
29	b1	615	CLA	C4-C3-C5-C6
29	b1	616	CLA	C11-C10-C8-C9
29	c1	501	CLA	CBD-CGD-O2D-CED
29	c1	502	CLA	CAD-CBD-CGD-O1D
29	c1	502	CLA	CAD-CBD-CGD-O2D
29	c1	504	CLA	CHA-CBD-CGD-O1D
29	c1	504	CLA	CHA-CBD-CGD-O2D
29	c1	504	CLA	CAD-CBD-CGD-O1D
29	c1	505	CLA	C1A-C2A-CAA-CBA
29	c1	505	CLA	C3A-C2A-CAA-CBA
29	c1	506	CLA	C2-C1-O2A-CGA
29	c1	506	CLA	CBD-CGD-O2D-CED
29	c1	509	CLA	C6-C7-C8-C9
29	c1	510	CLA	C2B-C3B-CAB-CBB
29	c1	510	CLA	C4B-C3B-CAB-CBB
29	c1	511	CLA	C1A-C2A-CAA-CBA
29	c1	511	CLA	CHA-CBD-CGD-O1D
29	c1	511	CLA	CHA-CBD-CGD-O2D
29	c1	512	CLA	CBA-CGA-O2A-C1
29	c1	512	CLA	O1A-CGA-O2A-C1
29	c1	512	CLA	CAD-CBD-CGD-O1D
29	c1	512	CLA	CAD-CBD-CGD-O2D
29	c1	513	CLA	C1A-C2A-CAA-CBA
29	c1	513	CLA	C3A-C2A-CAA-CBA
29	c1	513	CLA	C11-C10-C8-C9
29	d1	402	CLA	C2-C3-C5-C6
29	d1	402	CLA	C4-C3-C5-C6
29	n1	604	CLA	C14-C13-C15-C16
29	n1	610	CLA	C1A-C2A-CAA-CBA
29	n1	610	CLA	C2B-C3B-CAB-CBB
29	n1	610	CLA	C4B-C3B-CAB-CBB
29	n1	610	CLA	CBD-CGD-O2D-CED
29	n1	611	CLA	CBD-CGD-O2D-CED
29	n1	612	CLA	CBD-CGD-O2D-CED
29	n1	613	CLA	CHA-CBD-CGD-O1D
29	n1	613	CLA	CHA-CBD-CGD-O2D
29	n1	613	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	n1	614	CLA	C1A-C2A-CAA-CBA
29	g1	602	CLA	C1A-C2A-CAA-CBA
29	g1	602	CLA	C3A-C2A-CAA-CBA
29	g1	602	CLA	CBD-CGD-O2D-CED
29	g1	603	CLA	CBD-CGD-O2D-CED
29	g1	604	CLA	C2-C1-O2A-CGA
29	g1	610	CLA	C1A-C2A-CAA-CBA
29	g1	610	CLA	CHA-CBD-CGD-O1D
29	g1	610	CLA	CHA-CBD-CGD-O2D
29	g1	611	CLA	CHA-CBD-CGD-O1D
29	g1	611	CLA	CHA-CBD-CGD-O2D
29	g1	611	CLA	CBD-CGD-O2D-CED
29	g1	611	CLA	C11-C10-C8-C7
29	g1	612	CLA	CHA-CBD-CGD-O2D
29	g1	612	CLA	CBD-CGD-O2D-CED
29	g1	613	CLA	C2B-C3B-CAB-CBB
29	g1	613	CLA	C4B-C3B-CAB-CBB
29	r1	602	CLA	C6-C7-C8-C9
29	r1	603	CLA	C1A-C2A-CAA-CBA
29	r1	603	CLA	C3A-C2A-CAA-CBA
29	r1	603	CLA	CBA-CGA-O2A-C1
29	r1	603	CLA	O1A-CGA-O2A-C1
29	r1	603	CLA	CBD-CGD-O2D-CED
29	r1	604	CLA	CHA-CBD-CGD-O1D
29	r1	604	CLA	CHA-CBD-CGD-O2D
29	r1	608	CLA	C1A-C2A-CAA-CBA
29	r1	608	CLA	C3A-C2A-CAA-CBA
29	r1	608	CLA	CHA-CBD-CGD-O1D
29	r1	608	CLA	CBD-CGD-O2D-CED
29	r1	609	CLA	CBD-CGD-O2D-CED
29	r1	610	CLA	CHA-CBD-CGD-O1D
29	r1	610	CLA	CHA-CBD-CGD-O2D
29	r1	610	CLA	CBD-CGD-O2D-CED
29	r1	612	CLA	CBD-CGD-O2D-CED
29	s1	602	CLA	C2-C1-O2A-CGA
29	s1	602	CLA	CHA-CBD-CGD-O1D
29	s1	602	CLA	CHA-CBD-CGD-O2D
29	s1	603	CLA	C1A-C2A-CAA-CBA
29	s1	603	CLA	C3A-C2A-CAA-CBA
29	s1	603	CLA	C2B-C3B-CAB-CBB
29	s1	603	CLA	C4B-C3B-CAB-CBB
29	s1	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	s1	605	CLA	CBA-CGA-O2A-C1
29	s1	605	CLA	O1A-CGA-O2A-C1
29	s1	605	CLA	C2B-C3B-CAB-CBB
29	s1	605	CLA	C4B-C3B-CAB-CBB
29	s1	609	CLA	CBD-CGD-O2D-CED
29	s1	610	CLA	C1A-C2A-CAA-CBA
29	s1	610	CLA	C3A-C2A-CAA-CBA
29	s1	610	CLA	C2-C3-C5-C6
29	s1	610	CLA	C4-C3-C5-C6
29	s1	611	CLA	C1A-C2A-CAA-CBA
29	s1	611	CLA	C3A-C2A-CAA-CBA
29	s1	611	CLA	CHA-CBD-CGD-O1D
29	s1	611	CLA	CHA-CBD-CGD-O2D
29	s1	611	CLA	CBD-CGD-O2D-CED
29	s1	613	CLA	CBD-CGD-O2D-CED
29	s1	614	CLA	C3A-C2A-CAA-CBA
29	s1	614	CLA	C2B-C3B-CAB-CBB
29	s1	614	CLA	C4B-C3B-CAB-CBB
29	s1	617	CLA	C1A-C2A-CAA-CBA
29	s1	617	CLA	C2-C1-O2A-CGA
29	s1	617	CLA	CHA-CBD-CGD-O1D
29	s1	617	CLA	CHA-CBD-CGD-O2D
29	y1	603	CLA	CHA-CBD-CGD-O1D
29	y1	603	CLA	CHA-CBD-CGD-O2D
29	y1	604	CLA	CHA-CBD-CGD-O1D
29	y1	604	CLA	CHA-CBD-CGD-O2D
29	y1	608	CLA	C2-C1-O2A-CGA
29	y1	608	CLA	CHA-CBD-CGD-O1D
29	y1	608	CLA	CHA-CBD-CGD-O2D
29	y1	608	CLA	CBD-CGD-O2D-CED
29	y1	610	CLA	CBD-CGD-O2D-CED
29	y1	611	CLA	C1A-C2A-CAA-CBA
29	y1	611	CLA	CHA-CBD-CGD-O1D
29	y1	611	CLA	CHA-CBD-CGD-O2D
29	y1	614	CLA	C2B-C3B-CAB-CBB
29	y1	614	CLA	C4B-C3B-CAB-CBB
30	A	409	PHO	C3A-C2A-CAA-CBA
30	a	408	PHO	C1A-C2A-CAA-CBA
30	a	409	PHO	C3A-C2A-CAA-CBA
31	A	411	BCR	C11-C12-C13-C35
31	A	411	BCR	C17-C18-C19-C20
31	A	411	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	B	618	BCR	C11-C10-C9-C8
31	B	618	BCR	C11-C10-C9-C34
31	B	618	BCR	C10-C11-C12-C13
31	B	618	BCR	C11-C12-C13-C14
31	B	618	BCR	C11-C12-C13-C35
31	B	618	BCR	C17-C18-C19-C20
31	B	618	BCR	C36-C18-C19-C20
31	B	618	BCR	C37-C22-C23-C24
31	B	619	BCR	C7-C8-C9-C10
31	B	619	BCR	C7-C8-C9-C34
31	B	619	BCR	C17-C18-C19-C20
31	B	619	BCR	C36-C18-C19-C20
31	B	619	BCR	C37-C22-C23-C24
31	C	514	BCR	C11-C10-C9-C8
31	C	514	BCR	C11-C10-C9-C34
31	C	514	BCR	C10-C11-C12-C13
31	C	514	BCR	C21-C22-C23-C24
31	C	514	BCR	C37-C22-C23-C24
31	C	515	BCR	C11-C10-C9-C8
31	C	515	BCR	C11-C10-C9-C34
31	C	515	BCR	C9-C10-C11-C12
31	C	515	BCR	C10-C11-C12-C13
31	C	515	BCR	C17-C18-C19-C20
31	C	515	BCR	C36-C18-C19-C20
31	C	515	BCR	C23-C24-C25-C30
31	C	516	BCR	C5-C6-C7-C8
31	C	516	BCR	C7-C8-C9-C34
31	C	516	BCR	C11-C10-C9-C8
31	C	516	BCR	C11-C10-C9-C34
31	C	516	BCR	C11-C12-C13-C14
31	C	516	BCR	C11-C12-C13-C35
31	C	517	BCR	C11-C10-C9-C8
31	C	517	BCR	C11-C10-C9-C34
31	C	517	BCR	C17-C18-C19-C20
31	C	517	BCR	C36-C18-C19-C20
31	D	404	BCR	C11-C10-C9-C8
31	D	404	BCR	C11-C10-C9-C34
31	D	404	BCR	C10-C11-C12-C13
31	D	404	BCR	C23-C24-C25-C26
31	a	411	BCR	C1-C6-C7-C8
31	a	411	BCR	C11-C10-C9-C8
31	a	411	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
31	a	411	BCR	C10-C11-C12-C13
31	a	411	BCR	C17-C18-C19-C20
31	a	411	BCR	C36-C18-C19-C20
31	b	618	BCR	C11-C10-C9-C8
31	b	618	BCR	C11-C10-C9-C34
31	b	618	BCR	C10-C11-C12-C13
31	c	514	BCR	C11-C10-C9-C8
31	c	514	BCR	C11-C10-C9-C34
31	c	514	BCR	C9-C10-C11-C12
31	c	514	BCR	C10-C11-C12-C13
31	c	514	BCR	C11-C12-C13-C14
31	c	514	BCR	C11-C12-C13-C35
31	c	514	BCR	C36-C18-C19-C20
31	c	514	BCR	C23-C24-C25-C30
31	c	515	BCR	C7-C8-C9-C10
31	c	515	BCR	C7-C8-C9-C34
31	c	515	BCR	C11-C10-C9-C8
31	c	515	BCR	C11-C10-C9-C34
31	c	515	BCR	C17-C18-C19-C20
31	c	515	BCR	C36-C18-C19-C20
31	c	515	BCR	C19-C20-C21-C22
31	c	515	BCR	C23-C24-C25-C30
31	c	516	BCR	C1-C6-C7-C8
31	c	516	BCR	C5-C6-C7-C8
31	c	516	BCR	C7-C8-C9-C10
31	c	516	BCR	C7-C8-C9-C34
31	c	516	BCR	C11-C10-C9-C8
31	c	516	BCR	C11-C10-C9-C34
31	c	516	BCR	C10-C11-C12-C13
31	c	516	BCR	C36-C18-C19-C20
31	c	516	BCR	C23-C24-C25-C30
31	c	517	BCR	C11-C10-C9-C8
31	c	517	BCR	C11-C10-C9-C34
31	c	517	BCR	C10-C11-C12-C13
31	c	517	BCR	C17-C18-C19-C20
31	c	517	BCR	C36-C18-C19-C20
31	d	404	BCR	C11-C10-C9-C8
31	d	404	BCR	C11-C10-C9-C34
31	d	404	BCR	C10-C11-C12-C13
31	d	404	BCR	C36-C18-C19-C20
31	d	404	BCR	C21-C22-C23-C24
31	d	404	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
31	d	404	BCR	C23-C24-C25-C26
31	d	404	BCR	C23-C24-C25-C30
31	A1	411	BCR	C11-C10-C9-C8
31	A1	411	BCR	C11-C10-C9-C34
31	A1	411	BCR	C10-C11-C12-C13
31	A1	411	BCR	C17-C18-C19-C20
31	A1	411	BCR	C36-C18-C19-C20
31	B1	618	BCR	C11-C10-C9-C8
31	B1	618	BCR	C11-C10-C9-C34
31	B1	618	BCR	C10-C11-C12-C13
31	B1	618	BCR	C17-C18-C19-C20
31	B1	618	BCR	C36-C18-C19-C20
31	B1	619	BCR	C11-C10-C9-C8
31	B1	619	BCR	C11-C10-C9-C34
31	B1	619	BCR	C11-C12-C13-C14
31	B1	619	BCR	C11-C12-C13-C35
31	B1	619	BCR	C19-C20-C21-C22
31	C1	514	BCR	C11-C10-C9-C8
31	C1	514	BCR	C11-C10-C9-C34
31	C1	514	BCR	C9-C10-C11-C12
31	C1	514	BCR	C10-C11-C12-C13
31	C1	514	BCR	C11-C12-C13-C35
31	C1	515	BCR	C11-C10-C9-C8
31	C1	515	BCR	C11-C10-C9-C34
31	C1	515	BCR	C10-C11-C12-C13
31	C1	515	BCR	C17-C18-C19-C20
31	C1	515	BCR	C36-C18-C19-C20
31	C1	516	BCR	C1-C6-C7-C8
31	C1	516	BCR	C5-C6-C7-C8
31	C1	516	BCR	C7-C8-C9-C10
31	C1	516	BCR	C7-C8-C9-C34
31	C1	516	BCR	C11-C10-C9-C8
31	C1	516	BCR	C11-C10-C9-C34
31	C1	516	BCR	C10-C11-C12-C13
31	C1	516	BCR	C21-C22-C23-C24
31	C1	516	BCR	C37-C22-C23-C24
31	C1	517	BCR	C11-C10-C9-C8
31	C1	517	BCR	C11-C10-C9-C34
31	C1	517	BCR	C10-C11-C12-C13
31	C1	517	BCR	C17-C18-C19-C20
31	C1	517	BCR	C36-C18-C19-C20
31	D1	404	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	D1	404	BCR	C11-C10-C9-C34
31	D1	404	BCR	C10-C11-C12-C13
31	D1	404	BCR	C17-C18-C19-C20
31	D1	404	BCR	C36-C18-C19-C20
31	D1	404	BCR	C23-C24-C25-C26
31	D1	404	BCR	C23-C24-C25-C30
31	a1	411	BCR	C11-C10-C9-C8
31	a1	411	BCR	C11-C10-C9-C34
31	a1	411	BCR	C10-C11-C12-C13
31	a1	411	BCR	C19-C20-C21-C22
31	b1	618	BCR	C11-C10-C9-C8
31	b1	618	BCR	C11-C10-C9-C34
31	b1	618	BCR	C10-C11-C12-C13
31	b1	618	BCR	C11-C12-C13-C14
31	b1	618	BCR	C11-C12-C13-C35
31	b1	619	BCR	C7-C8-C9-C10
31	b1	619	BCR	C7-C8-C9-C34
31	b1	619	BCR	C11-C10-C9-C8
31	b1	619	BCR	C11-C10-C9-C34
31	b1	619	BCR	C10-C11-C12-C13
31	c1	514	BCR	C11-C10-C9-C8
31	c1	514	BCR	C11-C10-C9-C34
31	c1	514	BCR	C9-C10-C11-C12
31	c1	514	BCR	C10-C11-C12-C13
31	c1	515	BCR	C11-C10-C9-C8
31	c1	515	BCR	C11-C10-C9-C34
31	c1	515	BCR	C10-C11-C12-C13
31	c1	516	BCR	C5-C6-C7-C8
31	c1	516	BCR	C7-C8-C9-C10
31	c1	516	BCR	C7-C8-C9-C34
31	c1	516	BCR	C11-C10-C9-C8
31	c1	516	BCR	C11-C10-C9-C34
31	c1	516	BCR	C10-C11-C12-C13
31	c1	516	BCR	C17-C18-C19-C20
31	c1	516	BCR	C36-C18-C19-C20
31	c1	516	BCR	C21-C22-C23-C24
31	c1	516	BCR	C37-C22-C23-C24
31	c1	517	BCR	C11-C10-C9-C8
31	c1	517	BCR	C11-C10-C9-C34
31	c1	517	BCR	C10-C11-C12-C13
31	c1	517	BCR	C17-C18-C19-C20
31	c1	517	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	c1	517	BCR	C21-C22-C23-C24
31	c1	517	BCR	C37-C22-C23-C24
31	d1	404	BCR	C11-C10-C9-C8
31	d1	404	BCR	C11-C10-C9-C34
31	d1	404	BCR	C10-C11-C12-C13
31	d1	404	BCR	C11-C12-C13-C14
31	d1	404	BCR	C11-C12-C13-C35
31	d1	404	BCR	C13-C14-C15-C16
31	d1	404	BCR	C21-C22-C23-C24
31	d1	404	BCR	C37-C22-C23-C24
31	d1	404	BCR	C23-C24-C25-C26
31	d1	404	BCR	C23-C24-C25-C30
32	A	412	SQD	C5-C6-S-O7
32	A	412	SQD	C5-C6-S-O8
32	A	412	SQD	C5-C6-S-O9
32	B	621	SQD	C2-C1-O6-C44
32	B	621	SQD	O5-C1-O6-C44
32	B	621	SQD	O5-C5-C6-S
32	B	621	SQD	C5-C6-S-O7
32	B	621	SQD	C5-C6-S-O8
32	B	621	SQD	C5-C6-S-O9
32	B	626	SQD	C2-C1-O6-C44
32	B	626	SQD	O5-C1-O6-C44
32	B	626	SQD	C5-C6-S-O7
32	B	626	SQD	C5-C6-S-O8
32	B	626	SQD	C5-C6-S-O9
32	C	526	SQD	O5-C5-C6-S
32	C	526	SQD	C5-C6-S-O7
32	C	526	SQD	C5-C6-S-O8
32	C	526	SQD	C5-C6-S-O9
32	M	101	SQD	C5-C6-S-O7
32	M	101	SQD	C5-C6-S-O8
32	M	101	SQD	C5-C6-S-O9
32	a	412	SQD	O47-C45-C46-O48
32	a	412	SQD	O5-C5-C6-S
32	b	621	SQD	O5-C1-O6-C44
32	b	621	SQD	O5-C5-C6-S
32	b	626	SQD	C2-C1-O6-C44
32	b	626	SQD	O5-C1-O6-C44
32	m	101	SQD	C5-C6-S-O7
32	m	101	SQD	C5-C6-S-O8
32	m	101	SQD	C5-C6-S-O9

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Mol	Chain	Res	Type	Atoms
32	B1	621	SQD	C2-C1-O6-C44
32	B1	621	SQD	O5-C1-O6-C44
32	B1	621	SQD	O5-C5-C6-S
32	B1	626	SQD	C2-C1-O6-C44
32	B1	626	SQD	O5-C1-O6-C44
32	B1	626	SQD	C5-C6-S-O7
32	B1	626	SQD	C5-C6-S-O8
32	B1	626	SQD	C5-C6-S-O9
32	C1	526	SQD	O5-C5-C6-S
32	C1	526	SQD	C5-C6-S-O7
32	C1	526	SQD	C5-C6-S-O8
32	C1	526	SQD	C5-C6-S-O9
32	M1	101	SQD	C5-C6-S-O7
32	M1	101	SQD	C5-C6-S-O8
32	M1	101	SQD	C5-C6-S-O9
32	a1	412	SQD	O47-C45-C46-O48
32	a1	412	SQD	O5-C5-C6-S
32	b1	621	SQD	C2-C1-O6-C44
32	b1	621	SQD	O5-C1-O6-C44
32	c1	526	SQD	O5-C5-C6-S
32	m1	101	SQD	O5-C5-C6-S
32	m1	101	SQD	C5-C6-S-O8
33	A	413	LMG	O6-C1-O1-C7
33	B	622	LMG	O9-C10-O7-C8
33	B	622	LMG	C11-C10-O7-C8
33	W	201	LMG	O6-C1-O1-C7
33	W	201	LMG	C7-C8-O7-C10
33	W	201	LMG	C11-C10-O7-C8
33	a	413	LMG	O6-C1-O1-C7
33	b	622	LMG	O6-C1-O1-C7
33	b	622	LMG	O9-C10-O7-C8
33	b	622	LMG	C11-C10-O7-C8
33	B1	622	LMG	O6-C1-O1-C7
33	B1	622	LMG	O9-C10-O7-C8
33	W1	201	LMG	C11-C10-O7-C8
33	b1	622	LMG	O9-C10-O7-C8
33	c1	521	LMG	O10-C28-O8-C9
33	c1	523	LMG	C2-C1-O1-C7
33	c1	523	LMG	O6-C1-O1-C7
34	A	414	SPH	C1-C2-C3-O3
34	A	414	SPH	C1-C2-C3-C4
34	A	414	SPH	N2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
34	A	414	SPH	N2-C2-C3-C4
34	A	414	SPH	C2-C3-C4-C5
34	A	414	SPH	O3-C3-C4-C5
34	Y	625	SPH	C1-C2-C3-O3
34	Y	625	SPH	C1-C2-C3-C4
34	Y	625	SPH	N2-C2-C3-O3
34	Y	625	SPH	N2-C2-C3-C4
34	Y	625	SPH	C2-C3-C4-C5
34	a	414	SPH	O1-C1-C2-N2
34	a	414	SPH	O1-C1-C2-C3
34	a	414	SPH	C1-C2-C3-O3
34	a	414	SPH	C1-C2-C3-C4
34	a	414	SPH	N2-C2-C3-O3
34	a	414	SPH	N2-C2-C3-C4
34	y	625	SPH	C2-C3-C4-C5
34	y	625	SPH	O3-C3-C4-C5
34	A1	414	SPH	O1-C1-C2-N2
34	A1	414	SPH	O1-C1-C2-C3
34	A1	414	SPH	C1-C2-C3-O3
34	A1	414	SPH	C1-C2-C3-C4
34	A1	414	SPH	N2-C2-C3-O3
34	A1	414	SPH	N2-C2-C3-C4
34	Y1	625	SPH	O1-C1-C2-N2
34	Y1	625	SPH	O1-C1-C2-C3
34	Y1	625	SPH	C2-C3-C4-C5
34	Y1	625	SPH	O3-C3-C4-C5
34	a1	414	SPH	O1-C1-C2-N2
34	a1	414	SPH	C1-C2-C3-O3
34	y1	625	SPH	C1-C2-C3-O3
34	y1	625	SPH	C1-C2-C3-C4
34	y1	625	SPH	N2-C2-C3-C4
36	B	620	C7Z	C21-C26-C27-C28
36	B	620	C7Z	C27-C28-C29-C30
36	B	620	C7Z	C27-C28-C29-C39
36	b	620	C7Z	C5-C6-C7-C8
36	b	620	C7Z	C27-C28-C29-C30
36	b	620	C7Z	C27-C28-C29-C39
36	B1	620	C7Z	C27-C28-C29-C30
36	B1	620	C7Z	C27-C28-C29-C39
36	b1	620	C7Z	C11-C12-C13-C20
36	b1	620	C7Z	C11-C12-C13-C14
36	b1	620	C7Z	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
36	b1	620	C7Z	C27-C28-C29-C39
37	B	623	DGD	C2B-C1B-O2G-C2G
37	B	623	DGD	O1B-C1B-O2G-C2G
37	B	623	DGD	O6D-C1D-O3G-C3G
37	B	623	DGD	C2E-C1E-O5D-C6D
37	B	623	DGD	O6E-C1E-O5D-C6D
37	b	623	DGD	O1B-C1B-O2G-C2G
37	b	623	DGD	O6D-C1D-O3G-C3G
37	b	623	DGD	C2E-C1E-O5D-C6D
37	b	623	DGD	O6E-C1E-O5D-C6D
37	B1	623	DGD	O1B-C1B-O2G-C2G
37	B1	623	DGD	C2D-C1D-O3G-C3G
37	B1	623	DGD	O6D-C1D-O3G-C3G
37	B1	623	DGD	C2E-C1E-O5D-C6D
37	B1	623	DGD	O6E-C1E-O5D-C6D
37	b1	623	DGD	O1B-C1B-O2G-C2G
37	b1	623	DGD	O6D-C1D-O3G-C3G
37	b1	623	DGD	O6E-C1E-O5D-C6D
38	B	624	3PH	C1-O11-P-O13
38	B	624	3PH	C1-O11-P-O14
38	B	624	3PH	C1-O11-P-O12
38	T	101	3PH	C1-O11-P-O14
38	T	101	3PH	C1-O11-P-O12
38	T	101	3PH	C22-C21-O21-C2
38	S	626	3PH	C1-C2-O21-C21
38	S	626	3PH	O22-C21-O21-C2
38	b	624	3PH	C1-O11-P-O14
38	b	624	3PH	O22-C21-O21-C2
38	b	624	3PH	C22-C21-O21-C2
38	t	101	3PH	C1-O11-P-O13
38	t	101	3PH	C1-O11-P-O14
38	t	101	3PH	O22-C21-O21-C2
38	t	101	3PH	C22-C21-O21-C2
38	s	626	3PH	O22-C21-O21-C2
38	T1	101	3PH	C1-O11-P-O13
38	T1	101	3PH	C1-O11-P-O14
38	T1	101	3PH	C1-O11-P-O12
38	T1	101	3PH	C22-C21-O21-C2
38	S1	626	3PH	C1-O11-P-O13
38	S1	626	3PH	C1-O11-P-O14
38	S1	626	3PH	C1-O11-P-O12
38	S1	626	3PH	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
38	b1	624	3PH	C1-O11-P-O13
38	b1	624	3PH	C1-O11-P-O14
38	b1	624	3PH	O21-C2-C3-O31
38	b1	624	3PH	C22-C21-O21-C2
38	b1	624	3PH	O32-C31-O31-C3
38	b1	624	3PH	C32-C31-O31-C3
38	t1	101	3PH	O22-C21-O21-C2
38	s1	626	3PH	C1-O11-P-O13
38	s1	626	3PH	C1-O11-P-O14
38	s1	626	3PH	O22-C21-O21-C2
39	B	625	DGA	CG1-CG2-OG2-CB1
39	B	625	DGA	CG1-CG2-CG3-OXT
39	B	625	DGA	OG2-CG2-CG3-OXT
39	J	101	DGA	CG1-CG2-CG3-OXT
39	J	101	DGA	OG2-CG2-CG3-OXT
39	b	625	DGA	CG1-CG2-CG3-OXT
39	b	625	DGA	OG2-CG2-CG3-OXT
39	j	101	DGA	CG1-CG2-CG3-OXT
39	j	101	DGA	OG2-CG2-CG3-OXT
39	B1	625	DGA	OB1-CB1-OG2-CG2
39	b1	625	DGA	CB2-CB1-OG2-CG2
39	b1	625	DGA	OB1-CB1-OG2-CG2
39	c1	524	DGA	OG2-CG2-CG3-OXT
40	C	525	LHG	C3-O3-P-O4
40	C	525	LHG	C4-O6-P-O3
40	C	525	LHG	C4-O6-P-O4
40	C	525	LHG	C4-O6-P-O5
40	D	408	LHG	O1-C1-C2-C3
40	D	408	LHG	O2-C2-C3-O3
40	D	408	LHG	C3-O3-P-O4
40	D	408	LHG	C4-O6-P-O5
40	D	409	LHG	O1-C1-C2-C3
40	D	409	LHG	C1-C2-C3-O3
40	D	409	LHG	C3-O3-P-O5
40	D	410	LHG	O1-C1-C2-O2
40	D	410	LHG	O1-C1-C2-C3
40	D	410	LHG	C3-O3-P-O5
40	D	410	LHG	C4-O6-P-O5
40	D	410	LHG	O7-C5-C6-O8
40	L	101	LHG	C3-O3-P-O4
40	L	101	LHG	C3-O3-P-O5
40	L	101	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
40	L	101	LHG	C8-C7-O7-C5
40	N	624	LHG	C1-C2-C3-O3
40	N	624	LHG	C3-O3-P-O5
40	N	624	LHG	C4-O6-P-O3
40	N	624	LHG	C4-O6-P-O4
40	N	624	LHG	C4-O6-P-O5
40	N	624	LHG	O7-C5-C6-O8
40	G	624	LHG	O1-C1-C2-C3
40	G	624	LHG	C1-C2-C3-O3
40	G	624	LHG	C3-O3-P-O5
40	G	624	LHG	C4-O6-P-O4
40	G	624	LHG	O7-C5-C6-O8
40	S	624	LHG	O1-C1-C2-C3
40	S	624	LHG	C3-O3-P-O5
40	S	624	LHG	C4-O6-P-O4
40	S	624	LHG	C4-O6-P-O5
40	Y	624	LHG	C4-O6-P-O5
40	c	525	LHG	C1-C2-C3-O3
40	c	525	LHG	C4-O6-P-O4
40	d	408	LHG	O1-C1-C2-C3
40	d	408	LHG	C1-C2-C3-O3
40	d	408	LHG	C4-O6-P-O5
40	d	409	LHG	C3-O3-P-O6
40	d	409	LHG	C4-O6-P-O3
40	d	409	LHG	C4-O6-P-O4
40	d	409	LHG	C4-O6-P-O5
40	d	410	LHG	C1-C2-C3-O3
40	d	410	LHG	C3-O3-P-O4
40	d	410	LHG	C3-O3-P-O5
40	d	410	LHG	C3-O3-P-O6
40	d	410	LHG	C4-O6-P-O5
40	d	410	LHG	O7-C5-C6-O8
40	l	101	LHG	O1-C1-C2-C3
40	l	101	LHG	C3-O3-P-O4
40	l	101	LHG	C4-O6-P-O5
40	l	101	LHG	O9-C7-O7-C5
40	l	101	LHG	C8-C7-O7-C5
40	n	624	LHG	C1-C2-C3-O3
40	n	624	LHG	O2-C2-C3-O3
40	n	624	LHG	C3-O3-P-O6
40	n	624	LHG	C4-O6-P-O4
40	n	624	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
40	g	624	LHG	C4-O6-P-O5
40	s	624	LHG	O1-C1-C2-C3
40	s	624	LHG	O2-C2-C3-O3
40	s	624	LHG	C3-O3-P-O5
40	y	624	LHG	O1-C1-C2-C3
40	y	624	LHG	C3-O3-P-O5
40	D1	408	LHG	O1-C1-C2-C3
40	D1	408	LHG	C3-O3-P-O4
40	D1	408	LHG	C3-O3-P-O5
40	D1	408	LHG	C3-O3-P-O6
40	D1	409	LHG	O1-C1-C2-C3
40	D1	409	LHG	O2-C2-C3-O3
40	D1	409	LHG	C3-O3-P-O4
40	D1	409	LHG	C4-O6-P-O5
40	D1	410	LHG	O1-C1-C2-O2
40	D1	410	LHG	O1-C1-C2-C3
40	D1	410	LHG	C3-O3-P-O4
40	D1	410	LHG	C3-O3-P-O5
40	D1	410	LHG	C3-O3-P-O6
40	D1	410	LHG	C4-O6-P-O5
40	L1	101	LHG	O1-C1-C2-C3
40	L1	101	LHG	C4-O6-P-O4
40	L1	101	LHG	C5-C6-O8-C23
40	L1	101	LHG	O9-C7-O7-C5
40	L1	101	LHG	C8-C7-O7-C5
40	N1	624	LHG	O1-C1-C2-C3
40	N1	624	LHG	O2-C2-C3-O3
40	N1	624	LHG	C3-O3-P-O5
40	N1	624	LHG	C4-O6-P-O5
40	G1	624	LHG	O1-C1-C2-O2
40	G1	624	LHG	C4-O6-P-O5
40	G1	624	LHG	O7-C5-C6-O8
40	S1	624	LHG	C3-O3-P-O5
40	S1	624	LHG	C4-O6-P-O3
40	S1	624	LHG	C4-O6-P-O4
40	S1	624	LHG	C4-O6-P-O5
40	Y1	624	LHG	O1-C1-C2-C3
40	Y1	624	LHG	C1-C2-C3-O3
40	Y1	624	LHG	O2-C2-C3-O3
40	Y1	624	LHG	C3-O3-P-O5
40	c1	525	LHG	O1-C1-C2-O2
40	c1	525	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
40	d1	408	LHG	O1-C1-C2-C3
40	d1	408	LHG	C1-C2-C3-O3
40	d1	408	LHG	C3-O3-P-O4
40	d1	408	LHG	C3-O3-P-O5
40	d1	408	LHG	C4-O6-P-O5
40	d1	409	LHG	O1-C1-C2-O2
40	d1	409	LHG	O1-C1-C2-C3
40	d1	409	LHG	C1-C2-C3-O3
40	d1	409	LHG	C4-O6-P-O3
40	d1	410	LHG	O1-C1-C2-C3
40	d1	410	LHG	C3-O3-P-O4
40	d1	410	LHG	C3-O3-P-O5
40	d1	410	LHG	C3-O3-P-O6
40	d1	410	LHG	C4-O6-P-O5
40	d1	410	LHG	O7-C5-C6-O8
40	n1	624	LHG	O1-C1-C2-C3
40	n1	624	LHG	C4-O6-P-O4
40	n1	624	LHG	O7-C5-C6-O8
40	g1	624	LHG	O1-C1-C2-C3
40	g1	624	LHG	O2-C2-C3-O3
40	g1	624	LHG	C4-O6-P-O3
40	g1	624	LHG	C4-O6-P-O4
40	g1	624	LHG	C4-O6-P-O5
40	g1	624	LHG	O7-C5-C6-O8
40	g1	624	LHG	C8-C7-O7-C5
40	s1	624	LHG	O1-C1-C2-C3
40	s1	624	LHG	C1-C2-C3-O3
40	s1	624	LHG	C4-O6-P-O3
40	s1	624	LHG	C4-O6-P-O4
40	s1	624	LHG	C4-O6-P-O5
40	y1	624	LHG	O1-C1-C2-C3
40	y1	624	LHG	C4-O6-P-O5
41	C	527	LMK	C7-C8-O7-C10
41	C	527	LMK	C1-C2-C3-C4
41	C	527	LMK	C1-C2-C3-N4
41	C	527	LMK	C2-C3-N4-C5
41	C	527	LMK	C2-C3-N4-C6
41	C	527	LMK	C2-C3-N4-C46
41	C1	527	LMK	O9-C10-O7-C8
41	C1	527	LMK	C1-C2-C3-C4
41	C1	527	LMK	C1-C2-C3-N4
41	C1	527	LMK	C2-C3-N4-C5

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Mol	Chain	Res	Type	Atoms
41	C1	527	LMK	C2-C3-N4-C6
41	C1	527	LMK	C2-C3-N4-C46
43	D	405	PL9	C37-C38-C39-C41
43	d	405	PL9	C37-C38-C39-C40
43	D1	405	PL9	C7-C8-C9-C10
43	D1	405	PL9	C12-C11-C9-C8
43	D1	405	PL9	C18-C19-C21-C22
43	D1	405	PL9	C22-C23-C24-C26
43	D1	405	PL9	C27-C28-C29-C31
43	d1	405	PL9	C37-C38-C39-C40
43	d1	405	PL9	C37-C38-C39-C41
43	d1	405	PL9	C42-C43-C44-C46
45	H	101	RRX	C23-C24-C25-C26
45	h	101	RRX	C23-C24-C25-C26
45	h	101	RRX	C5-C6-C7-C8
45	H1	101	RRX	C23-C24-C25-C26
45	H1	101	RRX	C37-C22-C23-C24
45	H1	101	RRX	C21-C22-C23-C24
45	H1	101	RRX	C19-C20-C21-C22
45	h1	101	RRX	C23-C24-C25-C26
45	h1	101	RRX	C5-C6-C7-C8
46	I	101	GOL	C1-C2-C3-O3
47	I	102	4RF	O18-C19-C20-O21
47	I	102	4RF	C24-C22-O21-C20
47	K	101	4RF	O21-C20-C39-O40
47	i	101	4RF	O18-C19-C20-O21
47	i	101	4RF	O21-C20-C39-O40
47	i	101	4RF	C24-C22-O21-C20
47	i	101	4RF	C15-C16-O18-C19
47	I1	102	4RF	C24-C22-O21-C20
47	I1	102	4RF	C15-C16-O18-C19
47	I1	102	4RF	O17-C16-O18-C19
47	K1	101	4RF	O21-C20-C39-O40
47	i1	101	4RF	C24-C22-O21-C20
48	N	605	CHL	C2A-CAA-CBA-CGA
48	N	609	CHL	CHA-CBD-CGD-O1D
48	N	609	CHL	CHA-CBD-CGD-O2D
48	G	601	CHL	CHA-CBD-CGD-O1D
48	G	601	CHL	CHA-CBD-CGD-O2D
48	G	605	CHL	C1A-C2A-CAA-CBA
48	G	605	CHL	C3A-C2A-CAA-CBA
48	G	609	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
48	G	609	CHL	CHA-CBD-CGD-O2D
48	G	609	CHL	C4-C3-C5-C6
48	R	607	CHL	CHA-CBD-CGD-O1D
48	R	607	CHL	CHA-CBD-CGD-O2D
48	Y	601	CHL	CHA-CBD-CGD-O1D
48	Y	601	CHL	CHA-CBD-CGD-O2D
48	n	601	CHL	CHA-CBD-CGD-O1D
48	n	601	CHL	CHA-CBD-CGD-O2D
48	n	608	CHL	CHA-CBD-CGD-O1D
48	n	608	CHL	CHA-CBD-CGD-O2D
48	g	601	CHL	CHA-CBD-CGD-O1D
48	g	601	CHL	CHA-CBD-CGD-O2D
48	g	605	CHL	C1A-C2A-CAA-CBA
48	g	605	CHL	CHA-CBD-CGD-O1D
48	g	605	CHL	CHA-CBD-CGD-O2D
48	g	609	CHL	C2-C3-C5-C6
48	g	609	CHL	C4-C3-C5-C6
48	r	606	CHL	CHA-CBD-CGD-O1D
48	s	601	CHL	CHA-CBD-CGD-O1D
48	s	601	CHL	CHA-CBD-CGD-O2D
48	s	606	CHL	CHA-CBD-CGD-O1D
48	s	606	CHL	CHA-CBD-CGD-O2D
48	y	606	CHL	C2-C3-C5-C6
48	y	606	CHL	C4-C3-C5-C6
48	y	607	CHL	C14-C13-C15-C16
48	N1	608	CHL	CHA-CBD-CGD-O1D
48	N1	608	CHL	CHA-CBD-CGD-O2D
48	N1	609	CHL	CHA-CBD-CGD-O1D
48	N1	609	CHL	CHA-CBD-CGD-O2D
48	N1	609	CHL	CAD-CBD-CGD-O1D
48	N1	609	CHL	CAD-CBD-CGD-O2D
48	G1	601	CHL	CHA-CBD-CGD-O1D
48	G1	601	CHL	CHA-CBD-CGD-O2D
48	G1	605	CHL	CHA-CBD-CGD-O1D
48	G1	605	CHL	CHA-CBD-CGD-O2D
48	G1	607	CHL	C1A-C2A-CAA-CBA
48	G1	609	CHL	CHA-CBD-CGD-O1D
48	G1	609	CHL	CHA-CBD-CGD-O2D
48	G1	609	CHL	C2-C3-C5-C6
48	G1	609	CHL	C4-C3-C5-C6
48	R1	606	CHL	CHA-CBD-CGD-O1D
48	R1	606	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
48	S1	601	CHL	CHA-CBD-CGD-O1D
48	S1	601	CHL	CHA-CBD-CGD-O2D
48	S1	608	CHL	CHA-CBD-CGD-O1D
48	S1	608	CHL	CHA-CBD-CGD-O2D
48	Y1	601	CHL	CHA-CBD-CGD-O1D
48	Y1	601	CHL	CHA-CBD-CGD-O2D
48	Y1	609	CHL	CHA-CBD-CGD-O1D
48	Y1	609	CHL	CHA-CBD-CGD-O2D
48	n1	601	CHL	CHA-CBD-CGD-O1D
48	n1	601	CHL	C2-C3-C5-C6
48	n1	601	CHL	C4-C3-C5-C6
48	n1	606	CHL	C2A-CAA-CBA-CGA
48	g1	601	CHL	CHA-CBD-CGD-O1D
48	g1	601	CHL	CHA-CBD-CGD-O2D
48	g1	605	CHL	C1A-C2A-CAA-CBA
48	g1	605	CHL	CHA-CBD-CGD-O1D
48	g1	605	CHL	CHA-CBD-CGD-O2D
48	g1	607	CHL	C1A-C2A-CAA-CBA
48	g1	607	CHL	C3A-C2A-CAA-CBA
48	g1	609	CHL	CHA-CBD-CGD-O1D
48	g1	609	CHL	CHA-CBD-CGD-O2D
48	g1	609	CHL	C2-C3-C5-C6
48	g1	609	CHL	C4-C3-C5-C6
48	r1	606	CHL	CHA-CBD-CGD-O1D
48	r1	607	CHL	CHA-CBD-CGD-O1D
48	r1	607	CHL	CHA-CBD-CGD-O2D
48	s1	601	CHL	CHA-CBD-CGD-O1D
48	s1	601	CHL	CHA-CBD-CGD-O2D
48	s1	608	CHL	CHA-CBD-CGD-O1D
48	s1	608	CHL	CHA-CBD-CGD-O2D
48	y1	601	CHL	C3A-C2A-CAA-CBA
48	y1	601	CHL	CHA-CBD-CGD-O1D
48	y1	601	CHL	CHA-CBD-CGD-O2D
48	y1	607	CHL	C11-C10-C8-C9
49	N	621	LUT	C21-C26-C27-C28
49	G	621	LUT	C21-C26-C27-C28
49	S	621	LUT	C25-C26-C27-C28
49	Y	621	LUT	C21-C26-C27-C28
49	n	620	LUT	C31-C32-C33-C34
49	n	620	LUT	C31-C32-C33-C40
49	g	620	LUT	C25-C26-C27-C28
49	g	620	LUT	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
49	g	620	LUT	C31-C32-C33-C40
49	r	620	LUT	C11-C12-C13-C14
49	r	620	LUT	C11-C12-C13-C20
49	s	621	LUT	C31-C32-C33-C34
49	s	621	LUT	C31-C32-C33-C40
49	y	621	LUT	C21-C26-C27-C28
49	N1	620	LUT	C27-C28-C29-C39
49	N1	621	LUT	C7-C8-C9-C10
49	N1	621	LUT	C7-C8-C9-C19
49	G1	620	LUT	C1-C6-C7-C8
49	R1	620	LUT	C7-C8-C9-C10
49	R1	620	LUT	C7-C8-C9-C19
49	R1	620	LUT	C31-C32-C33-C34
49	R1	620	LUT	C31-C32-C33-C40
49	S1	620	LUT	C25-C26-C27-C28
49	S1	621	LUT	C11-C12-C13-C20
49	S1	621	LUT	C27-C28-C29-C39
49	Y1	620	LUT	C25-C26-C27-C28
49	Y1	620	LUT	C27-C28-C29-C30
49	Y1	620	LUT	C27-C28-C29-C39
49	Y1	620	LUT	C31-C32-C33-C34
49	Y1	620	LUT	C31-C32-C33-C40
49	Y1	621	LUT	C21-C26-C27-C28
49	n1	621	LUT	C1-C6-C7-C8
49	n1	621	LUT	C21-C26-C27-C28
49	g1	620	LUT	C27-C28-C29-C30
49	g1	620	LUT	C27-C28-C29-C39
49	g1	621	LUT	C21-C26-C27-C28
49	r1	620	LUT	C27-C28-C29-C30
49	r1	620	LUT	C27-C28-C29-C39
49	s1	620	LUT	C27-C28-C29-C30
49	s1	620	LUT	C27-C28-C29-C39
49	s1	621	LUT	C1-C6-C7-C8
49	s1	621	LUT	C11-C12-C13-C14
49	s1	621	LUT	C11-C12-C13-C20
49	y1	621	LUT	C21-C26-C27-C28
50	N	622	XAT	C27-C28-C29-C30
50	N	622	XAT	C27-C28-C29-C39
50	n	622	XAT	C11-C12-C13-C20
50	y	622	XAT	C20-C13-C14-C15
50	y	622	XAT	C14-C15-C35-C34
50	y	622	XAT	O24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
50	y	622	XAT	C31-C32-C33-C34
50	y	622	XAT	C31-C32-C33-C40
50	G1	622	XAT	C26-C27-C28-C29
50	R1	621	XAT	C31-C32-C33-C34
50	R1	621	XAT	C31-C32-C33-C40
50	Y1	622	XAT	C26-C27-C28-C29
50	n1	622	XAT	C27-C28-C29-C39
50	r1	621	XAT	C30-C31-C32-C33
50	y1	622	XAT	C31-C32-C33-C34
50	y1	622	XAT	C31-C32-C33-C40
51	R	622	NEX	C12-C13-C14-C15
51	R	622	NEX	C20-C13-C14-C15
51	R	622	NEX	C14-C15-C35-C34
51	R	622	NEX	C30-C31-C32-C33
51	Y	623	NEX	C11-C12-C13-C14
51	Y	623	NEX	C11-C12-C13-C20
51	g	623	NEX	C30-C31-C32-C33
51	g	623	NEX	C31-C32-C33-C34
51	g	623	NEX	C31-C32-C33-C40
51	r	622	NEX	C10-C11-C12-C13
51	r	622	NEX	C12-C13-C14-C15
51	r	622	NEX	C20-C13-C14-C15
51	r	622	NEX	C14-C15-C35-C34
51	s	623	NEX	C7-C8-C9-C19
51	G1	623	NEX	C10-C11-C12-C13
51	R1	622	NEX	C7-C8-C9-C19
51	R1	622	NEX	C10-C11-C12-C13
51	R1	622	NEX	C20-C13-C14-C15
51	R1	622	NEX	C14-C15-C35-C34
51	R1	622	NEX	C30-C31-C32-C33
51	S1	623	NEX	C28-C29-C30-C31
51	S1	623	NEX	C39-C29-C30-C31
51	Y1	623	NEX	C11-C12-C13-C20
51	Y1	623	NEX	C14-C15-C35-C34
51	r1	622	NEX	C12-C13-C14-C15
51	r1	622	NEX	C20-C13-C14-C15
51	r1	622	NEX	C28-C29-C30-C31
51	r1	622	NEX	C39-C29-C30-C31
51	r1	622	NEX	C30-C31-C32-C33
51	r1	622	NEX	C32-C33-C34-C35
51	r1	622	NEX	C40-C33-C34-C35
51	y1	623	NEX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
51	y1	623	NEX	C11-C12-C13-C20
52	r	625	LMT	O5'-C1'-O1'-C1
53	R	626	ERG	C16-C17-C20-C21
53	r	626	ERG	C13-C17-C20-C21
53	r	626	ERG	C16-C17-C20-C21
53	R1	626	ERG	C13-C17-C20-C21
53	R1	626	ERG	C16-C17-C20-C21
53	R1	626	ERG	C16-C17-C20-C22
53	r1	626	ERG	C13-C17-C20-C21
53	r1	626	ERG	C13-C17-C20-C22
53	r1	626	ERG	C16-C17-C20-C21
53	r1	626	ERG	C16-C17-C20-C22
53	r1	626	ERG	C22-C23-C24-C25
54	S	625	LPX	O1-C3-C4-C5
54	S	625	LPX	C3-O1-P1-O3
54	S	625	LPX	C3-O1-P1-O2
54	S	625	LPX	C3-O1-P1-O4
54	S	625	LPX	C1-O2-P1-O4
54	S	625	LPX	O2-C1-C2-N1
54	s	625	LPX	C3-C4-C5-O6
54	s	625	LPX	C1-O2-P1-O4
54	S1	625	LPX	O1-C3-C4-C5
54	S1	625	LPX	O1-C3-C4-O5
54	S1	625	LPX	C3-O1-P1-O2
54	S1	625	LPX	O2-C1-C2-N1
54	s1	625	LPX	O5-C4-C5-O6
54	s1	625	LPX	C3-C4-C5-O6
54	s1	625	LPX	C3-O1-P1-O4
54	s1	625	LPX	C1-O2-P1-O3
54	s1	625	LPX	O2-C1-C2-N1
55	Y	626	PTY	C3-O11-P1-O12
55	Y	626	PTY	C3-O11-P1-O14
55	Y	627	PTY	N1-C2-C3-O11
55	Y	627	PTY	C5-O14-P1-O11
55	y	626	PTY	C3-O11-P1-O12
55	y	626	PTY	C3-O11-P1-O13
55	y	626	PTY	C3-O11-P1-O14
55	y	626	PTY	C5-O14-P1-O13
55	y	627	PTY	N1-C2-C3-O11
55	y	627	PTY	O10-C8-O7-C6
55	y	627	PTY	C11-C8-O7-C6
55	y	627	PTY	C5-O14-P1-O11

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Mol	Chain	Res	Type	Atoms
55	y	627	PTY	C5-O14-P1-O12
55	y	627	PTY	C5-O14-P1-O13
55	Y1	626	PTY	N1-C2-C3-O11
55	Y1	626	PTY	C2-C3-O11-P1
55	Y1	627	PTY	N1-C2-C3-O11
55	Y1	627	PTY	C5-O14-P1-O12
55	Y1	627	PTY	C5-O14-P1-O13
55	y1	626	PTY	C11-C8-O7-C6
55	y1	626	PTY	C5-O14-P1-O11
55	y1	626	PTY	C5-O14-P1-O12
55	y1	627	PTY	C5-O14-P1-O13
55	Y1	627	PTY	C11-C8-O7-C6
55	y1	627	PTY	C11-C8-O7-C6
29	A	405	CLA	O1D-CGD-O2D-CED
29	R	603	CLA	O1D-CGD-O2D-CED
29	S	603	CLA	O1D-CGD-O2D-CED
29	S	613	CLA	O1D-CGD-O2D-CED
29	a	405	CLA	O1D-CGD-O2D-CED
29	b	602	CLA	O1D-CGD-O2D-CED
29	r	609	CLA	O1D-CGD-O2D-CED
29	B1	612	CLA	O1D-CGD-O2D-CED
29	B1	615	CLA	O1D-CGD-O2D-CED
29	N1	613	CLA	O1D-CGD-O2D-CED
29	R1	609	CLA	O1D-CGD-O2D-CED
29	S1	605	CLA	O1D-CGD-O2D-CED
29	Y1	608	CLA	O1D-CGD-O2D-CED
29	b1	608	CLA	O1D-CGD-O2D-CED
29	g1	610	CLA	O1D-CGD-O2D-CED
29	r1	609	CLA	O1D-CGD-O2D-CED
55	Y	627	PTY	C11-C8-O7-C6
55	Y1	627	PTY	O10-C8-O7-C6
29	B	612	CLA	O1D-CGD-O2D-CED
29	c	503	CLA	O1D-CGD-O2D-CED
29	r	603	CLA	O1D-CGD-O2D-CED
29	s	613	CLA	O1D-CGD-O2D-CED
29	A1	405	CLA	O1D-CGD-O2D-CED
29	B1	616	CLA	O1D-CGD-O2D-CED
29	C1	503	CLA	O1D-CGD-O2D-CED
29	N1	610	CLA	O1D-CGD-O2D-CED
29	R1	603	CLA	O1D-CGD-O2D-CED
29	R1	608	CLA	O1D-CGD-O2D-CED
29	R1	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	S1	611	CLA	O1D-CGD-O2D-CED
29	S1	617	CLA	O1D-CGD-O2D-CED
29	n1	610	CLA	O1D-CGD-O2D-CED
29	n1	613	CLA	O1D-CGD-O2D-CED
29	r1	608	CLA	O1D-CGD-O2D-CED
29	s1	613	CLA	O1D-CGD-O2D-CED
29	y1	608	CLA	O1D-CGD-O2D-CED
55	Y	627	PTY	C31-C30-O4-C1
29	A	405	CLA	CBD-CGD-O2D-CED
29	B	606	CLA	CBD-CGD-O2D-CED
29	B	611	CLA	CBD-CGD-O2D-CED
29	B	613	CLA	CBD-CGD-O2D-CED
29	B	615	CLA	CBD-CGD-O2D-CED
29	B	617	CLA	CBD-CGD-O2D-CED
29	C	501	CLA	CBD-CGD-O2D-CED
29	C	502	CLA	CBD-CGD-O2D-CED
29	C	506	CLA	CBD-CGD-O2D-CED
29	C	511	CLA	CBD-CGD-O2D-CED
29	C	513	CLA	CBD-CGD-O2D-CED
29	D	402	CLA	CBD-CGD-O2D-CED
29	N	611	CLA	CBD-CGD-O2D-CED
29	N	614	CLA	CBD-CGD-O2D-CED
29	G	602	CLA	CBD-CGD-O2D-CED
29	G	604	CLA	CBD-CGD-O2D-CED
29	G	612	CLA	CBD-CGD-O2D-CED
29	G	614	CLA	CBD-CGD-O2D-CED
29	R	603	CLA	CBD-CGD-O2D-CED
29	R	609	CLA	CBD-CGD-O2D-CED
29	R	612	CLA	CBD-CGD-O2D-CED
29	S	613	CLA	CBD-CGD-O2D-CED
29	S	614	CLA	CBD-CGD-O2D-CED
29	Y	603	CLA	CBD-CGD-O2D-CED
29	Y	608	CLA	CBD-CGD-O2D-CED
29	Y	612	CLA	CBD-CGD-O2D-CED
29	Y	613	CLA	CBD-CGD-O2D-CED
29	Y	614	CLA	CBD-CGD-O2D-CED
29	a	410	CLA	CBD-CGD-O2D-CED
29	b	602	CLA	CBD-CGD-O2D-CED
29	b	606	CLA	CBD-CGD-O2D-CED
29	b	607	CLA	CBD-CGD-O2D-CED
29	b	608	CLA	CBD-CGD-O2D-CED
29	b	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	b	615	CLA	CBD-CGD-O2D-CED
29	c	502	CLA	CBD-CGD-O2D-CED
29	c	503	CLA	CBD-CGD-O2D-CED
29	c	509	CLA	CBD-CGD-O2D-CED
29	c	510	CLA	CBD-CGD-O2D-CED
29	n	602	CLA	CBD-CGD-O2D-CED
29	g	603	CLA	CBD-CGD-O2D-CED
29	g	604	CLA	CBD-CGD-O2D-CED
29	g	613	CLA	CBD-CGD-O2D-CED
29	g	614	CLA	CBD-CGD-O2D-CED
29	r	602	CLA	CBD-CGD-O2D-CED
29	r	608	CLA	CBD-CGD-O2D-CED
29	r	612	CLA	CBD-CGD-O2D-CED
29	s	604	CLA	CBD-CGD-O2D-CED
29	s	612	CLA	CBD-CGD-O2D-CED
29	y	602	CLA	CBD-CGD-O2D-CED
29	y	604	CLA	CBD-CGD-O2D-CED
29	y	612	CLA	CBD-CGD-O2D-CED
29	y	614	CLA	CBD-CGD-O2D-CED
29	A1	410	CLA	CBD-CGD-O2D-CED
29	B1	606	CLA	CBD-CGD-O2D-CED
29	B1	610	CLA	CBD-CGD-O2D-CED
29	B1	611	CLA	CBD-CGD-O2D-CED
29	B1	612	CLA	CBD-CGD-O2D-CED
29	B1	615	CLA	CBD-CGD-O2D-CED
29	C1	503	CLA	CBD-CGD-O2D-CED
29	C1	507	CLA	CBD-CGD-O2D-CED
29	C1	511	CLA	CBD-CGD-O2D-CED
29	D1	402	CLA	CBD-CGD-O2D-CED
29	D1	403	CLA	CBD-CGD-O2D-CED
29	N1	602	CLA	CBD-CGD-O2D-CED
29	N1	610	CLA	CBD-CGD-O2D-CED
29	N1	611	CLA	CBD-CGD-O2D-CED
29	N1	613	CLA	CBD-CGD-O2D-CED
29	N1	614	CLA	CBD-CGD-O2D-CED
29	G1	602	CLA	CBD-CGD-O2D-CED
29	G1	604	CLA	CBD-CGD-O2D-CED
29	G1	610	CLA	CBD-CGD-O2D-CED
29	R1	608	CLA	CBD-CGD-O2D-CED
29	R1	609	CLA	CBD-CGD-O2D-CED
29	R1	612	CLA	CBD-CGD-O2D-CED
29	S1	605	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	S1	613	CLA	CBD-CGD-O2D-CED
29	S1	617	CLA	CBD-CGD-O2D-CED
29	Y1	604	CLA	CBD-CGD-O2D-CED
29	Y1	608	CLA	CBD-CGD-O2D-CED
29	Y1	612	CLA	CBD-CGD-O2D-CED
29	b1	603	CLA	CBD-CGD-O2D-CED
29	b1	608	CLA	CBD-CGD-O2D-CED
29	b1	611	CLA	CBD-CGD-O2D-CED
29	b1	617	CLA	CBD-CGD-O2D-CED
29	c1	502	CLA	CBD-CGD-O2D-CED
29	c1	503	CLA	CBD-CGD-O2D-CED
29	c1	509	CLA	CBD-CGD-O2D-CED
29	c1	511	CLA	CBD-CGD-O2D-CED
29	c1	513	CLA	CBD-CGD-O2D-CED
29	d1	403	CLA	CBD-CGD-O2D-CED
29	n1	602	CLA	CBD-CGD-O2D-CED
29	n1	604	CLA	CBD-CGD-O2D-CED
29	n1	613	CLA	CBD-CGD-O2D-CED
29	g1	604	CLA	CBD-CGD-O2D-CED
29	g1	610	CLA	CBD-CGD-O2D-CED
29	r1	602	CLA	CBD-CGD-O2D-CED
29	s1	602	CLA	CBD-CGD-O2D-CED
29	s1	604	CLA	CBD-CGD-O2D-CED
29	s1	605	CLA	CBD-CGD-O2D-CED
29	s1	612	CLA	CBD-CGD-O2D-CED
29	s1	614	CLA	CBD-CGD-O2D-CED
29	s1	617	CLA	CBD-CGD-O2D-CED
29	y1	602	CLA	CBD-CGD-O2D-CED
29	y1	603	CLA	CBD-CGD-O2D-CED
29	y1	604	CLA	CBD-CGD-O2D-CED
29	y1	613	CLA	CBD-CGD-O2D-CED
29	y1	614	CLA	CBD-CGD-O2D-CED
30	a	409	PHO	CBD-CGD-O2D-CED
30	A1	408	PHO	CBD-CGD-O2D-CED
30	a1	408	PHO	CBD-CGD-O2D-CED
30	a1	409	PHO	CBD-CGD-O2D-CED
29	A	406	CLA	O1A-CGA-O2A-C1
29	C	505	CLA	O1A-CGA-O2A-C1
29	C	512	CLA	O1A-CGA-O2A-C1
29	N	611	CLA	O1A-CGA-O2A-C1
29	G	602	CLA	O1A-CGA-O2A-C1
29	G	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	S	604	CLA	O1A-CGA-O2A-C1
29	Y	608	CLA	O1A-CGA-O2A-C1
29	b	603	CLA	O1A-CGA-O2A-C1
29	g	614	CLA	O1A-CGA-O2A-C1
29	r	603	CLA	O1A-CGA-O2A-C1
29	y	604	CLA	O1A-CGA-O2A-C1
29	D1	403	CLA	O1A-CGA-O2A-C1
29	N1	611	CLA	O1A-CGA-O2A-C1
29	G1	614	CLA	O1A-CGA-O2A-C1
29	R1	603	CLA	O1A-CGA-O2A-C1
29	S1	604	CLA	O1A-CGA-O2A-C1
29	S1	605	CLA	O1A-CGA-O2A-C1
29	a1	410	CLA	O1A-CGA-O2A-C1
29	g1	604	CLA	O1A-CGA-O2A-C1
29	r1	609	CLA	O1A-CGA-O2A-C1
29	y1	604	CLA	O1A-CGA-O2A-C1
29	y1	611	CLA	O1A-CGA-O2A-C1
29	y1	612	CLA	O1A-CGA-O2A-C1
32	c1	526	SQD	O10-C23-O48-C46
33	C1	521	LMG	O10-C28-O8-C9
33	W1	201	LMG	O10-C28-O8-C9
33	c1	523	LMG	O10-C28-O8-C9
40	L1	101	LHG	O10-C23-O8-C6
47	I	102	4RF	O17-C16-O18-C19
47	i	101	4RF	O17-C16-O18-C19
55	y	626	PTY	O30-C30-O4-C1
29	B	606	CLA	O1D-CGD-O2D-CED
29	B	617	CLA	O1D-CGD-O2D-CED
29	N	614	CLA	O1D-CGD-O2D-CED
29	R	609	CLA	O1D-CGD-O2D-CED
29	R	612	CLA	O1D-CGD-O2D-CED
29	Y	608	CLA	O1D-CGD-O2D-CED
29	b	606	CLA	O1D-CGD-O2D-CED
29	B1	610	CLA	O1D-CGD-O2D-CED
29	G1	610	CLA	O1D-CGD-O2D-CED
29	S1	613	CLA	O1D-CGD-O2D-CED
29	S1	614	CLA	O1D-CGD-O2D-CED
29	Y1	614	CLA	O1D-CGD-O2D-CED
29	b1	603	CLA	O1D-CGD-O2D-CED
29	c1	511	CLA	O1D-CGD-O2D-CED
29	n1	604	CLA	O1D-CGD-O2D-CED
29	g1	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	r1	603	CLA	O1D-CGD-O2D-CED
29	s1	612	CLA	O1D-CGD-O2D-CED
29	s1	614	CLA	O1D-CGD-O2D-CED
29	y1	613	CLA	O1D-CGD-O2D-CED
29	y1	614	CLA	O1D-CGD-O2D-CED
29	B	603	CLA	O1D-CGD-O2D-CED
29	B	607	CLA	O1D-CGD-O2D-CED
29	B	608	CLA	O1D-CGD-O2D-CED
29	C	503	CLA	O1D-CGD-O2D-CED
29	G	610	CLA	O1D-CGD-O2D-CED
29	G	614	CLA	O1D-CGD-O2D-CED
29	R	608	CLA	O1D-CGD-O2D-CED
29	R	610	CLA	O1D-CGD-O2D-CED
29	S	610	CLA	O1D-CGD-O2D-CED
29	S	617	CLA	O1D-CGD-O2D-CED
29	Y	610	CLA	O1D-CGD-O2D-CED
29	b	610	CLA	O1D-CGD-O2D-CED
29	b	611	CLA	O1D-CGD-O2D-CED
29	c	511	CLA	O1D-CGD-O2D-CED
29	d	403	CLA	O1D-CGD-O2D-CED
29	n	610	CLA	O1D-CGD-O2D-CED
29	n	613	CLA	O1D-CGD-O2D-CED
29	n	614	CLA	O1D-CGD-O2D-CED
29	g	610	CLA	O1D-CGD-O2D-CED
29	g	611	CLA	O1D-CGD-O2D-CED
29	g	613	CLA	O1D-CGD-O2D-CED
29	r	604	CLA	O1D-CGD-O2D-CED
29	s	614	CLA	O1D-CGD-O2D-CED
29	y	610	CLA	O1D-CGD-O2D-CED
29	A1	410	CLA	O1D-CGD-O2D-CED
29	B1	613	CLA	O1D-CGD-O2D-CED
29	B1	614	CLA	O1D-CGD-O2D-CED
29	C1	502	CLA	O1D-CGD-O2D-CED
29	C1	504	CLA	O1D-CGD-O2D-CED
29	C1	510	CLA	O1D-CGD-O2D-CED
29	C1	513	CLA	O1D-CGD-O2D-CED
29	N1	603	CLA	O1D-CGD-O2D-CED
29	G1	603	CLA	O1D-CGD-O2D-CED
29	G1	613	CLA	O1D-CGD-O2D-CED
29	R1	612	CLA	O1D-CGD-O2D-CED
29	S1	609	CLA	O1D-CGD-O2D-CED
29	a1	405	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	c1	501	CLA	O1D-CGD-O2D-CED
29	c1	503	CLA	O1D-CGD-O2D-CED
29	c1	506	CLA	O1D-CGD-O2D-CED
29	n1	611	CLA	O1D-CGD-O2D-CED
29	n1	612	CLA	O1D-CGD-O2D-CED
29	g1	611	CLA	O1D-CGD-O2D-CED
29	r1	610	CLA	O1D-CGD-O2D-CED
29	s1	603	CLA	O1D-CGD-O2D-CED
29	s1	609	CLA	O1D-CGD-O2D-CED
29	y1	610	CLA	O1D-CGD-O2D-CED
29	C	512	CLA	CBA-CGA-O2A-C1
29	G	611	CLA	CBA-CGA-O2A-C1
29	S	604	CLA	CBA-CGA-O2A-C1
29	Y	611	CLA	CBA-CGA-O2A-C1
29	b	603	CLA	CBA-CGA-O2A-C1
29	r	603	CLA	CBA-CGA-O2A-C1
29	y	604	CLA	CBA-CGA-O2A-C1
29	D1	403	CLA	CBA-CGA-O2A-C1
29	G1	614	CLA	CBA-CGA-O2A-C1
29	R1	603	CLA	CBA-CGA-O2A-C1
29	S1	604	CLA	CBA-CGA-O2A-C1
29	g1	602	CLA	CBA-CGA-O2A-C1
29	r1	609	CLA	CBA-CGA-O2A-C1
29	y1	611	CLA	CBA-CGA-O2A-C1
33	c1	523	LMG	C29-C28-O8-C9
40	L1	101	LHG	C24-C23-O8-C6
55	Y	627	PTY	O30-C30-O4-C1
33	c1	521	LMG	C4-C5-C6-O5
29	C	507	CLA	CBD-CGD-O2D-CED
29	C	510	CLA	CBD-CGD-O2D-CED
29	C	512	CLA	CBD-CGD-O2D-CED
29	D	403	CLA	CBD-CGD-O2D-CED
29	N	603	CLA	CBD-CGD-O2D-CED
29	N	604	CLA	CBD-CGD-O2D-CED
29	N	612	CLA	CBD-CGD-O2D-CED
29	N	613	CLA	CBD-CGD-O2D-CED
29	R	602	CLA	CBD-CGD-O2D-CED
29	R	604	CLA	CBD-CGD-O2D-CED
29	S	602	CLA	CBD-CGD-O2D-CED
29	S	604	CLA	CBD-CGD-O2D-CED
29	S	605	CLA	CBD-CGD-O2D-CED
29	S	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	Y	604	CLA	CBD-CGD-O2D-CED
29	b	603	CLA	CBD-CGD-O2D-CED
29	b	613	CLA	CBD-CGD-O2D-CED
29	b	614	CLA	CBD-CGD-O2D-CED
29	b	616	CLA	CBD-CGD-O2D-CED
29	c	512	CLA	CBD-CGD-O2D-CED
29	c	513	CLA	CBD-CGD-O2D-CED
29	n	603	CLA	CBD-CGD-O2D-CED
29	g	602	CLA	CBD-CGD-O2D-CED
29	g	612	CLA	CBD-CGD-O2D-CED
29	s	602	CLA	CBD-CGD-O2D-CED
29	s	605	CLA	CBD-CGD-O2D-CED
29	s	609	CLA	CBD-CGD-O2D-CED
29	A1	407	CLA	CBD-CGD-O2D-CED
29	B1	607	CLA	CBD-CGD-O2D-CED
29	B1	608	CLA	CBD-CGD-O2D-CED
29	B1	609	CLA	CBD-CGD-O2D-CED
29	C1	512	CLA	CBD-CGD-O2D-CED
29	G1	612	CLA	CBD-CGD-O2D-CED
29	G1	614	CLA	CBD-CGD-O2D-CED
29	R1	604	CLA	CBD-CGD-O2D-CED
29	S1	602	CLA	CBD-CGD-O2D-CED
29	S1	603	CLA	CBD-CGD-O2D-CED
29	S1	604	CLA	CBD-CGD-O2D-CED
29	Y1	602	CLA	CBD-CGD-O2D-CED
29	b1	613	CLA	CBD-CGD-O2D-CED
29	c1	507	CLA	CBD-CGD-O2D-CED
29	n1	614	CLA	CBD-CGD-O2D-CED
29	g1	613	CLA	CBD-CGD-O2D-CED
29	y1	612	CLA	CBD-CGD-O2D-CED
55	y1	627	PTY	O10-C8-O7-C6
29	B	603	CLA	O1A-CGA-O2A-C1
29	B	611	CLA	O1A-CGA-O2A-C1
29	D	403	CLA	O1A-CGA-O2A-C1
29	G	604	CLA	O1A-CGA-O2A-C1
29	G	614	CLA	O1A-CGA-O2A-C1
29	R	603	CLA	O1A-CGA-O2A-C1
29	R	608	CLA	O1A-CGA-O2A-C1
29	S	605	CLA	O1A-CGA-O2A-C1
29	S	613	CLA	O1A-CGA-O2A-C1
29	S	617	CLA	O1A-CGA-O2A-C1
29	Y	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	Y	611	CLA	O1A-CGA-O2A-C1
29	a	406	CLA	O1A-CGA-O2A-C1
29	c	506	CLA	O1A-CGA-O2A-C1
29	n	603	CLA	O1A-CGA-O2A-C1
29	g	604	CLA	O1A-CGA-O2A-C1
29	g	613	CLA	O1A-CGA-O2A-C1
29	r	608	CLA	O1A-CGA-O2A-C1
29	s	613	CLA	O1A-CGA-O2A-C1
29	y	611	CLA	O1A-CGA-O2A-C1
29	A1	406	CLA	O1A-CGA-O2A-C1
29	B1	603	CLA	O1A-CGA-O2A-C1
29	B1	611	CLA	O1A-CGA-O2A-C1
29	C1	505	CLA	O1A-CGA-O2A-C1
29	C1	512	CLA	O1A-CGA-O2A-C1
29	C1	513	CLA	O1A-CGA-O2A-C1
29	G1	604	CLA	O1A-CGA-O2A-C1
29	G1	611	CLA	O1A-CGA-O2A-C1
29	S1	613	CLA	O1A-CGA-O2A-C1
29	Y1	604	CLA	O1A-CGA-O2A-C1
29	Y1	608	CLA	O1A-CGA-O2A-C1
29	Y1	611	CLA	O1A-CGA-O2A-C1
29	Y1	612	CLA	O1A-CGA-O2A-C1
29	b1	611	CLA	O1A-CGA-O2A-C1
29	c1	506	CLA	O1A-CGA-O2A-C1
29	g1	602	CLA	O1A-CGA-O2A-C1
29	g1	611	CLA	O1A-CGA-O2A-C1
29	g1	613	CLA	O1A-CGA-O2A-C1
29	g1	614	CLA	O1A-CGA-O2A-C1
29	s1	613	CLA	O1A-CGA-O2A-C1
32	c	526	SQD	O10-C23-O48-C46
33	C	521	LMG	O10-C28-O8-C9
33	W	201	LMG	O10-C28-O8-C9
33	c	521	LMG	O10-C28-O8-C9
33	C1	523	LMG	O10-C28-O8-C9
33	w1	201	LMG	O10-C28-O8-C9
47	i1	101	4RF	O17-C16-O18-C19
29	B	614	CLA	O1D-CGD-O2D-CED
29	G	613	CLA	O1D-CGD-O2D-CED
29	d	402	CLA	O1D-CGD-O2D-CED
29	n	611	CLA	O1D-CGD-O2D-CED
29	s	617	CLA	O1D-CGD-O2D-CED
29	B1	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	B1	604	CLA	O1D-CGD-O2D-CED
29	C1	501	CLA	O1D-CGD-O2D-CED
29	R1	602	CLA	O1D-CGD-O2D-CED
29	Y1	613	CLA	O1D-CGD-O2D-CED
29	b1	602	CLA	O1D-CGD-O2D-CED
29	b1	604	CLA	O1D-CGD-O2D-CED
29	b1	606	CLA	O1D-CGD-O2D-CED
29	g1	602	CLA	O1D-CGD-O2D-CED
29	g1	603	CLA	O1D-CGD-O2D-CED
29	r1	612	CLA	O1D-CGD-O2D-CED
29	B	604	CLA	O1D-CGD-O2D-CED
29	B	610	CLA	O1D-CGD-O2D-CED
29	N	602	CLA	O1D-CGD-O2D-CED
29	G	611	CLA	O1D-CGD-O2D-CED
29	S	609	CLA	O1D-CGD-O2D-CED
29	b	617	CLA	O1D-CGD-O2D-CED
29	n	612	CLA	O1D-CGD-O2D-CED
29	g	603	CLA	O1D-CGD-O2D-CED
29	y	603	CLA	O1D-CGD-O2D-CED
29	y	613	CLA	O1D-CGD-O2D-CED
29	B1	617	CLA	O1D-CGD-O2D-CED
29	N1	612	CLA	O1D-CGD-O2D-CED
29	S1	612	CLA	O1D-CGD-O2D-CED
29	Y1	603	CLA	O1D-CGD-O2D-CED
29	b1	607	CLA	O1D-CGD-O2D-CED
29	g1	612	CLA	O1D-CGD-O2D-CED
29	s1	611	CLA	O1D-CGD-O2D-CED
55	y	627	PTY	C31-C30-O4-C1
29	A	410	CLA	CBD-CGD-O2D-CED
29	Y	602	CLA	CBD-CGD-O2D-CED
29	G1	611	CLA	CBD-CGD-O2D-CED
29	n1	603	CLA	CBD-CGD-O2D-CED
29	B	615	CLA	O1D-CGD-O2D-CED
29	G	603	CLA	O1D-CGD-O2D-CED
29	b	604	CLA	O1D-CGD-O2D-CED
29	r	608	CLA	O1D-CGD-O2D-CED
29	y	608	CLA	O1D-CGD-O2D-CED
29	C1	511	CLA	O1D-CGD-O2D-CED
29	b1	609	CLA	O1D-CGD-O2D-CED
29	n1	602	CLA	O1D-CGD-O2D-CED
32	B1	626	SQD	O49-C7-O47-C45
32	M1	101	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
33	W	201	LMG	O9-C10-O7-C8
33	W1	201	LMG	O9-C10-O7-C8
38	T	101	3PH	O22-C21-O21-C2
38	T1	101	3PH	O22-C21-O21-C2
38	b1	624	3PH	O22-C21-O21-C2
39	B	625	DGA	OB1-CB1-OG2-CG2
39	b	625	DGA	OB1-CB1-OG2-CG2
40	L	101	LHG	O9-C7-O7-C5
40	G	624	LHG	O9-C7-O7-C5
40	n	624	LHG	O9-C7-O7-C5
40	d1	410	LHG	O9-C7-O7-C5
40	n1	624	LHG	O9-C7-O7-C5
40	g1	624	LHG	O9-C7-O7-C5
40	y1	624	LHG	O9-C7-O7-C5
47	I	102	4RF	O23-C22-O21-C20
47	i	101	4RF	O23-C22-O21-C20
47	I1	102	4RF	O23-C22-O21-C20
47	i1	101	4RF	O23-C22-O21-C20
55	y1	626	PTY	O10-C8-O7-C6
29	B1	606	CLA	O1D-CGD-O2D-CED
29	D1	403	CLA	O1D-CGD-O2D-CED
29	B	605	CLA	C3-C5-C6-C7
29	C	505	CLA	C3-C5-C6-C7
29	C	506	CLA	C3-C5-C6-C7
29	S	603	CLA	C3-C5-C6-C7
29	S	604	CLA	C3-C5-C6-C7
29	Y	602	CLA	C3-C5-C6-C7
29	b	602	CLA	C3-C5-C6-C7
29	b	605	CLA	C3-C5-C6-C7
29	b	608	CLA	C3-C5-C6-C7
29	c	506	CLA	C3-C5-C6-C7
29	n	602	CLA	C3-C5-C6-C7
29	n	604	CLA	C3-C5-C6-C7
29	r	602	CLA	C3-C5-C6-C7
29	A1	410	CLA	C3-C5-C6-C7
29	N1	610	CLA	C3-C5-C6-C7
29	G1	603	CLA	C3-C5-C6-C7
29	R1	612	CLA	C3-C5-C6-C7
29	S1	602	CLA	C3-C5-C6-C7
29	S1	613	CLA	C3-C5-C6-C7
29	a1	410	CLA	C3-C5-C6-C7
29	b1	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	b1	605	CLA	C3-C5-C6-C7
29	b1	609	CLA	C3-C5-C6-C7
29	n1	610	CLA	C3-C5-C6-C7
29	s1	603	CLA	C3-C5-C6-C7
29	s1	604	CLA	C3-C5-C6-C7
29	s1	614	CLA	C3-C5-C6-C7
30	A	409	PHO	C3-C5-C6-C7
30	a	409	PHO	C3-C5-C6-C7
30	a1	409	PHO	C3-C5-C6-C7
48	g1	601	CHL	C3-C5-C6-C7
29	A	406	CLA	CBA-CGA-O2A-C1
29	B	603	CLA	CBA-CGA-O2A-C1
29	C	505	CLA	CBA-CGA-O2A-C1
29	N	611	CLA	CBA-CGA-O2A-C1
29	G	602	CLA	CBA-CGA-O2A-C1
29	G	614	CLA	CBA-CGA-O2A-C1
29	R	603	CLA	CBA-CGA-O2A-C1
29	S	617	CLA	CBA-CGA-O2A-C1
29	Y	603	CLA	CBA-CGA-O2A-C1
29	Y	608	CLA	CBA-CGA-O2A-C1
29	a	406	CLA	CBA-CGA-O2A-C1
29	n	603	CLA	CBA-CGA-O2A-C1
29	g	604	CLA	CBA-CGA-O2A-C1
29	g	614	CLA	CBA-CGA-O2A-C1
29	r	609	CLA	CBA-CGA-O2A-C1
29	s	613	CLA	CBA-CGA-O2A-C1
29	y	611	CLA	CBA-CGA-O2A-C1
29	y	612	CLA	CBA-CGA-O2A-C1
29	A1	406	CLA	CBA-CGA-O2A-C1
29	B1	603	CLA	CBA-CGA-O2A-C1
29	B1	610	CLA	CBA-CGA-O2A-C1
29	B1	614	CLA	CBA-CGA-O2A-C1
29	C1	505	CLA	CBA-CGA-O2A-C1
29	C1	512	CLA	CBA-CGA-O2A-C1
29	N1	611	CLA	CBA-CGA-O2A-C1
29	G1	604	CLA	CBA-CGA-O2A-C1
29	G1	611	CLA	CBA-CGA-O2A-C1
29	R1	602	CLA	CBA-CGA-O2A-C1
29	R1	608	CLA	CBA-CGA-O2A-C1
29	S1	605	CLA	CBA-CGA-O2A-C1
29	S1	613	CLA	CBA-CGA-O2A-C1
29	Y1	604	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	Y1	608	CLA	CBA-CGA-O2A-C1
29	Y1	611	CLA	CBA-CGA-O2A-C1
29	n1	603	CLA	CBA-CGA-O2A-C1
29	n1	611	CLA	CBA-CGA-O2A-C1
29	g1	604	CLA	CBA-CGA-O2A-C1
29	g1	611	CLA	CBA-CGA-O2A-C1
29	s1	613	CLA	CBA-CGA-O2A-C1
29	s1	614	CLA	CBA-CGA-O2A-C1
29	y1	604	CLA	CBA-CGA-O2A-C1
32	c	526	SQD	C24-C23-O48-C46
32	c1	526	SQD	C24-C23-O48-C46
33	C	521	LMG	C29-C28-O8-C9
33	W	201	LMG	C29-C28-O8-C9
33	C1	521	LMG	C29-C28-O8-C9
33	C1	523	LMG	C29-C28-O8-C9
33	W1	201	LMG	C29-C28-O8-C9
33	c1	521	LMG	C29-C28-O8-C9
33	w1	201	LMG	C29-C28-O8-C9
37	B	623	DGD	C2A-C1A-O1G-C1G
38	t	101	3PH	C32-C31-O31-C3
47	I	102	4RF	C15-C16-O18-C19
55	y	626	PTY	C31-C30-O4-C1
52	r1	625	LMT	O5B-C5B-C6B-O6B
29	n	602	CLA	C15-C16-C17-C18
33	B1	622	LMG	C11-C10-O7-C8
33	b1	622	LMG	C11-C10-O7-C8
37	b	623	DGD	C2B-C1B-O2G-C2G
37	B1	623	DGD	C2B-C1B-O2G-C2G
37	b1	623	DGD	C2B-C1B-O2G-C2G
38	t1	101	3PH	C22-C21-O21-C2
39	B1	625	DGA	CB2-CB1-OG2-CG2
40	G	624	LHG	C8-C7-O7-C5
40	n	624	LHG	C8-C7-O7-C5
40	d1	410	LHG	C8-C7-O7-C5
40	n1	624	LHG	C8-C7-O7-C5
40	y1	624	LHG	C8-C7-O7-C5
29	G	612	CLA	O1D-CGD-O2D-CED
29	b	612	CLA	O1D-CGD-O2D-CED
29	g	604	CLA	O1D-CGD-O2D-CED
29	s	612	CLA	O1D-CGD-O2D-CED
29	N1	614	CLA	O1D-CGD-O2D-CED
29	G1	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	d1	403	CLA	O1D-CGD-O2D-CED
29	y1	602	CLA	O1D-CGD-O2D-CED
29	C	509	CLA	CBD-CGD-O2D-CED
29	a	407	CLA	CBD-CGD-O2D-CED
29	b	609	CLA	CBD-CGD-O2D-CED
29	c	506	CLA	CBD-CGD-O2D-CED
29	a1	406	CLA	CBD-CGD-O2D-CED
29	a1	407	CLA	CBD-CGD-O2D-CED
29	b1	605	CLA	CBD-CGD-O2D-CED
29	b1	612	CLA	CBD-CGD-O2D-CED
30	A1	409	PHO	CBD-CGD-O2D-CED
55	Y1	627	PTY	O30-C30-O4-C1
29	B	606	CLA	C4-C3-C5-C6
29	C	501	CLA	C4-C3-C5-C6
29	D	402	CLA	C4-C3-C5-C6
29	b	603	CLA	C4-C3-C5-C6
29	b	615	CLA	C4-C3-C5-C6
29	g	602	CLA	C4-C3-C5-C6
29	r	608	CLA	C4-C3-C5-C6
29	Y1	612	CLA	C4-C3-C5-C6
48	N	601	CHL	C4-C3-C5-C6
48	N1	601	CHL	C4-C3-C5-C6
48	N1	606	CHL	C4-C3-C5-C6
29	C	501	CLA	C2-C3-C5-C6
29	d	403	CLA	C2-C3-C5-C6
29	C1	504	CLA	C2-C3-C5-C6
29	b1	606	CLA	C2-C3-C5-C6
29	b1	609	CLA	C2-C3-C5-C6
48	N	601	CHL	C2-C3-C5-C6
48	G	609	CHL	C2-C3-C5-C6
48	N1	606	CHL	C2-C3-C5-C6
29	c	507	CLA	CBD-CGD-O2D-CED
29	s	611	CLA	CBD-CGD-O2D-CED
29	y	611	CLA	CBD-CGD-O2D-CED
29	B1	605	CLA	CBD-CGD-O2D-CED
29	r1	604	CLA	CBD-CGD-O2D-CED
30	A	409	PHO	CBD-CGD-O2D-CED
29	R	603	CLA	C2A-CAA-CBA-CGA
29	R	608	CLA	C2A-CAA-CBA-CGA
29	R	609	CLA	C2A-CAA-CBA-CGA
29	S	614	CLA	C2A-CAA-CBA-CGA
29	Y	608	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	c	507	CLA	C2A-CAA-CBA-CGA
29	g	613	CLA	C2A-CAA-CBA-CGA
29	g	614	CLA	C2A-CAA-CBA-CGA
29	s	602	CLA	C2A-CAA-CBA-CGA
29	s	603	CLA	C2A-CAA-CBA-CGA
29	s	614	CLA	C2A-CAA-CBA-CGA
29	N1	604	CLA	C2A-CAA-CBA-CGA
29	G1	613	CLA	C2A-CAA-CBA-CGA
29	R1	609	CLA	C2A-CAA-CBA-CGA
29	R1	612	CLA	C2A-CAA-CBA-CGA
29	b1	613	CLA	C2A-CAA-CBA-CGA
29	b1	617	CLA	C2A-CAA-CBA-CGA
29	c1	507	CLA	C2A-CAA-CBA-CGA
29	n1	602	CLA	C2A-CAA-CBA-CGA
29	n1	611	CLA	C2A-CAA-CBA-CGA
29	g1	613	CLA	C2A-CAA-CBA-CGA
29	g1	614	CLA	C2A-CAA-CBA-CGA
29	r1	609	CLA	C2A-CAA-CBA-CGA
29	s1	602	CLA	C2A-CAA-CBA-CGA
29	s1	609	CLA	C2A-CAA-CBA-CGA
29	s1	612	CLA	C2A-CAA-CBA-CGA
29	s1	617	CLA	C2A-CAA-CBA-CGA
30	A	409	PHO	C2A-CAA-CBA-CGA
48	N	608	CHL	C2A-CAA-CBA-CGA
48	S	608	CHL	C2A-CAA-CBA-CGA
48	n	608	CHL	C2A-CAA-CBA-CGA
48	Y1	607	CHL	C2A-CAA-CBA-CGA
29	B1	604	CLA	O1A-CGA-O2A-C1
29	b	615	CLA	O1D-CGD-O2D-CED
33	A	413	LMG	C17-C18-C19-C20
33	A	413	LMG	C35-C36-C37-C38
33	A	413	LMG	C38-C39-C40-C41
33	B	622	LMG	C17-C18-C19-C20
33	C	521	LMG	C17-C18-C19-C20
33	C	521	LMG	C35-C36-C37-C38
33	C	523	LMG	C17-C18-C19-C20
33	C	523	LMG	C41-C42-C43-C44
33	D	411	LMG	C17-C18-C19-C20
33	D	411	LMG	C20-C21-C22-C23
33	H	102	LMG	C38-C39-C40-C41
33	W	201	LMG	C35-C36-C37-C38
33	W	201	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
33	a	413	LMG	C17-C18-C19-C20
33	a	413	LMG	C35-C36-C37-C38
33	a	413	LMG	C38-C39-C40-C41
33	b	622	LMG	C17-C18-C19-C20
33	c	521	LMG	C17-C18-C19-C20
33	c	521	LMG	C35-C36-C37-C38
33	c	523	LMG	C41-C42-C43-C44
33	d	411	LMG	C17-C18-C19-C20
33	d	411	LMG	C20-C21-C22-C23
33	h	102	LMG	C38-C39-C40-C41
33	w	201	LMG	C35-C36-C37-C38
33	A1	413	LMG	C17-C18-C19-C20
33	A1	413	LMG	C35-C36-C37-C38
33	A1	413	LMG	C38-C39-C40-C41
33	B1	622	LMG	C17-C18-C19-C20
33	C1	521	LMG	C17-C18-C19-C20
33	C1	521	LMG	C35-C36-C37-C38
33	C1	523	LMG	C17-C18-C19-C20
33	C1	523	LMG	C41-C42-C43-C44
33	D1	411	LMG	C17-C18-C19-C20
33	D1	411	LMG	C20-C21-C22-C23
33	H1	102	LMG	C38-C39-C40-C41
33	W1	201	LMG	C35-C36-C37-C38
33	W1	201	LMG	C38-C39-C40-C41
33	a1	413	LMG	C17-C18-C19-C20
33	a1	413	LMG	C35-C36-C37-C38
33	a1	413	LMG	C38-C39-C40-C41
33	b1	622	LMG	C17-C18-C19-C20
33	c1	521	LMG	C17-C18-C19-C20
33	c1	521	LMG	C35-C36-C37-C38
33	c1	523	LMG	C17-C18-C19-C20
33	c1	523	LMG	C41-C42-C43-C44
33	d1	411	LMG	C17-C18-C19-C20
33	d1	411	LMG	C20-C21-C22-C23
33	h1	102	LMG	C38-C39-C40-C41
33	w1	201	LMG	C35-C36-C37-C38
33	w1	201	LMG	C38-C39-C40-C41
37	C	518	DGD	C8B-C9B-CAB-CBB
37	C	519	DGD	C8A-C9A-CAA-CBA
37	C	519	DGD	CBB-CCB-CDB-CEB
37	C	520	DGD	CBB-CCB-CDB-CEB
37	c	518	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
37	c	519	DGD	C8A-C9A-CAA-CBA
37	c	519	DGD	CBB-CCB-CDB-CEB
37	c	520	DGD	CBB-CCB-CDB-CEB
37	C1	518	DGD	C8B-C9B-CAB-CBB
37	C1	519	DGD	C8A-C9A-CAA-CBA
37	C1	520	DGD	CBB-CCB-CDB-CEB
37	c1	518	DGD	C8B-C9B-CAB-CBB
37	c1	519	DGD	C8A-C9A-CAA-CBA
37	c1	519	DGD	CBB-CCB-CDB-CEB
37	c1	520	DGD	CBB-CCB-CDB-CEB
40	c	525	LHG	C11-C12-C13-C14
47	K1	101	4RF	C29-C30-C31-C32
29	R	602	CLA	C3-C5-C6-C7
29	R	612	CLA	C3-C5-C6-C7
29	S	610	CLA	C3-C5-C6-C7
29	c	504	CLA	C3-C5-C6-C7
29	c	511	CLA	C3-C5-C6-C7
29	n	603	CLA	C3-C5-C6-C7
29	r	608	CLA	C3-C5-C6-C7
29	s	609	CLA	C3-C5-C6-C7
29	y	603	CLA	C3-C5-C6-C7
29	B1	610	CLA	C3-C5-C6-C7
29	C1	511	CLA	C3-C5-C6-C7
29	c1	504	CLA	C3-C5-C6-C7
29	c1	505	CLA	C3-C5-C6-C7
29	c1	506	CLA	C3-C5-C6-C7
29	c1	507	CLA	C3-C5-C6-C7
29	r1	609	CLA	C3-C5-C6-C7
29	s1	610	CLA	C3-C5-C6-C7
29	y1	604	CLA	C3-C5-C6-C7
29	y1	613	CLA	C3-C5-C6-C7
29	B	611	CLA	CBA-CGA-O2A-C1
29	B	613	CLA	CBA-CGA-O2A-C1
29	C	506	CLA	CBA-CGA-O2A-C1
29	C	509	CLA	CBA-CGA-O2A-C1
29	D	403	CLA	CBA-CGA-O2A-C1
29	N	603	CLA	CBA-CGA-O2A-C1
29	G	604	CLA	CBA-CGA-O2A-C1
29	R	604	CLA	CBA-CGA-O2A-C1
29	R	608	CLA	CBA-CGA-O2A-C1
29	S	602	CLA	CBA-CGA-O2A-C1
29	S	605	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	S	613	CLA	CBA-CGA-O2A-C1
29	Y	604	CLA	CBA-CGA-O2A-C1
29	Y	613	CLA	CBA-CGA-O2A-C1
29	b	608	CLA	CBA-CGA-O2A-C1
29	c	506	CLA	CBA-CGA-O2A-C1
29	c	509	CLA	CBA-CGA-O2A-C1
29	n	611	CLA	CBA-CGA-O2A-C1
29	g	611	CLA	CBA-CGA-O2A-C1
29	g	613	CLA	CBA-CGA-O2A-C1
29	r	608	CLA	CBA-CGA-O2A-C1
29	y	603	CLA	CBA-CGA-O2A-C1
29	y	608	CLA	CBA-CGA-O2A-C1
29	B1	604	CLA	CBA-CGA-O2A-C1
29	B1	611	CLA	CBA-CGA-O2A-C1
29	C1	504	CLA	CBA-CGA-O2A-C1
29	C1	511	CLA	CBA-CGA-O2A-C1
29	C1	513	CLA	CBA-CGA-O2A-C1
29	N1	610	CLA	CBA-CGA-O2A-C1
29	R1	604	CLA	CBA-CGA-O2A-C1
29	R1	609	CLA	CBA-CGA-O2A-C1
29	S1	602	CLA	CBA-CGA-O2A-C1
29	S1	617	CLA	CBA-CGA-O2A-C1
29	Y1	603	CLA	CBA-CGA-O2A-C1
29	Y1	612	CLA	CBA-CGA-O2A-C1
29	Y1	613	CLA	CBA-CGA-O2A-C1
29	a1	407	CLA	CBA-CGA-O2A-C1
29	b1	604	CLA	CBA-CGA-O2A-C1
29	b1	611	CLA	CBA-CGA-O2A-C1
29	c1	506	CLA	CBA-CGA-O2A-C1
29	c1	509	CLA	CBA-CGA-O2A-C1
29	d1	403	CLA	CBA-CGA-O2A-C1
29	n1	602	CLA	CBA-CGA-O2A-C1
29	g1	613	CLA	CBA-CGA-O2A-C1
29	g1	614	CLA	CBA-CGA-O2A-C1
29	r1	608	CLA	CBA-CGA-O2A-C1
29	s1	610	CLA	CBA-CGA-O2A-C1
29	y1	603	CLA	CBA-CGA-O2A-C1
29	y1	612	CLA	CBA-CGA-O2A-C1
32	M	101	SQD	C24-C23-O48-C46
33	c	521	LMG	C29-C28-O8-C9
38	T1	101	3PH	C32-C31-O31-C3
38	t1	101	3PH	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
47	i1	101	4RF	C15-C16-O18-C19
55	Y1	627	PTY	C31-C30-O4-C1
33	c1	521	LMG	O6-C5-C6-O5
33	c	523	LMG	C17-C18-C19-C20
33	w	201	LMG	C38-C39-C40-C41
37	C1	519	DGD	CBB-CCB-CDB-CEB
29	C	511	CLA	O1D-CGD-O2D-CED
29	D	402	CLA	O1D-CGD-O2D-CED
29	N	611	CLA	O1D-CGD-O2D-CED
29	G	602	CLA	O1D-CGD-O2D-CED
29	G	604	CLA	O1D-CGD-O2D-CED
29	b	608	CLA	O1D-CGD-O2D-CED
37	c1	520	DGD	C4D-C5D-C6D-O5D
43	d1	405	PL9	C47-C48-C49-C51
29	N	610	CLA	CBD-CGD-O2D-CED
29	c	504	CLA	CBD-CGD-O2D-CED
29	C	501	CLA	O1D-CGD-O2D-CED
29	S	614	CLA	O1D-CGD-O2D-CED
29	Y	603	CLA	O1D-CGD-O2D-CED
29	Y	613	CLA	O1D-CGD-O2D-CED
29	Y	614	CLA	O1D-CGD-O2D-CED
29	n	602	CLA	O1D-CGD-O2D-CED
29	r	602	CLA	O1D-CGD-O2D-CED
29	D1	402	CLA	O1D-CGD-O2D-CED
29	G1	602	CLA	O1D-CGD-O2D-CED
29	Y1	604	CLA	O1D-CGD-O2D-CED
29	b1	617	CLA	O1D-CGD-O2D-CED
29	c1	502	CLA	O1D-CGD-O2D-CED
29	c1	509	CLA	O1D-CGD-O2D-CED
29	s1	605	CLA	O1D-CGD-O2D-CED
29	y1	604	CLA	O1D-CGD-O2D-CED
30	a1	409	PHO	O1D-CGD-O2D-CED
32	m	101	SQD	O49-C7-O47-C45
43	d	405	PL9	C37-C38-C39-C41
43	D1	405	PL9	C7-C8-C9-C11
29	C	509	CLA	O1A-CGA-O2A-C1
29	R	609	CLA	O1A-CGA-O2A-C1
29	S	609	CLA	O1A-CGA-O2A-C1
29	Y	603	CLA	O1A-CGA-O2A-C1
29	Y	612	CLA	O1A-CGA-O2A-C1
29	b	606	CLA	O1A-CGA-O2A-C1
29	c	509	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	n	611	CLA	O1A-CGA-O2A-C1
29	g	611	CLA	O1A-CGA-O2A-C1
29	s	617	CLA	O1A-CGA-O2A-C1
29	y	608	CLA	O1A-CGA-O2A-C1
29	y	612	CLA	O1A-CGA-O2A-C1
29	B1	610	CLA	O1A-CGA-O2A-C1
29	B1	614	CLA	O1A-CGA-O2A-C1
29	C1	509	CLA	O1A-CGA-O2A-C1
29	N1	610	CLA	O1A-CGA-O2A-C1
29	R1	602	CLA	O1A-CGA-O2A-C1
29	R1	604	CLA	O1A-CGA-O2A-C1
29	S1	609	CLA	O1A-CGA-O2A-C1
29	S1	617	CLA	O1A-CGA-O2A-C1
29	Y1	603	CLA	O1A-CGA-O2A-C1
29	c1	509	CLA	O1A-CGA-O2A-C1
29	n1	602	CLA	O1A-CGA-O2A-C1
29	n1	603	CLA	O1A-CGA-O2A-C1
29	n1	611	CLA	O1A-CGA-O2A-C1
29	r1	608	CLA	O1A-CGA-O2A-C1
29	s1	617	CLA	O1A-CGA-O2A-C1
29	y1	603	CLA	O1A-CGA-O2A-C1
32	M	101	SQD	O10-C23-O48-C46
38	b	624	3PH	O32-C31-O31-C3
38	t1	101	3PH	O32-C31-O31-C3
29	r	612	CLA	O1D-CGD-O2D-CED
29	y	602	CLA	O1D-CGD-O2D-CED
29	N1	602	CLA	O1D-CGD-O2D-CED
29	y1	603	CLA	O1D-CGD-O2D-CED
31	B	618	BCR	C9-C10-C11-C12
31	C	514	BCR	C13-C14-C15-C16
31	B1	618	BCR	C9-C10-C11-C12
31	D1	404	BCR	C9-C10-C11-C12
31	c1	514	BCR	C13-C14-C15-C16
31	c1	515	BCR	C9-C10-C11-C12
45	h1	101	RRX	C19-C20-C21-C22
45	h1	101	RRX	C15-C16-C17-C18
51	S	623	NEX	C9-C10-C11-C12
52	r	625	LMT	O5B-C5B-C6B-O6B
33	D1	411	LMG	C4-C5-C6-O5
29	a	406	CLA	CBD-CGD-O2D-CED
29	c	501	CLA	CBD-CGD-O2D-CED
29	n	604	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	N1	604	CLA	CBD-CGD-O2D-CED
29	B	613	CLA	O1D-CGD-O2D-CED
29	C	506	CLA	O1D-CGD-O2D-CED
29	C	513	CLA	O1D-CGD-O2D-CED
29	a	410	CLA	O1D-CGD-O2D-CED
29	c	502	CLA	O1D-CGD-O2D-CED
29	c	509	CLA	O1D-CGD-O2D-CED
29	s	604	CLA	O1D-CGD-O2D-CED
29	N1	611	CLA	O1D-CGD-O2D-CED
30	a1	408	PHO	O1D-CGD-O2D-CED
40	D	409	LHG	O2-C2-C3-O3
40	N	624	LHG	O2-C2-C3-O3
40	S	624	LHG	O2-C2-C3-O3
40	c	525	LHG	O2-C2-C3-O3
40	d	409	LHG	O2-C2-C3-O3
40	d	410	LHG	O2-C2-C3-O3
40	g	624	LHG	O2-C2-C3-O3
40	y	624	LHG	O2-C2-C3-O3
40	D1	408	LHG	O2-C2-C3-O3
40	G1	624	LHG	O2-C2-C3-O3
40	S1	624	LHG	O2-C2-C3-O3
40	d1	408	LHG	O2-C2-C3-O3
40	d1	409	LHG	O2-C2-C3-O3
40	n1	624	LHG	O2-C2-C3-O3
40	s1	624	LHG	O2-C2-C3-O3
54	S	625	LPX	O1-C3-C4-O5
54	s	625	LPX	O1-C3-C4-O5
54	s1	625	LPX	O1-C3-C4-O5
29	B	608	CLA	C3-C5-C6-C7
29	R	610	CLA	C3-C5-C6-C7
29	S	613	CLA	C3-C5-C6-C7
29	n	610	CLA	C3-C5-C6-C7
29	r	603	CLA	C3-C5-C6-C7
29	s	613	CLA	C3-C5-C6-C7
29	A1	406	CLA	C3-C5-C6-C7
29	C1	509	CLA	C3-C5-C6-C7
29	S1	610	CLA	C3-C5-C6-C7
29	Y1	614	CLA	C3-C5-C6-C7
29	r1	602	CLA	C3-C5-C6-C7
30	A1	409	PHO	C3-C5-C6-C7
29	B	608	CLA	CBA-CGA-O2A-C1
29	N	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	R	610	CLA	CBA-CGA-O2A-C1
29	S	610	CLA	CBA-CGA-O2A-C1
29	b	610	CLA	CBA-CGA-O2A-C1
29	s	602	CLA	CBA-CGA-O2A-C1
29	s	610	CLA	CBA-CGA-O2A-C1
29	s	617	CLA	CBA-CGA-O2A-C1
29	y	602	CLA	CBA-CGA-O2A-C1
29	A1	407	CLA	CBA-CGA-O2A-C1
29	C1	509	CLA	CBA-CGA-O2A-C1
29	c1	508	CLA	CBA-CGA-O2A-C1
29	s1	602	CLA	CBA-CGA-O2A-C1
29	s1	603	CLA	CBA-CGA-O2A-C1
29	s1	604	CLA	CBA-CGA-O2A-C1
29	s1	617	CLA	CBA-CGA-O2A-C1
29	y1	608	CLA	CBA-CGA-O2A-C1
29	y1	614	CLA	CBA-CGA-O2A-C1
32	m	101	SQD	C24-C23-O48-C46
32	M1	101	SQD	C24-C23-O48-C46
29	B	613	CLA	O1A-CGA-O2A-C1
29	C	506	CLA	O1A-CGA-O2A-C1
29	Y	613	CLA	O1A-CGA-O2A-C1
29	b	608	CLA	O1A-CGA-O2A-C1
29	s	602	CLA	O1A-CGA-O2A-C1
29	R1	608	CLA	O1A-CGA-O2A-C1
29	s1	614	CLA	O1A-CGA-O2A-C1
37	B	623	DGD	O1A-C1A-O1G-C1G
38	T	101	3PH	O32-C31-O31-C3
38	t	101	3PH	O32-C31-O31-C3
29	B	611	CLA	O1D-CGD-O2D-CED
29	C	502	CLA	O1D-CGD-O2D-CED
29	Y	612	CLA	O1D-CGD-O2D-CED
29	b	607	CLA	O1D-CGD-O2D-CED
29	y	604	CLA	O1D-CGD-O2D-CED
29	y	612	CLA	O1D-CGD-O2D-CED
29	C1	507	CLA	O1D-CGD-O2D-CED
29	b1	611	CLA	O1D-CGD-O2D-CED
54	s	625	LPX	O5-C4-C5-O6
32	m	101	SQD	C8-C7-O47-C45
32	B1	621	SQD	C8-C7-O47-C45
32	B1	626	SQD	C8-C7-O47-C45
32	M1	101	SQD	C8-C7-O47-C45
33	C	521	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
33	C1	523	LMG	C11-C10-O7-C8
39	B	625	DGA	CB2-CB1-OG2-CG2
39	b	625	DGA	CB2-CB1-OG2-CG2
43	d1	405	PL9	C47-C48-C49-C50
29	s	603	CLA	CBD-CGD-O2D-CED
29	B1	602	CLA	CBD-CGD-O2D-CED
29	b1	610	CLA	CBD-CGD-O2D-CED
29	g1	614	CLA	CBD-CGD-O2D-CED
29	s1	610	CLA	CBD-CGD-O2D-CED
33	H	102	LMG	O6-C5-C6-O5
37	c1	519	DGD	O6E-C5E-C6E-O5E
32	M1	101	SQD	C11-C10-C9-C8
40	C1	525	LHG	C11-C12-C13-C14
40	L1	101	LHG	C11-C12-C13-C14
47	I1	102	4RF	C33-C34-C35-C36
30	a	409	PHO	O1D-CGD-O2D-CED
29	S	602	CLA	O1A-CGA-O2A-C1
29	R1	609	CLA	O1A-CGA-O2A-C1
33	H1	102	LMG	C11-C12-C13-C14
40	C	525	LHG	C11-C12-C13-C14
52	r1	625	LMT	C4B-C5B-C6B-O6B
29	s1	604	CLA	O1D-CGD-O2D-CED
40	L	101	LHG	C7-C8-C9-C10
39	C	524	DGA	CCB-CDB-CEB-CFB
47	k1	101	4RF	C48-C49-C50-C51
29	N1	610	CLA	C5-C6-C7-C8
29	C	512	CLA	C3-C5-C6-C7
29	B1	617	CLA	C3-C5-C6-C7
29	c1	508	CLA	C3-C5-C6-C7
29	c1	512	CLA	C3-C5-C6-C7
48	S	608	CHL	C3-C5-C6-C7
29	R	609	CLA	CBA-CGA-O2A-C1
29	S	609	CLA	CBA-CGA-O2A-C1
29	Y	612	CLA	CBA-CGA-O2A-C1
29	b	606	CLA	CBA-CGA-O2A-C1
29	S1	609	CLA	CBA-CGA-O2A-C1
38	T	101	3PH	C32-C31-O31-C3
38	b	624	3PH	C32-C31-O31-C3
29	c	510	CLA	O1D-CGD-O2D-CED
29	y	614	CLA	O1D-CGD-O2D-CED
29	B1	611	CLA	O1D-CGD-O2D-CED
37	B1	623	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
52	R	625	LMT	O5'-C5'-C6'-O6'
32	B1	621	SQD	O49-C7-O47-C45
33	C1	523	LMG	O9-C10-O7-C8
40	s1	624	LHG	C9-C10-C11-C12
40	D1	410	LHG	C2-C3-O3-P
29	B	608	CLA	O1A-CGA-O2A-C1
29	R	604	CLA	O1A-CGA-O2A-C1
29	R	610	CLA	O1A-CGA-O2A-C1
29	b	610	CLA	O1A-CGA-O2A-C1
29	y	603	CLA	O1A-CGA-O2A-C1
29	A1	407	CLA	O1A-CGA-O2A-C1
29	C1	504	CLA	O1A-CGA-O2A-C1
29	C1	511	CLA	O1A-CGA-O2A-C1
29	S1	602	CLA	O1A-CGA-O2A-C1
29	Y1	613	CLA	O1A-CGA-O2A-C1
29	b1	604	CLA	O1A-CGA-O2A-C1
29	c1	508	CLA	O1A-CGA-O2A-C1
29	d1	403	CLA	O1A-CGA-O2A-C1
29	s1	602	CLA	O1A-CGA-O2A-C1
29	s1	610	CLA	O1A-CGA-O2A-C1
32	m	101	SQD	O10-C23-O48-C46
32	M1	101	SQD	O10-C23-O48-C46
38	T1	101	3PH	O32-C31-O31-C3
44	F	101	HEM	C3D-CAD-CBD-CGD
44	f	101	HEM	C3D-CAD-CBD-CGD
44	F1	101	HEM	C3D-CAD-CBD-CGD
29	r1	608	CLA	C5-C6-C7-C8
29	B	604	CLA	C4-C3-C5-C6
29	C	504	CLA	C4-C3-C5-C6
29	N	610	CLA	C4-C3-C5-C6
29	b	606	CLA	C4-C3-C5-C6
29	c	503	CLA	C4-C3-C5-C6
29	B1	606	CLA	C4-C3-C5-C6
29	N1	610	CLA	C4-C3-C5-C6
29	G1	602	CLA	C4-C3-C5-C6
29	Y1	602	CLA	C4-C3-C5-C6
29	b1	603	CLA	C4-C3-C5-C6
29	c1	503	CLA	C4-C3-C5-C6
29	g1	611	CLA	C4-C3-C5-C6
29	s1	614	CLA	C4-C3-C5-C6
43	D1	405	PL9	C20-C19-C21-C22
52	R	625	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
29	B	604	CLA	C2-C3-C5-C6
29	B	607	CLA	C2-C3-C5-C6
29	C	504	CLA	C2-C3-C5-C6
29	N	610	CLA	C2-C3-C5-C6
29	b	606	CLA	C2-C3-C5-C6
29	b	615	CLA	C2-C3-C5-C6
29	c	503	CLA	C2-C3-C5-C6
29	r	608	CLA	C2-C3-C5-C6
29	B1	606	CLA	C2-C3-C5-C6
29	B1	608	CLA	C2-C3-C5-C6
29	N1	610	CLA	C2-C3-C5-C6
29	G1	602	CLA	C2-C3-C5-C6
29	S1	602	CLA	C2-C3-C5-C6
29	Y1	602	CLA	C2-C3-C5-C6
29	a1	410	CLA	C2-C3-C5-C6
29	b1	603	CLA	C2-C3-C5-C6
29	c1	503	CLA	C2-C3-C5-C6
29	g1	611	CLA	C2-C3-C5-C6
29	s1	614	CLA	C2-C3-C5-C6
39	c1	524	DGA	CA1-CA2-CA3-CA4
55	y	627	PTY	O30-C30-O4-C1
29	A	407	CLA	C2A-CAA-CBA-CGA
29	S	602	CLA	C2A-CAA-CBA-CGA
29	a	407	CLA	C2A-CAA-CBA-CGA
29	G1	614	CLA	C2A-CAA-CBA-CGA
29	S1	602	CLA	C2A-CAA-CBA-CGA
29	Y1	610	CLA	C2A-CAA-CBA-CGA
29	b1	605	CLA	C2A-CAA-CBA-CGA
48	n	605	CHL	C2A-CAA-CBA-CGA
48	y	607	CHL	C2A-CAA-CBA-CGA
48	Y1	605	CHL	C2A-CAA-CBA-CGA
48	Y1	606	CHL	C2A-CAA-CBA-CGA
29	g	602	CLA	O1D-CGD-O2D-CED
29	B1	608	CLA	O1D-CGD-O2D-CED
29	Y1	612	CLA	O1D-CGD-O2D-CED
29	c1	513	CLA	O1D-CGD-O2D-CED
29	r1	602	CLA	O1D-CGD-O2D-CED
29	s1	617	CLA	O1D-CGD-O2D-CED
47	k	101	4RF	C48-C49-C50-C51
47	k1	101	4RF	C12-C13-C14-C15
33	D1	411	LMG	O6-C5-C6-O5
52	R1	625	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
29	N	603	CLA	O1A-CGA-O2A-C1
29	y	602	CLA	O1A-CGA-O2A-C1
29	C1	506	CLA	O1A-CGA-O2A-C1
29	a1	407	CLA	O1A-CGA-O2A-C1
29	s1	603	CLA	O1A-CGA-O2A-C1
29	s1	604	CLA	O1A-CGA-O2A-C1
29	y1	608	CLA	O1A-CGA-O2A-C1
32	c	526	SQD	O5-C1-O6-C44
33	B	622	LMG	O6-C1-O1-C7
33	W1	201	LMG	O6-C1-O1-C7
33	a1	413	LMG	O6-C1-O1-C7
52	R	625	LMT	O5'-C1'-O1'-C1
43	d	405	PL9	C39-C41-C42-C43
43	D1	405	PL9	C14-C16-C17-C18
43	d1	405	PL9	C39-C41-C42-C43
29	A	405	CLA	CBA-CGA-O2A-C1
29	C	511	CLA	CBA-CGA-O2A-C1
29	g	602	CLA	CBA-CGA-O2A-C1
29	r	604	CLA	CBA-CGA-O2A-C1
29	C1	506	CLA	CBA-CGA-O2A-C1
29	b1	606	CLA	CBA-CGA-O2A-C1
33	c	523	LMG	C29-C28-O8-C9
38	s1	626	3PH	C32-C31-O31-C3
40	D1	410	LHG	C24-C23-O8-C6
47	K	101	4RF	C31-C32-C33-C34
47	k	101	4RF	C12-C13-C14-C15
29	c	512	CLA	O1D-CGD-O2D-CED
29	g	614	CLA	O1D-CGD-O2D-CED
29	s1	602	CLA	O1D-CGD-O2D-CED
40	L1	101	LHG	C7-C8-C9-C10
29	N	603	CLA	O1D-CGD-O2D-CED
29	S	612	CLA	O1D-CGD-O2D-CED
29	b	614	CLA	O1D-CGD-O2D-CED
29	G1	614	CLA	O1D-CGD-O2D-CED
29	R1	604	CLA	O1D-CGD-O2D-CED
29	S1	603	CLA	O1D-CGD-O2D-CED
29	Y1	602	CLA	O1D-CGD-O2D-CED
29	b1	613	CLA	O1D-CGD-O2D-CED
30	A1	408	PHO	O1D-CGD-O2D-CED
29	S	610	CLA	O1A-CGA-O2A-C1
29	y1	614	CLA	O1A-CGA-O2A-C1
39	j1	101	DGA	CB2-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
40	S1	624	LHG	C8-C7-O7-C5
55	Y	627	PTY	O10-C8-O7-C6
43	D1	405	PL9	C32-C33-C34-C35
29	C	507	CLA	O1D-CGD-O2D-CED
29	C	512	CLA	O1D-CGD-O2D-CED
29	b	613	CLA	O1D-CGD-O2D-CED
29	B1	609	CLA	O1D-CGD-O2D-CED
29	S1	602	CLA	O1D-CGD-O2D-CED
29	c1	507	CLA	O1D-CGD-O2D-CED
29	n1	614	CLA	O1D-CGD-O2D-CED
29	s	609	CLA	O1D-CGD-O2D-CED
40	L	101	LHG	C1-C2-C3-O3
40	S	624	LHG	C1-C2-C3-O3
40	d	409	LHG	C1-C2-C3-O3
40	g	624	LHG	C1-C2-C3-O3
40	s	624	LHG	C1-C2-C3-O3
40	D1	408	LHG	C1-C2-C3-O3
40	D1	409	LHG	C1-C2-C3-O3
40	N1	624	LHG	C1-C2-C3-O3
40	G1	624	LHG	C1-C2-C3-O3
40	c1	525	LHG	C1-C2-C3-O3
40	g1	624	LHG	C1-C2-C3-O3
33	C	521	LMG	O9-C10-O7-C8
29	C	511	CLA	O1A-CGA-O2A-C1
29	N	610	CLA	O1A-CGA-O2A-C1
29	G	613	CLA	O1A-CGA-O2A-C1
29	r	604	CLA	O1A-CGA-O2A-C1
29	s	603	CLA	O1A-CGA-O2A-C1
29	s	610	CLA	O1A-CGA-O2A-C1
29	b1	612	CLA	O1A-CGA-O2A-C1
40	D1	410	LHG	O10-C23-O8-C6
29	R1	610	CLA	C3-C5-C6-C7
29	b1	610	CLA	C3-C5-C6-C7
29	n1	604	CLA	C3-C5-C6-C7
29	r1	603	CLA	C3-C5-C6-C7
29	s1	609	CLA	C3-C5-C6-C7
29	R	604	CLA	O1D-CGD-O2D-CED
29	S	604	CLA	O1D-CGD-O2D-CED
29	Y	604	CLA	O1D-CGD-O2D-CED
29	S1	604	CLA	O1D-CGD-O2D-CED
29	B	606	CLA	CBA-CGA-O2A-C1
29	C	513	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	N	602	CLA	CBA-CGA-O2A-C1
29	G	613	CLA	CBA-CGA-O2A-C1
29	S	603	CLA	CBA-CGA-O2A-C1
29	a	407	CLA	CBA-CGA-O2A-C1
29	a	410	CLA	CBA-CGA-O2A-C1
29	b	613	CLA	CBA-CGA-O2A-C1
29	c	511	CLA	CBA-CGA-O2A-C1
29	r	602	CLA	CBA-CGA-O2A-C1
29	s	603	CLA	CBA-CGA-O2A-C1
29	y	614	CLA	CBA-CGA-O2A-C1
29	B1	606	CLA	CBA-CGA-O2A-C1
29	B1	612	CLA	CBA-CGA-O2A-C1
29	B1	617	CLA	CBA-CGA-O2A-C1
29	N1	602	CLA	CBA-CGA-O2A-C1
29	N1	603	CLA	CBA-CGA-O2A-C1
29	G1	602	CLA	CBA-CGA-O2A-C1
29	G1	613	CLA	CBA-CGA-O2A-C1
29	R1	612	CLA	CBA-CGA-O2A-C1
29	S1	610	CLA	CBA-CGA-O2A-C1
29	b1	605	CLA	CBA-CGA-O2A-C1
29	b1	608	CLA	CBA-CGA-O2A-C1
29	b1	612	CLA	CBA-CGA-O2A-C1
29	b1	613	CLA	CBA-CGA-O2A-C1
29	c1	510	CLA	CBA-CGA-O2A-C1
29	c1	511	CLA	CBA-CGA-O2A-C1
29	r1	602	CLA	CBA-CGA-O2A-C1
29	r1	604	CLA	CBA-CGA-O2A-C1
30	A1	409	PHO	CBA-CGA-O2A-C1
32	A1	412	SQD	C24-C23-O48-C46
32	m1	101	SQD	C24-C23-O48-C46
37	C	520	DGD	C2A-C1A-O1G-C1G
37	c	520	DGD	C2A-C1A-O1G-C1G
37	C1	520	DGD	C2A-C1A-O1G-C1G
37	c1	520	DGD	C2A-C1A-O1G-C1G
38	S	626	3PH	C32-C31-O31-C3
38	s	626	3PH	C32-C31-O31-C3
40	L	101	LHG	C24-C23-O8-C6
40	d	410	LHG	C24-C23-O8-C6
40	C1	525	LHG	C24-C23-O8-C6
40	d1	408	LHG	C24-C23-O8-C6
47	k	101	4RF	C43-C41-O40-C39
55	y1	626	PTY	C31-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
29	A1	406	CLA	CBD-CGD-O2D-CED
29	c1	512	CLA	CBD-CGD-O2D-CED
52	R1	625	LMT	C4'-C5'-C6'-O6'
39	C1	524	DGA	CAA-CBA-CCA-CDA
29	S	602	CLA	O1D-CGD-O2D-CED
31	C	515	BCR	C19-C20-C21-C22
49	N	621	LUT	C29-C30-C31-C32
49	r1	620	LUT	C29-C30-C31-C32
47	i1	101	4RF	C13-C14-C15-C16
40	D1	409	LHG	C9-C10-C11-C12
29	b	609	CLA	C5-C6-C7-C8
29	b	615	CLA	C10-C11-C12-C13
29	B1	604	CLA	C13-C15-C16-C17
29	S1	609	CLA	C10-C11-C12-C13
33	H1	102	LMG	O6-C5-C6-O5
33	a1	413	LMG	O6-C5-C6-O5
32	m1	101	SQD	O10-C23-O48-C46
33	c	523	LMG	O10-C28-O8-C9
37	B1	623	DGD	C4E-C5E-C6E-O5E
52	r	625	LMT	C4B-C5B-C6B-O6B
32	b1	626	SQD	C11-C12-C13-C14
40	L1	101	LHG	O6-C4-C5-O7
33	a	413	LMG	O6-C5-C6-O5
52	R	625	LMT	C4'-C5'-C6'-O6'
37	c1	520	DGD	O6D-C5D-C6D-O5D
29	B	608	CLA	C10-C11-C12-C13
29	C	507	CLA	C13-C15-C16-C17
29	C	512	CLA	C5-C6-C7-C8
29	b	608	CLA	C5-C6-C7-C8
29	r	610	CLA	C10-C11-C12-C13
29	y	612	CLA	C5-C6-C7-C8
29	B1	602	CLA	C13-C15-C16-C17
29	B1	612	CLA	C8-C10-C11-C12
29	B1	613	CLA	C10-C11-C12-C13
29	B1	616	CLA	C8-C10-C11-C12
29	C1	503	CLA	C8-C10-C11-C12
29	Y1	602	CLA	C5-C6-C7-C8
29	Y1	613	CLA	C5-C6-C7-C8
29	c1	511	CLA	C8-C10-C11-C12
29	c1	513	CLA	C15-C16-C17-C18
29	d1	402	CLA	C10-C11-C12-C13
40	d	408	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
40	c1	525	LHG	O2-C2-C3-O3
29	N1	602	CLA	C3-C5-C6-C7
29	R1	602	CLA	C3-C5-C6-C7
37	C1	518	DGD	C1B-C2B-C3B-C4B
39	J1	101	DGA	CB1-CB2-CB3-CB4
40	D	410	LHG	C23-C24-C25-C26
40	G1	624	LHG	C7-C8-C9-C10
40	d1	410	LHG	C23-C24-C25-C26
32	a	412	SQD	C2-C1-O6-C44
32	c	526	SQD	C2-C1-O6-C44
33	B	622	LMG	C2-C1-O1-C7
33	b	622	LMG	C2-C1-O1-C7
37	B	623	DGD	C2D-C1D-O3G-C3G
37	b	623	DGD	C2D-C1D-O3G-C3G
37	C1	519	DGD	C2E-C1E-O5D-C6D
37	b1	623	DGD	C2D-C1D-O3G-C3G
37	b1	623	DGD	C2E-C1E-O5D-C6D
33	a1	413	LMG	O1-C7-C8-O7
33	d1	411	LMG	O1-C7-C8-O7
47	i1	101	4RF	O21-C20-C39-O40
39	c	524	DGA	CB9-CAB-CBB-CCB
47	I	102	4RF	C33-C34-C35-C36
47	i	101	4RF	C33-C34-C35-C36
29	S	603	CLA	O1A-CGA-O2A-C1
29	g	602	CLA	O1A-CGA-O2A-C1
29	B1	617	CLA	O1A-CGA-O2A-C1
29	N1	603	CLA	O1A-CGA-O2A-C1
29	r1	602	CLA	O1A-CGA-O2A-C1
52	R	625	LMT	O5B-C5B-C6B-O6B
29	s	603	CLA	C4-C3-C5-C6
48	s	608	CHL	C4-C3-C5-C6
29	D	402	CLA	C2-C3-C5-C6
29	Y1	612	CLA	C2-C3-C5-C6
48	N1	601	CHL	C2-C3-C5-C6
29	B	602	CLA	C11-C12-C13-C14
29	B	603	CLA	C14-C13-C15-C16
29	B	605	CLA	C6-C7-C8-C9
29	B	617	CLA	C14-C13-C15-C16
29	C	501	CLA	C11-C12-C13-C14
29	C	513	CLA	C11-C10-C8-C9
29	D	402	CLA	C6-C7-C8-C9
29	D	402	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	N	604	CLA	C11-C12-C13-C14
29	N	610	CLA	C11-C10-C8-C9
29	G	613	CLA	C11-C12-C13-C14
29	R	602	CLA	C6-C7-C8-C9
29	R	608	CLA	C11-C10-C8-C9
29	R	610	CLA	C6-C7-C8-C9
29	Y	603	CLA	C6-C7-C8-C9
29	Y	604	CLA	C11-C10-C8-C9
29	Y	614	CLA	C14-C13-C15-C16
29	b	603	CLA	C14-C13-C15-C16
29	b	605	CLA	C6-C7-C8-C9
29	b	606	CLA	C11-C10-C8-C9
29	b	607	CLA	C6-C7-C8-C9
29	b	616	CLA	C11-C10-C8-C9
29	c	501	CLA	C11-C12-C13-C14
29	c	504	CLA	C6-C7-C8-C9
29	c	505	CLA	C11-C10-C8-C9
29	c	513	CLA	C11-C10-C8-C9
29	g	611	CLA	C14-C13-C15-C16
29	r	610	CLA	C6-C7-C8-C9
29	s	603	CLA	C14-C13-C15-C16
29	s	609	CLA	C11-C10-C8-C9
29	y	604	CLA	C6-C7-C8-C9
29	A1	410	CLA	C6-C7-C8-C9
29	B1	602	CLA	C11-C12-C13-C14
29	B1	604	CLA	C11-C10-C8-C9
29	B1	606	CLA	C11-C10-C8-C9
29	B1	607	CLA	C6-C7-C8-C9
29	B1	610	CLA	C14-C13-C15-C16
29	B1	617	CLA	C14-C13-C15-C16
29	C1	508	CLA	C6-C7-C8-C9
29	C1	513	CLA	C11-C10-C8-C9
29	N1	604	CLA	C11-C12-C13-C14
29	R1	602	CLA	C6-C7-C8-C9
29	R1	612	CLA	C11-C10-C8-C9
29	S1	609	CLA	C11-C10-C8-C9
29	Y1	604	CLA	C11-C10-C8-C9
29	Y1	614	CLA	C6-C7-C8-C9
29	b1	602	CLA	C11-C12-C13-C14
29	b1	604	CLA	C11-C10-C8-C9
29	b1	608	CLA	C11-C10-C8-C9
29	b1	610	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	c1	501	CLA	C11-C12-C13-C14
29	c1	502	CLA	C6-C7-C8-C9
29	c1	504	CLA	C6-C7-C8-C9
29	c1	511	CLA	C11-C10-C8-C9
29	g1	602	CLA	C11-C12-C13-C14
29	g1	613	CLA	C11-C10-C8-C9
29	r1	612	CLA	C6-C7-C8-C9
29	r1	612	CLA	C11-C10-C8-C9
29	s1	609	CLA	C11-C10-C8-C9
29	s1	611	CLA	C6-C7-C8-C9
29	y1	612	CLA	C11-C12-C13-C14
30	a1	408	PHO	C6-C7-C8-C9
30	a1	409	PHO	C6-C7-C8-C9
48	N	605	CHL	C14-C13-C15-C16
48	N	609	CHL	C11-C12-C13-C14
48	G	607	CHL	C14-C13-C15-C16
48	Y	607	CHL	C6-C7-C8-C9
48	Y	607	CHL	C14-C13-C15-C16
48	Y	609	CHL	C11-C12-C13-C14
48	g	601	CHL	C14-C13-C15-C16
48	g	609	CHL	C14-C13-C15-C16
48	y	601	CHL	C11-C10-C8-C9
48	y	606	CHL	C11-C10-C8-C9
48	y	607	CHL	C6-C7-C8-C9
48	y	609	CHL	C11-C12-C13-C14
48	N1	606	CHL	C14-C13-C15-C16
48	G1	607	CHL	C11-C10-C8-C9
48	G1	607	CHL	C14-C13-C15-C16
48	Y1	607	CHL	C11-C10-C8-C9
48	Y1	609	CHL	C11-C12-C13-C14
48	g1	601	CHL	C14-C13-C15-C16
48	g1	609	CHL	C14-C13-C15-C16
48	s1	608	CHL	C11-C10-C8-C9
48	y1	609	CHL	C11-C12-C13-C14
29	N	612	CLA	O1D-CGD-O2D-CED
29	R	602	CLA	O1D-CGD-O2D-CED
29	c	513	CLA	O1D-CGD-O2D-CED
29	n	603	CLA	O1D-CGD-O2D-CED
29	s	605	CLA	O1D-CGD-O2D-CED
29	A1	407	CLA	O1D-CGD-O2D-CED
29	B1	607	CLA	O1D-CGD-O2D-CED
29	G1	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	Y	610	CLA	C5-C6-C7-C8
29	Y	611	CLA	C10-C11-C12-C13
29	Y	613	CLA	C2A-CAA-CBA-CGA
29	a	405	CLA	C2A-CAA-CBA-CGA
29	y	608	CLA	C2A-CAA-CBA-CGA
29	B1	604	CLA	C2A-CAA-CBA-CGA
29	Y1	613	CLA	C2A-CAA-CBA-CGA
29	b1	604	CLA	C2A-CAA-CBA-CGA
48	n	606	CHL	C2A-CAA-CBA-CGA
48	S1	601	CHL	C2A-CAA-CBA-CGA
48	n1	605	CHL	C2A-CAA-CBA-CGA
31	C	514	BCR	C36-C18-C19-C20
31	C	517	BCR	C37-C22-C23-C24
31	D	404	BCR	C36-C18-C19-C20
31	B1	618	BCR	C37-C22-C23-C24
31	C1	515	BCR	C7-C8-C9-C34
31	C1	515	BCR	C11-C12-C13-C35
31	C1	517	BCR	C37-C22-C23-C24
31	D1	404	BCR	C7-C8-C9-C34
31	D1	404	BCR	C37-C22-C23-C24
31	c1	514	BCR	C36-C18-C19-C20
31	c1	515	BCR	C7-C8-C9-C34
36	b	620	C7Z	C11-C12-C13-C20
36	B1	620	C7Z	C7-C8-C9-C19
36	b1	620	C7Z	C7-C8-C9-C19
45	H	101	RRX	C7-C8-C9-C34
45	h1	101	RRX	C36-C18-C19-C20
45	h1	101	RRX	C11-C12-C13-C35
49	Y	620	LUT	C27-C28-C29-C39
49	r	620	LUT	C7-C8-C9-C19
49	S1	621	LUT	C7-C8-C9-C19
49	n1	620	LUT	C27-C28-C29-C39
49	g1	621	LUT	C31-C32-C33-C40
49	s1	620	LUT	C31-C32-C33-C40
49	y1	620	LUT	C27-C28-C29-C39
50	R	621	XAT	C27-C28-C29-C39
50	r	621	XAT	C27-C28-C29-C39
51	y	623	NEX	C11-C12-C13-C20
31	C	516	BCR	C7-C8-C9-C10
31	C	516	BCR	C21-C22-C23-C24
31	C	517	BCR	C21-C22-C23-C24
31	B1	618	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	B1	618	BCR	C21-C22-C23-C24
31	C1	515	BCR	C7-C8-C9-C10
31	C1	515	BCR	C11-C12-C13-C14
31	C1	517	BCR	C21-C22-C23-C24
31	D1	404	BCR	C21-C22-C23-C24
31	c1	515	BCR	C7-C8-C9-C10
36	B	620	C7Z	C7-C8-C9-C10
36	B1	620	C7Z	C7-C8-C9-C10
36	b1	620	C7Z	C7-C8-C9-C10
45	H	101	RRX	C7-C8-C9-C10
45	h1	101	RRX	C17-C18-C19-C20
49	r	620	LUT	C7-C8-C9-C10
49	S1	621	LUT	C7-C8-C9-C10
49	g1	621	LUT	C31-C32-C33-C34
51	y1	623	NEX	C11-C12-C13-C14
29	D	403	CLA	O1D-CGD-O2D-CED
32	b	621	SQD	C8-C7-O47-C45
32	m1	101	SQD	C8-C7-O47-C45
33	c1	521	LMG	C11-C10-O7-C8
40	L1	101	LHG	C17-C18-C19-C20
40	c1	525	LHG	C33-C34-C35-C36
33	b1	622	LMG	C4-C5-C6-O5
32	B	626	SQD	C23-C24-C25-C26
33	D	411	LMG	C10-C11-C12-C13
39	j	101	DGA	CA1-CA2-CA3-CA4
40	D	408	LHG	C23-C24-C25-C26
40	D	410	LHG	C7-C8-C9-C10
40	d	410	LHG	C23-C24-C25-C26
29	a	410	CLA	O1A-CGA-O2A-C1
29	y	614	CLA	O1A-CGA-O2A-C1
29	G1	602	CLA	O1A-CGA-O2A-C1
29	R1	612	CLA	O1A-CGA-O2A-C1
29	S1	610	CLA	O1A-CGA-O2A-C1
29	b1	613	CLA	O1A-CGA-O2A-C1
29	c1	510	CLA	O1A-CGA-O2A-C1
29	c1	511	CLA	O1A-CGA-O2A-C1
29	r1	604	CLA	O1A-CGA-O2A-C1
38	S	626	3PH	O32-C31-O31-C3
47	k	101	4RF	O42-C41-O40-C39
29	N	610	CLA	C15-C16-C17-C18
29	G	603	CLA	C5-C6-C7-C8
29	Y	614	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	b	604	CLA	C15-C16-C17-C18
29	c	503	CLA	C15-C16-C17-C18
29	c	504	CLA	C13-C15-C16-C17
29	c	512	CLA	C13-C15-C16-C17
29	c	513	CLA	C10-C11-C12-C13
29	n	610	CLA	C15-C16-C17-C18
29	g	603	CLA	C8-C10-C11-C12
29	g	603	CLA	C10-C11-C12-C13
29	r	603	CLA	C5-C6-C7-C8
29	B1	614	CLA	C13-C15-C16-C17
29	R1	603	CLA	C5-C6-C7-C8
29	S1	611	CLA	C8-C10-C11-C12
29	Y1	610	CLA	C5-C6-C7-C8
29	b1	612	CLA	C15-C16-C17-C18
29	c1	506	CLA	C5-C6-C7-C8
29	g1	613	CLA	C10-C11-C12-C13
29	r1	603	CLA	C10-C11-C12-C13
29	y1	603	CLA	C13-C15-C16-C17
30	A	408	PHO	C15-C16-C17-C18
29	b	616	CLA	O1D-CGD-O2D-CED
29	s	602	CLA	O1D-CGD-O2D-CED
29	g1	613	CLA	O1D-CGD-O2D-CED
40	d1	409	LHG	C9-C10-C11-C12
47	k	101	4RF	C05-C06-C07-C08
37	B	623	DGD	C4D-C5D-C6D-O5D
52	r	625	LMT	O5'-C5'-C6'-O6'
52	r1	625	LMT	O5'-C5'-C6'-O6'
29	g	612	CLA	O1D-CGD-O2D-CED
29	S	609	CLA	C3-C5-C6-C7
29	S1	609	CLA	C3-C5-C6-C7
48	N	605	CHL	C3-C5-C6-C7
29	C	504	CLA	CBA-CGA-O2A-C1
29	a	405	CLA	CBA-CGA-O2A-C1
29	s	604	CLA	CBA-CGA-O2A-C1
29	y	610	CLA	CBA-CGA-O2A-C1
29	C1	503	CLA	CBA-CGA-O2A-C1
29	a1	405	CLA	CBA-CGA-O2A-C1
29	c1	513	CLA	CBA-CGA-O2A-C1
32	C1	526	SQD	C24-C23-O48-C46
38	B1	624	3PH	C32-C31-O31-C3
29	B	603	CLA	C8-C10-C11-C12
29	B	603	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	B	608	CLA	C13-C15-C16-C17
29	C	503	CLA	C15-C16-C17-C18
29	C	506	CLA	C5-C6-C7-C8
29	N	613	CLA	C5-C6-C7-C8
29	G	602	CLA	C15-C16-C17-C18
29	R	608	CLA	C10-C11-C12-C13
29	S	610	CLA	C13-C15-C16-C17
29	S	611	CLA	C8-C10-C11-C12
29	S	611	CLA	C15-C16-C17-C18
29	Y	614	CLA	C5-C6-C7-C8
29	b	606	CLA	C15-C16-C17-C18
29	b	610	CLA	C10-C11-C12-C13
29	b	615	CLA	C13-C15-C16-C17
29	c	509	CLA	C15-C16-C17-C18
29	n	604	CLA	C8-C10-C11-C12
29	g	613	CLA	C15-C16-C17-C18
29	s	609	CLA	C10-C11-C12-C13
29	s	611	CLA	C8-C10-C11-C12
29	y	602	CLA	C13-C15-C16-C17
29	y	603	CLA	C13-C15-C16-C17
29	B1	607	CLA	C13-C15-C16-C17
29	B1	609	CLA	C5-C6-C7-C8
29	C1	504	CLA	C15-C16-C17-C18
29	C1	508	CLA	C15-C16-C17-C18
29	C1	511	CLA	C10-C11-C12-C13
29	C1	511	CLA	C15-C16-C17-C18
29	N1	613	CLA	C5-C6-C7-C8
29	G1	602	CLA	C5-C6-C7-C8
29	G1	602	CLA	C8-C10-C11-C12
29	G1	603	CLA	C13-C15-C16-C17
29	S1	609	CLA	C8-C10-C11-C12
29	Y1	611	CLA	C10-C11-C12-C13
29	Y1	613	CLA	C15-C16-C17-C18
29	b1	604	CLA	C15-C16-C17-C18
29	b1	606	CLA	C15-C16-C17-C18
29	b1	614	CLA	C8-C10-C11-C12
29	c1	501	CLA	C10-C11-C12-C13
29	c1	508	CLA	C15-C16-C17-C18
29	n1	610	CLA	C8-C10-C11-C12
29	g1	611	CLA	C13-C15-C16-C17
29	r1	609	CLA	C10-C11-C12-C13
29	y1	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	y1	612	CLA	C13-C15-C16-C17
48	N	609	CHL	C13-C15-C16-C17
48	Y1	607	CHL	C5-C6-C7-C8
48	y1	607	CHL	C8-C10-C11-C12
33	d1	411	LMG	O6-C5-C6-O5
33	h1	102	LMG	C15-C16-C17-C18
32	a1	412	SQD	C23-C24-C25-C26
33	B	622	LMG	C10-C11-C12-C13
33	H1	102	LMG	C28-C29-C30-C31
37	c	519	DGD	C1A-C2A-C3A-C4A
38	S	626	3PH	C31-C32-C33-C34
38	s1	626	3PH	C31-C32-C33-C34
39	C1	524	DGA	CA1-CA2-CA3-CA4
39	j1	101	DGA	CA1-CA2-CA3-CA4
40	C	525	LHG	C23-C24-C25-C26
40	c	525	LHG	C7-C8-C9-C10
40	c	525	LHG	C23-C24-C25-C26
40	y	624	LHG	C7-C8-C9-C10
47	i1	101	4RF	C22-C24-C25-C26
55	y1	626	PTY	C30-C31-C32-C33
29	C	510	CLA	O1D-CGD-O2D-CED
29	A	407	CLA	CBD-CGD-O2D-CED
53	r	626	ERG	C17-C20-C22-C23
53	r1	626	ERG	C17-C20-C22-C23
51	N1	623	NEX	C14-C15-C35-C34
29	N	613	CLA	O1D-CGD-O2D-CED
29	B	608	CLA	C5-C6-C7-C8
29	B	610	CLA	C8-C10-C11-C12
29	B	612	CLA	C15-C16-C17-C18
29	C	501	CLA	C10-C11-C12-C13
29	C	502	CLA	C13-C15-C16-C17
29	N	603	CLA	C8-C10-C11-C12
29	N	613	CLA	C8-C10-C11-C12
29	S	603	CLA	C13-C15-C16-C17
29	S	609	CLA	C10-C11-C12-C13
29	Y	602	CLA	C10-C11-C12-C13
29	Y	603	CLA	C15-C16-C17-C18
29	Y	604	CLA	C13-C15-C16-C17
29	a	410	CLA	C8-C10-C11-C12
29	b	603	CLA	C10-C11-C12-C13
29	b	603	CLA	C13-C15-C16-C17
29	b	608	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	b	612	CLA	C13-C15-C16-C17
29	b	617	CLA	C5-C6-C7-C8
29	c	506	CLA	C5-C6-C7-C8
29	c	512	CLA	C10-C11-C12-C13
29	n	604	CLA	C10-C11-C12-C13
29	s	609	CLA	C8-C10-C11-C12
29	s	611	CLA	C13-C15-C16-C17
29	s	611	CLA	C15-C16-C17-C18
29	y	613	CLA	C5-C6-C7-C8
29	y	613	CLA	C15-C16-C17-C18
29	B1	603	CLA	C5-C6-C7-C8
29	B1	607	CLA	C5-C6-C7-C8
29	B1	607	CLA	C10-C11-C12-C13
29	B1	608	CLA	C5-C6-C7-C8
29	B1	609	CLA	C8-C10-C11-C12
29	B1	610	CLA	C8-C10-C11-C12
29	C1	512	CLA	C13-C15-C16-C17
29	C1	513	CLA	C8-C10-C11-C12
29	D1	403	CLA	C10-C11-C12-C13
29	N1	610	CLA	C13-C15-C16-C17
29	N1	613	CLA	C8-C10-C11-C12
29	G1	603	CLA	C15-C16-C17-C18
29	G1	611	CLA	C15-C16-C17-C18
29	R1	603	CLA	C10-C11-C12-C13
29	S1	610	CLA	C5-C6-C7-C8
29	S1	614	CLA	C5-C6-C7-C8
29	Y1	602	CLA	C15-C16-C17-C18
29	Y1	611	CLA	C5-C6-C7-C8
29	Y1	613	CLA	C10-C11-C12-C13
29	b1	602	CLA	C15-C16-C17-C18
29	b1	603	CLA	C15-C16-C17-C18
29	b1	604	CLA	C8-C10-C11-C12
29	b1	610	CLA	C5-C6-C7-C8
29	b1	610	CLA	C13-C15-C16-C17
29	b1	611	CLA	C15-C16-C17-C18
29	b1	613	CLA	C10-C11-C12-C13
29	b1	614	CLA	C13-C15-C16-C17
29	b1	615	CLA	C10-C11-C12-C13
29	c1	504	CLA	C15-C16-C17-C18
29	c1	506	CLA	C15-C16-C17-C18
29	c1	509	CLA	C15-C16-C17-C18
29	d1	403	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	g1	610	CLA	C10-C11-C12-C13
29	r1	610	CLA	C10-C11-C12-C13
29	s1	603	CLA	C13-C15-C16-C17
29	s1	611	CLA	C13-C15-C16-C17
29	s1	613	CLA	C5-C6-C7-C8
33	b	622	LMG	C19-C20-C21-C22
29	b	603	CLA	O1D-CGD-O2D-CED
29	C1	512	CLA	O1D-CGD-O2D-CED
40	C	525	LHG	O1-C1-C2-O2
40	D	409	LHG	O1-C1-C2-O2
40	G	624	LHG	O1-C1-C2-O2
40	d	408	LHG	O1-C1-C2-O2
40	D1	408	LHG	O1-C1-C2-O2
40	L1	101	LHG	O1-C1-C2-O2
40	d1	408	LHG	O1-C1-C2-O2
46	I	101	GOL	O2-C2-C3-O3
29	C	513	CLA	O1A-CGA-O2A-C1
29	G1	613	CLA	O1A-CGA-O2A-C1
37	c1	520	DGD	O1A-C1A-O1G-C1G
32	A	412	SQD	C7-C8-C9-C10
32	m	101	SQD	C7-C8-C9-C10
32	M1	101	SQD	C7-C8-C9-C10
33	C	523	LMG	C28-C29-C30-C31
33	H	102	LMG	C28-C29-C30-C31
33	b	622	LMG	C28-C29-C30-C31
33	c	523	LMG	C10-C11-C12-C13
33	d	411	LMG	C28-C29-C30-C31
37	c1	519	DGD	C1B-C2B-C3B-C4B
38	b	624	3PH	C31-C32-C33-C34
38	B1	624	3PH	C31-C32-C33-C34
38	T1	101	3PH	C31-C32-C33-C34
38	s1	626	3PH	C21-C22-C23-C24
39	C	524	DGA	CB1-CB2-CB3-CB4
39	c	524	DGA	CB1-CB2-CB3-CB4
39	j1	101	DGA	CB1-CB2-CB3-CB4
40	N	624	LHG	C7-C8-C9-C10
40	d	409	LHG	C7-C8-C9-C10
40	d	410	LHG	C7-C8-C9-C10
40	n	624	LHG	C7-C8-C9-C10
40	C1	525	LHG	C23-C24-C25-C26
40	D1	408	LHG	C7-C8-C9-C10
40	D1	409	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
40	D1	410	LHG	C23-C24-C25-C26
40	c1	525	LHG	C7-C8-C9-C10
40	d1	408	LHG	C7-C8-C9-C10
40	d1	408	LHG	C23-C24-C25-C26
40	d1	410	LHG	C7-C8-C9-C10
40	y1	624	LHG	C7-C8-C9-C10
47	i	101	4RF	C13-C14-C15-C16
47	i	101	4RF	C41-C43-C44-C45
47	k	101	4RF	C41-C43-C44-C45
47	I1	102	4RF	C13-C14-C15-C16
47	i1	101	4RF	C41-C43-C44-C45
55	y	626	PTY	C8-C11-C12-C13
33	C	521	LMG	O6-C5-C6-O5
40	C1	525	LHG	C33-C34-C35-C36
40	D1	410	LHG	C24-C25-C26-C27
47	k1	101	4RF	C05-C06-C07-C08
29	B	608	CLA	C8-C10-C11-C12
29	B	608	CLA	C15-C16-C17-C18
29	B	614	CLA	C13-C15-C16-C17
29	B	617	CLA	C8-C10-C11-C12
29	C	507	CLA	C8-C10-C11-C12
29	C	507	CLA	C15-C16-C17-C18
29	C	508	CLA	C10-C11-C12-C13
29	C	512	CLA	C13-C15-C16-C17
29	N	602	CLA	C8-C10-C11-C12
29	b	604	CLA	C8-C10-C11-C12
29	b	614	CLA	C5-C6-C7-C8
29	c	507	CLA	C8-C10-C11-C12
29	n	604	CLA	C15-C16-C17-C18
29	r	602	CLA	C8-C10-C11-C12
29	r	612	CLA	C10-C11-C12-C13
29	s	604	CLA	C5-C6-C7-C8
29	y	611	CLA	C5-C6-C7-C8
29	B1	603	CLA	C10-C11-C12-C13
29	C1	502	CLA	C13-C15-C16-C17
29	N1	604	CLA	C10-C11-C12-C13
29	G1	602	CLA	C13-C15-C16-C17
29	S1	611	CLA	C15-C16-C17-C18
29	S1	613	CLA	C5-C6-C7-C8
29	b1	607	CLA	C8-C10-C11-C12
29	b1	612	CLA	C5-C6-C7-C8
29	b1	617	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	b1	617	CLA	C13-C15-C16-C17
29	c1	513	CLA	C10-C11-C12-C13
29	g1	602	CLA	C13-C15-C16-C17
29	s1	602	CLA	C5-C6-C7-C8
29	s1	614	CLA	C5-C6-C7-C8
29	y1	613	CLA	C15-C16-C17-C18
48	n1	606	CHL	C5-C6-C7-C8
48	n1	609	CHL	C15-C16-C17-C18
29	c	504	CLA	CBA-CGA-O2A-C1
29	g	610	CLA	CBA-CGA-O2A-C1
33	d	411	LMG	C31-C32-C33-C34
37	C1	519	DGD	C5B-C6B-C7B-C8B
39	B1	625	DGA	CA3-CA4-CA5-CA6
40	C	525	LHG	C16-C17-C18-C19
40	S1	624	LHG	C9-C10-C11-C12
29	n1	603	CLA	O1D-CGD-O2D-CED
33	h	102	LMG	O6-C5-C6-O5
32	b	621	SQD	O49-C7-O47-C45
32	m1	101	SQD	O49-C7-O47-C45
29	B	602	CLA	C2-C1-O2A-CGA
29	B	613	CLA	C2-C1-O2A-CGA
29	B	614	CLA	C2-C1-O2A-CGA
29	G	614	CLA	C2-C1-O2A-CGA
29	Y	603	CLA	C2-C1-O2A-CGA
29	Y	614	CLA	C2-C1-O2A-CGA
29	b	605	CLA	C2-C1-O2A-CGA
29	b	613	CLA	C2-C1-O2A-CGA
29	b	614	CLA	C2-C1-O2A-CGA
29	n	610	CLA	C2-C1-O2A-CGA
29	g	602	CLA	C2-C1-O2A-CGA
29	g	614	CLA	C2-C1-O2A-CGA
29	y	604	CLA	C2-C1-O2A-CGA
29	y	608	CLA	C2-C1-O2A-CGA
29	B1	606	CLA	C2-C1-O2A-CGA
29	B1	607	CLA	C2-C1-O2A-CGA
29	C1	509	CLA	C2-C1-O2A-CGA
29	C1	512	CLA	C2-C1-O2A-CGA
29	N1	611	CLA	C2-C1-O2A-CGA
29	N1	613	CLA	C2-C1-O2A-CGA
29	G1	602	CLA	C2-C1-O2A-CGA
29	G1	604	CLA	C2-C1-O2A-CGA
29	R1	603	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	Y1	603	CLA	C2-C1-O2A-CGA
29	Y1	608	CLA	C2-C1-O2A-CGA
29	Y1	614	CLA	C2-C1-O2A-CGA
29	b1	602	CLA	C2-C1-O2A-CGA
29	b1	608	CLA	C2-C1-O2A-CGA
29	b1	611	CLA	C2-C1-O2A-CGA
29	b1	617	CLA	C2-C1-O2A-CGA
29	c1	510	CLA	C2-C1-O2A-CGA
29	n1	603	CLA	C2-C1-O2A-CGA
29	n1	611	CLA	C2-C1-O2A-CGA
29	g1	614	CLA	C2-C1-O2A-CGA
29	r1	604	CLA	C2-C1-O2A-CGA
29	s1	610	CLA	C2-C1-O2A-CGA
29	y1	603	CLA	C2-C1-O2A-CGA
30	A1	409	PHO	C2-C1-O2A-CGA
29	C	501	CLA	C15-C16-C17-C18
29	D	403	CLA	C13-C15-C16-C17
29	G	611	CLA	C5-C6-C7-C8
29	R	603	CLA	C10-C11-C12-C13
29	n	603	CLA	C15-C16-C17-C18
29	s	613	CLA	C5-C6-C7-C8
29	y	612	CLA	C13-C15-C16-C17
29	B1	614	CLA	C5-C6-C7-C8
29	C1	510	CLA	C5-C6-C7-C8
29	C1	510	CLA	C13-C15-C16-C17
29	S1	602	CLA	C8-C10-C11-C12
29	S1	603	CLA	C13-C15-C16-C17
29	a1	405	CLA	C5-C6-C7-C8
29	b1	606	CLA	C13-C15-C16-C17
29	b1	609	CLA	C13-C15-C16-C17
29	d1	402	CLA	C8-C10-C11-C12
48	g	607	CHL	C5-C6-C7-C8
37	b1	623	DGD	C4D-C5D-C6D-O5D
33	B	622	LMG	C28-C29-C30-C31
38	S1	626	3PH	C31-C32-C33-C34
39	c	524	DGA	CA1-CA2-CA3-CA4
39	j	101	DGA	CB1-CB2-CB3-CB4
40	S1	624	LHG	C23-C24-C25-C26
40	n1	624	LHG	C7-C8-C9-C10
48	G1	608	CHL	C2A-CAA-CBA-CGA
48	R1	606	CHL	C2A-CAA-CBA-CGA
32	b	626	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
33	h1	102	LMG	C11-C10-O7-C8
29	c	502	CLA	C13-C15-C16-C17
29	c	510	CLA	C8-C10-C11-C12
29	g	611	CLA	C15-C16-C17-C18
29	s	610	CLA	C10-C11-C12-C13
29	s	610	CLA	C13-C15-C16-C17
29	B1	602	CLA	C10-C11-C12-C13
29	S1	604	CLA	C5-C6-C7-C8
29	a1	406	CLA	C5-C6-C7-C8
29	a1	406	CLA	C13-C15-C16-C17
29	b1	604	CLA	C10-C11-C12-C13
29	b1	607	CLA	C13-C15-C16-C17
29	b1	616	CLA	C13-C15-C16-C17
29	n1	603	CLA	C8-C10-C11-C12
30	a	408	PHO	C8-C10-C11-C12
29	A	410	CLA	O1D-CGD-O2D-CED
29	C	501	CLA	C11-C10-C8-C7
29	C	505	CLA	C12-C13-C15-C16
29	C	509	CLA	C12-C13-C15-C16
29	C	513	CLA	C12-C13-C15-C16
29	b	608	CLA	C11-C12-C13-C15
29	g	603	CLA	C11-C12-C13-C15
29	s	603	CLA	C12-C13-C15-C16
29	B1	602	CLA	C11-C10-C8-C7
29	G1	603	CLA	C11-C12-C13-C15
29	Y1	613	CLA	C12-C13-C15-C16
29	b1	610	CLA	C11-C12-C13-C15
29	b1	610	CLA	C12-C13-C15-C16
29	g1	602	CLA	C11-C12-C13-C15
29	r1	609	CLA	C6-C7-C8-C10
29	y1	602	CLA	C11-C12-C13-C15
30	a1	408	PHO	C11-C12-C13-C15
48	N	609	CHL	C11-C12-C13-C15
48	Y	606	CHL	C12-C13-C15-C16
48	g	601	CHL	C11-C12-C13-C15
48	y	601	CHL	C11-C10-C8-C7
48	y	607	CHL	C6-C7-C8-C10
29	a	405	CLA	O1A-CGA-O2A-C1
29	b	613	CLA	O1A-CGA-O2A-C1
29	r	602	CLA	O1A-CGA-O2A-C1
29	B1	612	CLA	O1A-CGA-O2A-C1
29	N1	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	A1	412	SQD	O10-C23-O48-C46
37	C	520	DGD	O1A-C1A-O1G-C1G
38	s	626	3PH	O32-C31-O31-C3
40	L	101	LHG	O10-C23-O8-C6
40	d1	408	LHG	O10-C23-O8-C6
55	y1	626	PTY	O30-C30-O4-C1
31	C	514	BCR	C9-C10-C11-C12
31	a	411	BCR	C9-C10-C11-C12
31	b	618	BCR	C9-C10-C11-C12
31	b1	619	BCR	C19-C20-C21-C22
36	b1	620	C7Z	C29-C30-C31-C32
49	N1	620	LUT	C29-C30-C31-C32
49	G1	621	LUT	C29-C30-C31-C32
55	Y	626	PTY	C8-C11-C12-C13
29	b	615	CLA	C2A-CAA-CBA-CGA
29	g	610	CLA	C2A-CAA-CBA-CGA
29	s	613	CLA	C2A-CAA-CBA-CGA
29	A1	410	CLA	C2A-CAA-CBA-CGA
29	C1	507	CLA	C2A-CAA-CBA-CGA
29	R1	602	CLA	C2A-CAA-CBA-CGA
29	R1	604	CLA	C2A-CAA-CBA-CGA
29	c1	504	CLA	C2A-CAA-CBA-CGA
29	s1	613	CLA	C2A-CAA-CBA-CGA
48	N	606	CHL	C2A-CAA-CBA-CGA
48	Y	607	CHL	C2A-CAA-CBA-CGA
48	g	606	CHL	C2A-CAA-CBA-CGA
48	y	605	CHL	C2A-CAA-CBA-CGA
48	N1	608	CHL	C2A-CAA-CBA-CGA
29	N	604	CLA	O1D-CGD-O2D-CED
29	S	605	CLA	O1D-CGD-O2D-CED
29	Y	602	CLA	O1D-CGD-O2D-CED
29	a1	406	CLA	O1D-CGD-O2D-CED
29	b1	612	CLA	O1D-CGD-O2D-CED
29	y1	612	CLA	O1D-CGD-O2D-CED
29	B	607	CLA	C10-C11-C12-C13
29	D	403	CLA	C15-C16-C17-C18
29	G	602	CLA	C8-C10-C11-C12
29	Y	604	CLA	C15-C16-C17-C18
29	Y	611	CLA	C13-C15-C16-C17
29	b	602	CLA	C15-C16-C17-C18
29	d	403	CLA	C8-C10-C11-C12
29	g	611	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	r	610	CLA	C5-C6-C7-C8
29	r	612	CLA	C8-C10-C11-C12
29	y	610	CLA	C5-C6-C7-C8
29	B1	608	CLA	C8-C10-C11-C12
29	B1	608	CLA	C15-C16-C17-C18
29	B1	617	CLA	C8-C10-C11-C12
29	R1	612	CLA	C8-C10-C11-C12
29	S1	610	CLA	C13-C15-C16-C17
29	a1	410	CLA	C8-C10-C11-C12
29	b1	607	CLA	C5-C6-C7-C8
29	b1	614	CLA	C15-C16-C17-C18
29	c1	505	CLA	C10-C11-C12-C13
29	c1	512	CLA	C10-C11-C12-C13
29	n1	603	CLA	C5-C6-C7-C8
29	g1	611	CLA	C10-C11-C12-C13
29	y1	603	CLA	C15-C16-C17-C18
47	K1	101	4RF	C27-C28-C29-C30
40	C	525	LHG	C33-C34-C35-C36
29	B	606	CLA	O1A-CGA-O2A-C1
29	c	511	CLA	O1A-CGA-O2A-C1
29	b1	605	CLA	O1A-CGA-O2A-C1
30	A1	409	PHO	O1A-CGA-O2A-C1
37	c	520	DGD	O1A-C1A-O1G-C1G
32	b1	626	SQD	O5-C1-O6-C44
33	b1	622	LMG	O6-C1-O1-C7
37	C	519	DGD	O6E-C1E-O5D-C6D
37	c	519	DGD	O6E-C1E-O5D-C6D
37	C1	519	DGD	O6E-C1E-O5D-C6D
52	r1	625	LMT	O5'-C1'-O1'-C1
29	c	501	CLA	C10-C11-C12-C13
29	r	603	CLA	C8-C10-C11-C12
29	C1	512	CLA	C5-C6-C7-C8
29	N1	603	CLA	C8-C10-C11-C12
29	R1	603	CLA	C8-C10-C11-C12
29	Y1	604	CLA	C8-C10-C11-C12
29	c1	510	CLA	C15-C16-C17-C18
48	N	606	CHL	C5-C6-C7-C8
29	y	611	CLA	O1D-CGD-O2D-CED
29	G1	611	CLA	O1D-CGD-O2D-CED
37	c	518	DGD	C1B-C2B-C3B-C4B
47	I	102	4RF	C41-C43-C44-C45
31	C	517	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	b	619	BCR	C10-C11-C12-C13
31	c	515	BCR	C10-C11-C12-C13
31	B1	619	BCR	C10-C11-C12-C13
50	N1	622	XAT	C10-C11-C12-C13
50	Y1	622	XAT	C30-C31-C32-C33
51	N	623	NEX	C10-C11-C12-C13
51	G	623	NEX	C30-C31-C32-C33
51	R	622	NEX	C10-C11-C12-C13
51	S	623	NEX	C10-C11-C12-C13
51	y	623	NEX	C30-C31-C32-C33
51	G1	623	NEX	C30-C31-C32-C33
51	S1	623	NEX	C10-C11-C12-C13
51	g1	623	NEX	C10-C11-C12-C13
51	g1	623	NEX	C30-C31-C32-C33
37	c1	518	DGD	O6E-C5E-C6E-O5E
40	C	525	LHG	O2-C2-C3-O3
40	L	101	LHG	O2-C2-C3-O3
40	G	624	LHG	O2-C2-C3-O3
40	C1	525	LHG	O2-C2-C3-O3
33	c1	521	LMG	O9-C10-O7-C8
40	S1	624	LHG	O9-C7-O7-C5
29	R	603	CLA	C3-C5-C6-C7
29	y	611	CLA	C3-C5-C6-C7
29	S1	603	CLA	C3-C5-C6-C7
48	G1	601	CHL	C3-C5-C6-C7
29	G1	612	CLA	C2A-CAA-CBA-CGA
48	S1	606	CHL	C2A-CAA-CBA-CGA
29	B	602	CLA	C13-C15-C16-C17
29	C	501	CLA	C8-C10-C11-C12
29	C	513	CLA	C15-C16-C17-C18
29	D	403	CLA	C8-C10-C11-C12
29	N	604	CLA	C15-C16-C17-C18
29	G	611	CLA	C10-C11-C12-C13
29	R	608	CLA	C8-C10-C11-C12
29	S	610	CLA	C15-C16-C17-C18
29	S	611	CLA	C13-C15-C16-C17
29	Y	603	CLA	C13-C15-C16-C17
29	Y	611	CLA	C5-C6-C7-C8
29	Y	612	CLA	C10-C11-C12-C13
29	a	410	CLA	C5-C6-C7-C8
29	b	602	CLA	C10-C11-C12-C13
29	b	605	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	c	504	CLA	C10-C11-C12-C13
29	c	506	CLA	C15-C16-C17-C18
29	n	603	CLA	C5-C6-C7-C8
29	g	602	CLA	C8-C10-C11-C12
29	s	611	CLA	C5-C6-C7-C8
29	y	612	CLA	C15-C16-C17-C18
29	C1	506	CLA	C5-C6-C7-C8
29	C1	508	CLA	C13-C15-C16-C17
29	D1	403	CLA	C5-C6-C7-C8
29	G1	603	CLA	C10-C11-C12-C13
29	S1	610	CLA	C10-C11-C12-C13
29	Y1	602	CLA	C8-C10-C11-C12
29	b1	615	CLA	C5-C6-C7-C8
29	y1	602	CLA	C15-C16-C17-C18
29	y1	612	CLA	C8-C10-C11-C12
29	y1	614	CLA	C8-C10-C11-C12
48	N	609	CHL	C15-C16-C17-C18
48	g1	607	CHL	C5-C6-C7-C8
29	A	405	CLA	O1A-CGA-O2A-C1
29	N	602	CLA	O1A-CGA-O2A-C1
29	a	407	CLA	O1A-CGA-O2A-C1
29	s	604	CLA	O1A-CGA-O2A-C1
29	B1	606	CLA	O1A-CGA-O2A-C1
29	C1	503	CLA	O1A-CGA-O2A-C1
29	a1	405	CLA	O1A-CGA-O2A-C1
29	b1	608	CLA	O1A-CGA-O2A-C1
37	C1	520	DGD	O1A-C1A-O1G-C1G
38	s1	626	3PH	O32-C31-O31-C3
40	d	410	LHG	O10-C23-O8-C6
40	C1	525	LHG	O10-C23-O8-C6
39	b	625	DGA	CA1-CA2-CA3-CA4
47	k1	101	4RF	C41-C43-C44-C45
32	b	626	SQD	C11-C12-C13-C14
29	B	604	CLA	C13-C15-C16-C17
29	B	616	CLA	C8-C10-C11-C12
29	C	510	CLA	C13-C15-C16-C17
29	Y	613	CLA	C10-C11-C12-C13
29	b	602	CLA	C13-C15-C16-C17
29	b	607	CLA	C5-C6-C7-C8
29	b	610	CLA	C15-C16-C17-C18
29	c	501	CLA	C15-C16-C17-C18
29	n	602	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	n	603	CLA	C8-C10-C11-C12
29	n	613	CLA	C13-C15-C16-C17
29	y	614	CLA	C8-C10-C11-C12
29	B1	602	CLA	C5-C6-C7-C8
29	C1	507	CLA	C13-C15-C16-C17
29	C1	507	CLA	C15-C16-C17-C18
29	C1	508	CLA	C10-C11-C12-C13
29	S1	610	CLA	C8-C10-C11-C12
29	Y1	613	CLA	C8-C10-C11-C12
29	b1	602	CLA	C13-C15-C16-C17
29	b1	616	CLA	C8-C10-C11-C12
29	c1	506	CLA	C13-C15-C16-C17
29	c1	508	CLA	C5-C6-C7-C8
29	n1	613	CLA	C13-C15-C16-C17
29	g1	613	CLA	C15-C16-C17-C18
29	y1	603	CLA	C8-C10-C11-C12
48	n	609	CHL	C15-C16-C17-C18
32	M	101	SQD	C12-C13-C14-C15
32	a1	412	SQD	C15-C16-C17-C18
29	C	504	CLA	O1A-CGA-O2A-C1
29	g	610	CLA	O1A-CGA-O2A-C1
29	y	610	CLA	O1A-CGA-O2A-C1
29	b1	606	CLA	O1A-CGA-O2A-C1
29	c1	513	CLA	O1A-CGA-O2A-C1
32	C1	526	SQD	O10-C23-O48-C46
54	S1	625	LPX	O5-C4-C5-O6
32	c	526	SQD	C8-C7-O47-C45
33	C	523	LMG	C11-C10-O7-C8
33	a1	413	LMG	C11-C10-O7-C8
39	C1	524	DGA	CA3-CA4-CA5-CA6
40	y	624	LHG	C30-C31-C32-C33
29	a1	407	CLA	O1D-CGD-O2D-CED
29	B	602	CLA	C15-C16-C17-C18
29	D	403	CLA	C10-C11-C12-C13
29	N	602	CLA	C10-C11-C12-C13
29	G	611	CLA	C15-C16-C17-C18
29	R	608	CLA	C5-C6-C7-C8
29	S	611	CLA	C5-C6-C7-C8
29	Y	602	CLA	C8-C10-C11-C12
29	Y	604	CLA	C8-C10-C11-C12
29	Y	612	CLA	C5-C6-C7-C8
29	Y	612	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	b	608	CLA	C8-C10-C11-C12
29	b	610	CLA	C13-C15-C16-C17
29	b	615	CLA	C5-C6-C7-C8
29	c	505	CLA	C8-C10-C11-C12
29	c	507	CLA	C13-C15-C16-C17
29	d	403	CLA	C10-C11-C12-C13
29	s	602	CLA	C10-C11-C12-C13
29	y	612	CLA	C10-C11-C12-C13
29	B1	608	CLA	C10-C11-C12-C13
29	B1	614	CLA	C10-C11-C12-C13
29	C1	510	CLA	C15-C16-C17-C18
29	S1	602	CLA	C5-C6-C7-C8
29	Y1	611	CLA	C13-C15-C16-C17
29	b1	608	CLA	C10-C11-C12-C13
29	b1	617	CLA	C5-C6-C7-C8
29	c1	505	CLA	C5-C6-C7-C8
29	s1	609	CLA	C5-C6-C7-C8
29	s1	610	CLA	C10-C11-C12-C13
29	s1	611	CLA	C15-C16-C17-C18
29	y1	614	CLA	C5-C6-C7-C8
48	n	606	CHL	C5-C6-C7-C8
48	S1	608	CHL	C10-C11-C12-C13
40	C	525	LHG	C3-O3-P-O6
40	D	408	LHG	C3-O3-P-O6
40	D	408	LHG	C4-O6-P-O3
40	D	409	LHG	C3-O3-P-O6
40	D	410	LHG	C3-O3-P-O6
40	L	101	LHG	C3-O3-P-O6
40	G	624	LHG	C4-O6-P-O3
40	S	624	LHG	C4-O6-P-O3
40	Y	624	LHG	C4-O6-P-O3
40	c	525	LHG	C4-O6-P-O3
40	d	408	LHG	C3-O3-P-O6
40	d	408	LHG	C4-O6-P-O3
40	n	624	LHG	C4-O6-P-O3
40	s	624	LHG	C4-O6-P-O3
40	C1	525	LHG	C4-O6-P-O3
40	D1	409	LHG	C3-O3-P-O6
40	D1	409	LHG	C4-O6-P-O3
40	D1	410	LHG	C4-O6-P-O3
40	L1	101	LHG	C3-O3-P-O6
40	N1	624	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
40	G1	624	LHG	C4-O6-P-O3
40	c1	525	LHG	C4-O6-P-O3
40	d1	408	LHG	C3-O3-P-O6
40	d1	408	LHG	C4-O6-P-O3
40	d1	409	LHG	C3-O3-P-O6
40	d1	410	LHG	C4-O6-P-O3
40	n1	624	LHG	C4-O6-P-O3
54	s	625	LPX	C1-O2-P1-O1
54	s1	625	LPX	C3-O1-P1-O2
55	y	627	PTY	C3-O11-P1-O14
55	Y1	626	PTY	C3-O11-P1-O14
55	Y1	627	PTY	C5-O14-P1-O11
55	y1	626	PTY	C3-O11-P1-O14
55	y1	627	PTY	C3-O11-P1-O14
55	y1	627	PTY	C5-O14-P1-O11
33	b1	622	LMG	C28-C29-C30-C31
40	d	408	LHG	C23-C24-C25-C26
40	g	624	LHG	C7-C8-C9-C10
29	B	609	CLA	C3-C5-C6-C7
29	N	610	CLA	C3-C5-C6-C7
29	c1	503	CLA	C3-C5-C6-C7
40	d1	410	LHG	C29-C30-C31-C32
29	C	503	CLA	CBA-CGA-O2A-C1
29	G	603	CLA	CBA-CGA-O2A-C1
29	R	602	CLA	CBA-CGA-O2A-C1
29	c	513	CLA	CBA-CGA-O2A-C1
29	C1	510	CLA	CBA-CGA-O2A-C1
29	R1	610	CLA	CBA-CGA-O2A-C1
29	Y1	602	CLA	CBA-CGA-O2A-C1
29	c1	504	CLA	CBA-CGA-O2A-C1
29	r1	612	CLA	CBA-CGA-O2A-C1
39	C1	524	DGA	CA2-CA1-OG1-CG1
40	l	101	LHG	C24-C23-O8-C6
40	d1	409	LHG	C24-C23-O8-C6
47	k1	101	4RF	C15-C16-O18-C19
43	d1	405	PL9	C42-C43-C44-C45
29	C	509	CLA	O1D-CGD-O2D-CED
29	B	612	CLA	C8-C10-C11-C12
29	Y	613	CLA	C5-C6-C7-C8
29	Y	613	CLA	C15-C16-C17-C18
29	c	505	CLA	C10-C11-C12-C13
29	Y1	614	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	b1	608	CLA	C5-C6-C7-C8
29	s1	609	CLA	C10-C11-C12-C13
48	Y	606	CHL	C5-C6-C7-C8
48	N1	606	CHL	C5-C6-C7-C8
38	B1	624	3PH	O32-C31-O31-C3
33	a	413	LMG	C4-C5-C6-O5
29	c	506	CLA	O1D-CGD-O2D-CED
48	g	608	CHL	C2A-CAA-CBA-CGA
33	h1	102	LMG	C28-C29-C30-C31
37	c1	519	DGD	C1A-C2A-C3A-C4A
40	s	624	LHG	C7-C8-C9-C10
40	d1	409	LHG	C7-C8-C9-C10
47	I	102	4RF	C13-C14-C15-C16
29	b	609	CLA	O1D-CGD-O2D-CED
29	r1	604	CLA	O1D-CGD-O2D-CED
30	A	409	PHO	O1D-CGD-O2D-CED
40	C	525	LHG	C1-C2-C3-O3
40	D	408	LHG	C1-C2-C3-O3
40	l	101	LHG	C1-C2-C3-O3
40	y	624	LHG	C1-C2-C3-O3
40	C1	525	LHG	C1-C2-C3-O3
40	n1	624	LHG	C1-C2-C3-O3
54	s	625	LPX	O1-C3-C4-C5
32	M	101	SQD	O49-C7-O47-C45
32	b	626	SQD	O49-C7-O47-C45
32	c	526	SQD	O49-C7-O47-C45
33	C	523	LMG	O9-C10-O7-C8
33	A1	413	LMG	O9-C10-O7-C8
33	a1	413	LMG	O9-C10-O7-C8
33	h1	102	LMG	O9-C10-O7-C8
39	j1	101	DGA	OB1-CB1-OG2-CG2
29	S	602	CLA	C4-C3-C5-C6
29	S	611	CLA	C4-C3-C5-C6
29	b	614	CLA	C4-C3-C5-C6
29	N1	613	CLA	C4-C3-C5-C6
29	B	606	CLA	C2-C3-C5-C6
29	g	602	CLA	C2-C3-C5-C6
29	Y	602	CLA	C15-C16-C17-C18
29	Y	614	CLA	C13-C15-C16-C17
29	c	509	CLA	C10-C11-C12-C13
29	s	603	CLA	C8-C10-C11-C12
29	A1	406	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	B1	608	CLA	C13-C15-C16-C17
29	a1	406	CLA	C8-C10-C11-C12
29	r1	610	CLA	C5-C6-C7-C8
37	c1	518	DGD	C4A-C5A-C6A-C7A
29	C	501	CLA	C2A-CAA-CBA-CGA
29	C	505	CLA	C2A-CAA-CBA-CGA
29	G	613	CLA	C2A-CAA-CBA-CGA
29	S	613	CLA	C2A-CAA-CBA-CGA
29	Y	602	CLA	C2A-CAA-CBA-CGA
29	b	611	CLA	C2A-CAA-CBA-CGA
29	y	602	CLA	C2A-CAA-CBA-CGA
29	B1	614	CLA	C2A-CAA-CBA-CGA
29	C1	505	CLA	C2A-CAA-CBA-CGA
29	N1	602	CLA	C2A-CAA-CBA-CGA
29	S1	610	CLA	C2A-CAA-CBA-CGA
29	S1	614	CLA	C2A-CAA-CBA-CGA
29	Y1	602	CLA	C2A-CAA-CBA-CGA
29	Y1	608	CLA	C2A-CAA-CBA-CGA
29	a1	406	CLA	C2A-CAA-CBA-CGA
29	y1	608	CLA	C2A-CAA-CBA-CGA
48	S1	608	CHL	C2A-CAA-CBA-CGA
48	y1	607	CHL	C2A-CAA-CBA-CGA
29	N	610	CLA	C16-C17-C18-C20
29	b	607	CLA	C16-C17-C18-C20
29	B1	605	CLA	C16-C17-C18-C20
29	B1	611	CLA	C16-C17-C18-C20
29	b1	612	CLA	C16-C17-C18-C20
29	c1	501	CLA	C16-C17-C18-C19
29	c1	512	CLA	C16-C17-C18-C20
37	C1	518	DGD	O6E-C5E-C6E-O5E
48	G	601	CHL	C3-C5-C6-C7
30	A1	409	PHO	O1D-CGD-O2D-CED
29	A	407	CLA	CBA-CGA-O2A-C1
29	c	505	CLA	CBA-CGA-O2A-C1
29	d	403	CLA	CBA-CGA-O2A-C1
29	g	603	CLA	CBA-CGA-O2A-C1
29	r	610	CLA	CBA-CGA-O2A-C1
29	B1	608	CLA	CBA-CGA-O2A-C1
29	S1	614	CLA	CBA-CGA-O2A-C1
29	Y1	614	CLA	CBA-CGA-O2A-C1
29	b1	602	CLA	CBA-CGA-O2A-C1
29	c1	503	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	b	626	SQD	C24-C23-O48-C46
32	b1	621	SQD	C24-C23-O48-C46
38	B	624	3PH	C32-C31-O31-C3
47	K1	101	4RF	C43-C41-O40-C39
29	N	604	CLA	C13-C15-C16-C17
29	b	603	CLA	C15-C16-C17-C18
29	s	610	CLA	C15-C16-C17-C18
29	B1	606	CLA	C15-C16-C17-C18
29	C1	508	CLA	C8-C10-C11-C12
29	c1	512	CLA	C15-C16-C17-C18
39	c	524	DGA	CB7-CB8-CB9-CAB
31	C	514	BCR	C15-C16-C17-C18
31	c1	515	BCR	C19-C20-C21-C22
40	L	101	LHG	C23-C24-C25-C26
40	G1	624	LHG	C23-C24-C25-C26
32	B	626	SQD	C34-C35-C36-C37
38	S	626	3PH	C25-C26-C27-C28
39	J1	101	DGA	CB3-CB4-CB5-CB6
40	D	408	LHG	C28-C29-C30-C31
40	N	624	LHG	C25-C26-C27-C28
40	d	409	LHG	C24-C25-C26-C27
40	G1	624	LHG	C28-C29-C30-C31
40	c1	525	LHG	C13-C14-C15-C16
40	c1	525	LHG	C29-C30-C31-C32
41	c	527	LMK	C13-C14-C15-C27
52	R1	625	LMT	C4-C5-C6-C7
55	Y	626	PTY	C39-C40-C41-C42
32	M	101	SQD	C8-C7-O47-C45
33	A1	413	LMG	C11-C10-O7-C8
33	H1	102	LMG	C11-C10-O7-C8
33	w1	201	LMG	C11-C10-O7-C8
40	N	624	LHG	C8-C7-O7-C5
55	Y1	626	PTY	C11-C8-O7-C6
29	n1	602	CLA	C10-C11-C12-C13
29	n1	610	CLA	C5-C6-C7-C8
31	A	411	BCR	C11-C10-C9-C34
31	b	619	BCR	C11-C10-C9-C34
50	G	622	XAT	C20-C13-C14-C15
50	n	622	XAT	C40-C33-C34-C35
50	R1	621	XAT	C20-C13-C14-C15
50	n1	622	XAT	C20-C13-C14-C15
51	R	622	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
51	Y	623	NEX	C39-C29-C30-C31
51	n	623	NEX	C11-C10-C9-C19
51	g	623	NEX	C11-C10-C9-C19
51	g	623	NEX	C39-C29-C30-C31
51	s	623	NEX	C39-C29-C30-C31
51	N1	623	NEX	C20-C13-C14-C15
51	G1	623	NEX	C20-C13-C14-C15
51	G1	623	NEX	C39-C29-C30-C31
51	R1	622	NEX	C39-C29-C30-C31
51	R1	622	NEX	C40-C33-C34-C35
51	Y1	623	NEX	C39-C29-C30-C31
51	n1	623	NEX	C11-C10-C9-C19
51	n1	623	NEX	C39-C29-C30-C31
51	g1	623	NEX	C40-C33-C34-C35
51	y1	623	NEX	C40-C33-C34-C35
29	B	617	CLA	C3-C5-C6-C7
29	d	403	CLA	C3-C5-C6-C7
29	c1	511	CLA	C3-C5-C6-C7
32	M	101	SQD	C26-C27-C28-C29
32	c	526	SQD	C15-C16-C17-C18
32	A1	412	SQD	C15-C16-C17-C18
32	C1	526	SQD	C11-C10-C9-C8
32	m1	101	SQD	C12-C13-C14-C15
33	B	622	LMG	C31-C32-C33-C34
33	d1	411	LMG	C19-C20-C21-C22
37	C	519	DGD	C3A-C4A-C5A-C6A
37	c	519	DGD	CCB-CDB-CEB-CFB
37	c1	519	DGD	CCB-CDB-CEB-CFB
38	B	624	3PH	C3C-C3D-C3E-C3F
38	B1	624	3PH	C3C-C3D-C3E-C3F
38	T1	101	3PH	C2C-C2D-C2E-C2F
38	S1	626	3PH	C2B-C2C-C2D-C2E
38	s1	626	3PH	C2B-C2C-C2D-C2E
39	B	625	DGA	CA6-CA7-CA8-CA9
39	b	625	DGA	CA4-CA5-CA6-CA7
39	B1	625	DGA	CA4-CA5-CA6-CA7
39	C1	524	DGA	CA4-CA5-CA6-CA7
39	C1	524	DGA	CA9-CAA-CBA-CCA
40	D	408	LHG	C31-C32-C33-C34
40	D	409	LHG	C10-C11-C12-C13
40	G	624	LHG	C9-C10-C11-C12
40	G	624	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
40	y	624	LHG	C13-C14-C15-C16
40	y	624	LHG	C33-C34-C35-C36
40	C1	525	LHG	C28-C29-C30-C31
40	D1	408	LHG	C13-C14-C15-C16
40	N1	624	LHG	C13-C14-C15-C16
40	S1	624	LHG	C26-C27-C28-C29
40	Y1	624	LHG	C16-C17-C18-C19
40	d1	408	LHG	C30-C31-C32-C33
40	d1	409	LHG	C32-C33-C34-C35
47	K	101	4RF	C43-C44-C45-C46
47	k	101	4RF	C27-C28-C29-C30
52	r1	625	LMT	C11-C10-C9-C8
55	Y1	626	PTY	C40-C41-C42-C43
55	y1	626	PTY	C35-C36-C37-C38
29	c	504	CLA	O1D-CGD-O2D-CED
29	B1	605	CLA	O1D-CGD-O2D-CED
29	B	611	CLA	C16-C17-C18-C20
29	G	613	CLA	C16-C17-C18-C20
29	Y	604	CLA	C16-C17-C18-C19
29	b	617	CLA	C16-C17-C18-C20
29	c	513	CLA	C16-C17-C18-C19
29	d	403	CLA	C16-C17-C18-C20
29	B1	603	CLA	C16-C17-C18-C19
29	C1	505	CLA	C16-C17-C18-C19
29	S1	613	CLA	C6-C7-C8-C9
29	b1	602	CLA	C16-C17-C18-C19
29	c1	509	CLA	C16-C17-C18-C19
29	c1	510	CLA	C16-C17-C18-C20
29	n1	602	CLA	C16-C17-C18-C20
29	g1	602	CLA	C16-C17-C18-C19
29	b	612	CLA	CBA-CGA-O2A-C1
34	Y1	625	SPH	C14-C15-C16-C17
37	C	518	DGD	C3B-C4B-C5B-C6B
37	C1	520	DGD	C2A-C3A-C4A-C5A
37	C1	520	DGD	C9B-CAB-CBB-CCB
38	B	624	3PH	C28-C29-C2A-C2B
38	B	624	3PH	C3B-C3C-C3D-C3E
38	b	624	3PH	C23-C24-C25-C26
38	B1	624	3PH	C26-C27-C28-C29
39	b1	625	DGA	CA8-CA9-CAA-CBA
40	D	408	LHG	C25-C26-C27-C28
40	Y	624	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
40	g	624	LHG	C13-C14-C15-C16
40	y	624	LHG	C16-C17-C18-C19
40	N1	624	LHG	C31-C32-C33-C34
41	C	527	LMK	C12-C13-C14-C15
41	C	527	LMK	C31-C32-C33-C34
47	K	101	4RF	C10-C11-C12-C13
47	k	101	4RF	C46-C47-C48-C49
47	K1	101	4RF	C26-C27-C28-C29
52	R	625	LMT	C11-C10-C9-C8
54	S	625	LPX	C11-C12-C13-C14
54	S1	625	LPX	C10-C11-C12-C13
34	Y	625	SPH	O3-C3-C4-C5
34	A1	414	SPH	O3-C3-C4-C5
29	N	610	CLA	O1D-CGD-O2D-CED
29	c	507	CLA	O1D-CGD-O2D-CED
37	C	518	DGD	O6E-C5E-C6E-O5E
32	B	621	SQD	O49-C7-O47-C45
32	b1	621	SQD	O49-C7-O47-C45
33	w1	201	LMG	O9-C10-O7-C8
40	N	624	LHG	O9-C7-O7-C5
55	Y1	626	PTY	O10-C8-O7-C6
29	C	513	CLA	C8-C10-C11-C12
29	N	604	CLA	C10-C11-C12-C13
29	b	610	CLA	C5-C6-C7-C8
29	c	513	CLA	C8-C10-C11-C12
29	C1	508	CLA	C5-C6-C7-C8
29	C1	510	CLA	C8-C10-C11-C12
29	D1	403	CLA	C8-C10-C11-C12
29	R1	610	CLA	C5-C6-C7-C8
29	n1	604	CLA	C10-C11-C12-C13
29	y1	613	CLA	C5-C6-C7-C8
40	l	101	LHG	C23-C24-C25-C26
29	B	609	CLA	CBD-CGD-O2D-CED
29	y1	611	CLA	CBD-CGD-O2D-CED
38	B	624	3PH	C29-C2A-C2B-C2C
38	B1	624	3PH	C24-C25-C26-C27
39	B	625	DGA	CA4-CA5-CA6-CA7
39	C	524	DGA	CBB-CAB-CB9-CB8
39	C	524	DGA	CB9-CAB-CBB-CCB
39	b	625	DGA	CB9-CAB-CBB-CCB
40	C	525	LHG	C29-C30-C31-C32
40	c	525	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
40	d	408	LHG	C33-C34-C35-C36
40	l	101	LHG	C10-C11-C12-C13
40	g	624	LHG	C11-C10-C9-C8
40	D1	408	LHG	C11-C12-C13-C14
40	D1	408	LHG	C25-C26-C27-C28
40	N1	624	LHG	C9-C10-C11-C12
40	s1	624	LHG	C30-C31-C32-C33
47	I	102	4RF	C03-C04-C05-C06
29	s	611	CLA	O1D-CGD-O2D-CED
38	T1	101	3PH	C2-C1-O11-P
40	D1	409	LHG	C2-C3-O3-P
40	d1	410	LHG	C2-C3-O3-P
29	c	505	CLA	O1A-CGA-O2A-C1
32	B	626	SQD	C12-C13-C14-C15
32	A1	412	SQD	C24-C25-C26-C27
37	c	519	DGD	C3B-C4B-C5B-C6B
37	c	520	DGD	C9B-CAB-CBB-CCB
38	T	101	3PH	C22-C23-C24-C25
38	t1	101	3PH	C2A-C2B-C2C-C2D
39	b	625	DGA	CB2-CB3-CB4-CB5
39	b	625	DGA	CCB-CDB-CEB-CFB
39	c	524	DGA	CAB-CBB-CCB-CDB
40	N	624	LHG	C13-C14-C15-C16
40	Y1	624	LHG	C11-C10-C9-C8
40	n1	624	LHG	C11-C12-C13-C14
40	n1	624	LHG	C13-C14-C15-C16
40	n1	624	LHG	C33-C34-C35-C36
40	y1	624	LHG	C16-C17-C18-C19
41	c	527	LMK	C11-C12-C13-C14
41	c	527	LMK	C29-C30-C31-C32
55	Y1	626	PTY	C15-C16-C17-C18
32	b	621	SQD	C26-C27-C28-C29
33	d	411	LMG	C18-C19-C20-C21
33	B1	622	LMG	C31-C32-C33-C34
37	C	518	DGD	C3A-C4A-C5A-C6A
38	b1	624	3PH	C27-C28-C29-C2A
39	b	625	DGA	CB5-CB6-CB7-CB8
39	C1	524	DGA	CB6-CB7-CB8-CB9
40	D	409	LHG	C13-C14-C15-C16
40	D	410	LHG	C29-C30-C31-C32
40	N	624	LHG	C14-C15-C16-C17
40	G	624	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
40	N1	624	LHG	C14-C15-C16-C17
55	Y	626	PTY	C14-C15-C16-C17
55	Y1	626	PTY	C23-C24-C25-C26
29	s	610	CLA	C3-C5-C6-C7
29	C1	507	CLA	C3-C5-C6-C7
29	r1	608	CLA	C3-C5-C6-C7
32	B	621	SQD	C23-C24-C25-C26
32	C1	526	SQD	C7-C8-C9-C10
33	c1	523	LMG	C10-C11-C12-C13
39	J1	101	DGA	CA1-CA2-CA3-CA4
39	b1	625	DGA	CB1-CB2-CB3-CB4
40	D1	409	LHG	C7-C8-C9-C10
40	y1	624	LHG	C23-C24-C25-C26
47	I1	102	4RF	C41-C43-C44-C45
31	b	619	BCR	C11-C10-C9-C8
32	a1	412	SQD	C2-C1-O6-C44
32	b1	626	SQD	C2-C1-O6-C44
37	C	519	DGD	C2E-C1E-O5D-C6D
37	c	519	DGD	C2E-C1E-O5D-C6D
50	G	622	XAT	C12-C13-C14-C15
50	n	622	XAT	C32-C33-C34-C35
50	y	622	XAT	C12-C13-C14-C15
50	R1	621	XAT	C12-C13-C14-C15
50	n1	622	XAT	C12-C13-C14-C15
51	R	622	NEX	C28-C29-C30-C31
51	Y	623	NEX	C28-C29-C30-C31
51	n	623	NEX	C11-C10-C9-C8
51	g	623	NEX	C11-C10-C9-C8
51	g	623	NEX	C28-C29-C30-C31
51	s	623	NEX	C28-C29-C30-C31
51	N1	623	NEX	C12-C13-C14-C15
51	N1	623	NEX	C28-C29-C30-C31
51	G1	623	NEX	C12-C13-C14-C15
51	G1	623	NEX	C28-C29-C30-C31
51	R1	622	NEX	C12-C13-C14-C15
51	R1	622	NEX	C28-C29-C30-C31
51	R1	622	NEX	C32-C33-C34-C35
51	Y1	623	NEX	C28-C29-C30-C31
51	n1	623	NEX	C11-C10-C9-C8
51	n1	623	NEX	C28-C29-C30-C31
51	g1	623	NEX	C32-C33-C34-C35
51	y1	623	NEX	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
29	Y1	610	CLA	CBA-CGA-O2A-C1
32	b	621	SQD	C25-C26-C27-C28
32	A1	412	SQD	C26-C27-C28-C29
33	H	102	LMG	C12-C13-C14-C15
33	h	102	LMG	C31-C32-C33-C34
33	H1	102	LMG	C30-C31-C32-C33
37	C1	519	DGD	C4B-C5B-C6B-C7B
38	s	626	3PH	C26-C27-C28-C29
39	b	625	DGA	CEB-CFB-CGB-CHB
39	b1	625	DGA	CA2-CA3-CA4-CA5
39	b1	625	DGA	CB5-CB6-CB7-CB8
40	C	525	LHG	C30-C31-C32-C33
40	D	409	LHG	C25-C26-C27-C28
40	G	624	LHG	C11-C10-C9-C8
40	S	624	LHG	C12-C13-C14-C15
40	c	525	LHG	C26-C27-C28-C29
40	d	408	LHG	C25-C26-C27-C28
40	l	101	LHG	C34-C35-C36-C37
40	y	624	LHG	C11-C10-C9-C8
40	C1	525	LHG	C30-C31-C32-C33
40	D1	408	LHG	C30-C31-C32-C33
40	S1	624	LHG	C31-C32-C33-C34
40	Y1	624	LHG	C15-C16-C17-C18
40	d1	409	LHG	C34-C35-C36-C37
40	y1	624	LHG	C28-C29-C30-C31
40	y1	624	LHG	C29-C30-C31-C32
47	K1	101	4RF	C10-C11-C12-C13
47	i1	101	4RF	C07-C08-C09-C10
55	Y1	626	PTY	C39-C40-C41-C42
55	y1	626	PTY	C31-C32-C33-C34
29	B	603	CLA	C5-C6-C7-C8
29	B	604	CLA	C15-C16-C17-C18
29	C	511	CLA	C5-C6-C7-C8
29	y	604	CLA	C5-C6-C7-C8
29	B1	611	CLA	C8-C10-C11-C12
29	B1	612	CLA	C13-C15-C16-C17
29	N1	602	CLA	C15-C16-C17-C18
29	R1	602	CLA	C10-C11-C12-C13
29	a1	410	CLA	C10-C11-C12-C13
29	c1	503	CLA	C15-C16-C17-C18
29	c1	510	CLA	C13-C15-C16-C17
29	g1	613	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	b1	602	CLA	O1A-CGA-O2A-C1
29	r1	612	CLA	O1A-CGA-O2A-C1
40	l	101	LHG	O10-C23-O8-C6
29	C	501	CLA	C16-C17-C18-C20
29	C	509	CLA	C16-C17-C18-C20
29	G	602	CLA	C16-C17-C18-C20
29	G	610	CLA	C16-C17-C18-C19
29	Y	604	CLA	C16-C17-C18-C20
29	Y	614	CLA	C16-C17-C18-C19
29	b	605	CLA	C16-C17-C18-C20
29	c	509	CLA	C16-C17-C18-C19
29	c	510	CLA	C16-C17-C18-C20
29	n	602	CLA	C16-C17-C18-C20
29	s	604	CLA	C6-C7-C8-C9
29	B1	610	CLA	C16-C17-C18-C20
29	R1	608	CLA	C11-C12-C13-C14
29	R1	610	CLA	C11-C12-C13-C14
29	Y1	613	CLA	C16-C17-C18-C19
29	Y1	613	CLA	C16-C17-C18-C20
29	Y1	614	CLA	C16-C17-C18-C19
29	b1	610	CLA	C16-C17-C18-C20
29	g1	610	CLA	C16-C17-C18-C20
29	r1	608	CLA	C11-C12-C13-C15
29	y1	614	CLA	C16-C17-C18-C19
29	a	407	CLA	O1D-CGD-O2D-CED
29	n	604	CLA	O1D-CGD-O2D-CED
29	b1	605	CLA	O1D-CGD-O2D-CED
29	Y	604	CLA	C4-C3-C5-C6
29	c	510	CLA	C4-C3-C5-C6
29	c1	505	CLA	C4-C3-C5-C6
29	y1	613	CLA	C4-C3-C5-C6
43	d1	405	PL9	C40-C39-C41-C42
32	a1	412	SQD	C26-C27-C28-C29
33	w	201	LMG	C37-C38-C39-C40
33	B1	622	LMG	C18-C19-C20-C21
33	D1	411	LMG	C32-C33-C34-C35
33	c1	521	LMG	C12-C13-C14-C15
34	Y	625	SPH	C14-C15-C16-C17
38	S	626	3PH	C2A-C2B-C2C-C2D
38	s	626	3PH	C2C-C2D-C2E-C2F
38	s	626	3PH	C39-C3A-C3B-C3C
38	B1	624	3PH	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
38	B1	624	3PH	C32-C33-C34-C35
39	C	524	DGA	CA6-CA7-CA8-CA9
39	j	101	DGA	CA4-CA5-CA6-CA7
39	B1	625	DGA	CDB-CEB-CFB-CGB
40	Y	624	LHG	C26-C27-C28-C29
40	c	525	LHG	C29-C30-C31-C32
40	C1	525	LHG	C29-C30-C31-C32
41	c1	527	LMK	C31-C32-C33-C34
47	K	101	4RF	C05-C06-C07-C08
47	I1	102	4RF	C05-C06-C07-C08
52	r	625	LMT	C11-C10-C9-C8
55	Y	626	PTY	C40-C41-C42-C43
29	y	614	CLA	C2-C3-C5-C6
29	N1	613	CLA	C2-C3-C5-C6
29	y1	613	CLA	C2-C3-C5-C6
30	A	408	PHO	C2-C3-C5-C6
29	C	505	CLA	C11-C10-C8-C9
29	C	507	CLA	C6-C7-C8-C9
29	D	403	CLA	C11-C12-C13-C14
29	G	613	CLA	C6-C7-C8-C9
29	S	603	CLA	C6-C7-C8-C9
29	S	603	CLA	C11-C10-C8-C9
29	S	610	CLA	C14-C13-C15-C16
29	Y	602	CLA	C11-C10-C8-C9
29	b	602	CLA	C6-C7-C8-C9
29	b	616	CLA	C14-C13-C15-C16
29	c	503	CLA	C14-C13-C15-C16
29	c	509	CLA	C6-C7-C8-C9
29	c	512	CLA	C14-C13-C15-C16
29	d	403	CLA	C11-C10-C8-C9
29	n	610	CLA	C6-C7-C8-C9
29	n	610	CLA	C14-C13-C15-C16
29	n	613	CLA	C14-C13-C15-C16
29	g	611	CLA	C6-C7-C8-C9
29	r	603	CLA	C11-C10-C8-C9
29	r	610	CLA	C11-C10-C8-C9
29	B1	604	CLA	C14-C13-C15-C16
29	B1	605	CLA	C11-C12-C13-C14
29	B1	606	CLA	C11-C12-C13-C14
29	C1	503	CLA	C6-C7-C8-C9
29	C1	505	CLA	C14-C13-C15-C16
29	G1	610	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	G1	613	CLA	C6-C7-C8-C9
29	R1	610	CLA	C6-C7-C8-C9
29	Y1	610	CLA	C11-C12-C13-C14
29	b1	604	CLA	C6-C7-C8-C9
29	c1	509	CLA	C14-C13-C15-C16
29	c1	510	CLA	C14-C13-C15-C16
29	g1	602	CLA	C6-C7-C8-C9
29	g1	603	CLA	C6-C7-C8-C9
30	a1	408	PHO	C11-C12-C13-C14
30	a1	409	PHO	C11-C10-C8-C9
48	G	601	CHL	C11-C12-C13-C14
48	n	606	CHL	C14-C13-C15-C16
48	n	607	CHL	C11-C10-C8-C9
48	r1	606	CHL	C2A-CAA-CBA-CGA
37	c	519	DGD	C1B-C2B-C3B-C4B
38	t1	101	3PH	C31-C32-C33-C34
32	B	621	SQD	C24-C25-C26-C27
32	a	412	SQD	C33-C34-C35-C36
32	a1	412	SQD	C34-C35-C36-C37
32	b1	621	SQD	C11-C12-C13-C14
33	D	411	LMG	C15-C16-C17-C18
33	H1	102	LMG	C34-C35-C36-C37
34	y	625	SPH	C6-C7-C8-C9
34	y	625	SPH	C11-C12-C13-C14
34	y1	625	SPH	C7-C8-C9-C10
37	C1	520	DGD	C4A-C5A-C6A-C7A
38	B	624	3PH	C25-C26-C27-C28
38	t	101	3PH	C2E-C2F-C2G-C2H
38	s	626	3PH	C3B-C3C-C3D-C3E
38	b1	624	3PH	C24-C25-C26-C27
38	b1	624	3PH	C3E-C3F-C3G-C3H
38	t1	101	3PH	C2B-C2C-C2D-C2E
38	s1	626	3PH	C27-C28-C29-C2A
39	C	524	DGA	CA4-CA5-CA6-CA7
39	c1	524	DGA	CAA-CBA-CCA-CDA
39	c1	524	DGA	CB3-CB4-CB5-CB6
40	L	101	LHG	C9-C10-C11-C12
40	L	101	LHG	C31-C32-C33-C34
40	N	624	LHG	C28-C29-C30-C31
40	N	624	LHG	C33-C34-C35-C36
40	s	624	LHG	C11-C12-C13-C14
40	y	624	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
40	L1	101	LHG	C11-C10-C9-C8
40	G1	624	LHG	C16-C17-C18-C19
40	d1	408	LHG	C13-C14-C15-C16
40	g1	624	LHG	C11-C10-C9-C8
40	y1	624	LHG	C31-C32-C33-C34
47	I	102	4RF	C51-C52-C53-C54
47	I1	102	4RF	C49-C50-C51-C52
47	K1	101	4RF	C12-C13-C14-C15
52	R	625	LMT	C4-C5-C6-C7
55	y	626	PTY	C19-C20-C21-C22
29	B	615	CLA	C10-C11-C12-C13
29	b	607	CLA	C8-C10-C11-C12
29	B1	615	CLA	C15-C16-C17-C18
29	B1	617	CLA	C5-C6-C7-C8
29	N1	604	CLA	C15-C16-C17-C18
29	c1	510	CLA	C8-C10-C11-C12
29	s1	611	CLA	C8-C10-C11-C12
29	N	602	CLA	C2A-CAA-CBA-CGA
29	r	604	CLA	C2A-CAA-CBA-CGA
29	s	612	CLA	C2A-CAA-CBA-CGA
29	C1	502	CLA	C2A-CAA-CBA-CGA
29	S1	603	CLA	C2A-CAA-CBA-CGA
29	r1	610	CLA	C2A-CAA-CBA-CGA
30	a	409	PHO	C2A-CAA-CBA-CGA
48	N1	606	CHL	C2A-CAA-CBA-CGA
29	A	407	CLA	O1A-CGA-O2A-C1
29	c	504	CLA	O1A-CGA-O2A-C1
29	C1	510	CLA	O1A-CGA-O2A-C1
31	C	516	BCR	C37-C22-C23-C24
31	B1	618	BCR	C11-C12-C13-C35
36	B	620	C7Z	C7-C8-C9-C19
36	b	620	C7Z	C7-C8-C9-C19
45	H1	101	RRX	C7-C8-C9-C34
32	B	621	SQD	C11-C10-C9-C8
32	b	626	SQD	C17-C18-C19-C20
37	c1	520	DGD	C9B-CAB-CBB-CCB
38	B1	624	3PH	C3D-C3E-C3F-C3G
38	S1	626	3PH	C25-C26-C27-C28
39	B	625	DGA	CB3-CB4-CB5-CB6
39	C	524	DGA	CA2-CA3-CA4-CA5
40	S	624	LHG	C28-C29-C30-C31
40	c	525	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
40	d	409	LHG	C10-C11-C12-C13
40	D1	409	LHG	C11-C12-C13-C14
40	Y1	624	LHG	C31-C32-C33-C34
40	s1	624	LHG	C26-C27-C28-C29
41	c	527	LMK	C12-C13-C14-C15
47	I	102	4RF	C31-C32-C33-C34
47	k	101	4RF	C47-C48-C49-C50
47	K1	101	4RF	C46-C47-C48-C49
40	C	525	LHG	O1-C1-C2-C3
40	L	101	LHG	O1-C1-C2-C3
40	Y	624	LHG	O1-C1-C2-C3
40	d	409	LHG	O1-C1-C2-C3
40	n	624	LHG	O1-C1-C2-C3
40	g	624	LHG	O1-C1-C2-C3
40	C1	525	LHG	O1-C1-C2-C3
40	G1	624	LHG	O1-C1-C2-C3
40	c1	525	LHG	O1-C1-C2-C3
31	c	516	BCR	C17-C18-C19-C20
31	d	404	BCR	C17-C18-C19-C20
36	b	620	C7Z	C7-C8-C9-C10
45	H1	101	RRX	C7-C8-C9-C10
45	h1	101	RRX	C11-C12-C13-C14
51	Y1	623	NEX	C11-C12-C13-C14
29	B1	608	CLA	C3-C5-C6-C7
29	c	501	CLA	O1D-CGD-O2D-CED
32	B	626	SQD	O49-C7-O47-C45
29	C	511	CLA	C15-C16-C17-C18
29	S	602	CLA	C10-C11-C12-C13
29	Y	610	CLA	C13-C15-C16-C17
29	y	610	CLA	C13-C15-C16-C17
29	B1	606	CLA	C10-C11-C12-C13
29	a1	406	CLA	C10-C11-C12-C13
29	c1	513	CLA	C8-C10-C11-C12
29	n1	604	CLA	C15-C16-C17-C18
29	g1	603	CLA	C13-C15-C16-C17
29	y1	610	CLA	C5-C6-C7-C8
32	B	621	SQD	C8-C7-O47-C45
32	B	626	SQD	C8-C7-O47-C45
38	s1	626	3PH	C22-C21-O21-C2
40	G1	624	LHG	C8-C7-O7-C5
32	a1	412	SQD	C31-C32-C33-C34
39	C1	524	DGA	CA6-CA7-CA8-CA9

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Mol	Chain	Res	Type	Atoms
39	J1	101	DGA	CB6-CB7-CB8-CB9
39	c1	524	DGA	CBB-CAB-CB9-CB8
40	c	525	LHG	C24-C25-C26-C27
40	d	408	LHG	C11-C12-C13-C14
40	y	624	LHG	C11-C12-C13-C14
40	y	624	LHG	C28-C29-C30-C31
40	G1	624	LHG	C13-C14-C15-C16
40	s1	624	LHG	C24-C25-C26-C27
47	k1	101	4RF	C49-C50-C51-C52
47	k1	101	4RF	C52-C53-C54-C55
54	S1	625	LPX	C15-C16-C17-C18
55	Y1	626	PTY	C19-C20-C21-C22
33	a1	413	LMG	C4-C5-C6-O5
32	M	101	SQD	C7-C8-C9-C10
32	m1	101	SQD	C7-C8-C9-C10
40	d	409	LHG	C23-C24-C25-C26
40	d1	409	LHG	C23-C24-C25-C26
55	y	626	PTY	C30-C31-C32-C33
29	B1	614	CLA	C2C-C3C-CAC-CBC
32	A	412	SQD	C12-C13-C14-C15
32	a	412	SQD	C10-C11-C12-C13
32	c1	526	SQD	C17-C18-C19-C20
33	H	102	LMG	C13-C14-C15-C16
33	c	523	LMG	C18-C19-C20-C21
33	d	411	LMG	C19-C20-C21-C22
33	C1	523	LMG	C34-C35-C36-C37
33	h1	102	LMG	C12-C13-C14-C15
37	c	518	DGD	C3A-C4A-C5A-C6A
37	c	518	DGD	CAB-CBB-CCB-CDB
38	b	624	3PH	C28-C29-C2A-C2B
38	T1	101	3PH	C38-C39-C3A-C3B
38	s1	626	3PH	C29-C2A-C2B-C2C
39	b	625	DGA	CDB-CEB-CFB-CGB
39	j	101	DGA	CB7-CB8-CB9-CAB
39	b1	625	DGA	CB6-CB7-CB8-CB9
40	D	408	LHG	C24-C25-C26-C27
40	D1	408	LHG	C28-C29-C30-C31
40	D1	409	LHG	C17-C18-C19-C20
40	D1	410	LHG	C29-C30-C31-C32
40	G1	624	LHG	C11-C10-C9-C8
40	G1	624	LHG	C11-C12-C13-C14
40	d1	408	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
40	g1	624	LHG	C28-C29-C30-C31
40	s1	624	LHG	C11-C12-C13-C14
47	I	102	4RF	C27-C28-C29-C30
47	k	101	4RF	C09-C10-C11-C12
47	k1	101	4RF	C30-C31-C32-C33
52	R1	625	LMT	C3-C4-C5-C6
54	s	625	LPX	C11-C12-C13-C14
55	y	626	PTY	C17-C18-C19-C20
29	B	604	CLA	C4B-C3B-CAB-CBB
29	B	605	CLA	C4B-C3B-CAB-CBB
29	C	501	CLA	C4B-C3B-CAB-CBB
29	C	506	CLA	C4B-C3B-CAB-CBB
29	D	403	CLA	C4B-C3B-CAB-CBB
29	N	603	CLA	C4B-C3B-CAB-CBB
29	N	613	CLA	C4B-C3B-CAB-CBB
29	N	614	CLA	C4B-C3B-CAB-CBB
29	G	611	CLA	C4B-C3B-CAB-CBB
29	S	611	CLA	C4B-C3B-CAB-CBB
29	S	617	CLA	C4B-C3B-CAB-CBB
29	Y	612	CLA	C4B-C3B-CAB-CBB
29	Y	613	CLA	C4B-C3B-CAB-CBB
29	b	605	CLA	C4B-C3B-CAB-CBB
29	c	510	CLA	C4B-C3B-CAB-CBB
29	n	603	CLA	C4B-C3B-CAB-CBB
29	n	612	CLA	C4B-C3B-CAB-CBB
29	n	614	CLA	C4B-C3B-CAB-CBB
29	g	603	CLA	C4B-C3B-CAB-CBB
29	g	610	CLA	C4B-C3B-CAB-CBB
29	g	614	CLA	C4B-C3B-CAB-CBB
29	r	612	CLA	C4B-C3B-CAB-CBB
29	s	603	CLA	C4B-C3B-CAB-CBB
29	s	611	CLA	C4B-C3B-CAB-CBB
29	y	602	CLA	C4B-C3B-CAB-CBB
29	y	614	CLA	C4B-C3B-CAB-CBB
29	B1	607	CLA	C4B-C3B-CAB-CBB
29	C1	511	CLA	C4B-C3B-CAB-CBB
29	N1	611	CLA	C4B-C3B-CAB-CBB
29	G1	604	CLA	C4B-C3B-CAB-CBB
29	G1	611	CLA	C4B-C3B-CAB-CBB
29	R1	602	CLA	C4B-C3B-CAB-CBB
29	R1	609	CLA	C4B-C3B-CAB-CBB
29	S1	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	S1	604	CLA	C4B-C3B-CAB-CBB
29	S1	609	CLA	C4B-C3B-CAB-CBB
29	Y1	603	CLA	C4B-C3B-CAB-CBB
29	Y1	604	CLA	C4B-C3B-CAB-CBB
29	Y1	611	CLA	C4B-C3B-CAB-CBB
29	Y1	612	CLA	C4B-C3B-CAB-CBB
29	b1	603	CLA	C4B-C3B-CAB-CBB
29	b1	605	CLA	C4B-C3B-CAB-CBB
29	b1	609	CLA	C4B-C3B-CAB-CBB
29	c1	503	CLA	C4B-C3B-CAB-CBB
29	c1	505	CLA	C4B-C3B-CAB-CBB
29	c1	511	CLA	C4B-C3B-CAB-CBB
29	c1	513	CLA	C4B-C3B-CAB-CBB
29	d1	402	CLA	C4B-C3B-CAB-CBB
29	n1	612	CLA	C4B-C3B-CAB-CBB
29	n1	613	CLA	C4B-C3B-CAB-CBB
29	r1	609	CLA	C4B-C3B-CAB-CBB
29	s1	609	CLA	C4B-C3B-CAB-CBB
29	y1	604	CLA	C4B-C3B-CAB-CBB
29	B	611	CLA	C16-C17-C18-C19
29	G	610	CLA	C16-C17-C18-C20
29	G	613	CLA	C16-C17-C18-C19
29	R	603	CLA	C11-C12-C13-C14
29	S	604	CLA	C6-C7-C8-C9
29	S	604	CLA	C6-C7-C8-C10
29	b	602	CLA	C16-C17-C18-C20
29	b	607	CLA	C16-C17-C18-C19
29	c	501	CLA	C16-C17-C18-C19
29	c	501	CLA	C16-C17-C18-C20
29	d	403	CLA	C16-C17-C18-C19
29	n	603	CLA	C16-C17-C18-C19
29	g	602	CLA	C16-C17-C18-C19
29	y	614	CLA	C16-C17-C18-C19
29	y	614	CLA	C16-C17-C18-C20
29	A1	406	CLA	C16-C17-C18-C19
29	A1	406	CLA	C16-C17-C18-C20
29	B1	602	CLA	C16-C17-C18-C19
29	B1	602	CLA	C16-C17-C18-C20
29	B1	603	CLA	C16-C17-C18-C20
29	B1	608	CLA	C16-C17-C18-C20
29	B1	611	CLA	C16-C17-C18-C19
29	C1	505	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
29	C1	513	CLA	C16-C17-C18-C19
29	C1	513	CLA	C16-C17-C18-C20
29	G1	602	CLA	C16-C17-C18-C19
29	G1	602	CLA	C16-C17-C18-C20
29	c1	507	CLA	C16-C17-C18-C19
29	c1	507	CLA	C16-C17-C18-C20
29	c1	512	CLA	C16-C17-C18-C19
29	d1	402	CLA	C16-C17-C18-C20
29	n1	602	CLA	C16-C17-C18-C19
29	s1	613	CLA	C6-C7-C8-C10
48	S	608	CHL	C11-C12-C13-C14
48	s	608	CHL	C11-C12-C13-C15
29	B	604	CLA	C5-C6-C7-C8
29	C	504	CLA	C5-C6-C7-C8
29	D	402	CLA	C13-C15-C16-C17
29	b	603	CLA	C5-C6-C7-C8
29	c	508	CLA	C15-C16-C17-C18
29	C1	501	CLA	C13-C15-C16-C17
29	N1	602	CLA	C10-C11-C12-C13
29	N1	602	CLA	C13-C15-C16-C17
29	b1	606	CLA	C5-C6-C7-C8
29	b1	612	CLA	C8-C10-C11-C12
29	c1	509	CLA	C13-C15-C16-C17
29	r1	608	CLA	C10-C11-C12-C13
32	C	526	SQD	C29-C30-C31-C32
32	C1	526	SQD	C28-C29-C30-C31
33	d	411	LMG	C12-C13-C14-C15
33	W1	201	LMG	C29-C30-C31-C32
38	B	624	3PH	C2C-C2D-C2E-C2F
38	B	624	3PH	C3D-C3E-C3F-C3G
38	T	101	3PH	C24-C25-C26-C27
38	S	626	3PH	C35-C36-C37-C38
38	B1	624	3PH	C3A-C3B-C3C-C3D
39	B	625	DGA	CA9-CAA-CBA-CCA
39	b	625	DGA	CBB-CCB-CDB-CEB
40	S	624	LHG	C26-C27-C28-C29
40	d	409	LHG	C11-C12-C13-C14
40	l	101	LHG	C11-C10-C9-C8
40	n	624	LHG	C25-C26-C27-C28
40	D1	410	LHG	C31-C32-C33-C34
40	c1	525	LHG	C12-C13-C14-C15
40	d1	410	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
40	s1	624	LHG	C28-C29-C30-C31
47	i	101	4RF	C44-C45-C46-C47
47	K1	101	4RF	C07-C08-C09-C10
47	i1	101	4RF	C44-C45-C46-C47
52	r1	625	LMT	C5-C6-C7-C8
55	y	626	PTY	C15-C16-C17-C18
55	Y1	626	PTY	C36-C37-C38-C39
55	Y	626	PTY	N1-C2-C3-O11
29	Y1	610	CLA	CBD-CGD-O2D-CED
53	R	626	ERG	C13-C17-C20-C21
53	r	626	ERG	C13-C17-C20-C22
53	r	626	ERG	C16-C17-C20-C22
53	R1	626	ERG	C13-C17-C20-C22
32	B1	626	SQD	C14-C15-C16-C17
33	b1	622	LMG	C12-C13-C14-C15
37	c	520	DGD	C4A-C5A-C6A-C7A
38	T	101	3PH	C33-C34-C35-C36
38	b	624	3PH	C3E-C3F-C3G-C3H
38	t	101	3PH	C34-C35-C36-C37
38	b1	624	3PH	C34-C35-C36-C37
39	B	625	DGA	CB5-CB6-CB7-CB8
39	c	524	DGA	CB3-CB4-CB5-CB6
40	S	624	LHG	C11-C12-C13-C14
40	d	409	LHG	C28-C29-C30-C31
40	s	624	LHG	C31-C32-C33-C34
40	S1	624	LHG	C28-C29-C30-C31
40	d1	408	LHG	C11-C12-C13-C14
40	d1	409	LHG	C13-C14-C15-C16
47	k	101	4RF	C11-C12-C13-C14
47	k	101	4RF	C24-C25-C26-C27
47	k1	101	4RF	C28-C29-C30-C31
52	R	625	LMT	C5-C6-C7-C8
55	y1	626	PTY	C19-C20-C21-C22
32	b	621	SQD	C23-C24-C25-C26
37	C1	519	DGD	C1A-C2A-C3A-C4A
40	y	624	LHG	C23-C24-C25-C26
40	D1	410	LHG	C7-C8-C9-C10
29	y	604	CLA	C8-C10-C11-C12
29	c1	501	CLA	C8-C10-C11-C12
29	R	602	CLA	O1A-CGA-O2A-C1
29	c1	504	CLA	O1A-CGA-O2A-C1
32	b1	621	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
38	t	101	3PH	C2D-C2E-C2F-C2G
38	s	626	3PH	C24-C25-C26-C27
38	T1	101	3PH	C3A-C3B-C3C-C3D
39	B	625	DGA	CB9-CAB-CBB-CCB
39	b	625	DGA	CA6-CA7-CA8-CA9
39	c	524	DGA	CEB-CFB-CGB-CHB
39	B1	625	DGA	CA8-CA9-CAA-CBA
39	C1	524	DGA	CB2-CB3-CB4-CB5
39	c1	524	DGA	CA7-CA8-CA9-CAA
40	s	624	LHG	C26-C27-C28-C29
40	N1	624	LHG	C11-C12-C13-C14
40	d1	409	LHG	C31-C32-C33-C34
40	s1	624	LHG	C13-C14-C15-C16
47	i1	101	4RF	C51-C52-C53-C54
47	k1	101	4RF	C44-C45-C46-C47
52	r1	625	LMT	C3-C4-C5-C6
29	N1	604	CLA	O1D-CGD-O2D-CED
29	B	603	CLA	C3-C5-C6-C7
29	s	604	CLA	C3-C5-C6-C7
29	S1	611	CLA	C3-C5-C6-C7
37	B	623	DGD	O6E-C5E-C6E-O5E
29	b	614	CLA	CBA-CGA-O2A-C1
29	n	602	CLA	CBA-CGA-O2A-C1
40	D	410	LHG	C24-C23-O8-C6
32	b	621	SQD	C12-C13-C14-C15
33	W	201	LMG	C29-C30-C31-C32
33	h	102	LMG	C12-C13-C14-C15
37	C	519	DGD	C4A-C5A-C6A-C7A
38	b	624	3PH	C2E-C2F-C2G-C2H
38	s1	626	3PH	C37-C38-C39-C3A
39	c	524	DGA	CBB-CCB-CDB-CEB
39	j1	101	DGA	CB2-CB3-CB4-CB5
40	s	624	LHG	C13-C14-C15-C16
55	y1	626	PTY	C23-C24-C25-C26
29	B	609	CLA	C3A-C2A-CAA-CBA
29	C	513	CLA	C3A-C2A-CAA-CBA
29	N	603	CLA	C3A-C2A-CAA-CBA
29	N	614	CLA	C3A-C2A-CAA-CBA
29	G	603	CLA	C3A-C2A-CAA-CBA
29	Y	603	CLA	C3A-C2A-CAA-CBA
29	b	605	CLA	C3A-C2A-CAA-CBA
29	c	512	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	c	513	CLA	C3A-C2A-CAA-CBA
29	n	603	CLA	C3A-C2A-CAA-CBA
29	n	613	CLA	C3A-C2A-CAA-CBA
29	g	603	CLA	C3A-C2A-CAA-CBA
29	r	604	CLA	C3A-C2A-CAA-CBA
29	y	603	CLA	C3A-C2A-CAA-CBA
29	C1	501	CLA	C3A-C2A-CAA-CBA
29	C1	507	CLA	C3A-C2A-CAA-CBA
29	C1	512	CLA	C3A-C2A-CAA-CBA
29	C1	513	CLA	C3A-C2A-CAA-CBA
29	N1	603	CLA	C3A-C2A-CAA-CBA
29	N1	614	CLA	C3A-C2A-CAA-CBA
29	G1	603	CLA	C3A-C2A-CAA-CBA
29	Y1	603	CLA	C3A-C2A-CAA-CBA
29	b1	605	CLA	C3A-C2A-CAA-CBA
29	c1	507	CLA	C3A-C2A-CAA-CBA
29	c1	512	CLA	C3A-C2A-CAA-CBA
29	n1	603	CLA	C3A-C2A-CAA-CBA
29	n1	610	CLA	C3A-C2A-CAA-CBA
29	n1	613	CLA	C3A-C2A-CAA-CBA
29	n1	614	CLA	C3A-C2A-CAA-CBA
29	g1	603	CLA	C3A-C2A-CAA-CBA
29	s1	612	CLA	C3A-C2A-CAA-CBA
29	y1	603	CLA	C3A-C2A-CAA-CBA
30	a	408	PHO	C3A-C2A-CAA-CBA
48	G	606	CHL	C3A-C2A-CAA-CBA
48	g	605	CHL	C3A-C2A-CAA-CBA
48	g	607	CHL	C3A-C2A-CAA-CBA
48	N1	607	CHL	C3A-C2A-CAA-CBA
48	G1	605	CHL	C3A-C2A-CAA-CBA
48	G1	606	CHL	C3A-C2A-CAA-CBA
48	G1	607	CHL	C3A-C2A-CAA-CBA
29	Y	613	CLA	C8-C10-C11-C12
29	c	506	CLA	C13-C15-C16-C17
29	y	613	CLA	C10-C11-C12-C13
29	C1	505	CLA	C13-C15-C16-C17
31	C	514	BCR	C19-C20-C21-C22
32	b1	621	SQD	C25-C26-C27-C28
33	C	523	LMG	C18-C19-C20-C21
33	d	411	LMG	C13-C14-C15-C16
34	y1	625	SPH	C11-C10-C9-C8
38	T1	101	3PH	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
38	S1	626	3PH	C24-C25-C26-C27
39	B	625	DGA	CA3-CA4-CA5-CA6
40	D	408	LHG	C11-C12-C13-C14
40	S	624	LHG	C13-C14-C15-C16
40	Y	624	LHG	C11-C10-C9-C8
40	s	624	LHG	C30-C31-C32-C33
40	C1	525	LHG	C24-C25-C26-C27
40	D1	410	LHG	C25-C26-C27-C28
40	c1	525	LHG	C26-C27-C28-C29
40	c1	525	LHG	C28-C29-C30-C31
40	n1	624	LHG	C16-C17-C18-C19
47	k1	101	4RF	C09-C10-C11-C12
54	s	625	LPX	C15-C16-C17-C18
29	g1	614	CLA	O1D-CGD-O2D-CED
29	c	513	CLA	O1A-CGA-O2A-C1
29	B1	608	CLA	O1A-CGA-O2A-C1
29	Y1	602	CLA	O1A-CGA-O2A-C1
39	C1	524	DGA	OA1-CA1-OG1-CG1
47	k1	101	4RF	O17-C16-O18-C19
29	G	602	CLA	C16-C17-C18-C19
29	R	608	CLA	C11-C12-C13-C14
29	R	608	CLA	C11-C12-C13-C15
29	b	617	CLA	C16-C17-C18-C19
29	n	602	CLA	C16-C17-C18-C19
29	g	602	CLA	C16-C17-C18-C20
29	b1	602	CLA	C16-C17-C18-C20
29	c1	504	CLA	C16-C17-C18-C19
29	c1	509	CLA	C16-C17-C18-C20
29	d1	402	CLA	C16-C17-C18-C19
29	g1	602	CLA	C16-C17-C18-C20
29	g1	613	CLA	C16-C17-C18-C19
29	r1	608	CLA	C11-C12-C13-C14
29	s1	613	CLA	C6-C7-C8-C9
29	y1	612	CLA	C16-C17-C18-C19
29	y1	612	CLA	C16-C17-C18-C20
32	A1	412	SQD	C9-C10-C11-C12
32	B1	626	SQD	C15-C16-C17-C18
33	c1	523	LMG	C33-C34-C35-C36
37	C1	518	DGD	C3A-C4A-C5A-C6A
38	B	624	3PH	C2B-C2C-C2D-C2E
38	S	626	3PH	C24-C25-C26-C27
38	t1	101	3PH	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
39	B1	625	DGA	CDA-CEA-CFA-CGA
40	Y	624	LHG	C29-C30-C31-C32
40	Y	624	LHG	C31-C32-C33-C34
40	d	410	LHG	C25-C26-C27-C28
40	G1	624	LHG	C9-C10-C11-C12
47	I	102	4RF	C52-C53-C54-C55
47	k1	101	4RF	C24-C25-C26-C27
52	r	625	LMT	C4-C5-C6-C7
52	R1	625	LMT	C6-C7-C8-C9
33	b1	622	LMG	C7-C8-C9-O8
40	g	624	LHG	C4-C5-C6-O8
47	k1	101	4RF	O18-C19-C20-C39
40	G1	624	LHG	O9-C7-O7-C5
32	B	626	SQD	C28-C29-C30-C31
32	m	101	SQD	C27-C28-C29-C30
33	c1	523	LMG	C37-C38-C39-C40
39	B1	625	DGA	CB5-CB6-CB7-CB8
40	D1	410	LHG	C33-C34-C35-C36
55	y1	626	PTY	C17-C18-C19-C20
55	y1	626	PTY	C32-C33-C34-C35
53	R1	626	ERG	C17-C20-C22-C23
37	C1	520	DGD	O6D-C5D-C6D-O5D
50	Y	622	XAT	C14-C15-C35-C34
50	Y1	622	XAT	C14-C15-C35-C34
50	g1	622	XAT	C14-C15-C35-C34
51	G1	623	NEX	C14-C15-C35-C34
29	C1	512	CLA	C3-C5-C6-C7
40	g	624	LHG	C23-C24-C25-C26
34	A1	414	SPH	C6-C7-C8-C9
38	t	101	3PH	C32-C33-C34-C35
38	B1	624	3PH	C29-C2A-C2B-C2C
39	b1	625	DGA	CDB-CEB-CFB-CGB
39	c1	524	DGA	CA4-CA5-CA6-CA7
40	L1	101	LHG	C29-C30-C31-C32
40	S1	624	LHG	C14-C15-C16-C17
47	k1	101	4RF	C31-C32-C33-C34
52	R1	625	LMT	C5-C6-C7-C8
29	C	503	CLA	O1A-CGA-O2A-C1
29	R1	610	CLA	O1A-CGA-O2A-C1
47	K1	101	4RF	O42-C41-O40-C39
29	B	607	CLA	C5-C6-C7-C8
29	c	508	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	b	612	CLA	C4-C3-C5-C6
29	y	614	CLA	C4-C3-C5-C6
29	C1	501	CLA	C4-C3-C5-C6
29	y1	611	CLA	C4-C3-C5-C6
30	A	408	PHO	C4-C3-C5-C6
30	a	408	PHO	C4-C3-C5-C6
43	D	405	PL9	C40-C39-C41-C42
43	d	405	PL9	C40-C39-C41-C42
43	D1	405	PL9	C15-C14-C16-C17
39	J	101	DGA	CA2-CA1-OG1-CG1
29	Y	604	CLA	C2-C3-C5-C6
29	b	603	CLA	C2-C3-C5-C6
29	s	603	CLA	C2-C3-C5-C6
29	y1	611	CLA	C2-C3-C5-C6
30	a	408	PHO	C2-C3-C5-C6
32	b1	621	SQD	C8-C7-O47-C45
32	b1	626	SQD	C8-C7-O47-C45
33	h	102	LMG	C11-C10-O7-C8
33	C1	521	LMG	C11-C10-O7-C8
40	g	624	LHG	C8-C7-O7-C5
40	y	624	LHG	C8-C7-O7-C5
40	D1	409	LHG	C8-C7-O7-C5
40	N1	624	LHG	C8-C7-O7-C5
32	b1	621	SQD	C26-C27-C28-C29
37	C1	519	DGD	C3A-C4A-C5A-C6A
39	c1	524	DGA	CB5-CB6-CB7-CB8
40	d	409	LHG	C27-C28-C29-C30
40	y	624	LHG	C32-C33-C34-C35
40	N1	624	LHG	C25-C26-C27-C28
29	C	507	CLA	C2A-CAA-CBA-CGA
29	R	602	CLA	C2A-CAA-CBA-CGA
29	y	610	CLA	C2A-CAA-CBA-CGA
40	D	408	LHG	O1-C1-C2-O2
40	L	101	LHG	O1-C1-C2-O2
40	S	624	LHG	O1-C1-C2-O2
40	l	101	LHG	O1-C1-C2-O2
40	y	624	LHG	O1-C1-C2-O2
40	C1	525	LHG	O1-C1-C2-O2
40	D1	409	LHG	O1-C1-C2-O2
40	Y1	624	LHG	O1-C1-C2-O2
40	d1	410	LHG	O1-C1-C2-O2
40	n1	624	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
40	g1	624	LHG	O1-C1-C2-O2
40	s1	624	LHG	O1-C1-C2-O2
40	y1	624	LHG	O1-C1-C2-O2
41	C1	527	LMK	O9-C10-C11-C12
32	b	621	SQD	C10-C11-C12-C13
38	b	624	3PH	C24-C25-C26-C27
38	S1	626	3PH	C26-C27-C28-C29
39	c	524	DGA	CA6-CA7-CA8-CA9
39	j1	101	DGA	CB6-CB7-CB8-CB9
40	L	101	LHG	C28-C29-C30-C31
40	G	624	LHG	C26-C27-C28-C29
40	d	408	LHG	C30-C31-C32-C33
40	l	101	LHG	C25-C26-C27-C28
40	S1	624	LHG	C11-C12-C13-C14
54	s	625	LPX	C9-C10-C11-C12
55	Y1	626	PTY	C22-C23-C24-C25
55	y1	626	PTY	C21-C22-C23-C24
29	s1	610	CLA	O1D-CGD-O2D-CED
29	G	603	CLA	O1A-CGA-O2A-C1
29	d	403	CLA	O1A-CGA-O2A-C1
29	g	603	CLA	O1A-CGA-O2A-C1
29	Y1	614	CLA	O1A-CGA-O2A-C1
33	b1	622	LMG	O6-C5-C6-O5
29	c	512	CLA	C16-C17-C18-C19
29	r	602	CLA	C11-C12-C13-C14
29	s	610	CLA	C16-C17-C18-C19
29	c1	510	CLA	C16-C17-C18-C19
32	b	621	SQD	C13-C14-C15-C16
40	c	525	LHG	C33-C34-C35-C36
29	B	604	CLA	C2B-C3B-CAB-CBB
29	B	605	CLA	C2B-C3B-CAB-CBB
29	C	501	CLA	C2B-C3B-CAB-CBB
29	C	506	CLA	C2B-C3B-CAB-CBB
29	D	403	CLA	C2B-C3B-CAB-CBB
29	N	603	CLA	C2B-C3B-CAB-CBB
29	N	611	CLA	C2B-C3B-CAB-CBB
29	N	613	CLA	C2B-C3B-CAB-CBB
29	N	614	CLA	C2B-C3B-CAB-CBB
29	G	611	CLA	C2B-C3B-CAB-CBB
29	R	603	CLA	C2B-C3B-CAB-CBB
29	R	612	CLA	C2B-C3B-CAB-CBB
29	S	611	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	Y	603	CLA	C2B-C3B-CAB-CBB
29	Y	612	CLA	C2B-C3B-CAB-CBB
29	Y	613	CLA	C2B-C3B-CAB-CBB
29	c	510	CLA	C2B-C3B-CAB-CBB
29	n	603	CLA	C2B-C3B-CAB-CBB
29	n	612	CLA	C2B-C3B-CAB-CBB
29	n	614	CLA	C2B-C3B-CAB-CBB
29	g	603	CLA	C2B-C3B-CAB-CBB
29	g	610	CLA	C2B-C3B-CAB-CBB
29	g	614	CLA	C2B-C3B-CAB-CBB
29	r	603	CLA	C2B-C3B-CAB-CBB
29	r	604	CLA	C2B-C3B-CAB-CBB
29	r	612	CLA	C2B-C3B-CAB-CBB
29	s	603	CLA	C2B-C3B-CAB-CBB
29	s	605	CLA	C2B-C3B-CAB-CBB
29	s	611	CLA	C2B-C3B-CAB-CBB
29	y	602	CLA	C2B-C3B-CAB-CBB
29	y	603	CLA	C2B-C3B-CAB-CBB
29	y	614	CLA	C2B-C3B-CAB-CBB
29	B1	607	CLA	C2B-C3B-CAB-CBB
29	B1	617	CLA	C2B-C3B-CAB-CBB
29	C1	511	CLA	C2B-C3B-CAB-CBB
29	N1	611	CLA	C2B-C3B-CAB-CBB
29	N1	612	CLA	C2B-C3B-CAB-CBB
29	G1	604	CLA	C2B-C3B-CAB-CBB
29	G1	611	CLA	C2B-C3B-CAB-CBB
29	R1	602	CLA	C2B-C3B-CAB-CBB
29	R1	603	CLA	C2B-C3B-CAB-CBB
29	R1	609	CLA	C2B-C3B-CAB-CBB
29	S1	602	CLA	C2B-C3B-CAB-CBB
29	S1	604	CLA	C2B-C3B-CAB-CBB
29	S1	609	CLA	C2B-C3B-CAB-CBB
29	Y1	603	CLA	C2B-C3B-CAB-CBB
29	Y1	604	CLA	C2B-C3B-CAB-CBB
29	Y1	612	CLA	C2B-C3B-CAB-CBB
29	b1	603	CLA	C2B-C3B-CAB-CBB
29	b1	605	CLA	C2B-C3B-CAB-CBB
29	b1	609	CLA	C2B-C3B-CAB-CBB
29	b1	614	CLA	C2B-C3B-CAB-CBB
29	c1	503	CLA	C2B-C3B-CAB-CBB
29	c1	505	CLA	C2B-C3B-CAB-CBB
29	c1	511	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	c1	513	CLA	C2B-C3B-CAB-CBB
29	d1	402	CLA	C2B-C3B-CAB-CBB
29	n1	612	CLA	C2B-C3B-CAB-CBB
29	n1	613	CLA	C2B-C3B-CAB-CBB
29	r1	609	CLA	C2B-C3B-CAB-CBB
29	s1	609	CLA	C2B-C3B-CAB-CBB
29	y1	604	CLA	C2B-C3B-CAB-CBB
29	B	605	CLA	C5-C6-C7-C8
29	Y	612	CLA	C13-C15-C16-C17
29	g	603	CLA	C5-C6-C7-C8
29	G1	603	CLA	C8-C10-C11-C12
29	Y1	612	CLA	C8-C10-C11-C12
29	n1	602	CLA	C5-C6-C7-C8
33	c	523	LMG	C13-C14-C15-C16
40	C	525	LHG	C26-C27-C28-C29
40	n1	624	LHG	C25-C26-C27-C28
47	K1	101	4RF	C08-C09-C10-C11
54	S	625	LPX	C16-C17-C18-C19
29	c	509	CLA	C3-C5-C6-C7
29	a1	406	CLA	C3-C5-C6-C7
48	g	601	CHL	C3-C5-C6-C7
48	N1	607	CHL	C3-C5-C6-C7
29	s	603	CLA	O1D-CGD-O2D-CED
32	b1	626	SQD	C27-C28-C29-C30
34	Y1	625	SPH	C11-C10-C9-C8
39	b	625	DGA	CB4-CB5-CB6-CB7
40	L	101	LHG	C11-C10-C9-C8
40	g1	624	LHG	C31-C32-C33-C34
41	C1	527	LMK	C12-C13-C14-C15
52	R1	625	LMT	C11-C10-C9-C8
29	S1	614	CLA	O1A-CGA-O2A-C1
29	Y1	610	CLA	O1A-CGA-O2A-C1
29	c1	503	CLA	O1A-CGA-O2A-C1
32	b	626	SQD	O10-C23-O48-C46
38	B	624	3PH	O32-C31-O31-C3
29	S	613	CLA	C5-C6-C7-C8
29	y1	614	CLA	C15-C16-C17-C18
32	b1	626	SQD	C25-C26-C27-C28
33	C	523	LMG	C16-C17-C18-C19
39	c	524	DGA	CB6-CB7-CB8-CB9
39	C1	524	DGA	CBA-CCA-CDA-CEA
40	N	624	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
40	d	410	LHG	C31-C32-C33-C34
40	C1	525	LHG	C9-C10-C11-C12
40	L1	101	LHG	C28-C29-C30-C31
47	I	102	4RF	C46-C47-C48-C49
47	K	101	4RF	C32-C33-C34-C35
47	K	101	4RF	C46-C47-C48-C49
47	k	101	4RF	C30-C31-C32-C33
47	k1	101	4RF	C33-C34-C35-C36
32	b1	626	SQD	O49-C7-O47-C45
33	H1	102	LMG	O9-C10-O7-C8
40	g	624	LHG	O9-C7-O7-C5
40	N1	624	LHG	O9-C7-O7-C5
29	A	405	CLA	C2-C1-O2A-CGA
29	B	607	CLA	C2-C1-O2A-CGA
29	B	608	CLA	C2-C1-O2A-CGA
29	B	611	CLA	C2-C1-O2A-CGA
29	B	617	CLA	C2-C1-O2A-CGA
29	C	503	CLA	C2-C1-O2A-CGA
29	N	611	CLA	C2-C1-O2A-CGA
29	N	613	CLA	C2-C1-O2A-CGA
29	R	603	CLA	C2-C1-O2A-CGA
29	S	603	CLA	C2-C1-O2A-CGA
29	S	614	CLA	C2-C1-O2A-CGA
29	Y	608	CLA	C2-C1-O2A-CGA
29	b	608	CLA	C2-C1-O2A-CGA
29	b	617	CLA	C2-C1-O2A-CGA
29	c	503	CLA	C2-C1-O2A-CGA
29	n	611	CLA	C2-C1-O2A-CGA
29	g	611	CLA	C2-C1-O2A-CGA
29	A1	405	CLA	C2-C1-O2A-CGA
29	B1	611	CLA	C2-C1-O2A-CGA
29	B1	616	CLA	C2-C1-O2A-CGA
29	B1	617	CLA	C2-C1-O2A-CGA
29	C1	502	CLA	C2-C1-O2A-CGA
29	C1	504	CLA	C2-C1-O2A-CGA
29	C1	510	CLA	C2-C1-O2A-CGA
29	R1	612	CLA	C2-C1-O2A-CGA
29	S1	603	CLA	C2-C1-O2A-CGA
29	b1	614	CLA	C2-C1-O2A-CGA
29	c1	502	CLA	C2-C1-O2A-CGA
29	c1	509	CLA	C2-C1-O2A-CGA
29	n1	613	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	n1	614	CLA	C2-C1-O2A-CGA
29	g1	611	CLA	C2-C1-O2A-CGA
29	s1	611	CLA	C2-C1-O2A-CGA
29	s1	614	CLA	C2-C1-O2A-CGA
29	y1	604	CLA	C2-C1-O2A-CGA
48	Y1	607	CHL	C2-C1-O2A-CGA
32	B	621	SQD	C12-C13-C14-C15
32	a1	412	SQD	C10-C11-C12-C13
34	y	625	SPH	C11-C10-C9-C8
37	C	519	DGD	C6A-C7A-C8A-C9A
37	C	520	DGD	C9A-CAA-CBA-CCA
38	B	624	3PH	C2A-C2B-C2C-C2D
38	T	101	3PH	C32-C33-C34-C35
38	B1	624	3PH	C2E-C2F-C2G-C2H
38	S1	626	3PH	C29-C2A-C2B-C2C
39	B	625	DGA	CA7-CA8-CA9-CAA
39	J	101	DGA	CA4-CA5-CA6-CA7
39	j	101	DGA	CA2-CA3-CA4-CA5
40	N	624	LHG	C9-C10-C11-C12
40	d	408	LHG	C13-C14-C15-C16
40	N1	624	LHG	C16-C17-C18-C19
40	Y1	624	LHG	C29-C30-C31-C32
40	d1	409	LHG	C27-C28-C29-C30
40	y1	624	LHG	C13-C14-C15-C16
52	r1	625	LMT	C4-C5-C6-C7
29	a	405	CLA	C8-C10-C11-C12
29	b	606	CLA	C10-C11-C12-C13
29	s	611	CLA	C10-C11-C12-C13
29	B1	612	CLA	C5-C6-C7-C8
29	G1	613	CLA	C5-C6-C7-C8
29	Y1	603	CLA	C15-C16-C17-C18
29	b1	612	CLA	C10-C11-C12-C13
29	s1	611	CLA	C10-C11-C12-C13
29	b	612	CLA	O1A-CGA-O2A-C1
29	r	610	CLA	O1A-CGA-O2A-C1
40	d1	409	LHG	O10-C23-O8-C6
32	A	412	SQD	C14-C15-C16-C17
32	C1	526	SQD	C25-C26-C27-C28
33	H1	102	LMG	C12-C13-C14-C15
38	S1	626	3PH	C28-C29-C2A-C2B
38	S1	626	3PH	C34-C35-C36-C37
38	s1	626	3PH	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
39	J	101	DGA	CB7-CB8-CB9-CAB
39	c1	524	DGA	CA9-CAA-CBA-CCA
40	d	408	LHG	C26-C27-C28-C29
40	d	408	LHG	C29-C30-C31-C32
40	D1	408	LHG	C31-C32-C33-C34
40	D1	409	LHG	C13-C14-C15-C16
40	Y1	624	LHG	C33-C34-C35-C36
40	d1	409	LHG	C10-C11-C12-C13
29	C	501	CLA	C16-C17-C18-C19
29	s	604	CLA	C6-C7-C8-C10
29	C1	501	CLA	C16-C17-C18-C20
29	g1	610	CLA	C16-C17-C18-C19
37	C	518	DGD	C1B-C2B-C3B-C4B
37	c1	518	DGD	C1B-C2B-C3B-C4B
39	B1	625	DGA	CB1-CB2-CB3-CB4
31	A	411	BCR	C23-C24-C25-C26
31	A	411	BCR	C23-C24-C25-C30
31	C	514	BCR	C1-C6-C7-C8
31	C	514	BCR	C5-C6-C7-C8
31	C	516	BCR	C1-C6-C7-C8
31	C	516	BCR	C23-C24-C25-C26
31	C	516	BCR	C23-C24-C25-C30
31	C	517	BCR	C23-C24-C25-C26
31	C	517	BCR	C23-C24-C25-C30
31	D	404	BCR	C1-C6-C7-C8
31	D	404	BCR	C5-C6-C7-C8
31	D	404	BCR	C23-C24-C25-C30
31	a	411	BCR	C5-C6-C7-C8
31	a	411	BCR	C23-C24-C25-C26
31	a	411	BCR	C23-C24-C25-C30
31	c	514	BCR	C1-C6-C7-C8
31	c	514	BCR	C5-C6-C7-C8
31	c	514	BCR	C23-C24-C25-C26
31	c	516	BCR	C23-C24-C25-C26
31	d	404	BCR	C1-C6-C7-C8
31	d	404	BCR	C5-C6-C7-C8
31	B1	618	BCR	C23-C24-C25-C26
31	B1	618	BCR	C23-C24-C25-C30
31	C1	514	BCR	C1-C6-C7-C8
31	C1	514	BCR	C5-C6-C7-C8
31	C1	515	BCR	C23-C24-C25-C26
31	C1	515	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
31	C1	516	BCR	C23-C24-C25-C26
31	C1	516	BCR	C23-C24-C25-C30
31	C1	517	BCR	C23-C24-C25-C26
31	C1	517	BCR	C23-C24-C25-C30
31	D1	404	BCR	C1-C6-C7-C8
31	D1	404	BCR	C5-C6-C7-C8
31	a1	411	BCR	C23-C24-C25-C26
31	a1	411	BCR	C23-C24-C25-C30
31	b1	618	BCR	C23-C24-C25-C26
31	b1	618	BCR	C23-C24-C25-C30
31	c1	514	BCR	C1-C6-C7-C8
31	c1	514	BCR	C5-C6-C7-C8
31	c1	514	BCR	C23-C24-C25-C26
31	c1	514	BCR	C23-C24-C25-C30
31	c1	516	BCR	C1-C6-C7-C8
31	d1	404	BCR	C1-C6-C7-C8
31	d1	404	BCR	C5-C6-C7-C8
36	B	620	C7Z	C1-C6-C7-C8
36	b	620	C7Z	C1-C6-C7-C8
36	b	620	C7Z	C21-C26-C27-C28
36	b	620	C7Z	C25-C26-C27-C28
36	B1	620	C7Z	C1-C6-C7-C8
36	B1	620	C7Z	C21-C26-C27-C28
36	B1	620	C7Z	C25-C26-C27-C28
36	b1	620	C7Z	C1-C6-C7-C8
36	b1	620	C7Z	C5-C6-C7-C8
36	b1	620	C7Z	C25-C26-C27-C28
45	H1	101	RRX	C5-C6-C7-C8
49	G1	620	LUT	C5-C6-C7-C8
49	n1	621	LUT	C5-C6-C7-C8
49	g1	620	LUT	C1-C6-C7-C8
49	g1	620	LUT	C5-C6-C7-C8
49	s1	621	LUT	C5-C6-C7-C8
37	C	519	DGD	O6E-C5E-C6E-O5E
33	C	523	LMG	C12-C13-C14-C15
37	C1	519	DGD	CAB-CBB-CCB-CDB
40	S	624	LHG	C9-C10-C11-C12
40	n	624	LHG	C16-C17-C18-C19
40	g	624	LHG	C27-C28-C29-C30
54	S1	625	LPX	C17-C18-C19-C20
29	B	614	CLA	CBA-CGA-O2A-C1
29	B1	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	b1	623	DGD	C2A-C1A-O1G-C1G
39	J1	101	DGA	CA2-CA1-OG1-CG1
29	B	602	CLA	C10-C11-C12-C13
29	B	614	CLA	C8-C10-C11-C12
29	G	602	CLA	C13-C15-C16-C17
29	R	609	CLA	C8-C10-C11-C12
29	S	609	CLA	C5-C6-C7-C8
29	b	613	CLA	C10-C11-C12-C13
29	c	503	CLA	C13-C15-C16-C17
29	A1	405	CLA	C13-C15-C16-C17
29	A1	405	CLA	C15-C16-C17-C18
29	B1	610	CLA	C5-C6-C7-C8
29	Y1	612	CLA	C13-C15-C16-C17
29	b1	602	CLA	C10-C11-C12-C13
29	c1	511	CLA	C10-C11-C12-C13
37	C	518	DGD	O6D-C5D-C6D-O5D
37	c	519	DGD	C4B-C5B-C6B-C7B
38	s1	626	3PH	C3E-C3F-C3G-C3H
39	b	625	DGA	CB3-CB4-CB5-CB6
39	c1	524	DGA	CB7-CB8-CB9-CAB
40	G	624	LHG	C15-C16-C17-C18
40	c	525	LHG	C30-C31-C32-C33
47	I1	102	4RF	C51-C52-C53-C54
47	I1	102	4RF	C52-C53-C54-C55
47	k1	101	4RF	C32-C33-C34-C35
37	c1	518	DGD	C1A-C2A-C3A-C4A
38	B	624	3PH	C21-C22-C23-C24
40	n1	624	LHG	C23-C24-C25-C26
40	C	525	LHG	C25-C26-C27-C28
40	y	624	LHG	C9-C10-C11-C12
29	B	612	CLA	C13-C15-C16-C17
29	C	509	CLA	C15-C16-C17-C18
29	c	501	CLA	C8-C10-C11-C12
29	c	504	CLA	C8-C10-C11-C12
29	c	513	CLA	C13-C15-C16-C17
29	N1	604	CLA	C13-C15-C16-C17
29	c1	504	CLA	C8-C10-C11-C12
29	y1	611	CLA	C8-C10-C11-C12
32	A1	412	SQD	C13-C14-C15-C16
37	C1	519	DGD	C6B-C7B-C8B-C9B
40	L	101	LHG	C11-C12-C13-C14
40	n	624	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
40	N1	624	LHG	C28-C29-C30-C31
47	K	101	4RF	C03-C04-C05-C06
47	k1	101	4RF	C07-C08-C09-C10
29	G	613	CLA	C4-C3-C5-C6
29	A	410	CLA	C11-C10-C8-C7
29	B	603	CLA	C12-C13-C15-C16
29	B	605	CLA	C11-C12-C13-C15
29	B	607	CLA	C11-C12-C13-C15
29	B	609	CLA	C11-C12-C13-C15
29	B	610	CLA	C11-C12-C13-C15
29	B	612	CLA	C11-C10-C8-C7
29	B	617	CLA	C6-C7-C8-C10
29	C	507	CLA	C6-C7-C8-C10
29	C	513	CLA	C6-C7-C8-C10
29	D	402	CLA	C11-C12-C13-C15
29	D	402	CLA	C12-C13-C15-C16
29	D	403	CLA	C11-C12-C13-C15
29	G	613	CLA	C11-C12-C13-C15
29	R	603	CLA	C11-C10-C8-C7
29	S	603	CLA	C11-C10-C8-C7
29	Y	603	CLA	C6-C7-C8-C10
29	Y	614	CLA	C12-C13-C15-C16
29	a	410	CLA	C6-C7-C8-C10
29	b	602	CLA	C6-C7-C8-C10
29	b	604	CLA	C11-C12-C13-C15
29	b	605	CLA	C6-C7-C8-C10
29	b	612	CLA	C2-C3-C5-C6
29	b	616	CLA	C12-C13-C15-C16
29	c	503	CLA	C12-C13-C15-C16
29	c	509	CLA	C6-C7-C8-C10
29	c	510	CLA	C2-C3-C5-C6
29	c	512	CLA	C12-C13-C15-C16
29	c	513	CLA	C6-C7-C8-C10
29	d	403	CLA	C11-C10-C8-C7
29	n	603	CLA	C11-C10-C8-C7
29	n	610	CLA	C6-C7-C8-C10
29	g	603	CLA	C6-C7-C8-C10
29	g	611	CLA	C6-C7-C8-C10
29	g	613	CLA	C6-C7-C8-C10
29	r	603	CLA	C11-C10-C8-C7
29	r	610	CLA	C11-C10-C8-C7
29	s	602	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	y	604	CLA	C2-C3-C5-C6
29	A1	410	CLA	C6-C7-C8-C10
29	B1	606	CLA	C11-C12-C13-C15
29	B1	610	CLA	C11-C12-C13-C15
29	C1	503	CLA	C6-C7-C8-C10
29	C1	505	CLA	C11-C12-C13-C15
29	C1	505	CLA	C12-C13-C15-C16
29	C1	506	CLA	C6-C7-C8-C10
29	G1	611	CLA	C6-C7-C8-C10
29	G1	611	CLA	C11-C10-C8-C7
29	G1	613	CLA	C6-C7-C8-C10
29	R1	603	CLA	C2-C3-C5-C6
29	R1	609	CLA	C11-C10-C8-C7
29	R1	612	CLA	C11-C10-C8-C7
29	b1	602	CLA	C11-C12-C13-C15
29	b1	604	CLA	C6-C7-C8-C10
29	c1	503	CLA	C6-C7-C8-C10
29	c1	505	CLA	C2-C3-C5-C6
29	c1	508	CLA	C11-C12-C13-C15
29	c1	509	CLA	C12-C13-C15-C16
29	c1	510	CLA	C12-C13-C15-C16
29	c1	511	CLA	C11-C12-C13-C15
29	c1	513	CLA	C6-C7-C8-C10
29	n1	613	CLA	C2-C3-C5-C6
29	r1	612	CLA	C6-C7-C8-C10
29	r1	612	CLA	C11-C10-C8-C7
29	y1	602	CLA	C6-C7-C8-C10
29	y1	612	CLA	C12-C13-C15-C16
43	D	405	PL9	C43-C44-C46-C47
43	D1	405	PL9	C28-C29-C31-C32
48	G	601	CHL	C12-C13-C15-C16
48	n	607	CHL	C11-C10-C8-C7
48	g	609	CHL	C12-C13-C15-C16
48	s	608	CHL	C2-C3-C5-C6
48	y	606	CHL	C11-C10-C8-C7
48	g1	601	CHL	C12-C13-C15-C16
48	y1	609	CHL	C2-C3-C5-C6
29	s	611	CLA	C3-C5-C6-C7
29	b	614	CLA	O1A-CGA-O2A-C1
29	n	602	CLA	O1A-CGA-O2A-C1
29	B1	613	CLA	O1A-CGA-O2A-C1
39	J	101	DGA	OA1-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
33	C1	523	LMG	C16-C17-C18-C19
34	y1	625	SPH	C6-C7-C8-C9
38	B1	624	3PH	C37-C38-C39-C3A
47	k	101	4RF	C26-C27-C28-C29
29	B	611	CLA	C15-C16-C17-C18
29	C	502	CLA	C8-C10-C11-C12
29	N	603	CLA	C13-C15-C16-C17
29	R1	612	CLA	C5-C6-C7-C8
29	S1	611	CLA	C10-C11-C12-C13
29	r1	608	CLA	C8-C10-C11-C12
31	A	411	BCR	C19-C20-C21-C22
31	D	404	BCR	C9-C10-C11-C12
31	A1	411	BCR	C19-C20-C21-C22
31	c1	514	BCR	C19-C20-C21-C22
36	B	620	C7Z	C29-C30-C31-C32
49	g	621	LUT	C29-C30-C31-C32
49	y	621	LUT	C29-C30-C31-C32
50	y1	622	XAT	C29-C30-C31-C32
51	S1	623	NEX	C9-C10-C11-C12
29	c	510	CLA	C16-C17-C18-C19
29	C1	509	CLA	C16-C17-C18-C20
29	R1	610	CLA	C11-C12-C13-C15
29	A1	406	CLA	O1D-CGD-O2D-CED
29	B1	602	CLA	O1D-CGD-O2D-CED
29	b1	610	CLA	O1D-CGD-O2D-CED
33	C1	521	LMG	O9-C10-O7-C8
40	D1	409	LHG	O9-C7-O7-C5
55	y	626	PTY	O10-C8-O7-C6
38	b	624	3PH	C21-C22-C23-C24
40	d	408	LHG	C7-C8-C9-C10
40	n	624	LHG	C23-C24-C25-C26
40	g1	624	LHG	C7-C8-C9-C10
29	A	410	CLA	CBA-CGA-O2A-C1
29	B	612	CLA	CBA-CGA-O2A-C1
29	Y	614	CLA	CBA-CGA-O2A-C1
29	b	605	CLA	CBA-CGA-O2A-C1
29	c	503	CLA	CBA-CGA-O2A-C1
29	G1	603	CLA	CBA-CGA-O2A-C1
29	G1	610	CLA	CBA-CGA-O2A-C1
29	g1	603	CLA	CBA-CGA-O2A-C1
29	y1	602	CLA	CBA-CGA-O2A-C1
29	y1	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	c	519	DGD	C2A-C1A-O1G-C1G
37	c1	518	DGD	C2A-C1A-O1G-C1G
32	A	412	SQD	C31-C32-C33-C34
32	c	526	SQD	C11-C10-C9-C8
33	C1	523	LMG	C13-C14-C15-C16
34	Y	625	SPH	C11-C12-C13-C14
38	B1	624	3PH	C2D-C2E-C2F-C2G
40	g	624	LHG	C31-C32-C33-C34
47	k	101	4RF	C45-C46-C47-C48
47	i1	101	4RF	C52-C53-C54-C55
52	R1	625	LMT	C7-C8-C9-C10
29	N	613	CLA	C2A-CAA-CBA-CGA
29	G	610	CLA	C2A-CAA-CBA-CGA
29	S	603	CLA	C2A-CAA-CBA-CGA
29	b	617	CLA	C2A-CAA-CBA-CGA
29	g	602	CLA	C2A-CAA-CBA-CGA
29	r	602	CLA	C2A-CAA-CBA-CGA
29	y	613	CLA	C2A-CAA-CBA-CGA
29	B1	603	CLA	C2A-CAA-CBA-CGA
29	S1	613	CLA	C2A-CAA-CBA-CGA
29	s1	603	CLA	C2A-CAA-CBA-CGA
29	y1	602	CLA	C2A-CAA-CBA-CGA
29	y1	610	CLA	C2A-CAA-CBA-CGA
48	y1	605	CHL	C2A-CAA-CBA-CGA
29	a	406	CLA	O1D-CGD-O2D-CED
29	B	614	CLA	C5-C6-C7-C8
29	C	510	CLA	C15-C16-C17-C18
29	N	602	CLA	C13-C15-C16-C17
29	Y	612	CLA	C15-C16-C17-C18
29	n	610	CLA	C10-C11-C12-C13
29	n	613	CLA	C10-C11-C12-C13
29	r	610	CLA	C8-C10-C11-C12
29	C1	503	CLA	C15-C16-C17-C18
29	c1	509	CLA	C10-C11-C12-C13
32	B1	626	SQD	C32-C33-C34-C35
38	b1	624	3PH	C32-C33-C34-C35
39	j	101	DGA	CB6-CB7-CB8-CB9
40	D	408	LHG	C13-C14-C15-C16
40	l	101	LHG	C26-C27-C28-C29
47	K1	101	4RF	C25-C26-C27-C28
47	K1	101	4RF	C32-C33-C34-C35
47	k1	101	4RF	C03-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
33	d1	411	LMG	C22-C23-C24-C25
37	c1	519	DGD	C4A-C5A-C6A-C7A
38	B1	624	3PH	C39-C3A-C3B-C3C
38	s1	626	3PH	C36-C37-C38-C39
39	j1	101	DGA	CB3-CB4-CB5-CB6
40	d	409	LHG	C34-C35-C36-C37
40	g	624	LHG	C24-C25-C26-C27
40	D1	409	LHG	C28-C29-C30-C31
33	c	523	LMG	C28-C29-C30-C31
37	C	519	DGD	C1A-C2A-C3A-C4A
38	B	624	3PH	C31-C32-C33-C34
40	D	408	LHG	C7-C8-C9-C10
40	N	624	LHG	C23-C24-C25-C26
40	D1	408	LHG	C23-C24-C25-C26
40	N1	624	LHG	C7-C8-C9-C10
54	S1	625	LPX	C3-C4-C5-O6
29	B	613	CLA	C10-C11-C12-C13
29	g	602	CLA	C5-C6-C7-C8
32	b1	626	SQD	C12-C13-C14-C15
33	D1	411	LMG	C19-C20-C21-C22
34	y1	625	SPH	C9-C10-C11-C12
40	D	409	LHG	C11-C12-C13-C14
40	Y	624	LHG	C30-C31-C32-C33
40	L1	101	LHG	C25-C26-C27-C28
41	c1	527	LMK	C12-C13-C14-C15
47	K	101	4RF	C27-C28-C29-C30
47	i1	101	4RF	C27-C28-C29-C30
52	R1	625	LMT	O1'-C1-C2-C3
55	Y	626	PTY	C19-C20-C21-C22
38	B	624	3PH	C27-C28-C29-C2A
39	J	101	DGA	CB6-CB7-CB8-CB9
40	Y1	624	LHG	C13-C14-C15-C16
47	I1	102	4RF	C12-C13-C14-C15
47	K1	101	4RF	C43-C44-C45-C46
37	C1	518	DGD	C2A-C1A-O1G-C1G
55	Y	626	PTY	C31-C30-O4-C1
29	C	513	CLA	C16-C17-C18-C19
29	Y	610	CLA	C16-C17-C18-C20
29	s	602	CLA	C11-C12-C13-C15
29	D1	402	CLA	C16-C17-C18-C19
29	D1	403	CLA	C16-C17-C18-C20
29	R1	608	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
29	Y1	612	CLA	C16-C17-C18-C20
29	b1	608	CLA	C16-C17-C18-C20
29	b1	614	CLA	C16-C17-C18-C19
33	H	102	LMG	C4-C5-C6-O5
32	M1	101	SQD	O5-C1-O6-C44
37	C	518	DGD	O6E-C1E-O5D-C6D
29	A	405	CLA	C15-C16-C17-C18
29	A	410	CLA	C8-C10-C11-C12
29	g	613	CLA	C13-C15-C16-C17
29	b1	608	CLA	C13-C15-C16-C17
32	c	526	SQD	C12-C13-C14-C15
32	B1	626	SQD	C18-C19-C20-C21
40	c1	525	LHG	C11-C12-C13-C14
47	I1	102	4RF	C09-C10-C11-C12
47	K1	101	4RF	C24-C25-C26-C27
47	i1	101	4RF	C10-C11-C12-C13
55	y1	626	PTY	C38-C39-C40-C41
37	C	519	DGD	C1B-C2B-C3B-C4B
38	T	101	3PH	C31-C32-C33-C34
39	b	625	DGA	CB1-CB2-CB3-CB4
33	A	413	LMG	C11-C10-O7-C8
33	c	521	LMG	C11-C10-O7-C8
33	w	201	LMG	C11-C10-O7-C8
38	B	624	3PH	C22-C21-O21-C2
39	c	524	DGA	CB2-CB1-OG2-CG2
40	C	525	LHG	C8-C7-O7-C5
40	Y	624	LHG	C8-C7-O7-C5
40	s	624	LHG	C8-C7-O7-C5
40	D1	410	LHG	C8-C7-O7-C5
40	c1	525	LHG	C8-C7-O7-C5
47	K	101	4RF	C24-C22-O21-C20
55	y	626	PTY	C11-C8-O7-C6
51	Y	623	NEX	C30-C31-C32-C33
33	A1	413	LMG	C14-C15-C16-C17
34	a1	414	SPH	C14-C15-C16-C17
40	s	624	LHG	C33-C34-C35-C36
40	D1	409	LHG	C25-C26-C27-C28
29	B	606	CLA	C13-C15-C16-C17
29	N	610	CLA	C13-C15-C16-C17
29	Y	602	CLA	C13-C15-C16-C17
29	c	504	CLA	C5-C6-C7-C8
29	b1	603	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	g1	603	CLA	C15-C16-C17-C18
29	b1	615	CLA	CBD-CGD-O2D-CED
40	l	101	LHG	C9-C10-C11-C12
40	n	624	LHG	C24-C25-C26-C27
40	S1	624	LHG	C34-C35-C36-C37
33	c	521	LMG	O9-C10-O7-C8
33	h	102	LMG	O9-C10-O7-C8
40	C	525	LHG	O9-C7-O7-C5
40	D1	410	LHG	O9-C7-O7-C5
41	c	527	LMK	C2-C3-C4-O2
41	c1	527	LMK	C2-C3-C4-O2
29	G1	613	CLA	C3-C5-C6-C7
40	L1	101	LHG	C23-C24-C25-C26
32	c1	526	SQD	C18-C19-C20-C21
38	S1	626	3PH	C2D-C2E-C2F-C2G
55	y	626	PTY	C31-C32-C33-C34
53	r1	626	ERG	C21-C20-C22-C23
32	c1	526	SQD	C2-C1-O6-C44
29	C	509	CLA	C8-C10-C11-C12
29	c1	501	CLA	C15-C16-C17-C18
30	a1	408	PHO	C8-C10-C11-C12
33	A	413	LMG	O1-C7-C8-O7
33	a	413	LMG	O1-C7-C8-O7
40	N1	624	LHG	O7-C5-C6-O8
41	c	527	LMK	O1-C7-C8-O7
47	I	102	4RF	O21-C20-C39-O40
47	I1	102	4RF	O18-C19-C20-O21
37	C1	519	DGD	O6E-C5E-C6E-O5E
32	m	101	SQD	C26-C27-C28-C29
38	B	624	3PH	C24-C25-C26-C27
39	C1	524	DGA	CB5-CB6-CB7-CB8
40	D1	409	LHG	C34-C35-C36-C37
40	d1	408	LHG	C25-C26-C27-C28
40	g1	624	LHG	C17-C18-C19-C20
52	r	625	LMT	C6-C7-C8-C9
29	C	504	CLA	CBD-CGD-O2D-CED
29	c	509	CLA	C16-C17-C18-C20
29	b1	610	CLA	C16-C17-C18-C19
29	y1	614	CLA	C16-C17-C18-C20
32	b	621	SQD	C24-C25-C26-C27
33	B	622	LMG	C11-C12-C13-C14
34	a	414	SPH	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
39	C	524	DGA	CA9-CAA-CBA-CCA
47	k1	101	4RF	C11-C12-C13-C14
55	y1	626	PTY	C11-C12-C13-C14
33	D	411	LMG	O6-C5-C6-O5
29	N	613	CLA	C10-C11-C12-C13
29	B1	605	CLA	C15-C16-C17-C18
29	b1	606	CLA	C8-C10-C11-C12
29	r1	602	CLA	C8-C10-C11-C12
29	s1	603	CLA	C5-C6-C7-C8
48	G1	601	CHL	C5-C6-C7-C8
29	B	603	CLA	C4-C3-C5-C6
29	y	604	CLA	C4-C3-C5-C6
29	R1	603	CLA	C4-C3-C5-C6
29	b1	608	CLA	C4-C3-C5-C6
29	n1	613	CLA	C4-C3-C5-C6
40	D	409	LHG	C23-C24-C25-C26
29	G	613	CLA	C2-C3-C5-C6
29	S	602	CLA	C2-C3-C5-C6
29	S	611	CLA	C2-C3-C5-C6
29	b	614	CLA	C2-C3-C5-C6
30	a1	408	PHO	C2-C3-C5-C6
33	A	413	LMG	C36-C37-C38-C39
33	w1	201	LMG	C37-C38-C39-C40
39	C	524	DGA	CCA-CDA-CEA-CFA
47	i	101	4RF	C24-C25-C26-C27
47	k	101	4RF	C28-C29-C30-C31
54	s	625	LPX	C12-C13-C14-C15
29	A	410	CLA	C11-C10-C8-C9
29	B	605	CLA	C11-C12-C13-C14
29	B	609	CLA	C11-C12-C13-C14
29	B	617	CLA	C6-C7-C8-C9
29	C	505	CLA	C14-C13-C15-C16
29	C	509	CLA	C14-C13-C15-C16
29	C	513	CLA	C6-C7-C8-C9
29	D	402	CLA	C11-C12-C13-C14
29	G	610	CLA	C11-C12-C13-C14
29	G	611	CLA	C6-C7-C8-C9
29	G	611	CLA	C14-C13-C15-C16
29	R	603	CLA	C11-C10-C8-C9
29	Y	612	CLA	C6-C7-C8-C9
29	Y	613	CLA	C6-C7-C8-C9
29	b	615	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	c	503	CLA	C11-C12-C13-C14
29	c	509	CLA	C14-C13-C15-C16
29	c	513	CLA	C6-C7-C8-C9
29	c	513	CLA	C11-C12-C13-C14
29	n	603	CLA	C11-C10-C8-C9
29	n	604	CLA	C14-C13-C15-C16
29	g	603	CLA	C11-C12-C13-C14
29	g	610	CLA	C11-C10-C8-C9
29	g	613	CLA	C6-C7-C8-C9
29	s	602	CLA	C11-C10-C8-C9
29	y	610	CLA	C11-C12-C13-C14
29	y	613	CLA	C11-C12-C13-C14
29	C1	505	CLA	C11-C12-C13-C14
29	C1	512	CLA	C14-C13-C15-C16
29	G1	602	CLA	C6-C7-C8-C9
29	G1	611	CLA	C6-C7-C8-C9
29	R1	603	CLA	C11-C10-C8-C9
29	R1	609	CLA	C11-C10-C8-C9
29	R1	610	CLA	C11-C10-C8-C9
29	Y1	612	CLA	C14-C13-C15-C16
29	Y1	613	CLA	C14-C13-C15-C16
29	b1	610	CLA	C11-C12-C13-C14
29	c1	503	CLA	C6-C7-C8-C9
29	c1	508	CLA	C11-C12-C13-C14
29	c1	511	CLA	C11-C12-C13-C14
29	c1	513	CLA	C6-C7-C8-C9
29	g1	610	CLA	C11-C10-C8-C9
29	r1	608	CLA	C6-C7-C8-C9
29	r1	609	CLA	C11-C10-C8-C9
29	y1	602	CLA	C6-C7-C8-C9
29	y1	602	CLA	C11-C12-C13-C14
29	y1	612	CLA	C14-C13-C15-C16
29	y1	613	CLA	C11-C10-C8-C9
48	Y	606	CHL	C14-C13-C15-C16
48	g	601	CHL	C11-C12-C13-C14
48	N1	607	CHL	C11-C10-C8-C9
32	b	626	SQD	C12-C13-C14-C15
38	s	626	3PH	C23-C24-C25-C26
40	l	101	LHG	C28-C29-C30-C31
47	i	101	4RF	C49-C50-C51-C52
47	i1	101	4RF	C25-C26-C27-C28
29	n	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	y	614	CLA	C3-C5-C6-C7
29	G1	611	CLA	C3-C5-C6-C7
48	N	607	CHL	C3-C5-C6-C7
29	B	604	CLA	C2A-CAA-CBA-CGA
29	G	614	CLA	C2A-CAA-CBA-CGA
29	R	610	CLA	C2A-CAA-CBA-CGA
29	b	604	CLA	C2A-CAA-CBA-CGA
29	A1	407	CLA	C2A-CAA-CBA-CGA
48	R	607	CHL	C2A-CAA-CBA-CGA
48	r	607	CHL	C2A-CAA-CBA-CGA
29	B1	614	CLA	C4C-C3C-CAC-CBC
32	m1	101	SQD	C10-C11-C12-C13
38	T	101	3PH	C38-C39-C3A-C3B
39	c1	524	DGA	CBB-CCB-CDB-CEB
40	d	408	LHG	C24-C25-C26-C27
40	y1	624	LHG	C11-C10-C9-C8
55	y1	626	PTY	C24-C25-C26-C27
33	h1	102	LMG	O6-C5-C6-O5
37	c	518	DGD	O6E-C5E-C6E-O5E
31	D	404	BCR	C37-C22-C23-C24
29	c1	512	CLA	O1D-CGD-O2D-CED
29	b	614	CLA	C13-C15-C16-C17
29	r	608	CLA	C8-C10-C11-C12
29	g1	611	CLA	C15-C16-C17-C18
29	y1	611	CLA	C10-C11-C12-C13
33	C	521	LMG	C14-C15-C16-C17
33	H1	102	LMG	C14-C15-C16-C17
39	c	524	DGA	CDA-CEA-CFA-CGA
40	d1	409	LHG	C29-C30-C31-C32
40	y1	624	LHG	C33-C34-C35-C36
47	K	101	4RF	C11-C12-C13-C14
47	i1	101	4RF	C11-C12-C13-C14
54	s1	625	LPX	C15-C16-C17-C18
31	A	411	BCR	C11-C12-C13-C14
31	B	619	BCR	C21-C22-C23-C24
31	D	404	BCR	C21-C22-C23-C24
49	Y	620	LUT	C27-C28-C29-C30
49	N1	620	LUT	C27-C28-C29-C30
29	A	410	CLA	O1A-CGA-O2A-C1
29	B	614	CLA	O1A-CGA-O2A-C1
29	y1	602	CLA	O1A-CGA-O2A-C1
37	c	519	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
37	b1	623	DGD	O1A-C1A-O1G-C1G
37	c1	518	DGD	O1A-C1A-O1G-C1G
39	J1	101	DGA	OA1-CA1-OG1-CG1
40	D	410	LHG	O10-C23-O8-C6
29	A	407	CLA	C1A-C2A-CAA-CBA
29	B	602	CLA	C1A-C2A-CAA-CBA
29	B	604	CLA	C1A-C2A-CAA-CBA
29	B	610	CLA	C1A-C2A-CAA-CBA
29	C	503	CLA	C1A-C2A-CAA-CBA
29	C	511	CLA	C1A-C2A-CAA-CBA
29	D	403	CLA	C1A-C2A-CAA-CBA
29	N	603	CLA	C1A-C2A-CAA-CBA
29	G	603	CLA	C1A-C2A-CAA-CBA
29	G	610	CLA	C1A-C2A-CAA-CBA
29	G	611	CLA	C1A-C2A-CAA-CBA
29	G	614	CLA	C1A-C2A-CAA-CBA
29	R	602	CLA	C1A-C2A-CAA-CBA
29	R	603	CLA	C1A-C2A-CAA-CBA
29	S	602	CLA	C1A-C2A-CAA-CBA
29	S	604	CLA	C1A-C2A-CAA-CBA
29	S	609	CLA	C1A-C2A-CAA-CBA
29	S	610	CLA	C1A-C2A-CAA-CBA
29	S	617	CLA	C1A-C2A-CAA-CBA
29	Y	602	CLA	C1A-C2A-CAA-CBA
29	Y	603	CLA	C1A-C2A-CAA-CBA
29	Y	610	CLA	C1A-C2A-CAA-CBA
29	Y	611	CLA	C1A-C2A-CAA-CBA
29	Y	614	CLA	C1A-C2A-CAA-CBA
29	b	604	CLA	C1A-C2A-CAA-CBA
29	b	606	CLA	C1A-C2A-CAA-CBA
29	b	607	CLA	C1A-C2A-CAA-CBA
29	b	610	CLA	C1A-C2A-CAA-CBA
29	c	501	CLA	C1A-C2A-CAA-CBA
29	c	503	CLA	C1A-C2A-CAA-CBA
29	c	511	CLA	C1A-C2A-CAA-CBA
29	d	403	CLA	C1A-C2A-CAA-CBA
29	n	602	CLA	C1A-C2A-CAA-CBA
29	n	603	CLA	C1A-C2A-CAA-CBA
29	g	602	CLA	C1A-C2A-CAA-CBA
29	g	603	CLA	C1A-C2A-CAA-CBA
29	g	610	CLA	C1A-C2A-CAA-CBA
29	g	611	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	r	610	CLA	C1A-C2A-CAA-CBA
29	y	602	CLA	C1A-C2A-CAA-CBA
29	y	603	CLA	C1A-C2A-CAA-CBA
29	y	610	CLA	C1A-C2A-CAA-CBA
29	y	611	CLA	C1A-C2A-CAA-CBA
29	y	614	CLA	C1A-C2A-CAA-CBA
29	A1	407	CLA	C1A-C2A-CAA-CBA
29	B1	602	CLA	C1A-C2A-CAA-CBA
29	B1	605	CLA	C1A-C2A-CAA-CBA
29	B1	606	CLA	C1A-C2A-CAA-CBA
29	B1	610	CLA	C1A-C2A-CAA-CBA
29	B1	612	CLA	C1A-C2A-CAA-CBA
29	C1	503	CLA	C1A-C2A-CAA-CBA
29	C1	506	CLA	C1A-C2A-CAA-CBA
29	C1	507	CLA	C1A-C2A-CAA-CBA
29	C1	512	CLA	C1A-C2A-CAA-CBA
29	D1	402	CLA	C1A-C2A-CAA-CBA
29	N1	603	CLA	C1A-C2A-CAA-CBA
29	N1	613	CLA	C1A-C2A-CAA-CBA
29	G1	603	CLA	C1A-C2A-CAA-CBA
29	G1	610	CLA	C1A-C2A-CAA-CBA
29	R1	603	CLA	C1A-C2A-CAA-CBA
29	R1	608	CLA	C1A-C2A-CAA-CBA
29	R1	609	CLA	C1A-C2A-CAA-CBA
29	R1	610	CLA	C1A-C2A-CAA-CBA
29	R1	612	CLA	C1A-C2A-CAA-CBA
29	S1	602	CLA	C1A-C2A-CAA-CBA
29	S1	609	CLA	C1A-C2A-CAA-CBA
29	S1	610	CLA	C1A-C2A-CAA-CBA
29	S1	617	CLA	C1A-C2A-CAA-CBA
29	Y1	603	CLA	C1A-C2A-CAA-CBA
29	Y1	608	CLA	C1A-C2A-CAA-CBA
29	Y1	610	CLA	C1A-C2A-CAA-CBA
29	Y1	611	CLA	C1A-C2A-CAA-CBA
29	Y1	614	CLA	C1A-C2A-CAA-CBA
29	a1	405	CLA	C1A-C2A-CAA-CBA
29	b1	602	CLA	C1A-C2A-CAA-CBA
29	b1	610	CLA	C1A-C2A-CAA-CBA
29	c1	501	CLA	C1A-C2A-CAA-CBA
29	c1	503	CLA	C1A-C2A-CAA-CBA
29	c1	507	CLA	C1A-C2A-CAA-CBA
29	c1	512	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	n1	602	CLA	C1A-C2A-CAA-CBA
29	n1	603	CLA	C1A-C2A-CAA-CBA
29	n1	613	CLA	C1A-C2A-CAA-CBA
29	g1	603	CLA	C1A-C2A-CAA-CBA
29	g1	611	CLA	C1A-C2A-CAA-CBA
29	g1	614	CLA	C1A-C2A-CAA-CBA
29	r1	602	CLA	C1A-C2A-CAA-CBA
29	r1	610	CLA	C1A-C2A-CAA-CBA
29	s1	602	CLA	C1A-C2A-CAA-CBA
29	s1	605	CLA	C1A-C2A-CAA-CBA
29	s1	612	CLA	C1A-C2A-CAA-CBA
29	s1	614	CLA	C1A-C2A-CAA-CBA
29	y1	602	CLA	C1A-C2A-CAA-CBA
29	y1	603	CLA	C1A-C2A-CAA-CBA
29	y1	608	CLA	C1A-C2A-CAA-CBA
29	y1	610	CLA	C1A-C2A-CAA-CBA
29	y1	614	CLA	C1A-C2A-CAA-CBA
48	G	606	CHL	C1A-C2A-CAA-CBA
48	n	609	CHL	C1A-C2A-CAA-CBA
48	g	607	CHL	C1A-C2A-CAA-CBA
48	N1	607	CHL	C1A-C2A-CAA-CBA
48	G1	605	CHL	C1A-C2A-CAA-CBA
48	G1	606	CHL	C1A-C2A-CAA-CBA
48	G1	609	CHL	C1A-C2A-CAA-CBA
48	n1	608	CHL	C1A-C2A-CAA-CBA
48	s1	608	CHL	C1A-C2A-CAA-CBA
48	y1	601	CHL	C1A-C2A-CAA-CBA
48	y1	609	CHL	C1A-C2A-CAA-CBA
29	C	509	CLA	C16-C17-C18-C19
29	Y	614	CLA	C16-C17-C18-C20
29	b	602	CLA	C16-C17-C18-C19
29	n	610	CLA	C16-C17-C18-C19
29	r	602	CLA	C11-C12-C13-C15
29	s	610	CLA	C16-C17-C18-C20
29	B1	605	CLA	C16-C17-C18-C19
29	B1	608	CLA	C16-C17-C18-C19
29	C1	501	CLA	C16-C17-C18-C19
29	C1	509	CLA	C16-C17-C18-C19
29	D1	403	CLA	C16-C17-C18-C19
29	S1	613	CLA	C6-C7-C8-C10
29	Y1	612	CLA	C16-C17-C18-C19
29	Y1	614	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
29	b1	614	CLA	C16-C17-C18-C20
29	c1	501	CLA	C16-C17-C18-C20
29	n1	610	CLA	C16-C17-C18-C20
33	A	413	LMG	O9-C10-O7-C8
33	w	201	LMG	O9-C10-O7-C8
40	Y	624	LHG	O9-C7-O7-C5
40	s	624	LHG	O9-C7-O7-C5
40	y	624	LHG	O9-C7-O7-C5
40	c1	525	LHG	O9-C7-O7-C5
32	B	621	SQD	C9-C10-C11-C12
38	t	101	3PH	C22-C23-C24-C25
38	t1	101	3PH	C23-C24-C25-C26
38	t1	101	3PH	C3C-C3D-C3E-C3F
40	Y	624	LHG	C16-C17-C18-C19
31	b	619	BCR	C19-C20-C21-C22
36	b1	620	C7Z	C9-C10-C11-C12
49	G	621	LUT	C9-C10-C11-C12
49	G	621	LUT	C29-C30-C31-C32
49	n	621	LUT	C29-C30-C31-C32
49	N1	621	LUT	C29-C30-C31-C32
49	S1	621	LUT	C29-C30-C31-C32
49	s1	620	LUT	C33-C34-C35-C15
29	B	604	CLA	C10-C11-C12-C13
29	b	612	CLA	C15-C16-C17-C18
29	B1	615	CLA	C10-C11-C12-C13
29	c1	508	CLA	C10-C11-C12-C13
40	l	101	LHG	C3-O3-P-O6
40	g	624	LHG	C4-O6-P-O3
40	L1	101	LHG	C4-O6-P-O3
40	y1	624	LHG	C4-O6-P-O3
54	s	625	LPX	C3-O1-P1-O2
54	s1	625	LPX	C1-O2-P1-O1
55	y	626	PTY	C5-O14-P1-O11
32	C1	526	SQD	C17-C18-C19-C20
33	C1	523	LMG	C12-C13-C14-C15
34	a1	414	SPH	C7-C8-C9-C10
38	S	626	3PH	C27-C28-C29-C2A
40	G	624	LHG	C11-C12-C13-C14
40	n	624	LHG	C34-C35-C36-C37
40	d1	410	LHG	C11-C10-C9-C8
37	C1	519	DGD	C1B-C2B-C3B-C4B
40	G	624	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
40	g1	624	LHG	C23-C24-C25-C26
37	c	519	DGD	O6E-C5E-C6E-O5E
52	R1	625	LMT	O5B-C5B-C6B-O6B
30	A	408	PHO	C3-C5-C6-C7
32	C	526	SQD	C11-C10-C9-C8
32	A1	412	SQD	C31-C32-C33-C34
40	s	624	LHG	C14-C15-C16-C17
40	D1	409	LHG	C33-C34-C35-C36
41	c1	527	LMK	C11-C12-C13-C14
52	r	625	LMT	C3-C4-C5-C6
54	S1	625	LPX	C13-C14-C15-C16
29	B1	616	CLA	C10-C11-C12-C13
37	c	518	DGD	C2A-C1A-O1G-C1G
40	c	525	LHG	C24-C23-O8-C6
40	s1	624	LHG	C24-C23-O8-C6
47	I	102	4RF	C43-C41-O40-C39
33	B1	622	LMG	O6-C5-C6-O5
38	B	624	3PH	O11-C1-C2-C3
40	C	525	LHG	O6-C4-C5-C6
40	L	101	LHG	O6-C4-C5-C6
40	c	525	LHG	O6-C4-C5-C6
40	l	101	LHG	O6-C4-C5-C6
40	n	624	LHG	O6-C4-C5-C6
40	C1	525	LHG	O6-C4-C5-C6
40	L1	101	LHG	O6-C4-C5-C6
40	c1	525	LHG	O6-C4-C5-C6
40	d1	410	LHG	O6-C4-C5-C6
40	n1	624	LHG	O6-C4-C5-C6
55	y	627	PTY	O14-C5-C6-C1
32	b	626	SQD	C27-C28-C29-C30
33	c1	521	LMG	C18-C19-C20-C21
37	C1	518	DGD	C5A-C6A-C7A-C8A
37	C1	519	DGD	CCB-CDB-CEB-CFB
38	S	626	3PH	C22-C23-C24-C25
40	s	624	LHG	C12-C13-C14-C15
40	G1	624	LHG	C31-C32-C33-C34
40	c1	525	LHG	C11-C10-C9-C8
47	i	101	4RF	C46-C47-C48-C49
47	k	101	4RF	C32-C33-C34-C35
32	m	101	SQD	C23-C24-C25-C26
32	a1	412	SQD	C7-C8-C9-C10
33	h1	102	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
47	I1	102	4RF	C22-C24-C25-C26
37	C1	520	DGD	CCB-CDB-CEB-CFB
38	T	101	3PH	C2C-C2D-C2E-C2F
38	t1	101	3PH	C3B-C3C-C3D-C3E
39	J	101	DGA	CA2-CA3-CA4-CA5
40	L	101	LHG	C30-C31-C32-C33
40	d1	410	LHG	C30-C31-C32-C33
54	S	625	LPX	C12-C13-C14-C15
29	c	510	CLA	C13-C15-C16-C17
29	b1	604	CLA	C5-C6-C7-C8
29	D	402	CLA	C16-C17-C18-C20
29	N	610	CLA	C16-C17-C18-C19
29	b	605	CLA	C16-C17-C18-C19
29	c	512	CLA	C16-C17-C18-C20
29	c	513	CLA	C16-C17-C18-C20
29	s	602	CLA	C11-C12-C13-C14
29	g1	613	CLA	C16-C17-C18-C20
32	B	621	SQD	C10-C11-C12-C13
33	c1	521	LMG	C13-C14-C15-C16
40	s	624	LHG	C34-C35-C36-C37
32	A	412	SQD	C9-C10-C11-C12
37	C	519	DGD	C4B-C5B-C6B-C7B
38	B1	624	3PH	C2A-C2B-C2C-C2D
40	g1	624	LHG	C25-C26-C27-C28
47	i	101	4RF	C07-C08-C09-C10
55	y	626	PTY	C23-C24-C25-C26
29	C	503	CLA	C10-C11-C12-C13
29	g1	610	CLA	C8-C10-C11-C12
29	y1	612	CLA	C10-C11-C12-C13
32	B1	621	SQD	C11-C12-C13-C14
34	A1	414	SPH	C11-C10-C9-C8
38	T	101	3PH	C2D-C2E-C2F-C2G
40	l	101	LHG	C13-C14-C15-C16
40	n	624	LHG	C9-C10-C11-C12
40	c1	525	LHG	C14-C15-C16-C17
47	k1	101	4RF	C43-C44-C45-C46
29	Y	614	CLA	C4-C3-C5-C6
29	r1	609	CLA	C4-C3-C5-C6
43	d	405	PL9	C15-C14-C16-C17
48	y1	609	CHL	C4-C3-C5-C6
32	C	526	SQD	C13-C14-C15-C16
33	c	521	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
33	w1	201	LMG	C36-C37-C38-C39
34	A	414	SPH	C6-C7-C8-C9
38	t1	101	3PH	C22-C23-C24-C25
39	b	625	DGA	CA9-CAA-CBA-CCA
40	D1	408	LHG	C29-C30-C31-C32
40	D1	408	LHG	C34-C35-C36-C37
40	g1	624	LHG	C13-C14-C15-C16
47	i1	101	4RF	C09-C10-C11-C12
29	b	608	CLA	C15-C16-C17-C18
29	b	614	CLA	C8-C10-C11-C12
29	b	616	CLA	C8-C10-C11-C12
29	N1	604	CLA	C8-C10-C11-C12
29	R1	610	CLA	C10-C11-C12-C13
29	n1	604	CLA	C5-C6-C7-C8
29	r1	603	CLA	C8-C10-C11-C12
38	b1	624	3PH	C39-C3A-C3B-C3C
40	d1	410	LHG	C27-C28-C29-C30
47	K	101	4RF	C01-C02-C03-C04
47	K1	101	4RF	C49-C50-C51-C52
33	w	201	LMG	C28-C29-C30-C31
33	B1	622	LMG	C28-C29-C30-C31
47	K1	101	4RF	C13-C14-C15-C16
40	S	624	LHG	C8-C7-O7-C5
29	B	612	CLA	O1A-CGA-O2A-C1
29	Y	614	CLA	O1A-CGA-O2A-C1
29	c	503	CLA	O1A-CGA-O2A-C1
29	G1	603	CLA	O1A-CGA-O2A-C1
29	g1	603	CLA	O1A-CGA-O2A-C1
29	y1	610	CLA	O1A-CGA-O2A-C1
37	C1	518	DGD	O1A-C1A-O1G-C1G
33	D	411	LMG	C19-C20-C21-C22
38	t1	101	3PH	C37-C38-C39-C3A
38	s1	626	3PH	C2D-C2E-C2F-C2G
40	y	624	LHG	C26-C27-C28-C29
29	c1	507	CLA	C13-C15-C16-C17
48	S1	608	CHL	C5-C6-C7-C8
29	R	604	CLA	C2A-CAA-CBA-CGA
29	c	501	CLA	C2A-CAA-CBA-CGA
48	G	605	CHL	C2A-CAA-CBA-CGA
48	y	606	CHL	C2A-CAA-CBA-CGA
29	c	507	CLA	C16-C17-C18-C19
29	n	603	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
48	s	608	CHL	C11-C12-C13-C14
32	m	101	SQD	C44-C45-C46-O48
32	A1	412	SQD	O6-C44-C45-C46
32	C1	526	SQD	C44-C45-C46-O48
32	a1	412	SQD	C44-C45-C46-O48
32	b1	626	SQD	O6-C44-C45-C46
32	b1	626	SQD	C44-C45-C46-O48
33	a	413	LMG	C7-C8-C9-O8
33	c	523	LMG	C7-C8-C9-O8
33	A1	413	LMG	O1-C7-C8-C9
33	a1	413	LMG	O1-C7-C8-C9
33	c1	523	LMG	C7-C8-C9-O8
33	d1	411	LMG	O1-C7-C8-C9
37	b	623	DGD	O1G-C1G-C2G-C3G
37	c	520	DGD	O1G-C1G-C2G-C3G
37	c1	518	DGD	C2A-C3A-C4A-C5A
37	c1	520	DGD	O1G-C1G-C2G-C3G
38	S1	626	3PH	C35-C36-C37-C38
38	b1	624	3PH	C1-C2-C3-O31
39	c	524	DGA	OG1-CG1-CG2-CG3
39	C1	524	DGA	OG1-CG1-CG2-CG3
39	b1	625	DGA	OG1-CG1-CG2-CG3
40	C	525	LHG	C4-C5-C6-O8
40	L	101	LHG	C4-C5-C6-O8
40	Y	624	LHG	C4-C5-C6-O8
40	c	525	LHG	C4-C5-C6-O8
40	d	410	LHG	C4-C5-C6-O8
40	s	624	LHG	C4-C5-C6-O8
40	S1	624	LHG	C4-C5-C6-O8
40	g1	624	LHG	C4-C5-C6-O8
40	s1	624	LHG	C4-C5-C6-O8
41	c	527	LMK	C7-C8-C9-O8
41	C1	527	LMK	O1-C7-C8-C9
47	I	102	4RF	O18-C19-C20-C39
47	I	102	4RF	C19-C20-C39-O40
47	K	101	4RF	C19-C20-C39-O40
47	i	101	4RF	C12-C13-C14-C15
47	i	101	4RF	C19-C20-C39-O40
47	I1	102	4RF	O18-C19-C20-C39
47	i1	101	4RF	C19-C20-C39-O40
54	s1	625	LPX	C18-C19-C20-C21
55	Y	626	PTY	O4-C1-C6-C5

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Mol	Chain	Res	Type	Atoms
55	Y	627	PTY	O4-C1-C6-C5
55	y	626	PTY	O4-C1-C6-C5
55	y	627	PTY	O4-C1-C6-C5
29	n	603	CLA	C13-C15-C16-C17
29	n	613	CLA	C15-C16-C17-C18
29	B1	611	CLA	C15-C16-C17-C18
29	Y1	602	CLA	C13-C15-C16-C17
29	y1	612	CLA	C15-C16-C17-C18
32	A	412	SQD	C11-C10-C9-C8
38	t1	101	3PH	C38-C39-C3A-C3B
40	D	409	LHG	C28-C29-C30-C31
32	A1	412	SQD	C45-C44-O6-C1
33	W	201	LMG	C8-C7-O1-C1
33	w	201	LMG	C8-C7-O1-C1
33	W1	201	LMG	C8-C7-O1-C1
37	C	519	DGD	C2G-C3G-O3G-C1D
37	c	519	DGD	C5D-C6D-O5D-C1E
29	y1	611	CLA	O1D-CGD-O2D-CED
32	B	626	SQD	C35-C36-C37-C38
33	h1	102	LMG	C11-C12-C13-C14
34	y	625	SPH	C13-C14-C15-C16
37	c1	519	DGD	CDB-CEB-CFB-CGB
39	c1	524	DGA	CA8-CA9-CAA-CBA
40	L	101	LHG	C29-C30-C31-C32
40	L	101	LHG	C33-C34-C35-C36
40	d	408	LHG	C14-C15-C16-C17
40	g1	624	LHG	C35-C36-C37-C38
47	K	101	4RF	C29-C30-C31-C32
29	Y1	603	CLA	C13-C15-C16-C17
32	m	101	SQD	C24-C25-C26-C27
33	C	521	LMG	C19-C20-C21-C22
33	a	413	LMG	C15-C16-C17-C18
34	A1	414	SPH	C14-C15-C16-C17
38	b	624	3PH	C32-C33-C34-C35
38	s	626	3PH	C2B-C2C-C2D-C2E
39	B1	625	DGA	CB9-CAB-CBB-CCB
39	J1	101	DGA	CB5-CB6-CB7-CB8
40	L	101	LHG	C14-C15-C16-C17
40	l	101	LHG	C16-C17-C18-C19
40	n1	624	LHG	C28-C29-C30-C31
47	K	101	4RF	C09-C10-C11-C12
47	k1	101	4RF	C01-C02-C03-C04

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Mol	Chain	Res	Type	Atoms
53	r	626	ERG	C22-C23-C24-C28
33	c1	521	LMG	O7-C10-C11-C12
40	g1	624	LHG	O8-C23-C24-C25
48	N1	605	CHL	CAA-CBA-CGA-O2A
33	b1	622	LMG	C10-C11-C12-C13
40	G	624	LHG	C7-C8-C9-C10
32	c1	526	SQD	C19-C20-C21-C22
33	C	521	LMG	C32-C33-C34-C35
33	A1	413	LMG	C11-C12-C13-C14
38	B	624	3PH	C2F-C2G-C2H-C2I
38	b	624	3PH	C35-C36-C37-C38
38	t1	101	3PH	C2F-C2G-C2H-C2I
39	b	625	DGA	CA3-CA4-CA5-CA6
47	k	101	4RF	C33-C34-C35-C36
32	a	412	SQD	O5-C1-O6-C44
29	G	603	CLA	C8-C10-C11-C12
29	n1	602	CLA	C8-C10-C11-C12
33	a1	413	LMG	C29-C30-C31-C32
39	C1	524	DGA	CB4-CB5-CB6-CB7
40	D1	409	LHG	C19-C20-C21-C22
32	A	412	SQD	C24-C23-O48-C46
40	C	525	LHG	C24-C23-O8-C6
29	S	611	CLA	CBD-CGD-O2D-CED
33	d	411	LMG	O6-C5-C6-O5
37	b1	623	DGD	O6E-C5E-C6E-O5E
40	d	409	LHG	O1-C1-C2-O2
40	n	624	LHG	O1-C1-C2-O2
40	s	624	LHG	O1-C1-C2-O2
38	T	101	3PH	C2B-C2C-C2D-C2E
38	b1	624	3PH	C29-C2A-C2B-C2C
39	c	524	DGA	CA9-CAA-CBA-CCA
39	J1	101	DGA	CB7-CB8-CB9-CAB
40	L1	101	LHG	C35-C36-C37-C38
40	G1	624	LHG	C26-C27-C28-C29
29	c1	503	CLA	C13-C15-C16-C17
29	R	612	CLA	O1A-CGA-O2A-C1
29	b	605	CLA	O1A-CGA-O2A-C1
37	b	623	DGD	O6E-C5E-C6E-O5E
32	a1	412	SQD	C12-C13-C14-C15
37	C1	518	DGD	C2A-C3A-C4A-C5A
39	c1	524	DGA	CA2-CA3-CA4-CA5
40	D	408	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
40	N1	624	LHG	C35-C36-C37-C38
40	n1	624	LHG	O8-C23-C24-C25
33	c	523	LMG	C4-C5-C6-O5
33	a	413	LMG	C11-C10-O7-C8
40	y	624	LHG	C14-C15-C16-C17
40	S1	624	LHG	C15-C16-C17-C18
40	d1	408	LHG	C27-C28-C29-C30
47	K	101	4RF	C51-C52-C53-C54
29	C	505	CLA	C8-C10-C11-C12
29	b	611	CLA	C15-C16-C17-C18
33	C1	521	LMG	O6-C5-C6-O5
50	g1	622	XAT	C40-C33-C34-C35
51	N1	623	NEX	C39-C29-C30-C31
51	Y1	623	NEX	C11-C10-C9-C19
37	b1	623	DGD	O6D-C5D-C6D-O5D
29	y	613	CLA	C4-C3-C5-C6
30	a1	408	PHO	C4-C3-C5-C6
48	Y	609	CHL	C4-C3-C5-C6
48	S	606	CHL	C2A-CAA-CBA-CGA
32	a	412	SQD	C12-C13-C14-C15
33	C	523	LMG	C42-C43-C44-C45
33	w	201	LMG	C29-C30-C31-C32
37	C	520	DGD	CDB-CEB-CFB-CGB
47	K	101	4RF	C45-C46-C47-C48
55	y1	626	PTY	C22-C23-C24-C25
29	y	613	CLA	C2-C3-C5-C6
32	c	526	SQD	C23-C24-C25-C26
33	C	521	LMG	C28-C29-C30-C31
29	C	513	CLA	C16-C17-C18-C20
29	A1	410	CLA	C11-C12-C13-C15
29	N1	602	CLA	C16-C17-C18-C19
29	R	612	CLA	CBA-CGA-O2A-C1
29	c	510	CLA	CBA-CGA-O2A-C1
29	n1	610	CLA	CBA-CGA-O2A-C1
29	r1	610	CLA	CBA-CGA-O2A-C1
37	C	518	DGD	C2A-C1A-O1G-C1G
37	c1	519	DGD	C2A-C1A-O1G-C1G
39	C	524	DGA	CA2-CA1-OG1-CG1
32	B1	621	SQD	C14-C15-C16-C17
39	B1	625	DGA	CBA-CCA-CDA-CEA
40	L	101	LHG	C25-C26-C27-C28
40	n	624	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
40	D1	410	LHG	C11-C10-C9-C8
47	i	101	4RF	C30-C31-C32-C33
29	B	603	CLA	C13-C15-C16-C17
29	c	505	CLA	C5-C6-C7-C8
29	n	613	CLA	C8-C10-C11-C12
29	b1	604	CLA	C13-C15-C16-C17
29	s1	604	CLA	C5-C6-C7-C8
37	c1	518	DGD	C3A-C4A-C5A-C6A
37	c1	518	DGD	CCB-CDB-CEB-CFB
40	g	624	LHG	C28-C29-C30-C31
47	K	101	4RF	C44-C45-C46-C47
32	b	621	SQD	C46-C45-O47-C7
32	B1	621	SQD	C46-C45-O47-C7
32	M1	101	SQD	C46-C45-O47-C7
33	W1	201	LMG	C7-C8-O7-C10
38	s	626	3PH	C1-C2-O21-C21
38	T1	101	3PH	C3-C2-O21-C21
38	s1	626	3PH	C1-C2-O21-C21
29	N	611	CLA	C2A-CAA-CBA-CGA
29	b	605	CLA	C2A-CAA-CBA-CGA
29	r	609	CLA	C2A-CAA-CBA-CGA
29	c1	502	CLA	C2A-CAA-CBA-CGA
48	r1	607	CHL	C2A-CAA-CBA-CGA
29	B	616	CLA	C13-C15-C16-C17
29	C1	513	CLA	C10-C11-C12-C13
29	D1	402	CLA	C15-C16-C17-C18
29	R1	602	CLA	C8-C10-C11-C12
48	g	601	CHL	C5-C6-C7-C8
29	R	604	CLA	C2-C1-O2A-CGA
29	Y	604	CLA	C2-C1-O2A-CGA
29	b	616	CLA	C2-C1-O2A-CGA
29	r	603	CLA	C2-C1-O2A-CGA
29	s	609	CLA	C2-C1-O2A-CGA
29	B1	602	CLA	C2-C1-O2A-CGA
29	B1	603	CLA	C2-C1-O2A-CGA
29	B1	608	CLA	C2-C1-O2A-CGA
29	D1	403	CLA	C2-C1-O2A-CGA
29	R1	610	CLA	C2-C1-O2A-CGA
29	c1	503	CLA	C2-C1-O2A-CGA
29	r1	612	CLA	C2-C1-O2A-CGA
48	G	606	CHL	C2-C1-O2A-CGA
40	l	101	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
47	K1	101	4RF	C09-C10-C11-C12
40	l	101	LHG	C7-C8-C9-C10
29	b1	616	CLA	CBD-CGD-O2D-CED
29	a	405	CLA	C3-C5-C6-C7
34	y	625	SPH	C15-C16-C17-C18
38	T	101	3PH	C3A-C3B-C3C-C3D
39	c	524	DGA	CBB-CAB-CB9-CB8
40	d1	410	LHG	C32-C33-C34-C35
47	k1	101	4RF	C26-C27-C28-C29
55	y	626	PTY	C41-C42-C43-C44
29	A	407	CLA	O1D-CGD-O2D-CED
29	y	602	CLA	C15-C16-C17-C18
38	t	101	3PH	C1-O11-P-O12
38	s1	626	3PH	C1-O11-P-O12
40	C	525	LHG	C2-C3-O3-P
32	A	412	SQD	C16-C17-C18-C19
32	c	526	SQD	C14-C15-C16-C17
32	c	526	SQD	C17-C18-C19-C20
33	b	622	LMG	C11-C12-C13-C14
33	c	521	LMG	C29-C30-C31-C32
33	H1	102	LMG	C19-C20-C21-C22
38	T1	101	3PH	C24-C25-C26-C27
38	t1	101	3PH	C2D-C2E-C2F-C2G
40	n	624	LHG	C28-C29-C30-C31
47	i1	101	4RF	C02-C03-C04-C05
55	Y	626	PTY	C21-C22-C23-C24
30	A	409	PHO	CBA-CGA-O2A-C1
47	i	101	4RF	C43-C41-O40-C39
37	c	518	DGD	O1A-C1A-O1G-C1G
38	t	101	3PH	O11-C1-C2-O21
29	b1	608	CLA	C16-C17-C18-C19
29	c1	505	CLA	C16-C17-C18-C20
34	a	414	SPH	C14-C15-C16-C17
34	A1	414	SPH	C9-C10-C11-C12
40	L1	101	LHG	C19-C20-C21-C22
40	S1	624	LHG	C13-C14-C15-C16
47	i1	101	4RF	C33-C34-C35-C36
29	R	610	CLA	C8-C10-C11-C12
47	K	101	4RF	C12-C13-C14-C15
47	K	101	4RF	C35-C36-C37-C38
29	r1	610	CLA	O1A-CGA-O2A-C1
55	Y	626	PTY	O30-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
33	A1	413	LMG	C39-C40-C41-C42
39	c	524	DGA	CFA-CGA-CHA-CIA
34	A	414	SPH	C5-C6-C7-C8
29	B1	616	CLA	C13-C15-C16-C17
29	N1	610	CLA	C15-C16-C17-C18
31	A	411	BCR	C11-C10-C9-C8
32	b	621	SQD	C2-C1-O6-C44
33	A1	413	LMG	C2-C1-O1-C7
37	C	518	DGD	C2E-C1E-O5D-C6D
37	c1	519	DGD	C2E-C1E-O5D-C6D
50	g1	622	XAT	C32-C33-C34-C35
33	d	411	LMG	C33-C34-C35-C36
40	n1	624	LHG	C35-C36-C37-C38
55	y1	626	PTY	C41-C42-C43-C44
38	T1	101	3PH	O21-C2-C3-O31
40	Y	624	LHG	O7-C5-C6-O8
40	g	624	LHG	O7-C5-C6-O8
55	Y	626	PTY	O4-C1-C6-O7
32	B1	626	SQD	C35-C36-C37-C38
33	D	411	LMG	C32-C33-C34-C35
33	d1	411	LMG	C33-C34-C35-C36
38	T1	101	3PH	C25-C26-C27-C28
39	c1	524	DGA	CCA-CDA-CEA-CFA
40	G	624	LHG	C17-C18-C19-C20
47	i1	101	4RF	C32-C33-C34-C35
38	B	624	3PH	O22-C21-O21-C2
39	c	524	DGA	OB1-CB1-OG2-CG2
47	K	101	4RF	O23-C22-O21-C20
29	C	506	CLA	C10-C11-C12-C13
29	b1	602	CLA	C5-C6-C7-C8
29	g1	602	CLA	C8-C10-C11-C12
29	G1	610	CLA	O1A-CGA-O2A-C1
37	C	518	DGD	O1A-C1A-O1G-C1G
29	Y	610	CLA	C16-C17-C18-C19
29	D1	402	CLA	C16-C17-C18-C20
30	a	409	PHO	CHA-CBD-CGD-O1D
30	a	409	PHO	CHA-CBD-CGD-O2D
30	A1	408	PHO	CHA-CBD-CGD-O1D
30	A1	408	PHO	CHA-CBD-CGD-O2D
30	A1	409	PHO	CHA-CBD-CGD-O1D
30	A1	409	PHO	CHA-CBD-CGD-O2D
30	a1	409	PHO	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	a1	409	PHO	CHA-CBD-CGD-O2D
32	b1	626	SQD	C17-C18-C19-C20
33	A	413	LMG	C15-C16-C17-C18
33	w1	201	LMG	C11-C12-C13-C14
37	c1	519	DGD	C4B-C5B-C6B-C7B
38	t	101	3PH	C2B-C2C-C2D-C2E
38	T1	101	3PH	C2B-C2C-C2D-C2E
40	G1	624	LHG	C33-C34-C35-C36
40	c1	525	LHG	C25-C26-C27-C28
47	K1	101	4RF	C05-C06-C07-C08
47	k1	101	4RF	C34-C35-C36-C37
54	s1	625	LPX	C9-C10-C11-C12
29	C	510	CLA	C4-C3-C5-C6
29	N	603	CLA	C4-C3-C5-C6
29	S	610	CLA	C4-C3-C5-C6
29	b	602	CLA	C4-C3-C5-C6
29	y	603	CLA	C4-C3-C5-C6
43	D1	405	PL9	C30-C29-C31-C32
48	N	609	CHL	C4-C3-C5-C6
48	Y1	609	CHL	C4-C3-C5-C6
33	c	521	LMG	C13-C14-C15-C16
40	L1	101	LHG	C13-C14-C15-C16
29	B	603	CLA	C11-C10-C8-C7
29	B	604	CLA	C12-C13-C15-C16
29	B	605	CLA	C6-C7-C8-C10
29	B	605	CLA	C12-C13-C15-C16
29	B	613	CLA	C11-C10-C8-C7
29	B	616	CLA	C11-C12-C13-C15
29	C	504	CLA	C12-C13-C15-C16
29	C	507	CLA	C12-C13-C15-C16
29	C	512	CLA	C11-C10-C8-C7
29	C	513	CLA	C11-C12-C13-C15
29	N	603	CLA	C12-C13-C15-C16
29	N	604	CLA	C11-C10-C8-C7
29	N	604	CLA	C11-C12-C13-C15
29	G	602	CLA	C6-C7-C8-C10
29	G	610	CLA	C11-C12-C13-C15
29	G	611	CLA	C6-C7-C8-C10
29	G	613	CLA	C6-C7-C8-C10
29	R	610	CLA	C6-C7-C8-C10
29	R	610	CLA	C11-C10-C8-C7
29	S	609	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
29	S	610	CLA	C2-C3-C5-C6
29	Y	604	CLA	C11-C10-C8-C7
29	Y	612	CLA	C6-C7-C8-C10
29	Y	613	CLA	C11-C12-C13-C15
29	a	410	CLA	C11-C10-C8-C7
29	b	603	CLA	C6-C7-C8-C10
29	b	603	CLA	C12-C13-C15-C16
29	b	613	CLA	C6-C7-C8-C10
29	b	615	CLA	C6-C7-C8-C10
29	b	616	CLA	C11-C10-C8-C7
29	c	502	CLA	C11-C12-C13-C15
29	c	503	CLA	C11-C12-C13-C15
29	c	505	CLA	C12-C13-C15-C16
29	c	509	CLA	C12-C13-C15-C16
29	c	511	CLA	C11-C12-C13-C15
29	c	512	CLA	C6-C7-C8-C10
29	c	513	CLA	C11-C12-C13-C15
29	n	603	CLA	C6-C7-C8-C10
29	n	610	CLA	C11-C12-C13-C15
29	g	602	CLA	C6-C7-C8-C10
29	g	602	CLA	C12-C13-C15-C16
29	g	603	CLA	C12-C13-C15-C16
29	g	610	CLA	C11-C10-C8-C7
29	g	610	CLA	C12-C13-C15-C16
29	r	608	CLA	C6-C7-C8-C10
29	s	609	CLA	C11-C10-C8-C7
29	y	610	CLA	C11-C12-C13-C15
29	y	611	CLA	C11-C10-C8-C7
29	y	611	CLA	C12-C13-C15-C16
29	y	613	CLA	C11-C12-C13-C15
29	B1	605	CLA	C11-C12-C13-C15
29	B1	607	CLA	C6-C7-C8-C10
29	B1	607	CLA	C11-C10-C8-C7
29	B1	613	CLA	C12-C13-C15-C16
29	B1	617	CLA	C12-C13-C15-C16
29	C1	502	CLA	C11-C12-C13-C15
29	C1	504	CLA	C11-C10-C8-C7
29	C1	506	CLA	C11-C10-C8-C7
29	C1	508	CLA	C11-C10-C8-C7
29	C1	509	CLA	C12-C13-C15-C16
29	C1	511	CLA	C6-C7-C8-C10
29	C1	512	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	D1	402	CLA	C11-C12-C13-C15
29	D1	403	CLA	C11-C12-C13-C15
29	N1	610	CLA	C6-C7-C8-C10
29	G1	602	CLA	C6-C7-C8-C10
29	G1	610	CLA	C11-C10-C8-C7
29	R1	603	CLA	C11-C10-C8-C7
29	R1	610	CLA	C11-C10-C8-C7
29	S1	602	CLA	C11-C10-C8-C7
29	S1	609	CLA	C11-C10-C8-C7
29	S1	610	CLA	C11-C10-C8-C7
29	Y1	602	CLA	C6-C7-C8-C10
29	Y1	602	CLA	C11-C12-C13-C15
29	Y1	612	CLA	C12-C13-C15-C16
29	Y1	614	CLA	C6-C7-C8-C10
29	Y1	614	CLA	C11-C10-C8-C7
29	b1	602	CLA	C11-C10-C8-C7
29	b1	602	CLA	C12-C13-C15-C16
29	b1	613	CLA	C6-C7-C8-C10
29	b1	613	CLA	C12-C13-C15-C16
29	c1	504	CLA	C11-C10-C8-C7
29	c1	513	CLA	C12-C13-C15-C16
29	n1	602	CLA	C11-C10-C8-C7
29	n1	603	CLA	C12-C13-C15-C16
29	n1	610	CLA	C6-C7-C8-C10
29	g1	602	CLA	C6-C7-C8-C10
29	g1	610	CLA	C6-C7-C8-C10
29	g1	610	CLA	C11-C10-C8-C7
29	g1	611	CLA	C6-C7-C8-C10
29	g1	613	CLA	C12-C13-C15-C16
29	r1	603	CLA	C11-C10-C8-C7
29	r1	608	CLA	C6-C7-C8-C10
29	r1	609	CLA	C11-C10-C8-C7
29	s1	609	CLA	C11-C10-C8-C7
29	s1	610	CLA	C6-C7-C8-C10
29	s1	610	CLA	C11-C12-C13-C15
29	y1	603	CLA	C11-C12-C13-C15
29	y1	611	CLA	C11-C12-C13-C15
29	y1	613	CLA	C11-C10-C8-C7
29	y1	614	CLA	C11-C10-C8-C7
43	d1	405	PL9	C38-C39-C41-C42
48	N	606	CHL	C11-C10-C8-C7
48	N	607	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
48	G	601	CHL	C6-C7-C8-C10
48	G	607	CHL	C6-C7-C8-C10
48	Y	607	CHL	C6-C7-C8-C10
48	Y	609	CHL	C2-C3-C5-C6
48	n	606	CHL	C11-C10-C8-C7
48	g	601	CHL	C12-C13-C15-C16
48	y	609	CHL	C11-C12-C13-C15
48	N1	601	CHL	C12-C13-C15-C16
48	N1	607	CHL	C11-C10-C8-C7
48	G1	601	CHL	C11-C12-C13-C15
48	G1	607	CHL	C11-C10-C8-C7
48	Y1	606	CHL	C6-C7-C8-C10
48	Y1	609	CHL	C11-C12-C13-C15
48	n1	606	CHL	C11-C10-C8-C7
48	n1	607	CHL	C11-C12-C13-C15
48	s1	608	CHL	C11-C10-C8-C7
48	y1	607	CHL	C11-C10-C8-C7
33	H	102	LMG	O7-C10-C11-C12
29	C	508	CLA	C3-C5-C6-C7
29	n1	613	CLA	C3-C5-C6-C7
48	Y1	601	CHL	C3-C5-C6-C7
32	M1	101	SQD	C26-C27-C28-C29
32	m1	101	SQD	C11-C10-C9-C8
33	W	201	LMG	C31-C32-C33-C34
37	C	519	DGD	C3B-C4B-C5B-C6B
40	D	410	LHG	C27-C28-C29-C30
29	B	603	CLA	C11-C10-C8-C9
29	C	504	CLA	C14-C13-C15-C16
29	C	507	CLA	C14-C13-C15-C16
29	C	510	CLA	C14-C13-C15-C16
29	C	513	CLA	C11-C12-C13-C14
29	C	513	CLA	C14-C13-C15-C16
29	D	403	CLA	C11-C10-C8-C9
29	N	603	CLA	C14-C13-C15-C16
29	N	604	CLA	C11-C10-C8-C9
29	G	602	CLA	C6-C7-C8-C9
29	S	610	CLA	C11-C10-C8-C9
29	Y	602	CLA	C11-C12-C13-C14
29	Y	613	CLA	C11-C12-C13-C14
29	Y	613	CLA	C14-C13-C15-C16
29	a	410	CLA	C11-C10-C8-C9
29	b	603	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	b	614	CLA	C14-C13-C15-C16
29	b	615	CLA	C11-C10-C8-C9
29	c	502	CLA	C11-C12-C13-C14
29	c	505	CLA	C14-C13-C15-C16
29	c	507	CLA	C6-C7-C8-C9
29	c	512	CLA	C6-C7-C8-C9
29	d	402	CLA	C6-C7-C8-C9
29	d	402	CLA	C11-C12-C13-C14
29	n	610	CLA	C11-C12-C13-C14
29	g	602	CLA	C6-C7-C8-C9
29	g	602	CLA	C14-C13-C15-C16
29	g	603	CLA	C6-C7-C8-C9
29	g	603	CLA	C14-C13-C15-C16
29	y	611	CLA	C14-C13-C15-C16
29	y	612	CLA	C11-C10-C8-C9
29	B1	602	CLA	C11-C10-C8-C9
29	B1	607	CLA	C11-C10-C8-C9
29	B1	609	CLA	C11-C12-C13-C14
29	B1	612	CLA	C11-C12-C13-C14
29	B1	613	CLA	C14-C13-C15-C16
29	B1	615	CLA	C6-C7-C8-C9
29	B1	617	CLA	C6-C7-C8-C9
29	C1	504	CLA	C11-C10-C8-C9
29	C1	508	CLA	C11-C10-C8-C9
29	C1	509	CLA	C14-C13-C15-C16
29	D1	402	CLA	C11-C12-C13-C14
29	D1	403	CLA	C11-C12-C13-C14
29	N1	610	CLA	C11-C12-C13-C14
29	G1	603	CLA	C6-C7-C8-C9
29	G1	603	CLA	C14-C13-C15-C16
29	Y1	602	CLA	C11-C10-C8-C9
29	Y1	602	CLA	C11-C12-C13-C14
29	Y1	611	CLA	C11-C10-C8-C9
29	Y1	613	CLA	C11-C12-C13-C14
29	Y1	614	CLA	C11-C10-C8-C9
29	b1	602	CLA	C11-C10-C8-C9
29	b1	613	CLA	C14-C13-C15-C16
29	c1	504	CLA	C11-C10-C8-C9
29	n1	610	CLA	C6-C7-C8-C9
29	g1	610	CLA	C6-C7-C8-C9
29	g1	610	CLA	C14-C13-C15-C16
29	g1	611	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	g1	613	CLA	C14-C13-C15-C16
29	s1	610	CLA	C6-C7-C8-C9
29	s1	610	CLA	C11-C12-C13-C14
48	N	606	CHL	C11-C10-C8-C9
48	N	606	CHL	C14-C13-C15-C16
48	n	605	CHL	C11-C10-C8-C9
48	n	606	CHL	C11-C10-C8-C9
48	y	606	CHL	C6-C7-C8-C9
48	N1	606	CHL	C11-C10-C8-C9
48	G1	601	CHL	C11-C12-C13-C14
48	n1	606	CHL	C11-C10-C8-C9
48	n1	607	CHL	C11-C12-C13-C14
48	g1	607	CHL	C11-C10-C8-C9
51	G	623	NEX	C9-C10-C11-C12
37	b	623	DGD	C1B-C2B-C3B-C4B
32	c	526	SQD	C19-C20-C21-C22
32	a1	412	SQD	C25-C26-C27-C28
37	c1	519	DGD	C3B-C4B-C5B-C6B
29	G	610	CLA	CBA-CGA-O2A-C1
29	Y	602	CLA	CBA-CGA-O2A-C1
29	b	604	CLA	CBA-CGA-O2A-C1
29	r	612	CLA	CBA-CGA-O2A-C1
29	b1	610	CLA	CBA-CGA-O2A-C1
33	w	201	LMG	C29-C28-O8-C9
39	B1	625	DGA	CA2-CA1-OG1-CG1
40	d1	410	LHG	C24-C23-O8-C6
29	a	406	CLA	C10-C11-C12-C13
29	b	616	CLA	C10-C11-C12-C13
29	g	613	CLA	C10-C11-C12-C13
29	y1	610	CLA	C15-C16-C17-C18
29	b	607	CLA	C2A-CAA-CBA-CGA
29	C	508	CLA	C2C-C3C-CAC-CBC
33	h	102	LMG	C33-C34-C35-C36
37	c1	518	DGD	CDB-CEB-CFB-CGB
38	t	101	3PH	C27-C28-C29-C2A
38	S1	626	3PH	C32-C33-C34-C35
54	S1	625	LPX	C18-C19-C20-C21
37	C	518	DGD	C4D-C5D-C6D-O5D
31	C	517	BCR	C7-C8-C9-C34
31	b	618	BCR	C36-C18-C19-C20
31	c	516	BCR	C37-C22-C23-C24
45	H	101	RRX	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
45	h1	101	RRX	C37-C22-C23-C24
50	g	622	XAT	C11-C12-C13-C20
50	g1	622	XAT	C27-C28-C29-C39
50	g1	622	XAT	C31-C32-C33-C40
29	s	609	CLA	C5-C6-C7-C8
29	D	402	CLA	C16-C17-C18-C19
29	Y	613	CLA	C16-C17-C18-C19
29	A1	410	CLA	C11-C12-C13-C14
29	S1	610	CLA	C16-C17-C18-C19
29	n1	603	CLA	C16-C17-C18-C20
29	r1	612	CLA	C11-C12-C13-C15
32	C	526	SQD	C14-C15-C16-C17
33	C1	523	LMG	C42-C43-C44-C45
38	s	626	3PH	C25-C26-C27-C28
38	s	626	3PH	C27-C28-C29-C2A
40	g	624	LHG	C16-C17-C18-C19
40	d1	409	LHG	C28-C29-C30-C31
47	I1	102	4RF	C26-C27-C28-C29
31	c	514	BCR	C17-C18-C19-C20
31	c	516	BCR	C21-C22-C23-C24
31	c	517	BCR	C21-C22-C23-C24
36	b	620	C7Z	C11-C12-C13-C14
49	n1	620	LUT	C27-C28-C29-C30
50	n	622	XAT	C11-C12-C13-C14
50	r	621	XAT	C27-C28-C29-C30
50	n1	622	XAT	C27-C28-C29-C30
33	W	201	LMG	C32-C33-C34-C35
39	c1	524	DGA	CFA-CGA-CHA-CIA
40	D1	409	LHG	C35-C36-C37-C38
48	N	606	CHL	C3-C5-C6-C7
48	G1	607	CHL	C3-C5-C6-C7
29	b	609	CLA	C15-C16-C17-C18
29	c	510	CLA	C15-C16-C17-C18
29	g	610	CLA	C8-C10-C11-C12
29	s1	611	CLA	C5-C6-C7-C8
33	c1	523	LMG	C11-C10-O7-C8
33	H	102	LMG	C34-C35-C36-C37
33	d	411	LMG	C15-C16-C17-C18
33	B1	622	LMG	C33-C34-C35-C36
39	j1	101	DGA	CA5-CA6-CA7-CA8
40	c	525	LHG	C17-C18-C19-C20
54	s	625	LPX	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
32	A	412	SQD	O10-C23-O48-C46
47	I	102	4RF	O42-C41-O40-C39
29	S	614	CLA	CBA-CGA-O2A-C1
29	c	501	CLA	CBA-CGA-O2A-C1
32	C1	526	SQD	C9-C10-C11-C12
33	A	413	LMG	C14-C15-C16-C17
34	Y1	625	SPH	C6-C7-C8-C9
40	D1	408	LHG	C10-C11-C12-C13
47	I	102	4RF	C06-C07-C08-C09
29	N	610	CLA	C8-C10-C11-C12
29	g	602	CLA	C15-C16-C17-C18
29	S1	602	CLA	C10-C11-C12-C13
29	Y1	613	CLA	C13-C15-C16-C17
29	a1	405	CLA	C10-C11-C12-C13
29	d1	403	CLA	C13-C15-C16-C17
29	g1	602	CLA	C15-C16-C17-C18
48	S	608	CHL	C10-C11-C12-C13
32	C	526	SQD	C9-C10-C11-C12
32	a1	412	SQD	C28-C29-C30-C31
33	H1	102	LMG	C13-C14-C15-C16
38	T1	101	3PH	C22-C23-C24-C25
40	g	624	LHG	C9-C10-C11-C12
47	I	102	4RF	C24-C25-C26-C27
52	r	625	LMT	C5-C6-C7-C8
37	B	623	DGD	O6D-C5D-C6D-O5D
29	C1	506	CLA	CBD-CGD-O2D-CED
32	c1	526	SQD	C27-C28-C29-C30
29	B	603	CLA	C4B-C3B-CAB-CBB
29	B	617	CLA	C4B-C3B-CAB-CBB
29	C	513	CLA	C4B-C3B-CAB-CBB
29	N	611	CLA	C4B-C3B-CAB-CBB
29	Y	608	CLA	C4B-C3B-CAB-CBB
29	b	602	CLA	C4B-C3B-CAB-CBB
29	b	604	CLA	C4B-C3B-CAB-CBB
29	b	607	CLA	C4B-C3B-CAB-CBB
29	b	613	CLA	C4B-C3B-CAB-CBB
29	n	611	CLA	C4B-C3B-CAB-CBB
29	g	604	CLA	C4B-C3B-CAB-CBB
29	g	613	CLA	C4B-C3B-CAB-CBB
29	r	604	CLA	C4B-C3B-CAB-CBB
29	r	610	CLA	C4B-C3B-CAB-CBB
29	s	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	B1	613	CLA	C4B-C3B-CAB-CBB
29	B1	617	CLA	C4B-C3B-CAB-CBB
29	C1	502	CLA	C4B-C3B-CAB-CBB
29	C1	507	CLA	C4B-C3B-CAB-CBB
29	G1	602	CLA	C4B-C3B-CAB-CBB
29	G1	610	CLA	C4B-C3B-CAB-CBB
29	R1	610	CLA	C4B-C3B-CAB-CBB
29	S1	605	CLA	C4B-C3B-CAB-CBB
29	b1	604	CLA	C4B-C3B-CAB-CBB
29	n1	614	CLA	C4B-C3B-CAB-CBB
29	r1	602	CLA	C4B-C3B-CAB-CBB
29	r1	610	CLA	C4B-C3B-CAB-CBB
29	s1	610	CLA	C4B-C3B-CAB-CBB
29	s1	612	CLA	C4B-C3B-CAB-CBB
29	s1	613	CLA	C4B-C3B-CAB-CBB
29	y1	608	CLA	C4B-C3B-CAB-CBB
29	y1	613	CLA	C4B-C3B-CAB-CBB
29	S	611	CLA	C16-C17-C18-C20
29	n	604	CLA	C16-C17-C18-C20
29	A1	405	CLA	C16-C17-C18-C19
29	Y	611	CLA	C15-C16-C17-C18
29	c	504	CLA	C15-C16-C17-C18
29	C1	503	CLA	C5-C6-C7-C8
40	D	410	LHG	O6-C4-C5-C6
40	N	624	LHG	O6-C4-C5-C6
40	N1	624	LHG	O6-C4-C5-C6
40	G1	624	LHG	O6-C4-C5-C6
40	d1	409	LHG	O6-C4-C5-C6
55	y1	627	PTY	O14-C5-C6-C1
29	N	602	CLA	C3-C5-C6-C7
29	R	609	CLA	C3-C5-C6-C7
29	b1	608	CLA	C3-C5-C6-C7
40	d	409	LHG	C13-C14-C15-C16
47	K	101	4RF	C26-C27-C28-C29
32	b1	626	SQD	C7-C8-C9-C10
40	N1	624	LHG	C23-C24-C25-C26
55	y1	627	PTY	N1-C2-C3-O11
39	B1	625	DGA	CA9-CAA-CBA-CCA
54	s1	625	LPX	C13-C14-C15-C16
32	b	621	SQD	C24-C23-O48-C46
37	c1	519	DGD	O1A-C1A-O1G-C1G
29	S	603	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	y	602	CLA	C5-C6-C7-C8
29	B1	615	CLA	C5-C6-C7-C8
29	N1	603	CLA	C13-C15-C16-C17
29	b1	605	CLA	C13-C15-C16-C17
53	R	626	ERG	C16-C17-C20-C22
29	B	609	CLA	O1D-CGD-O2D-CED
47	i	101	4RF	C11-C12-C13-C14
47	i	101	4RF	C35-C36-C37-C38
29	B	610	CLA	C4-C3-C5-C6
29	B	615	CLA	C4-C3-C5-C6
29	s	602	CLA	C4-C3-C5-C6
43	D	405	PL9	C45-C44-C46-C47
48	y	609	CHL	C4-C3-C5-C6
37	c1	519	DGD	C4E-C5E-C6E-O5E
29	C	510	CLA	C2-C3-C5-C6
29	N	603	CLA	C2-C3-C5-C6
29	b	602	CLA	C2-C3-C5-C6
29	y	603	CLA	C2-C3-C5-C6
43	D	405	PL9	C38-C39-C41-C42
43	d	405	PL9	C38-C39-C41-C42
48	N	609	CHL	C2-C3-C5-C6
48	Y1	609	CHL	C2-C3-C5-C6
32	c	526	SQD	C13-C14-C15-C16
32	c1	526	SQD	C32-C33-C34-C35
33	D1	411	LMG	C22-C23-C24-C25
37	c	518	DGD	C4A-C5A-C6A-C7A
40	c1	525	LHG	C30-C31-C32-C33
29	b1	615	CLA	O1D-CGD-O2D-CED
29	g	603	CLA	C13-C15-C16-C17
29	y	603	CLA	C15-C16-C17-C18
33	a	413	LMG	O9-C10-O7-C8
29	n1	610	CLA	O1A-CGA-O2A-C1
47	K1	101	4RF	C44-C45-C46-C47
29	Y1	610	CLA	O1D-CGD-O2D-CED
29	c	507	CLA	C16-C17-C18-C20
29	b1	612	CLA	C16-C17-C18-C19
38	T1	101	3PH	C34-C35-C36-C37
38	b1	624	3PH	C33-C34-C35-C36
47	i	101	4RF	C09-C10-C11-C12
29	C	504	CLA	C8-C10-C11-C12
29	y1	612	CLA	C5-C6-C7-C8
29	g1	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
47	K	101	4RF	C43-C41-O40-C39
54	S	625	LPX	C7-C6-O6-C5
29	b	602	CLA	CAA-CBA-CGA-O2A
29	b1	602	CLA	CAA-CBA-CGA-O2A
40	G	624	LHG	O8-C23-C24-C25
32	b	626	SQD	C23-C24-C25-C26
38	t	101	3PH	C38-C39-C3A-C3B
38	s1	626	3PH	C2A-C2B-C2C-C2D
40	L	101	LHG	C13-C14-C15-C16
40	N	624	LHG	C35-C36-C37-C38
41	c1	527	LMK	C29-C30-C31-C32
47	i1	101	4RF	C05-C06-C07-C08
40	C1	525	LHG	C2-C3-O3-P
40	L1	101	LHG	C2-C3-O3-P
29	c	510	CLA	O1A-CGA-O2A-C1
40	c	525	LHG	O10-C23-O8-C6
29	N	613	CLA	C3A-C2A-CAA-CBA
29	b	609	CLA	C3A-C2A-CAA-CBA
29	b	610	CLA	C3A-C2A-CAA-CBA
29	r	612	CLA	C3A-C2A-CAA-CBA
29	B1	609	CLA	C3A-C2A-CAA-CBA
29	B1	616	CLA	C3A-C2A-CAA-CBA
29	N1	613	CLA	C3A-C2A-CAA-CBA
29	G1	612	CLA	C3A-C2A-CAA-CBA
29	S1	603	CLA	C3A-C2A-CAA-CBA
29	a1	405	CLA	C3A-C2A-CAA-CBA
29	b1	615	CLA	C3A-C2A-CAA-CBA
29	r1	612	CLA	C3A-C2A-CAA-CBA
48	Y	601	CHL	C3A-C2A-CAA-CBA
48	n	609	CHL	C3A-C2A-CAA-CBA
48	n1	601	CHL	C3A-C2A-CAA-CBA
48	g1	605	CHL	C3A-C2A-CAA-CBA
33	h1	102	LMG	C39-C40-C41-C42
37	C	520	DGD	CCB-CDB-CEB-CFB
40	y	624	LHG	C31-C32-C33-C34
40	c1	525	LHG	C24-C25-C26-C27
40	y1	624	LHG	C35-C36-C37-C38
31	A1	411	BCR	C9-C10-C11-C12
49	G	620	LUT	C29-C30-C31-C32
49	S1	620	LUT	C29-C30-C31-C32
49	g1	621	LUT	C9-C10-C11-C12
33	b1	622	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
37	c1	520	DGD	CCB-CDB-CEB-CFB
38	B	624	3PH	C26-C27-C28-C29
38	s	626	3PH	C22-C23-C24-C25
39	B1	625	DGA	CB6-CB7-CB8-CB9
40	D	409	LHG	C35-C36-C37-C38
40	d1	409	LHG	C19-C20-C21-C22
47	I	102	4RF	C07-C08-C09-C10
29	C	508	CLA	C13-C15-C16-C17
29	C1	509	CLA	C15-C16-C17-C18
29	b1	608	CLA	C8-C10-C11-C12
29	y1	604	CLA	C8-C10-C11-C12
48	G1	607	CHL	C5-C6-C7-C8
38	B	624	3PH	C39-C3A-C3B-C3C
39	B	625	DGA	CA2-CA3-CA4-CA5
39	j	101	DGA	CA5-CA6-CA7-CA8
39	B1	625	DGA	CA7-CA8-CA9-CAA
39	c1	524	DGA	CAB-CBB-CCB-CDB
40	Y	624	LHG	C35-C36-C37-C38
29	B1	610	CLA	C16-C17-C18-C19
29	C	510	CLA	CBA-CGA-O2A-C1
32	b1	626	SQD	C24-C23-O48-C46
39	b1	625	DGA	CA4-CA5-CA6-CA7
40	S	624	LHG	C29-C30-C31-C32
47	k1	101	4RF	C02-C03-C04-C05
29	B	606	CLA	C5-C6-C7-C8
29	a	406	CLA	C15-C16-C17-C18
29	b	615	CLA	C8-C10-C11-C12
29	y	603	CLA	C8-C10-C11-C12
32	B	626	SQD	O6-C44-C45-C46
32	M	101	SQD	C44-C45-C46-O48
32	a	412	SQD	O6-C44-C45-C46
32	a	412	SQD	C44-C45-C46-O48
33	A	413	LMG	O1-C7-C8-C9
33	B	622	LMG	C7-C8-C9-O8
33	a	413	LMG	O1-C7-C8-C9
33	b	622	LMG	C7-C8-C9-O8
33	w	201	LMG	O1-C7-C8-C9
33	B1	622	LMG	C7-C8-C9-O8
33	a1	413	LMG	C7-C8-C9-O8
37	B1	623	DGD	O1G-C1G-C2G-C3G
38	T1	101	3PH	C1-C2-C3-O31
38	S1	626	3PH	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
40	D	410	LHG	C4-C5-C6-O8
40	N	624	LHG	C4-C5-C6-O8
40	l	101	LHG	C4-C5-C6-O8
40	N1	624	LHG	C4-C5-C6-O8
40	c1	525	LHG	C4-C5-C6-O8
40	n1	624	LHG	C4-C5-C6-O8
41	c	527	LMK	O1-C7-C8-C9
47	i	101	4RF	O18-C19-C20-C39
47	K1	101	4RF	C19-C20-C39-O40
55	Y1	627	PTY	O4-C1-C6-C5
55	y1	627	PTY	O4-C1-C6-C5
38	t1	101	3PH	C32-C33-C34-C35
39	B	625	DGA	CAA-CBA-CCA-CDA
39	C	524	DGA	CB5-CB6-CB7-CB8
33	w	201	LMG	C10-C11-C12-C13
32	b1	626	SQD	C15-C16-C17-C18
38	t1	101	3PH	C27-C28-C29-C2A
40	Y	624	LHG	C11-C12-C13-C14
40	d	410	LHG	C34-C35-C36-C37
40	s1	624	LHG	C10-C11-C12-C13
40	s1	624	LHG	C33-C34-C35-C36
52	r	625	LMT	C9-C10-C11-C12
32	C1	526	SQD	C24-C25-C26-C27
32	c1	526	SQD	C15-C16-C17-C18
40	G	624	LHG	C30-C31-C32-C33
40	L1	101	LHG	C31-C32-C33-C34
29	Y	611	CLA	C3-C5-C6-C7
32	b1	626	SQD	C30-C31-C32-C33
39	J1	101	DGA	CA4-CA5-CA6-CA7
40	d	409	LHG	C33-C34-C35-C36
40	g1	624	LHG	C26-C27-C28-C29
55	Y	626	PTY	C37-C38-C39-C40
29	n	604	CLA	C4-C3-C5-C6
29	C1	505	CLA	C4-C3-C5-C6
48	S	608	CHL	C11-C12-C13-C15
38	T1	101	3PH	C29-C2A-C2B-C2C
38	b1	624	3PH	C25-C26-C27-C28
40	D	409	LHG	C19-C20-C21-C22
40	N1	624	LHG	C32-C33-C34-C35
33	h1	102	LMG	C19-C20-C21-C22
40	y	624	LHG	C10-C11-C12-C13
47	K	101	4RF	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
29	B1	611	CLA	C13-C15-C16-C17
40	y	624	LHG	C3-O3-P-O6
40	Y1	624	LHG	C3-O3-P-O6
41	C	527	LMK	C9-C8-O7-C10
41	C1	527	LMK	C9-C8-O7-C10
32	m	101	SQD	O47-C7-C8-C9
39	C	524	DGA	OA1-CA1-OG1-CG1
39	B1	625	DGA	OA1-CA1-OG1-CG1
40	C	525	LHG	O10-C23-O8-C6
38	S	626	3PH	C32-C33-C34-C35
29	C	504	CLA	O1D-CGD-O2D-CED
29	C1	504	CLA	C3-C5-C6-C7
29	B	602	CLA	C2A-CAA-CBA-CGA
29	r	603	CLA	C2A-CAA-CBA-CGA
29	N1	611	CLA	C2A-CAA-CBA-CGA
40	N	624	LHG	O1-C1-C2-O2
40	g	624	LHG	O1-C1-C2-O2
40	N1	624	LHG	O1-C1-C2-O2
32	B	621	SQD	C13-C14-C15-C16
38	b	624	3PH	C22-C23-C24-C25
38	B1	624	3PH	C34-C35-C36-C37
38	T1	101	3PH	C23-C24-C25-C26
40	l	101	LHG	C32-C33-C34-C35
40	n	624	LHG	C11-C12-C13-C14
40	L1	101	LHG	C33-C34-C35-C36
40	G1	624	LHG	C35-C36-C37-C38
40	c1	525	LHG	C34-C35-C36-C37
47	I1	102	4RF	C01-C02-C03-C04
47	K1	101	4RF	C31-C32-C33-C34
40	C	525	LHG	O6-C4-C5-O7
40	D	410	LHG	O6-C4-C5-O7
40	G	624	LHG	O6-C4-C5-O7
40	c	525	LHG	O6-C4-C5-O7
40	C1	525	LHG	O6-C4-C5-O7
40	N1	624	LHG	O6-C4-C5-O7
40	c1	525	LHG	O6-C4-C5-O7
40	g1	624	LHG	O6-C4-C5-O7
55	Y	627	PTY	O14-C5-C6-O7
53	R1	626	ERG	C23-C24-C25-C27
33	A1	413	LMG	C29-C28-O8-C9
32	M	101	SQD	C11-C12-C13-C14
29	b	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	b1	610	CLA	O1A-CGA-O2A-C1
40	s1	624	LHG	O10-C23-O8-C6
33	A1	413	LMG	C10-C11-C12-C13
47	k1	101	4RF	C13-C14-C15-C16
29	c1	504	CLA	C16-C17-C18-C20
29	y1	611	CLA	C15-C16-C17-C18
32	C1	526	SQD	C33-C34-C35-C36
38	t	101	3PH	C24-C25-C26-C27
39	j	101	DGA	CBB-CAB-CB9-CB8
29	B	603	CLA	C2B-C3B-CAB-CBB
29	C	513	CLA	C2B-C3B-CAB-CBB
29	S	617	CLA	C2B-C3B-CAB-CBB
29	b	602	CLA	C2B-C3B-CAB-CBB
29	b	604	CLA	C2B-C3B-CAB-CBB
29	b	613	CLA	C2B-C3B-CAB-CBB
29	n	611	CLA	C2B-C3B-CAB-CBB
29	g	604	CLA	C2B-C3B-CAB-CBB
29	r	610	CLA	C2B-C3B-CAB-CBB
29	B1	613	CLA	C2B-C3B-CAB-CBB
29	C1	502	CLA	C2B-C3B-CAB-CBB
29	C1	507	CLA	C2B-C3B-CAB-CBB
29	G1	610	CLA	C2B-C3B-CAB-CBB
29	Y1	611	CLA	C2B-C3B-CAB-CBB
29	n1	614	CLA	C2B-C3B-CAB-CBB
29	r1	610	CLA	C2B-C3B-CAB-CBB
29	s1	610	CLA	C2B-C3B-CAB-CBB
29	s1	612	CLA	C2B-C3B-CAB-CBB
29	s1	613	CLA	C2B-C3B-CAB-CBB
29	y1	613	CLA	C2B-C3B-CAB-CBB
32	A1	412	SQD	C16-C17-C18-C19
40	D	409	LHG	C30-C31-C32-C33
47	k	101	4RF	C01-C02-C03-C04
47	k	101	4RF	C03-C04-C05-C06
52	R	625	LMT	C3-C4-C5-C6
29	b	613	CLA	C8-C10-C11-C12
29	G	610	CLA	O1A-CGA-O2A-C1
30	A	409	PHO	O1A-CGA-O2A-C1
47	i	101	4RF	O42-C41-O40-C39
37	C	519	DGD	CAB-CBB-CCB-CDB
38	S	626	3PH	C37-C38-C39-C3A
38	S	626	3PH	C3F-C3G-C3H-C3I
40	l	101	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
40	S1	624	LHG	C33-C34-C35-C36
48	R	607	CHL	C2C-C3C-CAC-CBC
29	S1	614	CLA	C3-C5-C6-C7
32	m	101	SQD	C28-C29-C30-C31
38	B	624	3PH	C3E-C3F-C3G-C3H
40	C	525	LHG	C35-C36-C37-C38
40	C1	525	LHG	C26-C27-C28-C29
32	C1	526	SQD	O47-C45-C46-O48
32	b1	626	SQD	O47-C45-C46-O48
33	C	523	LMG	O1-C7-C8-O7
33	c	523	LMG	O1-C7-C8-O7
33	w	201	LMG	O1-C7-C8-O7
33	w1	201	LMG	O7-C8-C9-O8
37	c1	519	DGD	O1G-C1G-C2G-O2G
38	s	626	3PH	O21-C2-C3-O31
38	S1	626	3PH	O21-C2-C3-O31
39	c	524	DGA	OG1-CG1-CG2-OG2
40	L	101	LHG	O7-C5-C6-O8
40	l	101	LHG	O7-C5-C6-O8
40	n	624	LHG	O7-C5-C6-O8
40	s	624	LHG	O7-C5-C6-O8
40	D1	408	LHG	O7-C5-C6-O8
41	C	527	LMK	O1-C7-C8-O7
41	c1	527	LMK	O1-C7-C8-O7
55	Y	627	PTY	O4-C1-C6-O7
29	B	613	CLA	C13-C15-C16-C17
33	c	523	LMG	C14-C15-C16-C17
33	d	411	LMG	C22-C23-C24-C25
38	b	624	3PH	C39-C3A-C3B-C3C
40	g	624	LHG	C34-C35-C36-C37
55	Y	626	PTY	C36-C37-C38-C39
29	S	602	CLA	C11-C12-C13-C14
29	n1	610	CLA	C16-C17-C18-C19
33	b	622	LMG	C12-C13-C14-C15
33	h1	102	LMG	C29-C30-C31-C32
37	c	520	DGD	CCB-CDB-CEB-CFB
40	Y	624	LHG	C9-C10-C11-C12
32	M	101	SQD	O5-C1-O6-C44
39	B1	625	DGA	CG1-CG2-CG3-OXT
39	b1	625	DGA	CG1-CG2-CG3-OXT
40	S1	624	LHG	C1-C2-C3-O3
43	D	405	PL9	C39-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
43	d1	405	PL9	C19-C21-C22-C23
43	d1	405	PL9	C34-C36-C37-C38
54	s1	625	LPX	O1-C3-C4-C5
32	m1	101	SQD	C28-C29-C30-C31
38	T	101	3PH	C34-C35-C36-C37
39	c	524	DGA	CCB-CDB-CEB-CFB
39	B1	625	DGA	CEA-CFA-CGA-CHA
40	C	525	LHG	C24-C25-C26-C27
47	k	101	4RF	C44-C45-C46-C47
33	c1	523	LMG	O9-C10-O7-C8
29	B1	615	CLA	C4-C3-C5-C6
48	G	607	CHL	C4-C3-C5-C6
29	C	501	CLA	C2-C1-O2A-CGA
29	R	609	CLA	C2-C1-O2A-CGA
29	n	603	CLA	C2-C1-O2A-CGA
29	g	603	CLA	C2-C1-O2A-CGA
29	B1	604	CLA	C2-C1-O2A-CGA
29	B1	615	CLA	C2-C1-O2A-CGA
29	N1	604	CLA	C2-C1-O2A-CGA
29	b1	612	CLA	C2-C1-O2A-CGA
29	c1	505	CLA	C2-C1-O2A-CGA
48	R	607	CHL	C2-C1-O2A-CGA
43	d	405	PL9	C47-C48-C49-C51
48	y	609	CHL	C2-C3-C5-C6
32	M1	101	SQD	C28-C29-C30-C31
40	L	101	LHG	C10-C11-C12-C13
40	G1	624	LHG	C24-C25-C26-C27
52	r1	625	LMT	C9-C10-C11-C12
29	r	612	CLA	O1A-CGA-O2A-C1
29	c	512	CLA	C8-C10-C11-C12
29	B	607	CLA	C6-C7-C8-C9
29	B	614	CLA	C14-C13-C15-C16
29	B	616	CLA	C11-C12-C13-C14
29	C	511	CLA	C11-C12-C13-C14
29	N	602	CLA	C6-C7-C8-C9
29	S	609	CLA	C6-C7-C8-C9
29	S	610	CLA	C6-C7-C8-C9
29	Y	611	CLA	C6-C7-C8-C9
29	b	602	CLA	C14-C13-C15-C16
29	b	612	CLA	C11-C12-C13-C14
29	b	617	CLA	C14-C13-C15-C16
29	c	510	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	n	603	CLA	C14-C13-C15-C16
29	g	610	CLA	C14-C13-C15-C16
29	g	613	CLA	C11-C12-C13-C14
29	r	608	CLA	C6-C7-C8-C9
29	y	603	CLA	C14-C13-C15-C16
29	y	613	CLA	C11-C10-C8-C9
29	B1	616	CLA	C11-C10-C8-C9
29	B1	616	CLA	C14-C13-C15-C16
29	C1	501	CLA	C14-C13-C15-C16
29	C1	510	CLA	C14-C13-C15-C16
29	C1	513	CLA	C11-C12-C13-C14
29	D1	403	CLA	C6-C7-C8-C9
29	N1	610	CLA	C6-C7-C8-C9
29	Y1	612	CLA	C11-C10-C8-C9
29	b1	609	CLA	C6-C7-C8-C9
29	b1	610	CLA	C6-C7-C8-C9
29	b1	617	CLA	C14-C13-C15-C16
29	c1	507	CLA	C11-C12-C13-C14
29	c1	507	CLA	C14-C13-C15-C16
29	c1	511	CLA	C14-C13-C15-C16
29	n1	602	CLA	C11-C10-C8-C9
29	n1	603	CLA	C14-C13-C15-C16
29	g1	602	CLA	C14-C13-C15-C16
29	g1	603	CLA	C11-C12-C13-C14
29	r1	603	CLA	C11-C10-C8-C9
29	y1	603	CLA	C11-C12-C13-C14
29	y1	611	CLA	C14-C13-C15-C16
48	N	605	CHL	C11-C10-C8-C9
48	G	601	CHL	C14-C13-C15-C16
48	g	607	CHL	C11-C10-C8-C9
48	N1	607	CHL	C11-C12-C13-C14
48	G1	601	CHL	C6-C7-C8-C9
32	M	101	SQD	C24-C25-C26-C27
38	b	624	3PH	C26-C27-C28-C29
37	c1	519	DGD	C3A-C4A-C5A-C6A
38	B	624	3PH	C35-C36-C37-C38
29	C	510	CLA	C10-C11-C12-C13
29	g	603	CLA	C15-C16-C17-C18
29	y	613	CLA	C8-C10-C11-C12
29	Y1	604	CLA	C10-C11-C12-C13
29	y1	603	CLA	C5-C6-C7-C8
30	a1	408	PHO	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
48	S	608	CHL	C5-C6-C7-C8
48	Y1	607	CHL	C8-C10-C11-C12
30	A	409	PHO	C1A-C2A-CAA-CBA
30	a	409	PHO	C1A-C2A-CAA-CBA
40	D	410	LHG	C2-C3-O3-P
40	L	101	LHG	C2-C3-O3-P
40	S	624	LHG	C5-C4-O6-P
40	D1	409	LHG	C5-C4-O6-P
40	S1	624	LHG	C2-C3-O3-P
40	c1	525	LHG	C2-C3-O3-P
40	d1	408	LHG	C2-C3-O3-P
40	d1	409	LHG	C2-C3-O3-P
29	Y	602	CLA	O1A-CGA-O2A-C1
29	c	501	CLA	O1A-CGA-O2A-C1
33	w	201	LMG	O10-C28-O8-C9
38	b	624	3PH	C38-C39-C3A-C3B
40	D1	408	LHG	C24-C25-C26-C27
29	S1	617	CLA	C2A-CAA-CBA-CGA
29	r1	604	CLA	C2A-CAA-CBA-CGA
29	C	507	CLA	C16-C17-C18-C19
29	G	611	CLA	C16-C17-C18-C20
29	n	610	CLA	C16-C17-C18-C20
29	N1	602	CLA	C16-C17-C18-C20
29	Y1	611	CLA	C16-C17-C18-C19
38	t	101	3PH	C31-C32-C33-C34
29	c	508	CLA	C3-C5-C6-C7
31	C	514	BCR	C23-C24-C25-C26
31	C	515	BCR	C23-C24-C25-C26
31	C	517	BCR	C5-C6-C7-C8
31	b	619	BCR	C23-C24-C25-C26
31	c	515	BCR	C23-C24-C25-C26
31	B1	618	BCR	C5-C6-C7-C8
31	C1	514	BCR	C23-C24-C25-C26
31	b1	618	BCR	C5-C6-C7-C8
31	b1	619	BCR	C23-C24-C25-C26
31	b1	619	BCR	C23-C24-C25-C30
31	c1	515	BCR	C23-C24-C25-C26
31	c1	515	BCR	C23-C24-C25-C30
36	B	620	C7Z	C5-C6-C7-C8
49	N	620	LUT	C1-C6-C7-C8
49	N	620	LUT	C5-C6-C7-C8
49	S	620	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
49	S	620	LUT	C5-C6-C7-C8
49	Y	620	LUT	C1-C6-C7-C8
49	Y	620	LUT	C5-C6-C7-C8
49	g	621	LUT	C1-C6-C7-C8
49	G1	621	LUT	C1-C6-C7-C8
49	Y1	621	LUT	C1-C6-C7-C8
49	Y1	621	LUT	C5-C6-C7-C8
49	g1	621	LUT	C1-C6-C7-C8
49	g1	621	LUT	C5-C6-C7-C8
29	C	511	CLA	C8-C10-C11-C12
29	R	610	CLA	C5-C6-C7-C8
29	b	617	CLA	C8-C10-C11-C12
29	d	402	CLA	C15-C16-C17-C18
29	a1	405	CLA	C13-C15-C16-C17
29	c1	503	CLA	C8-C10-C11-C12
29	s1	610	CLA	C8-C10-C11-C12
48	n1	607	CHL	C5-C6-C7-C8
32	b1	626	SQD	C13-C14-C15-C16
33	W1	201	LMG	C33-C34-C35-C36
39	b1	625	DGA	CAA-CBA-CCA-CDA
40	l	101	LHG	C12-C13-C14-C15
47	I1	102	4RF	C27-C28-C29-C30
29	s	610	CLA	O1D-CGD-O2D-CED
33	C	521	LMG	O7-C10-C11-C12
31	c	517	BCR	C37-C22-C23-C24
31	c1	515	BCR	C11-C12-C13-C35
49	G1	620	LUT	C27-C28-C29-C39
48	R	606	CHL	C2A-CAA-CBA-CGA
33	w1	201	LMG	C39-C40-C41-C42
39	B	625	DGA	CFB-CGB-CHB-CIB
39	c1	524	DGA	CB2-CB3-CB4-CB5
31	B	618	BCR	C21-C22-C23-C24
31	C	514	BCR	C17-C18-C19-C20
31	C	517	BCR	C7-C8-C9-C10
31	D	404	BCR	C17-C18-C19-C20
31	C1	514	BCR	C11-C12-C13-C14
48	S1	607	CHL	C1A-C2A-CAA-CBA
49	S1	621	LUT	C11-C12-C13-C14
49	S1	621	LUT	C27-C28-C29-C30
49	s1	620	LUT	C31-C32-C33-C34
49	y1	620	LUT	C27-C28-C29-C30
51	y	623	NEX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	c	512	CLA	C15-C16-C17-C18
29	n	602	CLA	C13-C15-C16-C17
29	b1	615	CLA	C8-C10-C11-C12
29	d1	403	CLA	C15-C16-C17-C18
40	S	624	LHG	O9-C7-O7-C5
40	C1	525	LHG	O9-C7-O7-C5
51	r1	622	NEX	C14-C15-C35-C34
40	C1	525	LHG	C8-C7-O7-C5
33	d	411	LMG	C32-C33-C34-C35
37	c	519	DGD	CAB-CBB-CCB-CDB
38	S	626	3PH	C3B-C3C-C3D-C3E
40	G	624	LHG	C31-C32-C33-C34
40	n1	624	LHG	C34-C35-C36-C37
29	A1	410	CLA	C10-C11-C12-C13
48	Y1	606	CHL	C5-C6-C7-C8
32	A1	412	SQD	C11-C10-C9-C8
40	L1	101	LHG	C9-C10-C11-C12
29	S	611	CLA	C16-C17-C18-C19
29	B1	612	CLA	C16-C17-C18-C19
29	S1	610	CLA	C16-C17-C18-C20
29	r1	612	CLA	C11-C12-C13-C14
29	y1	613	CLA	C16-C17-C18-C19
34	A	414	SPH	C12-C13-C14-C15
40	C1	525	LHG	C35-C36-C37-C38
37	C1	520	DGD	C4D-C5D-C6D-O5D
29	b	604	CLA	C5-C6-C7-C8
29	b	608	CLA	C13-C15-C16-C17
29	y	612	CLA	C8-C10-C11-C12
29	c1	509	CLA	C5-C6-C7-C8
30	a1	408	PHO	C5-C6-C7-C8
53	r1	626	ERG	C22-C23-C24-C28
34	Y1	625	SPH	C12-C13-C14-C15
40	D1	409	LHG	C30-C31-C32-C33
29	c	506	CLA	C10-C11-C12-C13
29	b1	615	CLA	C13-C15-C16-C17
38	t	101	3PH	O11-C1-C2-C3
40	G	624	LHG	O6-C4-C5-C6
40	d	410	LHG	O6-C4-C5-C6
40	d1	408	LHG	O6-C4-C5-C6
40	g1	624	LHG	O6-C4-C5-C6
55	Y1	626	PTY	O14-C5-C6-C1
32	m1	101	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
40	l	101	LHG	O2-C2-C3-O3
29	C1	506	CLA	O1D-CGD-O2D-CED
33	D1	411	LMG	C18-C19-C20-C21
37	C1	519	DGD	C2A-C3A-C4A-C5A
29	B	602	CLA	C11-C12-C13-C15
29	B	604	CLA	C11-C12-C13-C15
29	B	607	CLA	C11-C10-C8-C7
29	B	608	CLA	C11-C10-C8-C7
29	B	615	CLA	C6-C7-C8-C10
29	B	617	CLA	C11-C12-C13-C15
29	C	502	CLA	C12-C13-C15-C16
29	C	509	CLA	C6-C7-C8-C10
29	C	509	CLA	C11-C10-C8-C7
29	C	510	CLA	C12-C13-C15-C16
29	C	511	CLA	C11-C12-C13-C15
29	D	402	CLA	C11-C10-C8-C7
29	D	403	CLA	C11-C10-C8-C7
29	N	602	CLA	C6-C7-C8-C10
29	G	603	CLA	C12-C13-C15-C16
29	R	602	CLA	C6-C7-C8-C10
29	S	602	CLA	C6-C7-C8-C10
29	S	610	CLA	C11-C10-C8-C7
29	Y	602	CLA	C11-C12-C13-C15
29	Y	611	CLA	C6-C7-C8-C10
29	Y	613	CLA	C6-C7-C8-C10
29	Y	613	CLA	C12-C13-C15-C16
29	b	602	CLA	C11-C10-C8-C7
29	b	602	CLA	C12-C13-C15-C16
29	b	607	CLA	C11-C12-C13-C15
29	b	608	CLA	C11-C10-C8-C7
29	b	613	CLA	C11-C10-C8-C7
29	b	616	CLA	C11-C12-C13-C15
29	b	617	CLA	C6-C7-C8-C10
29	c	501	CLA	C11-C12-C13-C15
29	c	507	CLA	C6-C7-C8-C10
29	c	510	CLA	C12-C13-C15-C16
29	c	513	CLA	C11-C10-C8-C7
29	d	402	CLA	C11-C12-C13-C15
29	n	613	CLA	C11-C10-C8-C7
29	n	613	CLA	C12-C13-C15-C16
29	g	611	CLA	C12-C13-C15-C16
29	g	613	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	r	602	CLA	C6-C7-C8-C10
29	r	609	CLA	C11-C10-C8-C7
29	r	612	CLA	C6-C7-C8-C10
29	y	603	CLA	C12-C13-C15-C16
29	y	604	CLA	C6-C7-C8-C10
29	y	612	CLA	C11-C10-C8-C7
29	y	613	CLA	C12-C13-C15-C16
29	A1	406	CLA	C12-C13-C15-C16
29	B1	603	CLA	C11-C10-C8-C7
29	B1	609	CLA	C11-C10-C8-C7
29	B1	609	CLA	C11-C12-C13-C15
29	B1	611	CLA	C11-C12-C13-C15
29	B1	615	CLA	C6-C7-C8-C10
29	B1	616	CLA	C11-C12-C13-C15
29	B1	617	CLA	C6-C7-C8-C10
29	C1	501	CLA	C12-C13-C15-C16
29	C1	510	CLA	C12-C13-C15-C16
29	C1	513	CLA	C11-C12-C13-C15
29	D1	403	CLA	C6-C7-C8-C10
29	D1	403	CLA	C11-C10-C8-C7
29	N1	602	CLA	C12-C13-C15-C16
29	N1	604	CLA	C6-C7-C8-C10
29	N1	604	CLA	C12-C13-C15-C16
29	N1	610	CLA	C11-C12-C13-C15
29	N1	610	CLA	C12-C13-C15-C16
29	G1	603	CLA	C6-C7-C8-C10
29	G1	610	CLA	C6-C7-C8-C10
29	S1	610	CLA	C11-C12-C13-C15
29	Y1	604	CLA	C11-C10-C8-C7
29	Y1	611	CLA	C6-C7-C8-C10
29	Y1	612	CLA	C11-C10-C8-C7
29	Y1	613	CLA	C11-C12-C13-C15
29	a1	405	CLA	C11-C10-C8-C7
29	a1	410	CLA	C11-C10-C8-C7
29	b1	603	CLA	C6-C7-C8-C10
29	b1	603	CLA	C11-C10-C8-C7
29	b1	609	CLA	C6-C7-C8-C10
29	b1	613	CLA	C11-C10-C8-C7
29	b1	616	CLA	C11-C10-C8-C7
29	c1	504	CLA	C6-C7-C8-C10
29	c1	507	CLA	C11-C12-C13-C15
29	c1	507	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	c1	513	CLA	C11-C10-C8-C7
29	n1	604	CLA	C12-C13-C15-C16
29	n1	610	CLA	C12-C13-C15-C16
29	n1	613	CLA	C11-C12-C13-C15
29	g1	602	CLA	C12-C13-C15-C16
29	g1	603	CLA	C11-C12-C13-C15
29	s1	603	CLA	C11-C10-C8-C7
29	s1	609	CLA	C6-C7-C8-C10
29	y1	604	CLA	C11-C10-C8-C7
29	y1	611	CLA	C12-C13-C15-C16
30	a1	408	PHO	C11-C10-C8-C7
30	a1	409	PHO	C11-C10-C8-C7
48	N	601	CHL	C12-C13-C15-C16
48	N	605	CHL	C11-C10-C8-C7
48	G	607	CHL	C2-C3-C5-C6
48	G	609	CHL	C11-C12-C13-C15
48	Y	606	CHL	C11-C10-C8-C7
48	Y	609	CHL	C12-C13-C15-C16
48	n	605	CHL	C11-C10-C8-C7
48	n	606	CHL	C11-C12-C13-C15
48	y	606	CHL	C6-C7-C8-C10
48	y	607	CHL	C11-C10-C8-C7
48	y	609	CHL	C12-C13-C15-C16
48	N1	605	CHL	C11-C10-C8-C7
48	N1	606	CHL	C11-C10-C8-C7
48	N1	606	CHL	C11-C12-C13-C15
48	N1	607	CHL	C11-C12-C13-C15
48	G1	601	CHL	C6-C7-C8-C10
48	G1	609	CHL	C11-C12-C13-C15
48	Y1	601	CHL	C6-C7-C8-C10
48	n1	601	CHL	C12-C13-C15-C16
48	n1	605	CHL	C12-C13-C15-C16
48	g1	601	CHL	C6-C7-C8-C10
48	g1	607	CHL	C11-C10-C8-C7
48	y1	606	CHL	C12-C13-C15-C16
29	S	614	CLA	O1A-CGA-O2A-C1
32	M	101	SQD	C28-C29-C30-C31
47	I	102	4RF	C44-C45-C46-C47
31	a	411	BCR	C19-C20-C21-C22
31	b	618	BCR	C13-C14-C15-C16
31	c	514	BCR	C13-C14-C15-C16
31	c	516	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	C1	514	BCR	C15-C16-C17-C18
31	C1	516	BCR	C9-C10-C11-C12
31	c1	516	BCR	C9-C10-C11-C12
31	c1	517	BCR	C15-C16-C17-C18
45	H	101	RRX	C19-C20-C21-C22
45	h	101	RRX	C19-C20-C21-C22
49	Y	621	LUT	C29-C30-C31-C32
49	n	620	LUT	C29-C30-C31-C32
49	s	621	LUT	C29-C30-C31-C32
49	g1	620	LUT	C29-C30-C31-C32
49	y1	621	LUT	C9-C10-C11-C12
51	G1	623	NEX	C13-C14-C15-C35
29	B	603	CLA	C16-C17-C18-C20
29	B	612	CLA	C16-C17-C18-C19
29	B	615	CLA	C16-C17-C18-C19
29	R	603	CLA	C11-C12-C13-C15
29	g	610	CLA	C16-C17-C18-C20
29	A1	405	CLA	C16-C17-C18-C20
29	n1	603	CLA	C16-C17-C18-C19
33	W1	201	LMG	O6-C5-C6-O5
33	H	102	LMG	C37-C38-C39-C40
38	t1	101	3PH	C26-C27-C28-C29
39	j1	101	DGA	CBB-CAB-CB9-CB8
32	m1	101	SQD	C23-C24-C25-C26
38	t	101	3PH	C21-C22-C23-C24
32	C	526	SQD	C15-C16-C17-C18
33	A	413	LMG	C31-C32-C33-C34
33	d	411	LMG	C34-C35-C36-C37
33	a1	413	LMG	C36-C37-C38-C39
47	I	102	4RF	C02-C03-C04-C05
29	B	615	CLA	C8-C10-C11-C12
29	N	602	CLA	C15-C16-C17-C18
29	n	604	CLA	C2A-CAA-CBA-CGA
29	n	611	CLA	C2A-CAA-CBA-CGA
29	r1	602	CLA	C2A-CAA-CBA-CGA
33	c1	523	LMG	C31-C32-C33-C34
34	a1	414	SPH	C12-C13-C14-C15
40	D	409	LHG	C29-C30-C31-C32
40	d	408	LHG	C34-C35-C36-C37
29	g	613	CLA	C8-C10-C11-C12
29	y	602	CLA	C10-C11-C12-C13
29	B1	603	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
38	B	624	3PH	C3F-C3G-C3H-C3I
38	b	624	3PH	C1-O11-P-O13
39	C	524	DGA	CB7-CB8-CB9-CAB
40	S	624	LHG	C30-C31-C32-C33
40	c	525	LHG	C25-C26-C27-C28
47	k	101	4RF	C49-C50-C51-C52
51	S	623	NEX	C11-C10-C9-C19
51	y	623	NEX	C11-C10-C9-C19
51	G1	623	NEX	C11-C10-C9-C19
51	G1	623	NEX	C40-C33-C34-C35
29	b1	611	CLA	C3-C5-C6-C7
48	G	609	CHL	C3-C5-C6-C7
29	S	602	CLA	C11-C12-C13-C15
29	Y	613	CLA	C16-C17-C18-C20
29	b	603	CLA	C16-C17-C18-C19
29	C1	510	CLA	C16-C17-C18-C19
30	A	408	PHO	C16-C17-C18-C20
29	Y	603	CLA	C8-C10-C11-C12
29	B	604	CLA	CBA-CGA-O2A-C1
29	B1	616	CLA	CBA-CGA-O2A-C1
39	c1	524	DGA	CA2-CA1-OG1-CG1
39	J	101	DGA	CB3-CB4-CB5-CB6
39	C1	524	DGA	CA2-CA3-CA4-CA5
40	n1	624	LHG	C14-C15-C16-C17
47	I	102	4RF	C47-C48-C49-C50
37	C	520	DGD	C1B-C2B-C3B-C4B
32	b	626	SQD	C19-C20-C21-C22
34	y1	625	SPH	C12-C13-C14-C15
38	t	101	3PH	C3A-C3B-C3C-C3D
39	B1	625	DGA	CA5-CA6-CA7-CA8
29	C	509	CLA	C10-C11-C12-C13
29	g1	602	CLA	C10-C11-C12-C13
39	c	524	DGA	CA7-CA8-CA9-CAA
40	d1	409	LHG	C35-C36-C37-C38
47	i1	101	4RF	C49-C50-C51-C52
29	B	606	CLA	CAD-CBD-CGD-O2D
29	C	503	CLA	CAD-CBD-CGD-O2D
29	N	602	CLA	CAD-CBD-CGD-O2D
29	N	614	CLA	CAD-CBD-CGD-O2D
29	G	602	CLA	CAD-CBD-CGD-O2D
29	G	603	CLA	CAD-CBD-CGD-O2D
29	G	612	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	b	615	CLA	CAD-CBD-CGD-O2D
29	c	507	CLA	CAD-CBD-CGD-O2D
29	n	602	CLA	CAD-CBD-CGD-O2D
29	n	612	CLA	CAD-CBD-CGD-O2D
29	g	603	CLA	CAD-CBD-CGD-O2D
29	g	604	CLA	CAD-CBD-CGD-O2D
29	g	614	CLA	CAD-CBD-CGD-O2D
29	r	602	CLA	CAD-CBD-CGD-O2D
29	r	612	CLA	CAD-CBD-CGD-O2D
29	y	602	CLA	CAD-CBD-CGD-O2D
29	y	614	CLA	CAD-CBD-CGD-O2D
29	B1	608	CLA	CAD-CBD-CGD-O2D
29	B1	617	CLA	CAD-CBD-CGD-O2D
29	C1	509	CLA	CAD-CBD-CGD-O2D
29	G1	604	CLA	CAD-CBD-CGD-O2D
29	R1	612	CLA	CAD-CBD-CGD-O2D
29	b1	611	CLA	CAD-CBD-CGD-O2D
29	b1	615	CLA	CAD-CBD-CGD-O2D
29	c1	504	CLA	CAD-CBD-CGD-O2D
29	c1	509	CLA	CAD-CBD-CGD-O2D
29	n1	602	CLA	CAD-CBD-CGD-O2D
29	r1	612	CLA	CAD-CBD-CGD-O2D
33	B	622	LMG	C9-C8-O7-C10
38	T	101	3PH	C3-C2-O21-C21
38	t	101	3PH	C3-C2-O21-C21
39	b	625	DGA	CG1-CG2-OG2-CB1
39	b1	625	DGA	CG1-CG2-OG2-CB1
48	N	605	CHL	CAD-CBD-CGD-O2D
48	N	608	CHL	CAD-CBD-CGD-O2D
48	Y	605	CHL	CAD-CBD-CGD-O2D
48	N1	606	CHL	CAD-CBD-CGD-O2D
48	G1	606	CHL	CAD-CBD-CGD-O2D
51	G1	623	NEX	C7-C8-C9-C19
32	C1	526	SQD	C12-C13-C14-C15
33	C1	523	LMG	C39-C40-C41-C42
38	b1	624	3PH	C2D-C2E-C2F-C2G
29	B1	609	CLA	C15-C16-C17-C18
29	R1	609	CLA	C10-C11-C12-C13
32	A	412	SQD	C24-C25-C26-C27
33	a	413	LMG	C39-C40-C41-C42
37	C	519	DGD	CDB-CEB-CFB-CGB
38	T1	101	3PH	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
39	c1	524	DGA	CFB-CGB-CHB-CIB
29	C	510	CLA	O1A-CGA-O2A-C1
29	B	617	CLA	CBA-CGA-O2A-C1
48	N	606	CHL	C4-C3-C5-C6
48	g	601	CHL	C4-C3-C5-C6
33	H	102	LMG	C29-C30-C31-C32
39	J	101	DGA	CB2-CB3-CB4-CB5
39	c	524	DGA	CFB-CGB-CHB-CIB
40	d1	409	LHG	C11-C12-C13-C14
33	H	102	LMG	O6-C1-O1-C7
37	c1	519	DGD	O6E-C1E-O5D-C6D
29	b1	608	CLA	C2-C3-C5-C6
32	C	526	SQD	O6-C44-C45-C46
32	C	526	SQD	C44-C45-C46-O48
32	m1	101	SQD	C44-C45-C46-O48
33	C	523	LMG	O1-C7-C8-C9
33	c	523	LMG	O1-C7-C8-C9
33	H1	102	LMG	C7-C8-C9-O8
33	d1	411	LMG	C7-C8-C9-O8
39	j	101	DGA	OG1-CG1-CG2-CG3
40	D	409	LHG	C4-C5-C6-O8
40	G	624	LHG	C4-C5-C6-O8
40	n	624	LHG	C4-C5-C6-O8
40	s	624	LHG	C2-C3-O3-P
40	C1	525	LHG	C4-C5-C6-O8
40	D1	408	LHG	C4-C5-C6-O8
40	G1	624	LHG	C4-C5-C6-O8
40	d1	408	LHG	C4-C5-C6-O8
40	d1	410	LHG	C4-C5-C6-O8
41	C	527	LMK	O1-C7-C8-C9
41	C1	527	LMK	C4-C3-N4-C6
41	c1	527	LMK	C7-C8-C9-O8
47	k	101	4RF	C19-C20-C39-O40
55	Y1	626	PTY	O4-C1-C6-C5
55	y1	626	PTY	O4-C1-C6-C5
33	A1	413	LMG	O10-C28-O8-C9
40	L	101	LHG	O6-C4-C5-O7
40	N	624	LHG	O6-C4-C5-O7
40	l	101	LHG	O6-C4-C5-O7
40	n	624	LHG	O6-C4-C5-O7
40	G1	624	LHG	O6-C4-C5-O7
40	d1	408	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
40	d1	409	LHG	O6-C4-C5-O7
40	n1	624	LHG	O6-C4-C5-O7
55	Y	626	PTY	O14-C5-C6-O7
55	y1	627	PTY	O14-C5-C6-O7
29	A	405	CLA	C5-C6-C7-C8
29	B1	612	CLA	C10-C11-C12-C13
48	N1	601	CHL	C3-C5-C6-C7
33	A1	413	LMG	O7-C10-C11-C12
29	g	614	CLA	O2A-C1-C2-C3
37	c	519	DGD	C2B-C3B-C4B-C5B
29	C1	508	CLA	CBA-CGA-O2A-C1
29	S	610	CLA	C2A-CAA-CBA-CGA
29	B1	602	CLA	C2A-CAA-CBA-CGA
48	Y	605	CHL	C2A-CAA-CBA-CGA
29	b1	605	CLA	C5-C6-C7-C8
32	M	101	SQD	C11-C10-C9-C8
32	C1	526	SQD	C19-C20-C21-C22
40	L1	101	LHG	C10-C11-C12-C13
29	B	605	CLA	C16-C17-C18-C19
29	a	406	CLA	C16-C17-C18-C20
29	n	604	CLA	C16-C17-C18-C19
30	A	408	PHO	C16-C17-C18-C19
33	c	523	LMG	C12-C13-C14-C15
37	C	519	DGD	C2A-C3A-C4A-C5A
40	d	409	LHG	C15-C16-C17-C18
40	n	624	LHG	C14-C15-C16-C17
55	y1	626	PTY	C37-C38-C39-C40
29	b1	616	CLA	O1D-CGD-O2D-CED
40	c	525	LHG	O9-C7-O7-C5
29	A	406	CLA	CHA-CBD-CGD-O1D
29	A	406	CLA	CHA-CBD-CGD-O2D
29	B	605	CLA	CHA-CBD-CGD-O1D
29	B	605	CLA	CHA-CBD-CGD-O2D
29	B	608	CLA	CHA-CBD-CGD-O1D
29	B	608	CLA	CHA-CBD-CGD-O2D
29	B	611	CLA	CHA-CBD-CGD-O1D
29	B	611	CLA	CHA-CBD-CGD-O2D
29	B	613	CLA	CHA-CBD-CGD-O1D
29	C	505	CLA	CHA-CBD-CGD-O2D
29	C	506	CLA	CHA-CBD-CGD-O1D
29	C	506	CLA	CHA-CBD-CGD-O2D
29	C	507	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	C	507	CLA	CHA-CBD-CGD-O2D
29	C	509	CLA	CHA-CBD-CGD-O1D
29	C	509	CLA	CHA-CBD-CGD-O2D
29	C	511	CLA	CHA-CBD-CGD-O1D
29	C	511	CLA	CHA-CBD-CGD-O2D
29	C	512	CLA	CHA-CBD-CGD-O1D
29	C	512	CLA	CHA-CBD-CGD-O2D
29	N	604	CLA	CHA-CBD-CGD-O1D
29	N	604	CLA	CHA-CBD-CGD-O2D
29	N	612	CLA	CHA-CBD-CGD-O1D
29	R	603	CLA	CHA-CBD-CGD-O1D
29	R	603	CLA	CHA-CBD-CGD-O2D
29	R	608	CLA	CHA-CBD-CGD-O2D
29	R	609	CLA	CHA-CBD-CGD-O1D
29	R	609	CLA	CHA-CBD-CGD-O2D
29	S	602	CLA	CHA-CBD-CGD-O1D
29	S	605	CLA	CHA-CBD-CGD-O1D
29	S	605	CLA	CHA-CBD-CGD-O2D
29	S	612	CLA	CHA-CBD-CGD-O1D
29	S	612	CLA	CHA-CBD-CGD-O2D
29	Y	602	CLA	CHA-CBD-CGD-O1D
29	Y	602	CLA	CHA-CBD-CGD-O2D
29	Y	612	CLA	CHA-CBD-CGD-O1D
29	Y	612	CLA	CHA-CBD-CGD-O2D
29	a	406	CLA	CHA-CBD-CGD-O1D
29	a	406	CLA	CHA-CBD-CGD-O2D
29	b	607	CLA	CHA-CBD-CGD-O1D
29	b	607	CLA	CHA-CBD-CGD-O2D
29	b	609	CLA	CHA-CBD-CGD-O1D
29	b	609	CLA	CHA-CBD-CGD-O2D
29	b	610	CLA	CHA-CBD-CGD-O1D
29	b	610	CLA	CHA-CBD-CGD-O2D
29	c	503	CLA	CHA-CBD-CGD-O1D
29	c	506	CLA	CHA-CBD-CGD-O1D
29	c	506	CLA	CHA-CBD-CGD-O2D
29	n	613	CLA	CHA-CBD-CGD-O1D
29	n	613	CLA	CHA-CBD-CGD-O2D
29	g	602	CLA	CHA-CBD-CGD-O1D
29	g	602	CLA	CHA-CBD-CGD-O2D
29	g	611	CLA	CHA-CBD-CGD-O1D
29	g	611	CLA	CHA-CBD-CGD-O2D
29	r	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	s	602	CLA	CHA-CBD-CGD-O1D
29	s	602	CLA	CHA-CBD-CGD-O2D
29	s	605	CLA	CHA-CBD-CGD-O1D
29	y	603	CLA	CHA-CBD-CGD-O1D
29	y	603	CLA	CHA-CBD-CGD-O2D
29	y	612	CLA	CHA-CBD-CGD-O1D
29	y	612	CLA	CHA-CBD-CGD-O2D
29	B1	602	CLA	CHA-CBD-CGD-O1D
29	B1	602	CLA	CHA-CBD-CGD-O2D
29	B1	604	CLA	CHA-CBD-CGD-O1D
29	B1	604	CLA	CHA-CBD-CGD-O2D
29	B1	605	CLA	CHA-CBD-CGD-O1D
29	B1	605	CLA	CHA-CBD-CGD-O2D
29	B1	609	CLA	CHA-CBD-CGD-O1D
29	B1	616	CLA	CHA-CBD-CGD-O2D
29	C1	502	CLA	CHA-CBD-CGD-O1D
29	C1	502	CLA	CHA-CBD-CGD-O2D
29	C1	505	CLA	CHA-CBD-CGD-O1D
29	C1	512	CLA	CHA-CBD-CGD-O1D
29	C1	512	CLA	CHA-CBD-CGD-O2D
29	G1	612	CLA	CHA-CBD-CGD-O1D
29	G1	612	CLA	CHA-CBD-CGD-O2D
29	G1	613	CLA	CHA-CBD-CGD-O1D
29	G1	613	CLA	CHA-CBD-CGD-O2D
29	S1	602	CLA	CHA-CBD-CGD-O1D
29	S1	602	CLA	CHA-CBD-CGD-O2D
29	S1	604	CLA	CHA-CBD-CGD-O1D
29	S1	611	CLA	CHA-CBD-CGD-O1D
29	S1	611	CLA	CHA-CBD-CGD-O2D
29	Y1	604	CLA	CHA-CBD-CGD-O1D
29	Y1	612	CLA	CHA-CBD-CGD-O1D
29	Y1	612	CLA	CHA-CBD-CGD-O2D
29	b1	605	CLA	CHA-CBD-CGD-O1D
29	b1	608	CLA	CHA-CBD-CGD-O2D
29	b1	610	CLA	CHA-CBD-CGD-O1D
29	b1	610	CLA	CHA-CBD-CGD-O2D
29	b1	612	CLA	CHA-CBD-CGD-O1D
29	b1	613	CLA	CHA-CBD-CGD-O1D
29	b1	613	CLA	CHA-CBD-CGD-O2D
29	c1	501	CLA	CHA-CBD-CGD-O1D
29	c1	501	CLA	CHA-CBD-CGD-O2D
29	c1	505	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	c1	505	CLA	CHA-CBD-CGD-O2D
29	g1	612	CLA	CHA-CBD-CGD-O1D
29	r1	603	CLA	CHA-CBD-CGD-O1D
29	r1	603	CLA	CHA-CBD-CGD-O2D
29	r1	608	CLA	CHA-CBD-CGD-O2D
29	s1	604	CLA	CHA-CBD-CGD-O1D
29	s1	604	CLA	CHA-CBD-CGD-O2D
29	s1	605	CLA	CHA-CBD-CGD-O1D
29	s1	605	CLA	CHA-CBD-CGD-O2D
29	y1	612	CLA	CHA-CBD-CGD-O1D
29	y1	612	CLA	CHA-CBD-CGD-O2D
48	G	605	CHL	CHA-CBD-CGD-O1D
48	G	605	CHL	CHA-CBD-CGD-O2D
48	r	606	CHL	CHA-CBD-CGD-O2D
48	N1	601	CHL	CHA-CBD-CGD-O1D
48	n1	601	CHL	CHA-CBD-CGD-O2D
48	n1	608	CHL	CHA-CBD-CGD-O1D
48	n1	608	CHL	CHA-CBD-CGD-O2D
48	r1	606	CHL	CHA-CBD-CGD-O2D
48	y1	609	CHL	CHA-CBD-CGD-O1D
48	y1	609	CHL	CHA-CBD-CGD-O2D
29	Y1	611	CLA	C15-C16-C17-C18
47	K1	101	4RF	C01-C02-C03-C04
29	C	501	CLA	O1A-CGA-O2A-C1
29	B1	616	CLA	O1A-CGA-O2A-C1
32	b	621	SQD	O10-C23-O48-C46
32	b1	626	SQD	O10-C23-O48-C46
40	d1	410	LHG	O10-C23-O8-C6
54	S	625	LPX	O7-C6-O6-C5
40	g1	624	LHG	C24-C25-C26-C27
32	M1	101	SQD	C2-C1-O6-C44
33	a	413	LMG	C2-C1-O1-C7
51	S	623	NEX	C11-C10-C9-C8
29	C1	503	CLA	C10-C11-C12-C13
32	B1	621	SQD	C25-C26-C27-C28
32	A	412	SQD	O6-C44-C45-O47
32	B	626	SQD	O6-C44-C45-O47
32	C	526	SQD	O6-C44-C45-O47
32	C	526	SQD	O47-C45-C46-O48
32	a	412	SQD	O6-C44-C45-O47
32	m	101	SQD	O47-C45-C46-O48
32	b1	626	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
33	b	622	LMG	O1-C7-C8-O7
33	c	523	LMG	O7-C8-C9-O8
33	A1	413	LMG	O1-C7-C8-O7
33	B1	622	LMG	O7-C8-C9-O8
37	B	623	DGD	O1G-C1G-C2G-O2G
37	b	623	DGD	O1G-C1G-C2G-O2G
37	c	520	DGD	O1G-C1G-C2G-O2G
37	B1	623	DGD	O1G-C1G-C2G-O2G
37	C1	520	DGD	O2G-C2G-C3G-O3G
39	j	101	DGA	OG1-CG1-CG2-OG2
40	C1	525	LHG	O7-C5-C6-O8
40	S1	624	LHG	O7-C5-C6-O8
40	c1	525	LHG	O7-C5-C6-O8
41	c	527	LMK	O7-C8-C9-O8
47	i1	101	4RF	O18-C19-C20-O21
47	k1	101	4RF	O18-C19-C20-O21
55	Y1	627	PTY	O4-C1-C6-O7
55	y1	626	PTY	O4-C1-C6-O7
55	y1	627	PTY	O4-C1-C6-O7
38	s1	626	3PH	C22-C23-C24-C25
29	C	505	CLA	C13-C15-C16-C17
29	g1	610	CLA	O1A-CGA-O2A-C1
39	B1	625	DGA	CB7-CB8-CB9-CAB
40	d1	408	LHG	C26-C27-C28-C29
40	d1	408	LHG	C33-C34-C35-C36
40	n1	624	LHG	C30-C31-C32-C33
29	s	614	CLA	C6-C7-C8-C10
29	y	603	CLA	C16-C17-C18-C19
29	Y1	611	CLA	C16-C17-C18-C20
34	y1	625	SPH	N2-C2-C3-O3
40	S1	624	LHG	O1-C1-C2-O2
32	B	626	SQD	C14-C15-C16-C17
37	c	519	DGD	C6B-C7B-C8B-C9B
39	J1	101	DGA	CB2-CB3-CB4-CB5
39	c1	524	DGA	CA3-CA4-CA5-CA6
29	d1	402	CLA	C3-C5-C6-C7
29	B	615	CLA	C5-C6-C7-C8
29	y	611	CLA	C4-C3-C5-C6
48	n1	609	CHL	C4-C3-C5-C6
37	C	519	DGD	C9A-CAA-CBA-CCA
47	k	101	4RF	C54-C55-C56-C57
29	C1	501	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
43	D1	405	PL9	C13-C14-C16-C17
48	g	601	CHL	C2-C3-C5-C6
32	C1	526	SQD	C32-C33-C34-C35
33	d1	411	LMG	O9-C10-O7-C8
29	B	604	CLA	C11-C12-C13-C14
29	B	606	CLA	C6-C7-C8-C9
29	B	607	CLA	C11-C10-C8-C9
29	B	608	CLA	C11-C10-C8-C9
29	B	608	CLA	C11-C12-C13-C14
29	B	615	CLA	C6-C7-C8-C9
29	B	617	CLA	C11-C12-C13-C14
29	C	511	CLA	C14-C13-C15-C16
29	B1	605	CLA	C14-C13-C15-C16
29	N1	603	CLA	C14-C13-C15-C16
29	N1	604	CLA	C14-C13-C15-C16
29	G1	610	CLA	C11-C12-C13-C14
29	Y1	611	CLA	C6-C7-C8-C9
29	a1	410	CLA	C11-C10-C8-C9
29	c1	512	CLA	C11-C10-C8-C9
29	g1	603	CLA	C14-C13-C15-C16
29	g1	611	CLA	C11-C10-C8-C9
29	y1	604	CLA	C11-C10-C8-C9
30	a1	408	PHO	C11-C10-C8-C9
48	N	607	CHL	C11-C12-C13-C14
48	n	607	CHL	C11-C12-C13-C14
48	N1	605	CHL	C11-C10-C8-C9
29	S	611	CLA	O1D-CGD-O2D-CED
33	w	201	LMG	C11-C12-C13-C14
40	C1	525	LHG	C34-C35-C36-C37
40	d1	409	LHG	C33-C34-C35-C36
37	c	520	DGD	O6D-C5D-C6D-O5D
29	B	604	CLA	O1A-CGA-O2A-C1
29	B	617	CLA	O1A-CGA-O2A-C1
39	c1	524	DGA	OA1-CA1-OG1-CG1
47	K	101	4RF	O42-C41-O40-C39
40	c1	525	LHG	C23-C24-C25-C26
40	d	409	LHG	C29-C30-C31-C32
32	B	621	SQD	C4-C5-C6-S
32	C	526	SQD	C4-C5-C6-S
32	b	621	SQD	C4-C5-C6-S
32	C1	526	SQD	C4-C5-C6-S
32	b1	626	SQD	C5-C6-S-O8

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Mol	Chain	Res	Type	Atoms
32	c1	526	SQD	C4-C5-C6-S
32	a	412	SQD	C9-C10-C11-C12
40	C	525	LHG	C28-C29-C30-C31
29	B1	608	CLA	C2A-CAA-CBA-CGA
48	g	605	CHL	C2A-CAA-CBA-CGA
48	S1	608	CHL	CAA-CBA-CGA-O2A
38	B	624	3PH	C2E-C2F-C2G-C2H
38	s1	626	3PH	C3A-C3B-C3C-C3D
39	B	625	DGA	CA8-CA9-CAA-CBA
31	b	618	BCR	C37-C22-C23-C24
49	G	620	LUT	C27-C28-C29-C39
50	Y	622	XAT	C31-C32-C33-C40
47	i	101	4RF	C47-C48-C49-C50
40	S1	624	LHG	O1-C1-C2-C3
46	I1	101	GOL	C1-C2-C3-O3
29	Y	613	CLA	C13-C15-C16-C17
29	c1	508	CLA	C8-C10-C11-C12
30	a1	408	PHO	C13-C15-C16-C17
34	Y1	625	SPH	C13-C14-C15-C16
39	B	625	DGA	CBB-CAB-CB9-CB8
47	k1	101	4RF	C35-C36-C37-C38
31	c1	515	BCR	C11-C12-C13-C14
49	G1	620	LUT	C27-C28-C29-C30
50	R	621	XAT	C27-C28-C29-C30
33	A	413	LMG	C37-C38-C39-C40
37	C1	519	DGD	C9B-CAB-CBB-CCB
38	T1	101	3PH	C26-C27-C28-C29
41	C	527	LMK	C34-C16-C17-C18
29	A	410	CLA	C1A-C2A-CAA-CBA
29	B	605	CLA	C1A-C2A-CAA-CBA
29	N	602	CLA	C1A-C2A-CAA-CBA
29	R	609	CLA	C1A-C2A-CAA-CBA
29	b	612	CLA	C1A-C2A-CAA-CBA
29	r	612	CLA	C1A-C2A-CAA-CBA
29	y	604	CLA	C1A-C2A-CAA-CBA
29	B1	616	CLA	C1A-C2A-CAA-CBA
29	C1	511	CLA	C1A-C2A-CAA-CBA
29	D1	403	CLA	C1A-C2A-CAA-CBA
29	G1	612	CLA	C1A-C2A-CAA-CBA
29	S1	604	CLA	C1A-C2A-CAA-CBA
29	r1	612	CLA	C1A-C2A-CAA-CBA
48	N	609	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
48	G	609	CHL	C1A-C2A-CAA-CBA
48	s	608	CHL	C1A-C2A-CAA-CBA
48	N1	606	CHL	C1A-C2A-CAA-CBA
29	B	613	CLA	C16-C17-C18-C19
29	B1	607	CLA	C16-C17-C18-C19
29	g	602	CLA	C13-C15-C16-C17
29	r	602	CLA	C10-C11-C12-C13
29	r	608	CLA	C5-C6-C7-C8
40	y	624	LHG	C34-C35-C36-C37
29	R	608	CLA	C2-C1-O2A-CGA
29	n	613	CLA	C2-C1-O2A-CGA
29	s	610	CLA	C2-C1-O2A-CGA
29	R1	604	CLA	C2-C1-O2A-CGA
29	a1	405	CLA	C2-C1-O2A-CGA
29	a1	406	CLA	C2-C1-O2A-CGA
29	c1	501	CLA	C2-C1-O2A-CGA
29	r1	609	CLA	C2-C1-O2A-CGA
29	r1	610	CLA	C2-C1-O2A-CGA
29	C	501	CLA	CBA-CGA-O2A-C1
29	b	615	CLA	CBA-CGA-O2A-C1
38	S	626	3PH	C34-C35-C36-C37
38	t1	101	3PH	C3A-C3B-C3C-C3D
40	s	624	LHG	C28-C29-C30-C31
40	d1	410	LHG	C9-C10-C11-C12
40	d1	410	LHG	C34-C35-C36-C37
31	d	404	BCR	C19-C20-C21-C22
45	H1	101	RRX	C9-C10-C11-C12
49	Y1	620	LUT	C9-C10-C11-C12
49	Y1	621	LUT	C33-C34-C35-C15
49	n1	621	LUT	C29-C30-C31-C32
41	c	527	LMK	C10-C11-C12-C13
29	b1	611	CLA	C13-C15-C16-C17
40	D	409	LHG	C4-O6-P-O3
40	D	410	LHG	C4-O6-P-O3
40	L	101	LHG	C4-O6-P-O3
40	N	624	LHG	C3-O3-P-O6
40	S	624	LHG	C3-O3-P-O6
40	s	624	LHG	C3-O3-P-O6
40	C1	525	LHG	C3-O3-P-O6
40	N1	624	LHG	C3-O3-P-O6
40	S1	624	LHG	C3-O3-P-O6
40	s1	624	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
32	b1	626	SQD	C14-C15-C16-C17
37	C	519	DGD	CDA-CEA-CFA-CGA
38	b1	624	3PH	C3D-C3E-C3F-C3G
40	L	101	LHG	C27-C28-C29-C30
40	n	624	LHG	C31-C32-C33-C34
54	s	625	LPX	C18-C19-C20-C21
29	r	609	CLA	C4-C3-C5-C6
29	y1	603	CLA	C4-C3-C5-C6
33	w1	201	LMG	O7-C10-C11-C12
29	Y1	611	CLA	C3-C5-C6-C7
29	b1	604	CLA	C3-C5-C6-C7
40	l	101	LHG	C2-C3-O3-P
40	D1	408	LHG	C2-C3-O3-P
40	s1	624	LHG	C2-C3-O3-P
29	B	603	CLA	C2-C3-C5-C6
29	B	610	CLA	C2-C3-C5-C6
29	r1	609	CLA	C2-C3-C5-C6
32	m1	101	SQD	C26-C27-C28-C29
39	c	524	DGA	CA2-CA3-CA4-CA5
39	j1	101	DGA	CA4-CA5-CA6-CA7
29	G	603	CLA	C4B-C3B-CAB-CBB
29	G	612	CLA	C4B-C3B-CAB-CBB
29	R	608	CLA	C4B-C3B-CAB-CBB
29	b	616	CLA	C4B-C3B-CAB-CBB
29	c	501	CLA	C4B-C3B-CAB-CBB
29	c	504	CLA	C4B-C3B-CAB-CBB
29	g	611	CLA	C4B-C3B-CAB-CBB
29	g	612	CLA	C4B-C3B-CAB-CBB
29	C1	504	CLA	C4B-C3B-CAB-CBB
29	G1	603	CLA	C4B-C3B-CAB-CBB
29	R1	612	CLA	C4B-C3B-CAB-CBB
29	S1	603	CLA	C4B-C3B-CAB-CBB
29	b1	617	CLA	C4B-C3B-CAB-CBB
29	c1	501	CLA	C4B-C3B-CAB-CBB
29	c1	504	CLA	C4B-C3B-CAB-CBB
29	n1	611	CLA	C4B-C3B-CAB-CBB
29	s1	611	CLA	C4B-C3B-CAB-CBB
29	y1	603	CLA	C4B-C3B-CAB-CBB
40	D	408	LHG	C4-O6-P-O4
40	D	409	LHG	C3-O3-P-O4
40	D	410	LHG	C3-O3-P-O4
40	Y	624	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
40	d	408	LHG	C3-O3-P-O5
40	d	408	LHG	C4-O6-P-O4
40	d	409	LHG	C3-O3-P-O5
40	l	101	LHG	C3-O3-P-O5
40	n	624	LHG	C3-O3-P-O4
40	g	624	LHG	C4-O6-P-O4
40	s	624	LHG	C4-O6-P-O5
40	C1	525	LHG	C4-O6-P-O4
40	D1	409	LHG	C4-O6-P-O4
40	D1	410	LHG	C4-O6-P-O4
40	L1	101	LHG	C3-O3-P-O5
40	L1	101	LHG	C4-O6-P-O5
40	N1	624	LHG	C4-O6-P-O4
40	G1	624	LHG	C4-O6-P-O4
40	d1	408	LHG	C4-O6-P-O4
40	d1	409	LHG	C3-O3-P-O5
40	d1	409	LHG	C4-O6-P-O4
40	d1	410	LHG	C4-O6-P-O4
40	y1	624	LHG	C4-O6-P-O4
54	S1	625	LPX	C3-O1-P1-O3
54	s1	625	LPX	C3-O1-P1-O3
55	Y	626	PTY	C3-O11-P1-O13
55	Y	627	PTY	C5-O14-P1-O12
55	y	627	PTY	C3-O11-P1-O12
55	Y1	626	PTY	C3-O11-P1-O13
55	y1	626	PTY	C3-O11-P1-O12
55	y1	626	PTY	C5-O14-P1-O13
55	y1	627	PTY	C3-O11-P1-O13
29	c	505	CLA	C16-C17-C18-C20
29	y	613	CLA	C16-C17-C18-C19
29	C1	503	CLA	C16-C17-C18-C20
29	R1	602	CLA	C11-C12-C13-C14
29	R1	612	CLA	C11-C12-C13-C15
29	a1	405	CLA	C16-C17-C18-C20
29	b1	605	CLA	C16-C17-C18-C20
29	s1	614	CLA	C6-C7-C8-C9
33	B1	622	LMG	C19-C20-C21-C22
33	w1	201	LMG	C34-C35-C36-C37
38	s	626	3PH	C35-C36-C37-C38
29	N1	611	CLA	O2A-C1-C2-C3
29	G1	604	CLA	O2A-C1-C2-C3
29	n1	611	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
29	A	410	CLA	C10-C11-C12-C13
29	B	612	CLA	C5-C6-C7-C8
29	B	617	CLA	C15-C16-C17-C18
29	r1	609	CLA	C5-C6-C7-C8
29	B	602	CLA	CBA-CGA-O2A-C1
38	s1	626	3PH	O11-C1-C2-C3
40	D1	410	LHG	O6-C4-C5-C6
55	Y	627	PTY	O14-C5-C6-C1
55	y1	626	PTY	O14-C5-C6-C1
33	h1	102	LMG	C16-C17-C18-C19
38	T	101	3PH	C3B-C3C-C3D-C3E
39	c	524	DGA	CA4-CA5-CA6-CA7
39	j1	101	DGA	CB4-CB5-CB6-CB7
47	i1	101	4RF	C48-C49-C50-C51
34	A1	414	SPH	C15-C16-C17-C18
55	y1	626	PTY	C36-C37-C38-C39
29	R	609	CLA	C5-C6-C7-C8
48	g	609	CHL	C13-C15-C16-C17
53	R	626	ERG	C21-C20-C22-C23
43	D	405	PL9	C47-C48-C49-C51
29	G1	603	CLA	C2A-CAA-CBA-CGA
29	Y1	604	CLA	C3-C5-C6-C7
29	b	602	CLA	C5-C6-C7-C8
32	C	526	SQD	C32-C33-C34-C35
37	c	519	DGD	C5A-C6A-C7A-C8A
40	d	408	LHG	C32-C33-C34-C35
55	y	626	PTY	C32-C33-C34-C35
32	B	621	SQD	C28-C29-C30-C31
33	a1	413	LMG	C33-C34-C35-C36
38	B	624	3PH	C23-C24-C25-C26
29	B	605	CLA	CAD-CBD-CGD-O1D
29	B	608	CLA	CAD-CBD-CGD-O1D
29	B	613	CLA	CAD-CBD-CGD-O1D
29	B	617	CLA	CAD-CBD-CGD-O1D
29	C	505	CLA	CAD-CBD-CGD-O1D
29	C	506	CLA	CAD-CBD-CGD-O1D
29	C	512	CLA	CAD-CBD-CGD-O1D
29	G	604	CLA	CAD-CBD-CGD-O1D
29	b	610	CLA	CAD-CBD-CGD-O1D
29	c	501	CLA	CAD-CBD-CGD-O1D
29	c	503	CLA	CAD-CBD-CGD-O1D
29	c	505	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	c	506	CLA	CAD-CBD-CGD-O1D
29	B1	602	CLA	CAD-CBD-CGD-O1D
29	B1	605	CLA	CAD-CBD-CGD-O1D
29	C1	502	CLA	CAD-CBD-CGD-O1D
29	C1	503	CLA	CAD-CBD-CGD-O1D
29	C1	505	CLA	CAD-CBD-CGD-O1D
29	b1	605	CLA	CAD-CBD-CGD-O1D
29	b1	610	CLA	CAD-CBD-CGD-O1D
29	b1	613	CLA	CAD-CBD-CGD-O1D
29	c1	501	CLA	CAD-CBD-CGD-O1D
29	c1	505	CLA	CAD-CBD-CGD-O1D
29	c1	506	CLA	CAD-CBD-CGD-O1D
29	g1	604	CLA	CAD-CBD-CGD-O1D
32	b	626	SQD	C5-C6-S-O7
32	b1	626	SQD	C5-C6-S-O7
32	m1	101	SQD	C5-C6-S-O7
32	m1	101	SQD	C5-C6-S-O9
41	C1	527	LMK	C29-C28-O8-C9
48	N	609	CHL	CAD-CBD-CGD-O1D
48	n	601	CHL	CAD-CBD-CGD-O1D
48	r	606	CHL	CAD-CBD-CGD-O1D
48	N1	601	CHL	CAD-CBD-CGD-O1D
48	R1	606	CHL	CAD-CBD-CGD-O1D
48	n1	601	CHL	CAD-CBD-CGD-O1D
48	r1	606	CHL	CAD-CBD-CGD-O1D
51	s	623	NEX	C7-C8-C9-C10
51	R1	622	NEX	C7-C8-C9-C10
51	s1	623	NEX	C7-C8-C9-C10
55	Y	626	PTY	C2-C3-O11-P1
55	y	626	PTY	C2-C3-O11-P1
55	y1	626	PTY	C2-C3-O11-P1
33	B1	622	LMG	C10-C11-C12-C13
41	C	527	LMK	C28-C29-C30-C31
33	h1	102	LMG	O7-C10-C11-C12
29	B	606	CLA	C8-C10-C11-C12
29	G1	611	CLA	C13-C15-C16-C17
38	B1	624	3PH	C3B-C3C-C3D-C3E
40	L	101	LHG	C19-C20-C21-C22
33	H1	102	LMG	C4-C5-C6-O5
29	B	602	CLA	O1A-CGA-O2A-C1
29	s1	611	CLA	O1A-CGA-O2A-C1
37	C1	520	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
37	c1	519	DGD	C7A-C8A-C9A-CAA
29	C	505	CLA	C5-C6-C7-C8
29	S	603	CLA	C8-C10-C11-C12
37	C1	518	DGD	C9B-CAB-CBB-CCB
40	G	624	LHG	C24-C25-C26-C27
32	c1	526	SQD	C7-C8-C9-C10
33	C1	523	LMG	C10-C11-C12-C13
37	C1	518	DGD	C6B-C7B-C8B-C9B
29	s1	611	CLA	CBA-CGA-O2A-C1
47	K1	101	4RF	C15-C16-O18-C19
29	C1	508	CLA	O1A-CGA-O2A-C1
33	B	622	LMG	C15-C16-C17-C18
33	b1	622	LMG	C13-C14-C15-C16
39	b1	625	DGA	CDA-CEA-CFA-CGA
48	N	606	CHL	C16-C17-C18-C19
48	N1	605	CHL	C4-C3-C5-C6
29	B	602	CLA	C12-C13-C15-C16
29	B	606	CLA	C12-C13-C15-C16
29	B	608	CLA	C11-C12-C13-C15
29	B	608	CLA	C12-C13-C15-C16
29	B	614	CLA	C11-C10-C8-C7
29	C	501	CLA	C11-C12-C13-C15
29	C	511	CLA	C12-C13-C15-C16
29	G	610	CLA	C6-C7-C8-C10
29	Y	603	CLA	C11-C12-C13-C15
29	Y	610	CLA	C12-C13-C15-C16
29	b	605	CLA	C12-C13-C15-C16
29	c	501	CLA	C12-C13-C15-C16
29	c	504	CLA	C6-C7-C8-C10
29	c	504	CLA	C12-C13-C15-C16
29	c	507	CLA	C12-C13-C15-C16
29	n	603	CLA	C12-C13-C15-C16
29	s	609	CLA	C6-C7-C8-C10
29	s	610	CLA	C11-C10-C8-C7
29	s	610	CLA	C11-C12-C13-C15
29	y	613	CLA	C11-C10-C8-C7
29	B1	602	CLA	C6-C7-C8-C10
29	B1	605	CLA	C12-C13-C15-C16
29	B1	606	CLA	C11-C10-C8-C7
29	B1	608	CLA	C12-C13-C15-C16
29	B1	610	CLA	C12-C13-C15-C16
29	B1	617	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
29	C1	505	CLA	C6-C7-C8-C10
29	N1	603	CLA	C12-C13-C15-C16
29	N1	604	CLA	C11-C12-C13-C15
29	G1	602	CLA	C12-C13-C15-C16
29	G1	610	CLA	C11-C12-C13-C15
29	G1	611	CLA	C11-C12-C13-C15
29	S1	603	CLA	C11-C12-C13-C15
29	S1	611	CLA	C11-C10-C8-C7
29	Y1	602	CLA	C12-C13-C15-C16
29	Y1	603	CLA	C12-C13-C15-C16
29	a1	406	CLA	C11-C12-C13-C15
29	b1	608	CLA	C11-C10-C8-C7
29	b1	616	CLA	C11-C12-C13-C15
29	c1	501	CLA	C11-C12-C13-C15
29	c1	501	CLA	C12-C13-C15-C16
29	c1	503	CLA	C12-C13-C15-C16
29	c1	504	CLA	C12-C13-C15-C16
29	c1	509	CLA	C6-C7-C8-C10
29	c1	509	CLA	C11-C10-C8-C7
29	c1	512	CLA	C11-C10-C8-C7
29	d1	403	CLA	C11-C10-C8-C7
29	d1	403	CLA	C11-C12-C13-C15
29	n1	602	CLA	C11-C12-C13-C15
29	g1	603	CLA	C12-C13-C15-C16
29	y1	610	CLA	C12-C13-C15-C16
30	A	409	PHO	C6-C7-C8-C10
30	a1	409	PHO	C6-C7-C8-C10
38	B	624	3PH	O11-C1-C2-O21
38	s1	626	3PH	O11-C1-C2-O21
40	d	410	LHG	O6-C4-C5-O7
40	d1	410	LHG	O6-C4-C5-O7
48	N	605	CHL	C11-C12-C13-C15
48	Y	607	CHL	C11-C10-C8-C7
48	n	607	CHL	C11-C12-C13-C15
48	g	601	CHL	C6-C7-C8-C10
48	g	607	CHL	C11-C10-C8-C7
48	g	609	CHL	C11-C12-C13-C15
48	y	601	CHL	C3A-C2A-CAA-CBA
48	y	606	CHL	C11-C12-C13-C15
48	y	607	CHL	C12-C13-C15-C16
48	N1	609	CHL	C12-C13-C15-C16
48	G1	607	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
48	Y1	607	CHL	C11-C10-C8-C7
48	n1	601	CHL	C11-C12-C13-C15
48	g1	609	CHL	C12-C13-C15-C16
48	y1	609	CHL	C11-C12-C13-C15
49	R	620	LUT	C25-C26-C27-C28
49	S	620	LUT	C25-C26-C27-C28
49	Y	620	LUT	C25-C26-C27-C28
49	y	620	LUT	C25-C26-C27-C28
49	R1	620	LUT	C25-C26-C27-C28
49	g1	620	LUT	C25-C26-C27-C28
49	r1	620	LUT	C25-C26-C27-C28
49	s1	621	LUT	C25-C26-C27-C28
49	y1	620	LUT	C25-C26-C27-C28
55	y	626	PTY	O14-C5-C6-O7
55	y	627	PTY	O14-C5-C6-O7
55	Y1	626	PTY	O14-C5-C6-O7
55	y1	626	PTY	O14-C5-C6-O7
38	B1	624	3PH	C28-C29-C2A-C2B
29	B	613	CLA	C3-C5-C6-C7
29	b	615	CLA	O1A-CGA-O2A-C1
36	b	620	C7Z	C13-C14-C15-C35
32	b1	621	SQD	O47-C7-C8-C9
33	C1	521	LMG	O7-C10-C11-C12
32	c	526	SQD	C18-C19-C20-C21
37	c1	520	DGD	CAB-CBB-CCB-CDB
29	G	613	CLA	C13-C15-C16-C17
40	S	624	LHG	C23-C24-C25-C26
40	D	410	LHG	C8-C7-O7-C5
40	d1	410	LHG	O2-C2-C3-O3
32	B	621	SQD	C26-C27-C28-C29
38	s1	626	3PH	C35-C36-C37-C38
39	j	101	DGA	CB4-CB5-CB6-CB7
39	J1	101	DGA	CA2-CA3-CA4-CA5
29	N1	602	CLA	C8-C10-C11-C12
29	A	405	CLA	C2A-CAA-CBA-CGA
29	B	610	CLA	C2A-CAA-CBA-CGA
29	n	602	CLA	C2A-CAA-CBA-CGA
29	r	610	CLA	C2A-CAA-CBA-CGA
48	G	607	CHL	C2A-CAA-CBA-CGA
34	A	414	SPH	C11-C12-C13-C14
38	T1	101	3PH	C2F-C2G-C2H-C2I
40	D	409	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
40	g1	624	LHG	C16-C17-C18-C19
29	Y	614	CLA	C3-C5-C6-C7
29	A1	405	CLA	CAA-CBA-CGA-O2A
48	g	606	CHL	CAA-CBA-CGA-O2A
29	R1	608	CLA	C8-C10-C11-C12
32	C1	526	SQD	O6-C44-C45-C46
33	B	622	LMG	O1-C7-C8-C9
33	H	102	LMG	C7-C8-C9-O8
33	h1	102	LMG	C40-C41-C42-C43
33	w1	201	LMG	C7-C8-C9-O8
34	a1	414	SPH	C1-C2-C3-C4
37	c1	519	DGD	O1G-C1G-C2G-C3G
40	D	409	LHG	C34-C35-C36-C37
40	d	410	LHG	C11-C10-C9-C8
40	d1	408	LHG	C34-C35-C36-C37
32	A1	412	SQD	O6-C44-C45-O47
32	C1	526	SQD	O6-C44-C45-O47
33	B	622	LMG	O7-C8-C9-O8
33	H	102	LMG	O7-C8-C9-O8
33	b	622	LMG	O7-C8-C9-O8
33	b1	622	LMG	O7-C8-C9-O8
33	c1	523	LMG	O7-C8-C9-O8
37	c1	520	DGD	O1G-C1G-C2G-O2G
38	t1	101	3PH	O21-C2-C3-O31
39	C1	524	DGA	OG1-CG1-CG2-OG2
39	b1	625	DGA	OG1-CG1-CG2-OG2
40	s1	624	LHG	O7-C5-C6-O8
41	C1	527	LMK	O1-C7-C8-O7
47	k	101	4RF	O21-C20-C39-O40
55	y	626	PTY	O4-C1-C6-O7
55	y	627	PTY	O4-C1-C6-O7
32	A	412	SQD	C28-C29-C30-C31
32	m1	101	SQD	C11-C12-C13-C14
33	C1	521	LMG	C29-C30-C31-C32
33	A	413	LMG	C29-C30-C31-C32
40	y1	624	LHG	C26-C27-C28-C29
40	N1	624	LHG	C12-C13-C14-C15
33	w1	201	LMG	C8-C7-O1-C1
37	C	519	DGD	C5D-C6D-O5D-C1E
37	c	519	DGD	C2G-C3G-O3G-C1D
37	C1	519	DGD	C5D-C6D-O5D-C1E
37	c1	519	DGD	C5D-C6D-O5D-C1E

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Mol	Chain	Res	Type	Atoms
29	s1	617	CLA	CAA-CBA-CGA-O2A
29	C	507	CLA	C16-C17-C18-C20
29	b	603	CLA	C16-C17-C18-C20
29	c1	505	CLA	C16-C17-C18-C19
29	G	602	CLA	C5-C6-C7-C8
29	b	614	CLA	C15-C16-C17-C18
29	c	512	CLA	C5-C6-C7-C8
47	i	101	4RF	C53-C54-C55-C56
38	T	101	3PH	C2-C1-O11-P
40	c	525	LHG	C2-C3-O3-P
29	B1	617	CLA	C15-C16-C17-C18
29	G1	613	CLA	C4-C3-C5-C6
29	s1	611	CLA	C4-C3-C5-C6
48	n1	605	CHL	C4-C3-C5-C6
39	j	101	DGA	CA2-CA1-OG1-CG1
40	g1	624	LHG	C24-C23-O8-C6
37	C	520	DGD	C4A-C5A-C6A-C7A
37	C	520	DGD	C5A-C6A-C7A-C8A
40	L1	101	LHG	C26-C27-C28-C29
29	Y	614	CLA	C2-C3-C5-C6
48	Y1	607	CHL	C2-C3-C5-C6
40	L	101	LHG	C35-C36-C37-C38
47	i	101	4RF	C03-C04-C05-C06
29	c	505	CLA	C13-C15-C16-C17
29	B1	605	CLA	C10-C11-C12-C13
29	C	502	CLA	C6-C7-C8-C9
29	C	502	CLA	C14-C13-C15-C16
29	C	504	CLA	C11-C10-C8-C9
29	C	509	CLA	C11-C10-C8-C9
29	D	402	CLA	C11-C10-C8-C9
29	G	603	CLA	C14-C13-C15-C16
29	b	602	CLA	C11-C10-C8-C9
29	b	607	CLA	C11-C12-C13-C14
29	b	609	CLA	C11-C10-C8-C9
29	b	612	CLA	C14-C13-C15-C16
29	b	613	CLA	C11-C10-C8-C9
29	b	616	CLA	C11-C12-C13-C14
29	b	617	CLA	C6-C7-C8-C9
29	c	511	CLA	C11-C12-C13-C14
29	c	513	CLA	C14-C13-C15-C16
29	n	613	CLA	C11-C10-C8-C9
29	r	609	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	r	612	CLA	C6-C7-C8-C9
29	s	610	CLA	C11-C10-C8-C9
29	y	613	CLA	C14-C13-C15-C16
29	A1	406	CLA	C14-C13-C15-C16
29	B1	603	CLA	C11-C10-C8-C9
29	B1	609	CLA	C11-C10-C8-C9
29	B1	611	CLA	C11-C12-C13-C14
29	B1	616	CLA	C11-C12-C13-C14
29	C1	502	CLA	C11-C12-C13-C14
29	C1	511	CLA	C6-C7-C8-C9
29	D1	403	CLA	C11-C10-C8-C9
29	N1	602	CLA	C14-C13-C15-C16
29	N1	610	CLA	C14-C13-C15-C16
29	G1	602	CLA	C14-C13-C15-C16
29	G1	610	CLA	C6-C7-C8-C9
29	S1	610	CLA	C11-C12-C13-C14
29	a1	405	CLA	C11-C10-C8-C9
29	b1	603	CLA	C6-C7-C8-C9
29	b1	603	CLA	C11-C10-C8-C9
29	b1	613	CLA	C11-C10-C8-C9
29	n1	610	CLA	C14-C13-C15-C16
48	G	607	CHL	C6-C7-C8-C9
48	G	609	CHL	C11-C12-C13-C14
48	G	609	CHL	C14-C13-C15-C16
48	Y	609	CHL	C11-C10-C8-C9
48	Y	609	CHL	C14-C13-C15-C16
48	n	606	CHL	C11-C12-C13-C14
48	y	607	CHL	C11-C10-C8-C9
48	N1	606	CHL	C11-C12-C13-C14
48	Y1	601	CHL	C6-C7-C8-C9
48	n1	601	CHL	C14-C13-C15-C16
48	n1	605	CHL	C14-C13-C15-C16
48	n1	606	CHL	C14-C13-C15-C16
48	g1	601	CHL	C6-C7-C8-C9
48	y1	606	CHL	C11-C10-C8-C9
47	K1	101	4RF	O17-C16-O18-C19
39	C	524	DGA	CAB-CBB-CCB-CDB
39	c	524	DGA	CEA-CFA-CGA-CHA
29	B1	606	CLA	C3-C5-C6-C7
29	c1	501	CLA	C3-C5-C6-C7
30	a1	408	PHO	C3-C5-C6-C7
32	a1	412	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
33	d	411	LMG	O6-C1-O1-C7
32	b1	621	SQD	C23-C24-C25-C26
29	s1	614	CLA	C2A-CAA-CBA-CGA
46	I1	101	GOL	O2-C2-C3-O3
47	i	101	4RF	C25-C26-C27-C28
49	r	620	LUT	C33-C34-C35-C15
51	R1	622	NEX	C13-C14-C15-C35
32	B	626	SQD	C32-C33-C34-C35
34	a	414	SPH	C6-C7-C8-C9
40	n	624	LHG	C33-C34-C35-C36
49	N1	620	LUT	C31-C32-C33-C40
40	Y	624	LHG	C32-C33-C34-C35
39	B	625	DGA	CA1-CA2-CA3-CA4
29	s1	609	CLA	C11-C12-C13-C14
39	b	625	DGA	CA2-CA3-CA4-CA5
40	N1	624	LHG	C30-C31-C32-C33
31	c1	514	BCR	C17-C18-C19-C20
29	n1	613	CLA	C8-C10-C11-C12
32	B	626	SQD	C15-C16-C17-C18
38	B	624	3PH	C3A-C3B-C3C-C3D
39	B	625	DGA	CBA-CCA-CDA-CEA
40	D	409	LHG	C33-C34-C35-C36
40	S1	624	LHG	C24-C25-C26-C27
55	y	626	PTY	C40-C41-C42-C43
29	B	617	CLA	C2B-C3B-CAB-CBB
29	C	502	CLA	C2B-C3B-CAB-CBB
29	C	503	CLA	C2B-C3B-CAB-CBB
29	G	603	CLA	C2B-C3B-CAB-CBB
29	G	612	CLA	C2B-C3B-CAB-CBB
29	S	605	CLA	C2B-C3B-CAB-CBB
29	Y	608	CLA	C2B-C3B-CAB-CBB
29	b	607	CLA	C2B-C3B-CAB-CBB
29	c	501	CLA	C2B-C3B-CAB-CBB
29	c	504	CLA	C2B-C3B-CAB-CBB
29	c	505	CLA	C2B-C3B-CAB-CBB
29	c	507	CLA	C2B-C3B-CAB-CBB
29	g	613	CLA	C2B-C3B-CAB-CBB
29	s	602	CLA	C2B-C3B-CAB-CBB
29	s	609	CLA	C2B-C3B-CAB-CBB
29	B1	614	CLA	C2B-C3B-CAB-CBB
29	C1	510	CLA	C2B-C3B-CAB-CBB
29	G1	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	G1	603	CLA	C2B-C3B-CAB-CBB
29	R1	610	CLA	C2B-C3B-CAB-CBB
29	R1	612	CLA	C2B-C3B-CAB-CBB
29	S1	605	CLA	C2B-C3B-CAB-CBB
29	Y1	613	CLA	C2B-C3B-CAB-CBB
29	b1	604	CLA	C2B-C3B-CAB-CBB
29	c1	504	CLA	C2B-C3B-CAB-CBB
29	n1	602	CLA	C2B-C3B-CAB-CBB
29	g1	611	CLA	C2B-C3B-CAB-CBB
29	g1	614	CLA	C2B-C3B-CAB-CBB
29	r1	602	CLA	C2B-C3B-CAB-CBB
29	s1	611	CLA	C2B-C3B-CAB-CBB
29	y1	602	CLA	C2B-C3B-CAB-CBB
29	y1	608	CLA	C2B-C3B-CAB-CBB
39	j1	101	DGA	OA1-CA1-OG1-CG1
29	C1	505	CLA	C10-C11-C12-C13
51	y	623	NEX	C39-C29-C30-C31
34	A	414	SPH	C11-C10-C9-C8
47	K1	101	4RF	C35-C36-C37-C38
29	B	616	CLA	C4-C3-C5-C6
29	C	506	CLA	C4-C3-C5-C6
48	n	605	CHL	C4-C3-C5-C6
40	N	624	LHG	C16-C17-C18-C19
40	S	624	LHG	C31-C32-C33-C34
40	d1	408	LHG	C32-C33-C34-C35
29	y	611	CLA	C2-C3-C5-C6
29	g1	603	CLA	C5-C6-C7-C8
47	k	101	4RF	C13-C14-C15-C16
29	G	611	CLA	C16-C17-C18-C19
29	R1	602	CLA	C11-C12-C13-C15
33	c	523	LMG	C30-C31-C32-C33
33	A1	413	LMG	C16-C17-C18-C19
40	l	101	LHG	C17-C18-C19-C20
41	C1	527	LMK	C31-C32-C33-C34
40	d	410	LHG	C29-C30-C31-C32
29	c1	506	CLA	C8-C10-C11-C12
29	N	611	CLA	C1-C2-C3-C4
29	G	604	CLA	C1-C2-C3-C4
29	G	614	CLA	C1-C2-C3-C4
29	n	611	CLA	C1-C2-C3-C4
29	g	604	CLA	C1-C2-C3-C4
29	g	614	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
29	N1	611	CLA	C1-C2-C3-C4
29	G1	604	CLA	C1-C2-C3-C4
29	G1	614	CLA	C1-C2-C3-C4
29	n1	611	CLA	C1-C2-C3-C4
29	g1	604	CLA	C1-C2-C3-C4
29	g1	614	CLA	C1-C2-C3-C4
34	A1	414	SPH	C2-C3-C4-C5
48	N	608	CHL	C1-C2-C3-C4
48	G	606	CHL	C1-C2-C3-C4
48	R	607	CHL	C1-C2-C3-C4
48	n	608	CHL	C1-C2-C3-C4
48	g	606	CHL	C1-C2-C3-C4
48	r	607	CHL	C1-C2-C3-C4
48	N1	608	CHL	C1-C2-C3-C4
48	G1	606	CHL	C1-C2-C3-C4
48	R1	607	CHL	C1-C2-C3-C4
48	n1	608	CHL	C1-C2-C3-C4
48	g1	606	CHL	C1-C2-C3-C4
48	r1	607	CHL	C1-C2-C3-C4
34	y1	625	SPH	C14-C15-C16-C17
39	c	524	DGA	CB4-CB5-CB6-CB7
39	b1	625	DGA	CFB-CGB-CHB-CIB
29	D	402	CLA	CAA-CBA-CGA-O2A
33	h	102	LMG	C15-C16-C17-C18
29	C	505	CLA	C15-C16-C17-C18
29	B1	607	CLA	C15-C16-C17-C18
32	B	621	SQD	C46-C45-O47-C7
32	M	101	SQD	C46-C45-O47-C7
32	m	101	SQD	C46-C45-O47-C7
32	b1	621	SQD	C46-C45-O47-C7
32	m1	101	SQD	C46-C45-O47-C7
33	b	622	LMG	C9-C8-O7-C10
33	C1	523	LMG	C7-C8-O7-C10
39	B1	625	DGA	CG1-CG2-OG2-CB1
40	L	101	LHG	C6-C5-O7-C7
55	y	626	PTY	O14-C5-C6-C1
29	B	615	CLA	C2A-CAA-CBA-CGA
29	s	611	CLA	C2A-CAA-CBA-CGA
29	B1	607	CLA	C2A-CAA-CBA-CGA
29	G1	610	CLA	C2A-CAA-CBA-CGA
29	c1	510	CLA	C2A-CAA-CBA-CGA
48	N1	607	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
48	n1	608	CHL	C2A-CAA-CBA-CGA
32	c1	526	SQD	C16-C17-C18-C19
41	C	527	LMK	C13-C14-C15-C27
40	D	410	LHG	O9-C7-O7-C5
39	j1	101	DGA	CA2-CA1-OG1-CG1
29	a	405	CLA	C10-C11-C12-C13
29	B	610	CLA	C2-C1-O2A-CGA
29	C	513	CLA	C2-C1-O2A-CGA
29	N	602	CLA	C2-C1-O2A-CGA
29	N	604	CLA	C2-C1-O2A-CGA
29	S	611	CLA	C2-C1-O2A-CGA
29	y	602	CLA	C2-C1-O2A-CGA
29	N1	614	CLA	C2-C1-O2A-CGA
29	S1	617	CLA	C2-C1-O2A-CGA
29	r1	603	CLA	C2-C1-O2A-CGA
30	a	409	PHO	C2-C1-O2A-CGA
48	N	609	CHL	C2-C1-O2A-CGA
48	Y	601	CHL	C2-C1-O2A-CGA
48	y	601	CHL	C2-C1-O2A-CGA
48	Y1	609	CHL	C2-C1-O2A-CGA
48	n1	608	CHL	C2-C1-O2A-CGA
38	b1	624	3PH	C35-C36-C37-C38
40	d1	410	LHG	C31-C32-C33-C34
29	g	613	CLA	C16-C17-C18-C19
40	S1	624	LHG	C7-C8-C9-C10
32	C1	526	SQD	C34-C35-C36-C37
38	t	101	3PH	C35-C36-C37-C38
40	C	525	LHG	C12-C13-C14-C15
32	M	101	SQD	O47-C7-C8-C9
48	G	607	CHL	CAA-CBA-CGA-O2A
29	b1	614	CLA	C5-C6-C7-C8
29	A	406	CLA	C3-C5-C6-C7
32	b	626	SQD	C16-C17-C18-C19
40	S	624	LHG	C14-C15-C16-C17
29	B	610	CLA	C5-C6-C7-C8
41	C	527	LMK	C30-C31-C32-C33
31	B	619	BCR	C19-C20-C21-C22
53	R	626	ERG	C22-C23-C24-C28
29	n1	613	CLA	O1A-CGA-O2A-C1
39	j	101	DGA	OA1-CA1-OG1-CG1
32	b1	621	SQD	C14-C15-C16-C17
34	y	625	SPH	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
48	g1	601	CHL	C16-C17-C18-C19
40	s1	624	LHG	C23-C24-C25-C26
48	g1	606	CHL	O2A-C1-C2-C3
29	B	605	CLA	C4-C3-C5-C6
29	C1	506	CLA	C4-C3-C5-C6
29	c1	513	CLA	C4-C3-C5-C6
29	n1	610	CLA	C4-C3-C5-C6
38	t	101	3PH	C23-C24-C25-C26
39	C1	524	DGA	CB9-CAB-CBB-CCB
31	C	514	BCR	C23-C24-C25-C30
31	C	517	BCR	C1-C6-C7-C8
31	b	619	BCR	C23-C24-C25-C30
31	B1	618	BCR	C1-C6-C7-C8
31	C1	514	BCR	C23-C24-C25-C30
31	b1	618	BCR	C1-C6-C7-C8
49	N	621	LUT	C1-C6-C7-C8
49	N	621	LUT	C5-C6-C7-C8
49	S	621	LUT	C5-C6-C7-C8
49	g	621	LUT	C5-C6-C7-C8
49	N1	620	LUT	C5-C6-C7-C8
49	G1	621	LUT	C5-C6-C7-C8
49	n1	620	LUT	C1-C6-C7-C8
49	n1	620	LUT	C5-C6-C7-C8
29	s	602	CLA	C2-C3-C5-C6
29	B1	615	CLA	C2-C3-C5-C6
29	C1	505	CLA	C2-C3-C5-C6
29	y1	603	CLA	C2-C3-C5-C6
48	N	606	CHL	C2-C3-C5-C6
48	n1	609	CHL	C2-C3-C5-C6
40	g	624	LHG	C35-C36-C37-C38
40	N1	624	LHG	C33-C34-C35-C36
40	g1	624	LHG	O10-C23-O8-C6
55	Y	626	PTY	C35-C36-C37-C38
29	b1	615	CLA	CBA-CGA-O2A-C1
40	N	624	LHG	O8-C23-C24-C25
39	C	524	DGA	CEA-CFA-CGA-CHA
39	B1	625	DGA	CFB-CGB-CHB-CIB
29	B	613	CLA	C16-C17-C18-C20
29	g	610	CLA	C16-C17-C18-C19
29	a1	405	CLA	C16-C17-C18-C19
29	n1	604	CLA	C16-C17-C18-C20
29	C1	513	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	d1	411	LMG	C11-C10-O7-C8
47	I1	102	4RF	C46-C47-C48-C49
29	B	606	CLA	C2A-CAA-CBA-CGA
29	B	613	CLA	C2A-CAA-CBA-CGA
29	B1	613	CLA	C2A-CAA-CBA-CGA
29	R1	608	CLA	C2A-CAA-CBA-CGA
30	a1	408	PHO	C2A-CAA-CBA-CGA
48	G1	601	CHL	C2A-CAA-CBA-CGA
51	y	623	NEX	C28-C29-C30-C31
51	G1	623	NEX	C11-C10-C9-C8
51	s1	623	NEX	C28-C29-C30-C31
33	a	413	LMG	C31-C32-C33-C34
55	y	626	PTY	C13-C14-C15-C16
32	A	412	SQD	O47-C45-C46-O48
33	B	622	LMG	O1-C7-C8-O7
33	a	413	LMG	O7-C8-C9-O8
33	a1	413	LMG	O7-C8-C9-O8
37	c	519	DGD	O1G-C1G-C2G-O2G
39	j1	101	DGA	OG1-CG1-CG2-OG2
40	C	525	LHG	O7-C5-C6-O8
40	c	525	LHG	O7-C5-C6-O8
29	n1	604	CLA	C8-C10-C11-C12
33	B	622	LMG	C14-C15-C16-C17
33	C	521	LMG	C31-C32-C33-C34
39	J1	101	DGA	CA5-CA6-CA7-CA8
40	D1	409	LHG	C31-C32-C33-C34
40	G	624	LHG	C3-O3-P-O6
40	Y	624	LHG	C3-O3-P-O6
40	c	525	LHG	C3-O3-P-O6
40	l	101	LHG	C4-O6-P-O3
40	g	624	LHG	C3-O3-P-O6
40	G1	624	LHG	C3-O3-P-O6
40	c1	525	LHG	C3-O3-P-O6
40	n1	624	LHG	C3-O3-P-O6
40	g1	624	LHG	C3-O3-P-O6
40	y1	624	LHG	C3-O3-P-O6
54	S	625	LPX	C1-O2-P1-O1
55	Y	626	PTY	C5-O14-P1-O11
55	Y	627	PTY	C3-O11-P1-O14
55	Y1	626	PTY	C5-O14-P1-O11
55	Y1	627	PTY	C3-O11-P1-O14
32	C1	526	SQD	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
38	T	101	3PH	C3F-C3G-C3H-C3I
40	C	525	LHG	C17-C18-C19-C20
37	C	520	DGD	O6D-C5D-C6D-O5D
33	A	413	LMG	C34-C35-C36-C37
55	Y	626	PTY	C23-C24-C25-C26
37	C1	520	DGD	C1A-C2A-C3A-C4A
47	I	102	4RF	C22-C24-C25-C26
53	R1	626	ERG	C23-C24-C25-C26
40	Y	624	LHG	C19-C20-C21-C22
40	c	525	LHG	C14-C15-C16-C17
54	S1	625	LPX	C7-C6-O6-C5
32	A	412	SQD	O6-C44-C45-C46
33	b	622	LMG	O1-C7-C8-C9
29	Y	603	CLA	C4-C3-C5-C6
29	Y1	603	CLA	C4-C3-C5-C6
34	A1	414	SPH	C7-C8-C9-C10
47	I	102	4RF	C29-C30-C31-C32
47	k	101	4RF	C34-C35-C36-C37
29	A	405	CLA	C12-C13-C15-C16
29	A	406	CLA	C11-C10-C8-C7
29	B	615	CLA	C2-C3-C5-C6
29	D	402	CLA	C6-C7-C8-C10
29	b	612	CLA	C12-C13-C15-C16
29	n	610	CLA	C12-C13-C15-C16
29	s	611	CLA	C11-C12-C13-C15
29	B1	602	CLA	C11-C12-C13-C15
29	B1	616	CLA	C11-C10-C8-C7
29	B1	616	CLA	C12-C13-C15-C16
29	Y1	610	CLA	C11-C12-C13-C15
29	Y1	611	CLA	C11-C10-C8-C7
29	b1	614	CLA	C11-C10-C8-C7
29	g1	603	CLA	C6-C7-C8-C10
29	g1	610	CLA	C12-C13-C15-C16
30	a	408	PHO	C11-C12-C13-C15
43	D	405	PL9	C13-C14-C16-C17
43	D	405	PL9	C18-C19-C21-C22
48	Y	601	CHL	C6-C7-C8-C10
48	g	607	CHL	C12-C13-C15-C16
40	g1	624	LHG	C33-C34-C35-C36
47	I1	102	4RF	C53-C54-C55-C56
29	B	605	CLA	C14-C13-C15-C16
29	B	613	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	C	501	CLA	C11-C10-C8-C9
29	C	512	CLA	C11-C10-C8-C9
29	G	610	CLA	C6-C7-C8-C9
29	R	610	CLA	C11-C10-C8-C9
29	S	602	CLA	C6-C7-C8-C9
29	Y	603	CLA	C11-C12-C13-C14
29	a	410	CLA	C6-C7-C8-C9
29	c	502	CLA	C6-C7-C8-C9
29	c	507	CLA	C14-C13-C15-C16
29	g	613	CLA	C14-C13-C15-C16
29	B1	602	CLA	C6-C7-C8-C9
29	C1	506	CLA	C11-C10-C8-C9
29	G1	611	CLA	C11-C10-C8-C9
29	S1	610	CLA	C11-C10-C8-C9
29	Y1	602	CLA	C6-C7-C8-C9
29	Y1	602	CLA	C14-C13-C15-C16
29	a1	410	CLA	C6-C7-C8-C9
29	b1	602	CLA	C14-C13-C15-C16
29	b1	616	CLA	C11-C12-C13-C14
29	c1	503	CLA	C14-C13-C15-C16
29	n1	602	CLA	C11-C12-C13-C14
29	r1	609	CLA	C6-C7-C8-C9
29	s1	603	CLA	C11-C10-C8-C9
29	y1	610	CLA	C14-C13-C15-C16
29	y1	611	CLA	C11-C12-C13-C14
29	y1	614	CLA	C11-C10-C8-C9
48	N	601	CHL	C14-C13-C15-C16
48	G	601	CHL	C6-C7-C8-C9
48	y	609	CHL	C14-C13-C15-C16
48	G1	607	CHL	C6-C7-C8-C9
48	G1	609	CHL	C11-C12-C13-C14
48	Y1	606	CHL	C6-C7-C8-C9
48	y1	606	CHL	C14-C13-C15-C16
29	b1	603	CLA	C13-C15-C16-C17
31	c	514	BCR	C15-C16-C17-C18
31	C1	517	BCR	C9-C10-C11-C12
49	S	621	LUT	C29-C30-C31-C32
49	r	620	LUT	C9-C10-C11-C12
49	y1	621	LUT	C33-C34-C35-C15
50	Y1	622	XAT	C13-C14-C15-C35
51	S	623	NEX	C33-C34-C35-C15
29	B1	613	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	y1	613	CLA	C16-C17-C18-C20
32	B	626	SQD	C27-C28-C29-C30
32	b1	621	SQD	C10-C11-C12-C13
54	S	625	LPX	C10-C11-C12-C13
32	C	526	SQD	C28-C29-C30-C31
40	y	624	LHG	C24-C25-C26-C27
40	y1	624	LHG	C11-C12-C13-C14
32	C	526	SQD	C24-C23-O48-C46
32	m	101	SQD	O49-C7-C8-C9
33	a	413	LMG	C11-C12-C13-C14
38	B1	624	3PH	C36-C37-C38-C39
55	Y1	626	PTY	C24-C25-C26-C27
33	D	411	LMG	C33-C34-C35-C36
33	w	201	LMG	C33-C34-C35-C36
34	A	414	SPH	C15-C16-C17-C18
37	c	518	DGD	CCB-CDB-CEB-CFB
40	D	410	LHG	C10-C11-C12-C13
40	l	101	LHG	C11-C12-C13-C14
40	D1	409	LHG	C14-C15-C16-C17
40	n1	624	LHG	C17-C18-C19-C20
29	n	602	CLA	C8-C10-C11-C12
29	c	505	CLA	C16-C17-C18-C19
29	y	613	CLA	C16-C17-C18-C20
29	b1	609	CLA	C16-C17-C18-C19
29	s1	614	CLA	C6-C7-C8-C10
32	C1	526	SQD	C35-C36-C37-C38
40	d	409	LHG	C30-C31-C32-C33
47	k1	101	4RF	C43-C41-O40-C39
40	d	409	LHG	C2-C3-O3-P
40	D1	408	LHG	C5-C4-O6-P
40	G1	624	LHG	C2-C3-O3-P
47	k1	101	4RF	C45-C46-C47-C48
29	Y1	610	CLA	C10-C11-C12-C13
29	c1	504	CLA	C13-C15-C16-C17
49	G	620	LUT	C27-C28-C29-C30
50	g	622	XAT	C11-C12-C13-C14
50	g1	622	XAT	C27-C28-C29-C30
32	B1	621	SQD	C26-C27-C28-C29
33	b1	622	LMG	C33-C34-C35-C36
37	c1	518	DGD	CAB-CBB-CCB-CDB
38	S1	626	3PH	C3C-C3D-C3E-C3F
38	s1	626	3PH	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
40	d1	410	LHG	C1-C2-C3-O3
33	H1	102	LMG	C15-C16-C17-C18
29	n	603	CLA	C4-C3-C5-C6
29	y	612	CLA	C4-C3-C5-C6
38	B1	624	3PH	C21-C22-C23-C24
29	n	604	CLA	C2-C3-C5-C6
29	n	613	CLA	C2-C3-C5-C6
48	n	605	CHL	C2-C3-C5-C6
38	T	101	3PH	C25-C26-C27-C28
29	s1	609	CLA	C11-C12-C13-C15
29	c	508	CLA	CBA-CGA-O2A-C1
30	a	408	PHO	C10-C11-C12-C13
29	b1	615	CLA	O1A-CGA-O2A-C1
47	k1	101	4RF	O42-C41-O40-C39
52	r	625	LMT	C4'-C5'-C6'-O6'
33	h	102	LMG	C11-C12-C13-C14
33	b1	622	LMG	C19-C20-C21-C22
41	C1	527	LMK	C2-C1-O1-C7
33	D1	411	LMG	C16-C17-C18-C19
38	s	626	3PH	C28-C29-C2A-C2B
39	C1	524	DGA	CBB-CCB-CDB-CEB
29	s	610	CLA	CBD-CGD-O2D-CED
33	h1	102	LMG	C29-C28-O8-C9
55	Y	626	PTY	C30-C31-C32-C33
32	b1	621	SQD	C27-C28-C29-C30
40	D	408	LHG	C11-C10-C9-C8
29	C	502	CLA	C4B-C3B-CAB-CBB
29	C	503	CLA	C4B-C3B-CAB-CBB
29	R	602	CLA	C4B-C3B-CAB-CBB
29	S	604	CLA	C4B-C3B-CAB-CBB
29	S	605	CLA	C4B-C3B-CAB-CBB
29	a	407	CLA	C4B-C3B-CAB-CBB
29	b	603	CLA	C4B-C3B-CAB-CBB
29	c	502	CLA	C4B-C3B-CAB-CBB
29	c	505	CLA	C4B-C3B-CAB-CBB
29	c	507	CLA	C4B-C3B-CAB-CBB
29	n	604	CLA	C4B-C3B-CAB-CBB
29	n	610	CLA	C4B-C3B-CAB-CBB
29	s	609	CLA	C4B-C3B-CAB-CBB
29	B1	614	CLA	C4B-C3B-CAB-CBB
29	C1	510	CLA	C4B-C3B-CAB-CBB
29	Y1	613	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	n1	602	CLA	C4B-C3B-CAB-CBB
29	n1	604	CLA	C4B-C3B-CAB-CBB
29	g1	611	CLA	C4B-C3B-CAB-CBB
29	g1	614	CLA	C4B-C3B-CAB-CBB
29	y1	602	CLA	C4B-C3B-CAB-CBB
29	r	608	CLA	C2A-CAA-CBA-CGA
29	s	605	CLA	C2A-CAA-CBA-CGA
48	n	607	CHL	C2A-CAA-CBA-CGA
48	N1	605	CHL	CAA-CBA-CGA-O1A
32	m1	101	SQD	O5-C1-O6-C44
37	C1	519	DGD	O6D-C1D-O3G-C3G
31	D	404	BCR	C19-C20-C21-C22
31	d	404	BCR	C9-C10-C11-C12
31	C1	515	BCR	C19-C20-C21-C22
31	C1	516	BCR	C19-C20-C21-C22
31	b1	618	BCR	C19-C20-C21-C22
36	b	620	C7Z	C9-C10-C11-C12
49	R1	620	LUT	C29-C30-C31-C32
49	Y1	621	LUT	C13-C14-C15-C35
49	y1	621	LUT	C29-C30-C31-C32
50	Y	622	XAT	C13-C14-C15-C35
51	r	622	NEX	C33-C34-C35-C15
51	N1	623	NEX	C13-C14-C15-C35
51	R1	622	NEX	C9-C10-C11-C12
51	R1	622	NEX	C29-C30-C31-C32
51	n1	623	NEX	C9-C10-C11-C12
32	C	526	SQD	O10-C23-O48-C46
29	C	509	CLA	C5-C6-C7-C8
29	G	602	CLA	C10-C11-C12-C13
29	b	615	CLA	C15-C16-C17-C18
47	i1	101	4RF	C31-C32-C33-C34
38	S1	626	3PH	C3D-C3E-C3F-C3G
40	D	410	LHG	C26-C27-C28-C29
40	L	101	LHG	C12-C13-C14-C15
31	C1	514	BCR	C18-C19-C20-C21
50	y1	622	XAT	C10-C11-C12-C13
51	G	623	NEX	C10-C11-C12-C13
51	r	622	NEX	C30-C31-C32-C33
51	y1	623	NEX	C30-C31-C32-C33
54	S1	625	LPX	O7-C6-O6-C5
29	c1	505	CLA	C15-C16-C17-C18
53	R	626	ERG	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
29	C	508	CLA	C16-C17-C18-C20
32	B1	621	SQD	O47-C7-C8-C9
38	S1	626	3PH	O31-C31-C32-C33
29	B1	602	CLA	C3-C5-C6-C7
32	B	626	SQD	C31-C32-C33-C34
40	D1	409	LHG	C29-C30-C31-C32
29	R	608	CLA	C4-C3-C5-C6
29	n	613	CLA	C4-C3-C5-C6
29	B1	610	CLA	C4-C3-C5-C6
29	g1	613	CLA	C4-C3-C5-C6
48	y1	601	CHL	C4-C3-C5-C6
48	G	601	CHL	C5-C6-C7-C8
32	m1	101	SQD	C9-C10-C11-C12
33	C1	523	LMG	C36-C37-C38-C39
40	D	409	LHG	C24-C25-C26-C27
47	k	101	4RF	C53-C54-C55-C56
33	h1	102	LMG	O10-C28-O8-C9
33	d	411	LMG	C11-C12-C13-C14
29	B	617	CLA	C13-C15-C16-C17
29	S	614	CLA	C5-C6-C7-C8
40	D1	408	LHG	O9-C7-O7-C5
33	c	521	LMG	C36-C37-C38-C39
39	c1	524	DGA	CA6-CA7-CA8-CA9
40	S1	624	LHG	C35-C36-C37-C38
47	k1	101	4RF	C46-C47-C48-C49
55	Y1	626	PTY	C37-C38-C39-C40
29	b	610	CLA	C2-C1-O2A-CGA
29	y	610	CLA	C2-C1-O2A-CGA
29	G1	610	CLA	C2-C1-O2A-CGA
29	c1	513	CLA	C2-C1-O2A-CGA
29	y1	610	CLA	C2-C1-O2A-CGA
48	n	608	CHL	C2-C1-O2A-CGA
48	g	606	CHL	C2-C1-O2A-CGA
48	y	606	CHL	C2-C1-O2A-CGA
48	Y1	606	CHL	C2-C1-O2A-CGA
48	n1	607	CHL	C2-C1-O2A-CGA
38	S	626	3PH	C26-C27-C28-C29
39	b	625	DGA	CFB-CGB-CHB-CIB
29	B1	612	CLA	C16-C17-C18-C20
33	D	411	LMG	C12-C13-C14-C15
33	d1	411	LMG	C11-C12-C13-C14
43	D1	405	PL9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
53	R1	626	ERG	C22-C23-C24-C28
32	M	101	SQD	C2-C1-O6-C44
29	c	505	CLA	C2A-CAA-CBA-CGA
29	s	604	CLA	C2A-CAA-CBA-CGA
29	G1	602	CLA	C2A-CAA-CBA-CGA
29	S1	611	CLA	C2A-CAA-CBA-CGA
29	c1	506	CLA	C2A-CAA-CBA-CGA
38	b	624	3PH	O21-C2-C3-O31
40	D1	410	LHG	O7-C5-C6-O8
48	Y	606	CHL	C2A-CAA-CBA-CGA
48	G1	607	CHL	C2A-CAA-CBA-CGA
48	R1	607	CHL	C2A-CAA-CBA-CGA
48	n1	607	CHL	C2A-CAA-CBA-CGA
32	c	526	SQD	C30-C31-C32-C33
38	S1	626	3PH	C39-C3A-C3B-C3C
29	n1	613	CLA	CBA-CGA-O2A-C1
55	Y1	626	PTY	C30-C31-C32-C33
32	C	526	SQD	C18-C19-C20-C21
33	B	622	LMG	C33-C34-C35-C36
38	S1	626	3PH	C3E-C3F-C3G-C3H
39	c	524	DGA	CA8-CA9-CAA-CBA
40	s1	624	LHG	C25-C26-C27-C28
40	n1	624	LHG	O10-C23-C24-C25
29	g	612	CLA	C3A-C2A-CAA-CBA
29	b1	607	CLA	C3A-C2A-CAA-CBA
29	c1	511	CLA	C3A-C2A-CAA-CBA
29	s1	609	CLA	C3A-C2A-CAA-CBA
48	g	601	CHL	C3A-C2A-CAA-CBA
48	n1	609	CHL	C3A-C2A-CAA-CBA
29	b1	616	CLA	C16-C17-C18-C20
29	r1	610	CLA	C11-C12-C13-C15
29	s1	611	CLA	C16-C17-C18-C19
37	c	519	DGD	C3A-C4A-C5A-C6A
48	n	608	CHL	O2A-C1-C2-C3
29	R1	609	CLA	CAA-CBA-CGA-O2A
39	c1	524	DGA	CEB-CFB-CGB-CHB
40	s	624	LHG	C32-C33-C34-C35
40	C1	525	LHG	C25-C26-C27-C28
29	d	402	CLA	CBA-CGA-O2A-C1
29	c	503	CLA	C8-C10-C11-C12
32	B	626	SQD	C18-C19-C20-C21
40	y	624	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
41	c	527	LMK	C32-C33-C34-C16
47	k	101	4RF	C51-C52-C53-C54
48	y	605	CHL	CAA-CBA-CGA-O1A
40	D1	408	LHG	C26-C27-C28-C29
40	g1	624	LHG	C29-C30-C31-C32
41	C1	527	LMK	C28-C29-C30-C31
29	B	610	CLA	C14-C13-C15-C16
29	B	616	CLA	C6-C7-C8-C9
29	G	602	CLA	C11-C12-C13-C14
29	a	406	CLA	C14-C13-C15-C16
29	b	604	CLA	C11-C10-C8-C9
29	b	614	CLA	C11-C12-C13-C14
29	r	603	CLA	C6-C7-C8-C9
29	A1	406	CLA	C6-C7-C8-C9
29	B1	603	CLA	C11-C12-C13-C14
29	B1	603	CLA	C14-C13-C15-C16
29	B1	614	CLA	C11-C12-C13-C14
29	D1	402	CLA	C6-C7-C8-C9
29	G1	611	CLA	C14-C13-C15-C16
29	S1	603	CLA	C11-C12-C13-C14
29	S1	611	CLA	C11-C10-C8-C9
29	S1	611	CLA	C14-C13-C15-C16
29	Y1	613	CLA	C6-C7-C8-C9
29	b1	604	CLA	C14-C13-C15-C16
29	b1	615	CLA	C11-C10-C8-C9
29	n1	613	CLA	C14-C13-C15-C16
29	g1	603	CLA	C11-C10-C8-C9
29	r1	603	CLA	C6-C7-C8-C9
29	y1	603	CLA	C6-C7-C8-C9
29	y1	611	CLA	C6-C7-C8-C9
30	A	409	PHO	C6-C7-C8-C9
30	a	409	PHO	C6-C7-C8-C9
48	N	607	CHL	C14-C13-C15-C16
48	Y	601	CHL	C6-C7-C8-C9
48	Y	606	CHL	C11-C12-C13-C14
48	g	601	CHL	C6-C7-C8-C9
48	g	601	CHL	C11-C10-C8-C9
48	g	609	CHL	C6-C7-C8-C9
48	n1	601	CHL	C11-C10-C8-C9
32	B1	626	SQD	C9-C10-C11-C12
33	c1	523	LMG	C16-C17-C18-C19
39	C	524	DGA	CB6-CB7-CB8-CB9

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Mol	Chain	Res	Type	Atoms
48	y	605	CHL	CAA-CBA-CGA-O2A
33	B1	622	LMG	C14-C15-C16-C17
40	N	624	LHG	C31-C32-C33-C34
47	I	102	4RF	C32-C33-C34-C35
29	S	613	CLA	C2C-C3C-CAC-CBC
37	B1	623	DGD	C2A-C3A-C4A-C5A
39	c1	524	DGA	CDB-CEB-CFB-CGB
40	n	624	LHG	C30-C31-C32-C33
48	y1	609	CHL	C2C-C3C-CAC-CBC
29	c	506	CLA	C8-C10-C11-C12
29	c	509	CLA	C13-C15-C16-C17
33	w1	201	LMG	O1-C7-C8-C9
49	n	621	LUT	C21-C26-C27-C28
49	g	621	LUT	C21-C26-C27-C28
49	s1	620	LUT	C21-C26-C27-C28
50	y1	622	XAT	C40-C33-C34-C35
51	N	623	NEX	C39-C29-C30-C31
51	G	623	NEX	C39-C29-C30-C31
51	R	622	NEX	C40-C33-C34-C35
51	S	623	NEX	C39-C29-C30-C31
51	Y	623	NEX	C20-C13-C14-C15
51	n	623	NEX	C39-C29-C30-C31
51	r	622	NEX	C39-C29-C30-C31
51	r	622	NEX	C40-C33-C34-C35
51	g1	623	NEX	C39-C29-C30-C31
51	s1	623	NEX	C39-C29-C30-C31
29	N	613	CLA	C3-C5-C6-C7
29	G	613	CLA	C3-C5-C6-C7
32	c1	526	SQD	O49-C7-O47-C45
33	W1	201	LMG	C32-C33-C34-C35
40	S	624	LHG	C15-C16-C17-C18
32	M1	101	SQD	O47-C7-C8-C9
29	n	612	CLA	CAA-CBA-CGA-O1A
29	y1	604	CLA	C2A-CAA-CBA-CGA
29	g1	613	CLA	C5-C6-C7-C8
40	g1	624	LHG	O10-C23-C24-C25
33	B	622	LMG	C29-C30-C31-C32
47	K	101	4RF	C04-C05-C06-C07
29	C1	503	CLA	C16-C17-C18-C19
29	R1	612	CLA	C11-C12-C13-C14
29	b1	605	CLA	C16-C17-C18-C19
29	n1	604	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
53	r	626	ERG	C22-C23-C24-C25
40	S1	624	LHG	C24-C23-O8-C6
33	c	523	LMG	O6-C1-O1-C7
33	C1	523	LMG	O6-C1-O1-C7
32	A	412	SQD	C33-C34-C35-C36
33	C1	523	LMG	C18-C19-C20-C21
33	a1	413	LMG	C13-C14-C15-C16
38	t1	101	3PH	C28-C29-C2A-C2B
40	d	410	LHG	C26-C27-C28-C29
55	Y	626	PTY	C25-C26-C27-C28
29	C	509	CLA	C13-C15-C16-C17
40	D	410	LHG	C30-C31-C32-C33
49	N1	620	LUT	C31-C32-C33-C34
32	a	412	SQD	C29-C30-C31-C32
32	B1	626	SQD	C11-C12-C13-C14
33	a	413	LMG	C30-C31-C32-C33
33	c1	521	LMG	C34-C35-C36-C37
55	Y1	626	PTY	C38-C39-C40-C41
29	n	612	CLA	CAA-CBA-CGA-O2A
37	b	623	DGD	C1G-C2G-O2G-C1B
37	b1	623	DGD	C1G-C2G-O2G-C1B
40	l	101	LHG	C6-C5-O7-C7
29	N1	603	CLA	C4-C3-C5-C6
29	B	612	CLA	C1A-C2A-CAA-CBA
29	N	613	CLA	C1A-C2A-CAA-CBA
29	a	410	CLA	C1A-C2A-CAA-CBA
29	b	609	CLA	C1A-C2A-CAA-CBA
29	c	506	CLA	C1A-C2A-CAA-CBA
29	d	402	CLA	C1A-C2A-CAA-CBA
29	g	612	CLA	C1A-C2A-CAA-CBA
29	r	602	CLA	C1A-C2A-CAA-CBA
29	s	602	CLA	C1A-C2A-CAA-CBA
29	C1	504	CLA	C1A-C2A-CAA-CBA
29	G1	611	CLA	C1A-C2A-CAA-CBA
29	a1	410	CLA	C1A-C2A-CAA-CBA
29	b1	612	CLA	C1A-C2A-CAA-CBA
29	c1	506	CLA	C1A-C2A-CAA-CBA
48	N	606	CHL	C1A-C2A-CAA-CBA
48	N	607	CHL	C1A-C2A-CAA-CBA
48	Y	601	CHL	C1A-C2A-CAA-CBA
48	g	608	CHL	C1A-C2A-CAA-CBA
48	r	607	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
48	y	601	CHL	C1A-C2A-CAA-CBA
48	n1	601	CHL	C1A-C2A-CAA-CBA
48	n1	609	CHL	C1A-C2A-CAA-CBA
40	n	624	LHG	C29-C30-C31-C32
55	Y	626	PTY	C15-C16-C17-C18
48	Y1	606	CHL	C16-C17-C18-C20
29	B	602	CLA	C11-C10-C8-C7
29	B	613	CLA	C6-C7-C8-C10
29	B	617	CLA	C12-C13-C15-C16
29	C	506	CLA	C2-C3-C5-C6
29	N	603	CLA	C11-C12-C13-C15
29	N	604	CLA	C6-C7-C8-C10
29	G	603	CLA	C11-C10-C8-C7
29	R	602	CLA	C11-C10-C8-C7
29	Y	602	CLA	C12-C13-C15-C16
29	a	405	CLA	C11-C10-C8-C7
29	b	606	CLA	C11-C10-C8-C7
29	c	502	CLA	C11-C10-C8-C7
29	c	507	CLA	C11-C12-C13-C15
29	c	508	CLA	C11-C10-C8-C7
29	y	613	CLA	C6-C7-C8-C10
29	C1	513	CLA	C12-C13-C15-C16
29	S1	610	CLA	C6-C7-C8-C10
29	b1	604	CLA	C11-C10-C8-C7
29	b1	605	CLA	C11-C10-C8-C7
29	b1	617	CLA	C6-C7-C8-C10
29	c1	513	CLA	C11-C12-C13-C15
29	s1	611	CLA	C6-C7-C8-C10
29	y1	611	CLA	C11-C10-C8-C7
43	d1	405	PL9	C12-C11-C9-C8
48	N	607	CHL	C12-C13-C15-C16
48	G	601	CHL	C11-C12-C13-C15
48	y	601	CHL	C12-C13-C15-C16
48	N1	605	CHL	C11-C12-C13-C15
48	N1	606	CHL	C12-C13-C15-C16
48	S1	608	CHL	C11-C10-C8-C7
29	C1	510	CLA	C3-C5-C6-C7
33	C	523	LMG	C30-C31-C32-C33
55	Y1	626	PTY	C33-C34-C35-C36
31	c	517	BCR	C9-C10-C11-C12
51	Y	623	NEX	C9-C10-C11-C12
51	Y1	623	NEX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
41	c1	527	LMK	C9-C8-O7-C10
47	K1	101	4RF	C34-C35-C36-C37
47	i1	101	4RF	C24-C25-C26-C27
29	N	613	CLA	CAA-CBA-CGA-O2A
48	S	601	CHL	CAA-CBA-CGA-O2A
40	D	409	LHG	C15-C16-C17-C18
40	G	624	LHG	C10-C11-C12-C13
29	B	607	CLA	C16-C17-C18-C19
29	b	608	CLA	C16-C17-C18-C20
29	s1	603	CLA	C16-C17-C18-C20
33	b	622	LMG	C31-C32-C33-C34
33	h1	102	LMG	C33-C34-C35-C36
29	b1	615	CLA	C3-C5-C6-C7
40	d	408	LHG	C2-C3-O3-P
29	S	611	CLA	C2A-CAA-CBA-CGA
29	B1	606	CLA	C2A-CAA-CBA-CGA
48	g	607	CHL	C2A-CAA-CBA-CGA
37	C	519	DGD	O6D-C5D-C6D-O5D
41	c	527	LMK	O10-C28-C29-C30
29	R	612	CLA	C10-C11-C12-C13
29	C1	504	CLA	C5-C6-C7-C8
29	a1	410	CLA	C5-C6-C7-C8
32	B	626	SQD	C19-C20-C21-C22
40	n	624	LHG	C32-C33-C34-C35
47	K	101	4RF	C50-C51-C52-C53
53	R1	626	ERG	C28-C24-C25-C26
29	S	612	CLA	CAA-CBA-CGA-O1A
38	S1	626	3PH	C2A-C2B-C2C-C2D
55	Y	626	PTY	C12-C13-C14-C15
32	C	526	SQD	O49-C7-O47-C45
29	b	605	CLA	C5-C6-C7-C8
30	a	408	PHO	CBA-CGA-O2A-C1
40	D	410	LHG	C34-C35-C36-C37
55	Y	626	PTY	O14-C5-C6-C1
38	t	101	3PH	C29-C2A-C2B-C2C
40	D	408	LHG	C30-C31-C32-C33
47	k1	101	4RF	C27-C28-C29-C30
29	g	613	CLA	C16-C17-C18-C20
29	C1	510	CLA	C16-C17-C18-C20
29	c1	507	CLA	C8-C10-C11-C12
38	T1	101	3PH	C2E-C2F-C2G-C2H
29	B	612	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	S1	604	CLA	C4-C3-C5-C6
29	c1	506	CLA	C4-C3-C5-C6
29	y1	614	CLA	C4-C3-C5-C6
48	Y1	601	CHL	C4-C3-C5-C6
33	C	521	LMG	C37-C38-C39-C40
33	b1	622	LMG	C11-C12-C13-C14
39	C1	524	DGA	CFA-CGA-CHA-CIA
47	I1	102	4RF	C10-C11-C12-C13
55	Y1	626	PTY	C11-C12-C13-C14
29	C	502	CLA	C10-C11-C12-C13
29	B	616	CLA	C2-C3-C5-C6
29	Y	603	CLA	C2-C3-C5-C6
29	Y1	603	CLA	C2-C3-C5-C6
43	d	405	PL9	C28-C29-C31-C32
29	B	610	CLA	C2B-C3B-CAB-CBB
29	N	604	CLA	C2B-C3B-CAB-CBB
29	R	608	CLA	C2B-C3B-CAB-CBB
29	S	604	CLA	C2B-C3B-CAB-CBB
29	S	610	CLA	C2B-C3B-CAB-CBB
29	a	407	CLA	C2B-C3B-CAB-CBB
29	b	616	CLA	C2B-C3B-CAB-CBB
29	b	617	CLA	C2B-C3B-CAB-CBB
29	n	604	CLA	C2B-C3B-CAB-CBB
29	n	610	CLA	C2B-C3B-CAB-CBB
29	g	611	CLA	C2B-C3B-CAB-CBB
29	g	612	CLA	C2B-C3B-CAB-CBB
29	C1	504	CLA	C2B-C3B-CAB-CBB
29	R1	604	CLA	C2B-C3B-CAB-CBB
29	S1	603	CLA	C2B-C3B-CAB-CBB
29	b1	617	CLA	C2B-C3B-CAB-CBB
29	c1	501	CLA	C2B-C3B-CAB-CBB
29	n1	611	CLA	C2B-C3B-CAB-CBB
29	y1	603	CLA	C2B-C3B-CAB-CBB
40	L1	101	LHG	C12-C13-C14-C15
40	Y1	624	LHG	C17-C18-C19-C20
29	R1	609	CLA	C5-C6-C7-C8
32	B1	626	SQD	C7-C8-C9-C10
40	Y	624	LHG	C7-C8-C9-C10
40	Y1	624	LHG	O9-C7-O7-C5
38	b	624	3PH	C2A-C2B-C2C-C2D
33	c1	521	LMG	O9-C10-C11-C12
33	B1	622	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
34	a1	414	SPH	N2-C2-C3-C4
51	N	623	NEX	C28-C29-C30-C31
51	G	623	NEX	C28-C29-C30-C31
51	S	623	NEX	C28-C29-C30-C31
51	n	623	NEX	C28-C29-C30-C31
51	r	622	NEX	C28-C29-C30-C31
51	Y1	623	NEX	C11-C10-C9-C8
51	g1	623	NEX	C28-C29-C30-C31
29	y	602	CLA	C8-C10-C11-C12
30	a	409	PHO	C8-C10-C11-C12
48	S	601	CHL	CAA-CBA-CGA-O1A
48	s	601	CHL	CAA-CBA-CGA-O2A
32	M	101	SQD	O47-C45-C46-O48
32	m1	101	SQD	O47-C45-C46-O48
33	C1	521	LMG	O7-C8-C9-O8
33	d1	411	LMG	O7-C8-C9-O8
55	Y1	626	PTY	O4-C1-C6-O7
40	y1	624	LHG	C30-C31-C32-C33
47	k	101	4RF	C22-C24-C25-C26
31	c	516	BCR	C15-C16-C17-C18
49	N1	621	LUT	C33-C34-C35-C15
49	R1	620	LUT	C33-C34-C35-C15
49	Y1	621	LUT	C29-C30-C31-C32
49	n1	620	LUT	C29-C30-C31-C32
50	g	622	XAT	C9-C10-C11-C12
51	N	623	NEX	C29-C30-C31-C32
29	S	612	CLA	CAA-CBA-CGA-O2A
29	B1	604	CLA	C10-C11-C12-C13
29	c1	502	CLA	C13-C15-C16-C17
48	N1	601	CHL	C10-C11-C12-C13
39	J1	101	DGA	CA6-CA7-CA8-CA9
32	C	526	SQD	C31-C32-C33-C34
32	c1	526	SQD	C34-C35-C36-C37
34	a	414	SPH	C11-C10-C9-C8
39	c	524	DGA	CA3-CA4-CA5-CA6
40	g1	624	LHG	C34-C35-C36-C37
47	k1	101	4RF	C29-C30-C31-C32
33	w	201	LMG	O6-C1-O1-C7
29	B	605	CLA	C10-C11-C12-C13
37	c	519	DGD	C6A-C7A-C8A-C9A
39	c	524	DGA	CA5-CA6-CA7-CA8
40	D	408	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
40	C1	525	LHG	C17-C18-C19-C20
40	s1	624	LHG	C27-C28-C29-C30
30	a	408	PHO	O1A-CGA-O2A-C1
39	C1	524	DGA	CG1-CG2-CG3-OXT
39	c1	524	DGA	CG1-CG2-CG3-OXT
43	d1	405	PL9	C14-C16-C17-C18
33	c1	523	LMG	C30-C31-C32-C33
37	C	520	DGD	C4B-C5B-C6B-C7B
29	R1	609	CLA	C4-C3-C5-C6
29	b1	612	CLA	C4-C3-C5-C6
43	d1	405	PL9	C32-C33-C34-C35
48	N1	607	CHL	C4-C3-C5-C6
32	c	526	SQD	C27-C28-C29-C30
38	t1	101	3PH	C3F-C3G-C3H-C3I
29	A	410	CLA	C2-C1-O2A-CGA
29	B	605	CLA	C2-C1-O2A-CGA
29	a	410	CLA	C2-C1-O2A-CGA
29	b	606	CLA	C2-C1-O2A-CGA
29	c	513	CLA	C2-C1-O2A-CGA
29	b1	609	CLA	C2-C1-O2A-CGA
29	b1	610	CLA	C2-C1-O2A-CGA
48	n	601	CHL	C2-C1-O2A-CGA
48	g	601	CHL	C2-C1-O2A-CGA
48	g	609	CHL	C2-C1-O2A-CGA
29	G1	613	CLA	C2-C3-C5-C6
43	d1	405	PL9	C13-C14-C16-C17
48	N1	605	CHL	C2-C3-C5-C6
48	Y1	601	CHL	C2-C3-C5-C6
38	t1	101	3PH	C2E-C2F-C2G-C2H
29	d	402	CLA	O1A-CGA-O2A-C1
29	g1	611	CLA	C5-C6-C7-C8
41	c1	527	LMK	C14-C15-C27-C35
55	y1	626	PTY	C20-C21-C22-C23
29	S	614	CLA	CAA-CBA-CGA-O2A
40	g	624	LHG	O8-C23-C24-C25
29	A	405	CLA	C14-C13-C15-C16
29	C	512	CLA	C11-C12-C13-C14
29	b	608	CLA	C11-C12-C13-C14
29	b	611	CLA	C11-C12-C13-C14
29	d	403	CLA	C14-C13-C15-C16
29	n	604	CLA	C6-C7-C8-C9
29	y	602	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	B1	610	CLA	C11-C12-C13-C14
29	b1	611	CLA	C11-C12-C13-C14
29	s1	602	CLA	C11-C10-C8-C9
48	S1	608	CHL	C11-C10-C8-C9
48	y1	606	CHL	C11-C12-C13-C14
34	Y	625	SPH	C13-C14-C15-C16
34	a	414	SPH	C12-C13-C14-C15
37	C	519	DGD	C2B-C3B-C4B-C5B
37	c1	520	DGD	C4B-C5B-C6B-C7B
29	D	402	CLA	C3-C5-C6-C7
29	C	503	CLA	C5-C6-C7-C8
38	S	626	3PH	C22-C21-O21-C2
40	D1	408	LHG	C8-C7-O7-C5
29	N1	613	CLA	CAA-CBA-CGA-O2A
32	B	621	SQD	O47-C7-C8-C9
33	c	521	LMG	O7-C10-C11-C12
33	b	622	LMG	C22-C23-C24-C25
37	C	519	DGD	CCA-CDA-CEA-CFA
47	K	101	4RF	C33-C34-C35-C36
33	C	523	LMG	O6-C5-C6-O5
29	C1	510	CLA	C10-C11-C12-C13
29	R1	608	CLA	C10-C11-C12-C13
48	N1	609	CHL	C13-C15-C16-C17
29	C	502	CLA	C2A-CAA-CBA-CGA
29	y1	613	CLA	C2A-CAA-CBA-CGA
30	a	408	PHO	C2A-CAA-CBA-CGA
48	S	601	CHL	C2A-CAA-CBA-CGA
48	N1	605	CHL	C2A-CAA-CBA-CGA
48	s	601	CHL	CAA-CBA-CGA-O1A
40	Y	624	LHG	C34-C35-C36-C37
29	c	508	CLA	O1A-CGA-O2A-C1
31	A	411	BCR	C1-C6-C7-C8
31	A	411	BCR	C5-C6-C7-C8
31	B	619	BCR	C23-C24-C25-C30
31	c	517	BCR	C23-C24-C25-C30
31	A1	411	BCR	C23-C24-C25-C30
45	H	101	RRX	C23-C24-C25-C30
49	G	621	LUT	C1-C6-C7-C8
49	R	620	LUT	C1-C6-C7-C8
49	S	621	LUT	C1-C6-C7-C8
49	Y	621	LUT	C1-C6-C7-C8
49	s	620	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
49	y	620	LUT	C1-C6-C7-C8
49	N1	620	LUT	C1-C6-C7-C8
49	S1	620	LUT	C1-C6-C7-C8
49	Y1	620	LUT	C1-C6-C7-C8
29	y1	613	CLA	C13-C15-C16-C17
29	A1	410	CLA	C2C-C3C-CAC-CBC
47	I	102	4RF	C26-C27-C28-C29
49	y	620	LUT	C27-C28-C29-C39
29	A	406	CLA	C15-C16-C17-C18
40	N	624	LHG	O1-C1-C2-C3
33	b1	622	LMG	C14-C15-C16-C17
37	C	519	DGD	CCB-CDB-CEB-CFB
52	r	625	LMT	C7-C8-C9-C10
40	S1	624	LHG	O10-C23-O8-C6
31	B	618	BCR	C15-C16-C17-C18
31	B1	618	BCR	C13-C14-C15-C16
31	b1	619	BCR	C9-C10-C11-C12
49	N1	620	LUT	C33-C34-C35-C15
32	M	101	SQD	C10-C11-C12-C13
33	b1	622	LMG	C15-C16-C17-C18
29	r1	603	CLA	C4-C3-C5-C6
29	s1	613	CLA	C4-C3-C5-C6
43	d1	405	PL9	C12-C11-C9-C10
43	d1	405	PL9	C15-C14-C16-C17
48	n	609	CHL	C4-C3-C5-C6
48	g	607	CHL	C4-C3-C5-C6
48	N1	609	CHL	C4-C3-C5-C6
49	y	620	LUT	C27-C28-C29-C30
50	g1	622	XAT	C31-C32-C33-C34
29	C	508	CLA	C16-C17-C18-C19
29	B1	613	CLA	C16-C17-C18-C20
29	C	510	CLA	C5-C6-C7-C8
29	N1	613	CLA	C15-C16-C17-C18
29	c1	502	CLA	C2C-C3C-CAC-CBC
29	n	603	CLA	C2-C3-C5-C6
29	C1	506	CLA	C2-C3-C5-C6
29	s1	611	CLA	C2-C3-C5-C6
48	n1	605	CHL	C2-C3-C5-C6
29	D1	402	CLA	CAA-CBA-CGA-O2A
38	T	101	3PH	C23-C24-C25-C26
39	j1	101	DGA	CA7-CA8-CA9-CAA
33	a1	413	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
37	C	518	DGD	C5D-C6D-O5D-C1E
40	c	525	LHG	C8-C7-O7-C5
40	d	409	LHG	C8-C7-O7-C5
37	C1	520	DGD	C3A-C4A-C5A-C6A
33	d1	411	LMG	C4-C5-C6-O5
37	c1	519	DGD	C9A-CAA-CBA-CCA
33	d1	411	LMG	O10-C28-O8-C9
29	s1	602	CLA	CAA-CBA-CGA-O2A
33	a1	413	LMG	C14-C15-C16-C17
33	d1	411	LMG	C14-C15-C16-C17
29	A	410	CLA	C11-C12-C13-C14
29	B	602	CLA	C16-C17-C18-C20
29	B	603	CLA	C16-C17-C18-C19
29	y	612	CLA	C16-C17-C18-C19
29	r1	603	CLA	C11-C12-C13-C15
29	B	610	CLA	C3-C5-C6-C7
29	c	501	CLA	C3-C5-C6-C7
34	A1	414	SPH	C4-C5-C6-C7
29	B1	613	CLA	C8-C10-C11-C12
29	G1	602	CLA	C15-C16-C17-C18
38	T	101	3PH	O11-C1-C2-O21
40	D1	410	LHG	O6-C4-C5-O7
33	d	411	LMG	C10-C11-C12-C13
39	B	625	DGA	CDA-CEA-CFA-CGA
29	s	612	CLA	CAA-CBA-CGA-O2A
48	s1	601	CHL	CAA-CBA-CGA-O2A
29	N	603	CLA	C2A-CAA-CBA-CGA
29	N	604	CLA	C2A-CAA-CBA-CGA
29	B1	610	CLA	C2A-CAA-CBA-CGA
29	R1	603	CLA	C2A-CAA-CBA-CGA
37	C	518	DGD	C4A-C5A-C6A-C7A
40	c1	525	LHG	C17-C18-C19-C20
40	g1	624	LHG	C30-C31-C32-C33
29	s1	614	CLA	CAA-CBA-CGA-O2A
54	s	625	LPX	C6-C7-C8-C9
40	d	409	LHG	O9-C7-O7-C5
29	s	605	CLA	C4C-C3C-CAC-CBC
41	C1	527	LMK	O7-C10-C11-C12
29	C1	501	CLA	C3-C5-C6-C7
29	B	610	CLA	C4B-C3B-CAB-CBB
29	N	604	CLA	C4B-C3B-CAB-CBB
29	S	610	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	b	617	CLA	C4B-C3B-CAB-CBB
29	y	610	CLA	C4B-C3B-CAB-CBB
29	R1	604	CLA	C4B-C3B-CAB-CBB
29	y1	611	CLA	C4B-C3B-CAB-CBB
29	y1	612	CLA	C4B-C3B-CAB-CBB
29	B	612	CLA	C16-C17-C18-C20
32	A	412	SQD	C32-C33-C34-C35
34	a1	414	SPH	C11-C10-C9-C8
40	s1	624	LHG	C35-C36-C37-C38
47	K	101	4RF	C54-C55-C56-C57
47	i	101	4RF	C26-C27-C28-C29
38	B	624	3PH	C2D-C2E-C2F-C2G
38	T	101	3PH	C3C-C3D-C3E-C3F
38	s	626	3PH	C31-C32-C33-C34
29	C	512	CLA	C4-C3-C5-C6
29	R	609	CLA	C4-C3-C5-C6
29	C1	510	CLA	C4-C3-C5-C6
48	y1	606	CHL	C4-C3-C5-C6
40	Y1	624	LHG	C8-C7-O7-C5
29	b1	602	CLA	CAA-CBA-CGA-O1A
29	g	613	CLA	C11-C12-C13-C15
29	y	602	CLA	C11-C12-C13-C15
29	y	614	CLA	C6-C7-C8-C10
29	N1	603	CLA	C2-C3-C5-C6
29	a1	410	CLA	C6-C7-C8-C10
29	b1	608	CLA	C11-C12-C13-C15
29	b1	612	CLA	C2-C3-C5-C6
29	n1	613	CLA	C12-C13-C15-C16
29	y1	614	CLA	C2-C3-C5-C6
48	n	609	CHL	C2-C3-C5-C6
48	G1	607	CHL	C11-C12-C13-C15
29	b1	613	CLA	C15-C16-C17-C18
40	l	101	LHG	C33-C34-C35-C36
39	B1	625	DGA	OG2-CG2-CG3-OXT
39	C1	524	DGA	OG2-CG2-CG3-OXT
39	b1	625	DGA	OG2-CG2-CG3-OXT
33	H	102	LMG	O9-C10-C11-C12
36	b	620	C7Z	C33-C34-C35-C15
50	y	622	XAT	C9-C10-C11-C12
38	B	624	3PH	O31-C31-C32-C33
48	n1	607	CHL	CAA-CBA-CGA-O2A
33	W	201	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
29	B	606	CLA	C16-C17-C18-C19
38	S1	626	3PH	C2-C1-O11-P
40	L1	101	LHG	C1-C2-C3-O3
32	a	412	SQD	C26-C27-C28-C29
33	H1	102	LMG	O7-C8-C9-O8
37	C1	519	DGD	O1G-C1G-C2G-O2G
29	Y	610	CLA	CBA-CGA-O2A-C1
39	c1	524	DGA	CCB-CDB-CEB-CFB
40	G	624	LHG	C35-C36-C37-C38
29	b	602	CLA	CAA-CBA-CGA-O1A
33	c	521	LMG	C33-C34-C35-C36
29	y	604	CLA	C13-C15-C16-C17
29	b1	602	CLA	C8-C10-C11-C12
48	s1	601	CHL	CAA-CBA-CGA-O1A
48	r	607	CHL	O2A-C1-C2-C3
48	n1	608	CHL	O2A-C1-C2-C3
29	R	612	CLA	CAA-CBA-CGA-O2A
29	g	613	CLA	CAA-CBA-CGA-O2A
29	g	614	CLA	CAA-CBA-CGA-O2A
29	Y1	613	CLA	CAA-CBA-CGA-O2A
37	C1	518	DGD	O1G-C1A-C2A-C3A
38	s	626	3PH	O21-C21-C22-C23
39	c	524	DGA	OG2-CB1-CB2-CB3
40	D1	409	LHG	O7-C7-C8-C9
33	C1	521	LMG	C33-C34-C35-C36
29	B	607	CLA	O1A-CGA-O2A-C1
29	b1	609	CLA	C10-C11-C12-C13
48	n	607	CHL	C8-C10-C11-C12
29	b1	606	CLA	C16-C17-C18-C19
29	b1	609	CLA	C16-C17-C18-C20
29	c1	513	CLA	C16-C17-C18-C19
43	D1	405	PL9	C2-C3-C7-C8
33	C	523	LMG	C36-C37-C38-C39
29	N1	610	CLA	C8-C10-C11-C12
32	c1	526	SQD	C9-C10-C11-C12
38	T	101	3PH	C1-O11-P-O13
39	J1	101	DGA	CA7-CA8-CA9-CAA
47	i	101	4RF	C08-C09-C10-C11
50	y	622	XAT	C40-C33-C34-C35
50	y1	622	XAT	C20-C13-C14-C15
51	g	623	NEX	C20-C13-C14-C15
51	y1	623	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	b1	608	CLA	CAA-CBA-CGA-O2A
29	b1	615	CLA	CAA-CBA-CGA-O2A
29	c1	505	CLA	CAA-CBA-CGA-O2A
30	A	409	PHO	CAA-CBA-CGA-O2A
37	b	623	DGD	O1G-C1A-C2A-C3A
38	S1	626	3PH	O21-C21-C22-C23
38	t1	101	3PH	O31-C31-C32-C33
40	D	408	LHG	O7-C7-C8-C9
29	s	605	CLA	C2C-C3C-CAC-CBC
47	I1	102	4RF	C03-C04-C05-C06
29	c	506	CLA	C4-C3-C5-C6
29	c	513	CLA	C4-C3-C5-C6
30	A1	408	PHO	C4-C3-C5-C6
48	y	601	CHL	C4-C3-C5-C6
48	S1	608	CHL	C4-C3-C5-C6
48	g1	607	CHL	C4-C3-C5-C6
29	N	603	CLA	C10-C11-C12-C13
29	B	612	CLA	C2-C3-C5-C6
29	r	609	CLA	C2-C3-C5-C6
29	c1	506	CLA	C2-C3-C5-C6
29	n1	610	CLA	C2-C3-C5-C6
29	r1	603	CLA	C2-C3-C5-C6
43	d1	405	PL9	C28-C29-C31-C32
48	N1	607	CHL	C2-C3-C5-C6
33	h1	102	LMG	C34-C35-C36-C37
38	B1	624	3PH	C33-C34-C35-C36
29	B	615	CLA	C16-C17-C18-C20
29	Y1	610	CLA	C16-C17-C18-C19
30	a1	409	PHO	C16-C17-C18-C19
38	b1	624	3PH	O21-C21-C22-C23
29	S	613	CLA	C4C-C3C-CAC-CBC
29	A	406	CLA	C11-C10-C8-C9
29	B	602	CLA	C14-C13-C15-C16
29	B	606	CLA	C14-C13-C15-C16
29	B	608	CLA	C14-C13-C15-C16
29	B	610	CLA	C11-C12-C13-C14
29	N	604	CLA	C6-C7-C8-C9
29	G	611	CLA	C11-C10-C8-C9
29	Y	602	CLA	C14-C13-C15-C16
29	Y	604	CLA	C6-C7-C8-C9
29	Y	610	CLA	C14-C13-C15-C16
29	b	605	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	c	501	CLA	C14-C13-C15-C16
29	c	504	CLA	C14-C13-C15-C16
29	c	507	CLA	C11-C12-C13-C14
29	c	508	CLA	C11-C10-C8-C9
29	y	611	CLA	C11-C10-C8-C9
29	y	613	CLA	C6-C7-C8-C9
29	B1	605	CLA	C6-C7-C8-C9
29	B1	608	CLA	C14-C13-C15-C16
29	B1	617	CLA	C11-C12-C13-C14
29	C1	505	CLA	C6-C7-C8-C9
29	C1	506	CLA	C6-C7-C8-C9
29	N1	604	CLA	C6-C7-C8-C9
29	G1	611	CLA	C11-C12-C13-C14
29	R1	612	CLA	C6-C7-C8-C9
29	S1	610	CLA	C6-C7-C8-C9
29	Y1	603	CLA	C14-C13-C15-C16
29	a1	406	CLA	C14-C13-C15-C16
29	b1	617	CLA	C6-C7-C8-C9
29	b1	617	CLA	C11-C12-C13-C14
29	c1	501	CLA	C14-C13-C15-C16
29	c1	504	CLA	C14-C13-C15-C16
29	c1	509	CLA	C11-C10-C8-C9
29	c1	511	CLA	C6-C7-C8-C9
29	c1	513	CLA	C14-C13-C15-C16
29	d1	403	CLA	C11-C10-C8-C9
29	d1	403	CLA	C11-C12-C13-C14
29	s1	602	CLA	C6-C7-C8-C9
48	N	605	CHL	C11-C12-C13-C14
48	Y	606	CHL	C11-C10-C8-C9
48	Y	607	CHL	C11-C10-C8-C9
48	y	606	CHL	C11-C12-C13-C14
48	N1	601	CHL	C14-C13-C15-C16
29	b	613	CLA	C3-C5-C6-C7
40	g1	624	LHG	C18-C19-C20-C21
29	G	612	CLA	C3A-C2A-CAA-CBA
29	b	617	CLA	C3A-C2A-CAA-CBA
29	s	605	CLA	C3A-C2A-CAA-CBA
29	y	608	CLA	C3A-C2A-CAA-CBA
29	S1	605	CLA	C3A-C2A-CAA-CBA
29	b1	603	CLA	C3A-C2A-CAA-CBA
29	s1	617	CLA	C3A-C2A-CAA-CBA
29	y1	613	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	A	408	PHO	C3A-C2A-CAA-CBA
30	A1	409	PHO	C3A-C2A-CAA-CBA
48	N	607	CHL	C3A-C2A-CAA-CBA
48	g	608	CHL	C3A-C2A-CAA-CBA
48	G1	609	CHL	C3A-C2A-CAA-CBA
48	n1	608	CHL	C3A-C2A-CAA-CBA
48	g1	601	CHL	C3A-C2A-CAA-CBA
39	b	625	DGA	CBB-CAB-CB9-CB8
40	y1	624	LHG	C17-C18-C19-C20
48	g1	605	CHL	C2-C1-O2A-CGA
29	Y	613	CLA	CAA-CBA-CGA-O2A
29	B1	603	CLA	CAA-CBA-CGA-O2A
29	n1	604	CLA	CAA-CBA-CGA-O2A
33	C	523	LMG	O7-C10-C11-C12
33	d	411	LMG	O7-C10-C11-C12
48	y	606	CHL	CAA-CBA-CGA-O2A
32	a1	412	SQD	C32-C33-C34-C35
33	A1	413	LMG	C34-C35-C36-C37
40	y	624	LHG	C27-C28-C29-C30
40	s1	624	LHG	C11-C10-C9-C8
29	s	612	CLA	CAA-CBA-CGA-O1A
29	C	502	CLA	CAD-CBD-CGD-O2D
29	C	504	CLA	CAD-CBD-CGD-O2D
29	C	510	CLA	CAD-CBD-CGD-O2D
29	R	602	CLA	CAD-CBD-CGD-O2D
29	Y	603	CLA	CAD-CBD-CGD-O2D
29	Y	614	CLA	CAD-CBD-CGD-O2D
29	b	605	CLA	CAD-CBD-CGD-O2D
29	b	606	CLA	CAD-CBD-CGD-O2D
29	c	510	CLA	CAD-CBD-CGD-O2D
29	c	512	CLA	CAD-CBD-CGD-O2D
29	n	611	CLA	CAD-CBD-CGD-O2D
29	r	603	CLA	CAD-CBD-CGD-O2D
29	C1	506	CLA	CAD-CBD-CGD-O2D
29	N1	602	CLA	CAD-CBD-CGD-O2D
29	N1	604	CLA	CAD-CBD-CGD-O2D
29	G1	603	CLA	CAD-CBD-CGD-O2D
29	G1	614	CLA	CAD-CBD-CGD-O2D
29	n1	603	CLA	CAD-CBD-CGD-O2D
29	n1	612	CLA	CAD-CBD-CGD-O2D
29	g1	602	CLA	CAD-CBD-CGD-O2D
29	g1	614	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	y1	614	CLA	CAD-CBD-CGD-O2D
30	a	408	PHO	CAD-CBD-CGD-O2D
34	y1	625	SPH	O3-C3-C4-C5
37	b1	623	DGD	C3G-C2G-O2G-C1B
38	t1	101	3PH	C1-C2-O21-C21
38	t1	101	3PH	C3-C2-O21-C21
40	l	101	LHG	C4-C5-O7-C7
48	G	606	CHL	CAD-CBD-CGD-O2D
48	S	606	CHL	CAD-CBD-CGD-O2D
48	g	607	CHL	CAD-CBD-CGD-O2D
48	g	609	CHL	CAD-CBD-CGD-O2D
48	S1	606	CHL	CAD-CBD-CGD-O2D
29	B	602	CLA	C16-C17-C18-C19
29	r1	610	CLA	C11-C12-C13-C14
29	s1	603	CLA	C16-C17-C18-C19
47	k	101	4RF	C31-C32-C33-C34
49	S1	620	LUT	C9-C10-C11-C12
29	b	608	CLA	C2A-CAA-CBA-CGA
29	Y1	612	CLA	C3-C5-C6-C7
29	g1	613	CLA	C3-C5-C6-C7
32	A1	412	SQD	C33-C34-C35-C36
32	B1	626	SQD	C12-C13-C14-C15
29	c	505	CLA	C2-C1-O2A-CGA
29	C1	501	CLA	C2-C1-O2A-CGA
29	d1	403	CLA	C2-C1-O2A-CGA
29	n1	612	CLA	CAA-CBA-CGA-O2A
39	c	524	DGA	CB2-CB3-CB4-CB5
29	C	503	CLA	CAA-CBA-CGA-O2A
29	c	503	CLA	CAA-CBA-CGA-O2A
29	c1	512	CLA	CAA-CBA-CGA-O2A
33	c	523	LMG	O7-C10-C11-C12
33	W1	201	LMG	O7-C10-C11-C12
39	b1	625	DGA	OG1-CA1-CA2-CA3
48	n1	605	CHL	CAA-CBA-CGA-O2A
29	b1	614	CLA	O1D-CGD-O2D-CED
29	c	511	CLA	C4-C3-C5-C6
43	d1	405	PL9	C35-C34-C36-C37
30	a1	408	PHO	C16-C17-C18-C19
29	c1	502	CLA	C4C-C3C-CAC-CBC
40	s	624	LHG	C9-C10-C11-C12
29	c	508	CLA	C8-C10-C11-C12
29	S1	604	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
43	D1	405	PL9	C33-C34-C36-C37
48	g	607	CHL	C2-C3-C5-C6
48	N1	609	CHL	C2-C3-C5-C6
29	y	613	CLA	CAA-CBA-CGA-O2A
29	B1	609	CLA	CAA-CBA-CGA-O2A
29	B1	615	CLA	CAA-CBA-CGA-O2A
30	A1	409	PHO	CAA-CBA-CGA-O2A
32	b	621	SQD	O47-C7-C8-C9
39	b1	625	DGA	OG2-CB1-CB2-CB3
40	N	624	LHG	O7-C7-C8-C9
40	c	525	LHG	O7-C7-C8-C9
33	C	523	LMG	C13-C14-C15-C16
33	c	523	LMG	C31-C32-C33-C34
38	t1	101	3PH	C33-C34-C35-C36
40	Y	624	LHG	C10-C11-C12-C13
31	C	514	BCR	C11-C12-C13-C14
31	b	618	BCR	C17-C18-C19-C20
31	b	618	BCR	C21-C22-C23-C24
31	C1	516	BCR	C17-C18-C19-C20
31	D1	404	BCR	C7-C8-C9-C10
45	H	101	RRX	C17-C18-C19-C20
45	h1	101	RRX	C21-C22-C23-C24
49	R1	620	LUT	C27-C28-C29-C30
50	Y	622	XAT	C31-C32-C33-C34
34	a1	414	SPH	C4-C5-C6-C7
34	A1	414	SPH	C5-C6-C7-C8
38	b	624	3PH	C3D-C3E-C3F-C3G
37	B	623	DGD	O1G-C1G-C2G-C3G
37	C1	520	DGD	C1G-C2G-C3G-O3G
38	t1	101	3PH	C1-C2-C3-O31
41	C	527	LMK	C4-C3-N4-C5
41	C	527	LMK	C4-C3-N4-C6
41	c	527	LMK	C11-C10-O7-C8
41	c1	527	LMK	O1-C7-C8-C9
41	c1	527	LMK	C11-C10-O7-C8
50	Y	622	XAT	O24-C26-C27-C28
50	G1	622	XAT	O24-C26-C27-C28
51	S	623	NEX	O24-C26-C27-C28
51	g1	623	NEX	O24-C26-C27-C28
51	y1	623	NEX	O24-C26-C27-C28
48	Y1	605	CHL	CAA-CBA-CGA-O1A
47	i	101	4RF	C48-C49-C50-C51

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Mol	Chain	Res	Type	Atoms
29	B	607	CLA	CBA-CGA-O2A-C1
52	r1	625	LMT	C4'-C5'-C6'-O6'
29	a	410	CLA	C10-C11-C12-C13
29	G	611	CLA	C3-C5-C6-C7
29	b	610	CLA	C3-C5-C6-C7
29	B	608	CLA	CAA-CBA-CGA-O2A
29	G	613	CLA	CAA-CBA-CGA-O2A
29	G	614	CLA	CAA-CBA-CGA-O2A
29	c	505	CLA	CAA-CBA-CGA-O2A
29	C1	502	CLA	CAA-CBA-CGA-O2A
29	R1	604	CLA	CAA-CBA-CGA-O2A
29	b1	603	CLA	CAA-CBA-CGA-O2A
29	r1	604	CLA	CAA-CBA-CGA-O2A
29	y1	613	CLA	CAA-CBA-CGA-O2A
32	A	412	SQD	O47-C7-C8-C9
37	C	518	DGD	O2G-C1B-C2B-C3B
40	S	624	LHG	O8-C23-C24-C25
40	y	624	LHG	O8-C23-C24-C25
48	g1	605	CHL	CAA-CBA-CGA-O2A
38	T1	101	3PH	C3C-C3D-C3E-C3F
40	d	408	LHG	C11-C10-C9-C8
40	L1	101	LHG	C14-C15-C16-C17
38	s	626	3PH	C21-C22-C23-C24
48	R	607	CHL	O2A-C1-C2-C3
40	G	624	LHG	O10-C23-C24-C25
33	b1	622	LMG	C16-C17-C18-C19
29	b	616	CLA	C13-C15-C16-C17
30	A	408	PHO	O2A-C1-C2-C3
48	y	607	CHL	O2A-C1-C2-C3
48	G1	609	CHL	O2A-C1-C2-C3
48	Y1	607	CHL	O2A-C1-C2-C3
32	A	412	SQD	C15-C16-C17-C18
32	B1	626	SQD	C31-C32-C33-C34
38	T1	101	3PH	C2A-C2B-C2C-C2D
33	d1	411	LMG	C29-C28-O8-C9
29	Y	610	CLA	C2A-CAA-CBA-CGA
29	r	612	CLA	C2A-CAA-CBA-CGA
29	S	610	CLA	C8-C10-C11-C12
29	c	507	CLA	C15-C16-C17-C18
29	d	403	CLA	C13-C15-C16-C17
48	G	607	CHL	C5-C6-C7-C8
32	a1	412	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
37	C	519	DGD	C5A-C6A-C7A-C8A
29	N	604	CLA	CAA-CBA-CGA-O2A
29	b	607	CLA	O1A-CGA-O2A-C1
29	n1	612	CLA	CAA-CBA-CGA-O1A
32	c	526	SQD	C35-C36-C37-C38
39	B	625	DGA	CDB-CEB-CFB-CGB
40	Y	624	LHG	C15-C16-C17-C18
34	Y	625	SPH	C4-C5-C6-C7
29	b	612	CLA	C16-C17-C18-C19
29	r1	603	CLA	C11-C12-C13-C14
29	A	405	CLA	CHA-CBD-CGD-O2D
29	B	609	CLA	CHA-CBD-CGD-O1D
29	B	609	CLA	CHA-CBD-CGD-O2D
29	B	614	CLA	CHA-CBD-CGD-O1D
29	B	614	CLA	CHA-CBD-CGD-O2D
29	B	617	CLA	CHA-CBD-CGD-O1D
29	D	402	CLA	CHA-CBD-CGD-O1D
29	D	402	CLA	CHA-CBD-CGD-O2D
29	N	610	CLA	CHA-CBD-CGD-O1D
29	N	610	CLA	CHA-CBD-CGD-O2D
29	G	604	CLA	CHA-CBD-CGD-O1D
29	G	610	CLA	CHA-CBD-CGD-O1D
29	G	610	CLA	CHA-CBD-CGD-O2D
29	R	604	CLA	CHA-CBD-CGD-O1D
29	R	604	CLA	CHA-CBD-CGD-O2D
29	R	612	CLA	CHA-CBD-CGD-O1D
29	S	604	CLA	CHA-CBD-CGD-O2D
29	S	613	CLA	CHA-CBD-CGD-O1D
29	S	613	CLA	CHA-CBD-CGD-O2D
29	b	604	CLA	CHA-CBD-CGD-O1D
29	b	604	CLA	CHA-CBD-CGD-O2D
29	b	611	CLA	CHA-CBD-CGD-O1D
29	b	611	CLA	CHA-CBD-CGD-O2D
29	c	503	CLA	CHA-CBD-CGD-O2D
29	d	402	CLA	CHA-CBD-CGD-O1D
29	d	402	CLA	CHA-CBD-CGD-O2D
29	n	610	CLA	CHA-CBD-CGD-O1D
29	n	610	CLA	CHA-CBD-CGD-O2D
29	g	612	CLA	CHA-CBD-CGD-O1D
29	g	612	CLA	CHA-CBD-CGD-O2D
29	r	603	CLA	CHA-CBD-CGD-O2D
29	s	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	y	604	CLA	CHA-CBD-CGD-O1D
29	y	611	CLA	CHA-CBD-CGD-O1D
29	y	611	CLA	CHA-CBD-CGD-O2D
29	A1	406	CLA	CHA-CBD-CGD-O1D
29	A1	406	CLA	CHA-CBD-CGD-O2D
29	B1	610	CLA	CHA-CBD-CGD-O1D
29	B1	610	CLA	CHA-CBD-CGD-O2D
29	B1	611	CLA	CHA-CBD-CGD-O1D
29	C1	503	CLA	CHA-CBD-CGD-O1D
29	C1	505	CLA	CHA-CBD-CGD-O2D
29	N1	610	CLA	CHA-CBD-CGD-O1D
29	N1	610	CLA	CHA-CBD-CGD-O2D
29	N1	611	CLA	CHA-CBD-CGD-O1D
29	N1	611	CLA	CHA-CBD-CGD-O2D
29	N1	612	CLA	CHA-CBD-CGD-O1D
29	G1	602	CLA	CHA-CBD-CGD-O1D
29	G1	611	CLA	CHA-CBD-CGD-O1D
29	G1	611	CLA	CHA-CBD-CGD-O2D
29	R1	602	CLA	CHA-CBD-CGD-O1D
29	R1	609	CLA	CHA-CBD-CGD-O1D
29	R1	609	CLA	CHA-CBD-CGD-O2D
29	S1	604	CLA	CHA-CBD-CGD-O2D
29	S1	612	CLA	CHA-CBD-CGD-O1D
29	S1	612	CLA	CHA-CBD-CGD-O2D
29	Y1	602	CLA	CHA-CBD-CGD-O1D
29	Y1	602	CLA	CHA-CBD-CGD-O2D
29	a1	407	CLA	CHA-CBD-CGD-O1D
29	a1	407	CLA	CHA-CBD-CGD-O2D
29	b1	605	CLA	CHA-CBD-CGD-O2D
29	b1	606	CLA	CHA-CBD-CGD-O2D
29	b1	617	CLA	CHA-CBD-CGD-O1D
29	b1	617	CLA	CHA-CBD-CGD-O2D
29	c1	502	CLA	CHA-CBD-CGD-O1D
29	c1	502	CLA	CHA-CBD-CGD-O2D
29	c1	506	CLA	CHA-CBD-CGD-O1D
29	c1	507	CLA	CHA-CBD-CGD-O1D
29	c1	508	CLA	CHA-CBD-CGD-O1D
29	c1	508	CLA	CHA-CBD-CGD-O2D
29	n1	604	CLA	CHA-CBD-CGD-O1D
29	n1	610	CLA	CHA-CBD-CGD-O1D
29	n1	610	CLA	CHA-CBD-CGD-O2D
29	n1	614	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	n1	614	CLA	CHA-CBD-CGD-O2D
29	g1	604	CLA	CHA-CBD-CGD-O1D
29	g1	604	CLA	CHA-CBD-CGD-O2D
29	g1	613	CLA	CHA-CBD-CGD-O2D
29	r1	609	CLA	CHA-CBD-CGD-O2D
29	s1	603	CLA	CHA-CBD-CGD-O1D
29	s1	609	CLA	CHA-CBD-CGD-O1D
29	s1	609	CLA	CHA-CBD-CGD-O2D
29	s1	612	CLA	CHA-CBD-CGD-O2D
29	s1	613	CLA	CHA-CBD-CGD-O1D
29	s1	613	CLA	CHA-CBD-CGD-O2D
29	y1	602	CLA	CHA-CBD-CGD-O1D
29	y1	602	CLA	CHA-CBD-CGD-O2D
29	y1	610	CLA	CHA-CBD-CGD-O1D
29	y1	610	CLA	CHA-CBD-CGD-O2D
29	y1	613	CLA	CHA-CBD-CGD-O1D
29	y1	613	CLA	CHA-CBD-CGD-O2D
31	C	516	BCR	C13-C14-C15-C16
31	c1	517	BCR	C9-C10-C11-C12
41	C	527	LMK	C2-C3-C4-O3
41	C1	527	LMK	C2-C3-C4-O3
48	y	601	CHL	CHA-CBD-CGD-O1D
48	y	601	CHL	CHA-CBD-CGD-O2D
48	N1	601	CHL	CHA-CBD-CGD-O2D
48	R1	607	CHL	CHA-CBD-CGD-O1D
48	R1	607	CHL	CHA-CBD-CGD-O2D
48	Y1	607	CHL	CHA-CBD-CGD-O1D
48	Y1	607	CHL	CHA-CBD-CGD-O2D
48	y1	605	CHL	CHA-CBD-CGD-O1D
48	y1	605	CHL	CHA-CBD-CGD-O2D
49	n1	621	LUT	C33-C34-C35-C15
29	c1	502	CLA	CAA-CBA-CGA-O2A
38	s1	626	3PH	O21-C21-C22-C23
39	C1	524	DGA	OG2-CB1-CB2-CB3
29	s1	605	CLA	C2C-C3C-CAC-CBC
38	B1	624	3PH	C27-C28-C29-C2A
40	S1	624	LHG	C29-C30-C31-C32
29	c	506	CLA	C2-C3-C5-C6
29	C1	510	CLA	C2-C3-C5-C6
30	A1	408	PHO	C2-C3-C5-C6
48	g1	607	CHL	C2-C3-C5-C6
29	A1	405	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	c	523	LMG	C2-C1-O1-C7
51	y1	623	NEX	C28-C29-C30-C31
48	G	608	CHL	C2A-CAA-CBA-CGA
39	B	625	DGA	CCB-CDB-CEB-CFB
40	d1	410	LHG	C24-C25-C26-C27
29	b	608	CLA	C16-C17-C18-C19
29	G1	613	CLA	C16-C17-C18-C20
29	d	402	CLA	C13-C15-C16-C17
29	C1	501	CLA	C15-C16-C17-C18
29	A	406	CLA	CAA-CBA-CGA-O2A
29	b	603	CLA	CAA-CBA-CGA-O2A
29	b	609	CLA	CAA-CBA-CGA-O2A
29	r	612	CLA	CAA-CBA-CGA-O2A
38	t	101	3PH	O31-C31-C32-C33
39	c1	524	DGA	OG1-CA1-CA2-CA3
40	Y	624	LHG	O8-C23-C24-C25
40	d1	408	LHG	O7-C7-C8-C9
40	y1	624	LHG	O8-C23-C24-C25
55	y	626	PTY	O4-C30-C31-C32
33	C	523	LMG	C11-C12-C13-C14
39	B1	625	DGA	CFA-CGA-CHA-CIA
47	k1	101	4RF	C08-C09-C10-C11
40	D	409	LHG	C7-C8-C9-C10
40	N	624	LHG	C34-C35-C36-C37
40	S	624	LHG	C32-C33-C34-C35
29	b	603	CLA	C8-C10-C11-C12
29	B1	603	CLA	C8-C10-C11-C12
29	C1	504	CLA	C10-C11-C12-C13
29	s1	605	CLA	C4C-C3C-CAC-CBC
33	D1	411	LMG	C21-C22-C23-C24
40	Y	624	LHG	C33-C34-C35-C36
29	b	612	CLA	C8-C10-C11-C12
29	B	603	CLA	CAA-CBA-CGA-O2A
29	B	609	CLA	CAA-CBA-CGA-O2A
29	R	604	CLA	CAA-CBA-CGA-O2A
29	a	405	CLA	CAA-CBA-CGA-O2A
29	b	608	CLA	CAA-CBA-CGA-O2A
29	B1	608	CLA	CAA-CBA-CGA-O2A
29	n1	614	CLA	CAA-CBA-CGA-O2A
29	g1	603	CLA	CAA-CBA-CGA-O2A
33	D	411	LMG	O7-C10-C11-C12
33	h1	102	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
37	c	519	DGD	O2G-C1B-C2B-C3B
40	d	408	LHG	O8-C23-C24-C25
47	K	101	4RF	C14-C15-C16-O18
47	K1	101	4RF	O21-C22-C24-C25
55	Y	626	PTY	O4-C30-C31-C32
38	S	626	3PH	C33-C34-C35-C36
38	S1	626	3PH	C38-C39-C3A-C3B
38	s1	626	3PH	C26-C27-C28-C29
40	c	525	LHG	C12-C13-C14-C15
29	B	607	CLA	C2A-CAA-CBA-CGA
29	c	502	CLA	C2A-CAA-CBA-CGA
48	Y1	605	CHL	CAA-CBA-CGA-O2A
30	A	409	PHO	CHA-CBD-CGD-O1D
30	A	409	PHO	CHA-CBD-CGD-O2D
34	a1	414	SPH	N2-C2-C3-O3
41	C	527	LMK	O9-C10-C11-C12
44	f1	101	HEM	C4D-C3D-CAD-CBD
29	G1	613	CLA	C15-C16-C17-C18
29	s1	610	CLA	C5-C6-C7-C8
37	C	520	DGD	CAA-CBA-CCA-CDA
40	g	624	LHG	C26-C27-C28-C29
33	h1	102	LMG	C30-C31-C32-C33
32	C	526	SQD	C8-C7-O47-C45
32	c1	526	SQD	C8-C7-O47-C45
29	B	610	CLA	CAA-CBA-CGA-O2A
29	c	513	CLA	CAA-CBA-CGA-O2A
29	d	402	CLA	CAA-CBA-CGA-O2A
29	g	603	CLA	CAA-CBA-CGA-O2A
29	g1	613	CLA	CAA-CBA-CGA-O2A
39	j1	101	DGA	OG1-CA1-CA2-CA3
47	K1	101	4RF	O40-C41-C43-C44
32	c1	526	SQD	C11-C10-C9-C8
47	i1	101	4RF	C46-C47-C48-C49
29	A1	406	CLA	C4-C3-C5-C6
29	c1	511	CLA	C4-C3-C5-C6
37	c1	519	DGD	C2B-C3B-C4B-C5B
40	D	410	LHG	C31-C32-C33-C34
39	b1	625	DGA	CEB-CFB-CGB-CHB
29	C	504	CLA	C11-C10-C8-C7
29	N	613	CLA	C12-C13-C15-C16
29	R	608	CLA	C11-C10-C8-C7
29	y	614	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	A1	406	CLA	C11-C10-C8-C7
29	B1	610	CLA	C2-C3-C5-C6
29	B1	615	CLA	C11-C10-C8-C7
29	c1	502	CLA	C6-C7-C8-C10
29	r1	602	CLA	C6-C7-C8-C10
30	a1	408	PHO	C6-C7-C8-C10
48	N1	605	CHL	C6-C7-C8-C10
48	N1	609	CHL	C11-C12-C13-C15
48	Y1	609	CHL	C12-C13-C15-C16
43	d1	405	PL9	C4-C3-C7-C8
32	b1	626	SQD	C19-C20-C21-C22
38	B1	624	3PH	C22-C23-C24-C25
39	j	101	DGA	OB1-CB1-OG2-CG2
33	c	521	LMG	O6-C1-O1-C7
29	B	615	CLA	CAA-CBA-CGA-O2A
32	c1	526	SQD	O47-C7-C8-C9
33	a	413	LMG	O7-C10-C11-C12
33	B1	622	LMG	O8-C28-C29-C30
47	I	102	4RF	C14-C15-C16-O18
54	s1	625	LPX	O6-C6-C7-C8
29	c1	509	CLA	C4C-C3C-CAC-CBC
40	N1	624	LHG	C15-C16-C17-C18
29	N	613	CLA	C14-C13-C15-C16
29	c	502	CLA	C11-C10-C8-C9
29	n	603	CLA	C6-C7-C8-C9
29	s	609	CLA	C6-C7-C8-C9
29	s	610	CLA	C11-C12-C13-C14
29	s	611	CLA	C11-C12-C13-C14
29	y	614	CLA	C11-C10-C8-C9
29	B1	612	CLA	C14-C13-C15-C16
29	a1	406	CLA	C11-C12-C13-C14
29	s1	609	CLA	C6-C7-C8-C9
48	N1	609	CHL	C14-C13-C15-C16
48	g1	601	CHL	C11-C12-C13-C14
29	b1	603	CLA	CAA-CBA-CGA-O1A
29	b1	615	CLA	CAA-CBA-CGA-O1A
36	B	620	C7Z	C9-C10-C11-C12
29	c	502	CLA	C2B-C3B-CAB-CBB
29	y	610	CLA	C2B-C3B-CAB-CBB
48	N	607	CHL	C2B-C3B-CAB-CBB
48	Y	607	CHL	C2B-C3B-CAB-CBB
48	g	607	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
48	s	606	CHL	C2B-C3B-CAB-CBB
48	N1	607	CHL	C2B-C3B-CAB-CBB
48	N1	608	CHL	C2B-C3B-CAB-CBB
48	Y1	607	CHL	C2B-C3B-CAB-CBB
48	g1	607	CHL	C2B-C3B-CAB-CBB
48	N1	608	CHL	O2A-C1-C2-C3
29	B	605	CLA	O1A-CGA-O2A-C1
29	Y	610	CLA	O1A-CGA-O2A-C1
29	S1	612	CLA	CAA-CBA-CGA-O2A
33	w1	201	LMG	C28-C29-C30-C31
33	B	622	LMG	C18-C19-C20-C21
40	y1	624	LHG	C34-C35-C36-C37
37	C1	519	DGD	C2A-C1A-O1G-C1G
29	S	610	CLA	CAA-CBA-CGA-O2A
29	b	615	CLA	CAA-CBA-CGA-O2A
29	b1	607	CLA	CAA-CBA-CGA-O2A
39	C	524	DGA	OG1-CA1-CA2-CA3
39	j1	101	DGA	OG2-CB1-CB2-CB3
40	L1	101	LHG	O7-C7-C8-C9
29	Y	613	CLA	CAA-CBA-CGA-O1A
32	M	101	SQD	C4-C5-C6-S
32	b	626	SQD	C5-C6-S-O8
32	m	101	SQD	C4-C5-C6-S
32	b1	626	SQD	C4-C5-C6-S
29	G1	603	CLA	C16-C17-C18-C19
32	b	621	SQD	C11-C10-C9-C8
33	a1	413	LMG	C32-C33-C34-C35
37	C	518	DGD	C6B-C7B-C8B-C9B
29	a1	405	CLA	C3-C5-C6-C7
29	B	610	CLA	O1A-CGA-O2A-C1
29	y	613	CLA	O1A-CGA-O2A-C1
37	C1	519	DGD	O1A-C1A-O1G-C1G
34	y1	625	SPH	C13-C14-C15-C16
38	b1	624	3PH	C2A-C2B-C2C-C2D
29	n1	602	CLA	C15-C16-C17-C18
29	A	406	CLA	C2A-CAA-CBA-CGA
29	C	512	CLA	C2A-CAA-CBA-CGA
29	a	406	CLA	C2A-CAA-CBA-CGA
29	b	606	CLA	C2A-CAA-CBA-CGA
29	C1	506	CLA	C2A-CAA-CBA-CGA
29	R1	610	CLA	C2A-CAA-CBA-CGA
29	g	613	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
29	c1	505	CLA	CAA-CBA-CGA-O1A
33	C	523	LMG	O9-C10-C11-C12
33	C1	523	LMG	C30-C31-C32-C33
40	Y1	624	LHG	C27-C28-C29-C30
29	g1	614	CLA	CAA-CBA-CGA-O2A
32	a1	412	SQD	O47-C7-C8-C9
38	S	626	3PH	O21-C21-C22-C23
40	N1	624	LHG	O7-C7-C8-C9
33	C	521	LMG	C13-C14-C15-C16
47	K	101	4RF	C24-C25-C26-C27
47	I1	102	4RF	C32-C33-C34-C35
40	d	409	LHG	C24-C23-O8-C6
33	H1	102	LMG	C37-C38-C39-C40
31	C1	516	BCR	C36-C18-C19-C20
32	M	101	SQD	C23-C24-C25-C26
49	R1	620	LUT	C27-C28-C29-C39
50	Y	622	XAT	C27-C28-C29-C39
29	g	614	CLA	CAA-CBA-CGA-O1A
29	b1	608	CLA	CAA-CBA-CGA-O1A
37	C1	518	DGD	O1A-C1A-C2A-C3A
38	S1	626	3PH	O22-C21-C22-C23
38	t1	101	3PH	O32-C31-C32-C33
30	a1	409	PHO	C16-C17-C18-C20
40	d1	410	LHG	C33-C34-C35-C36
48	Y1	607	CHL	C4-C3-C5-C6
44	f1	101	HEM	C2D-C3D-CAD-CBD
40	c1	525	LHG	O7-C7-C8-C9
41	C	527	LMK	C11-C12-C13-C14
32	b1	621	SQD	O49-C7-C8-C9
33	C	521	LMG	O9-C10-C11-C12
33	A1	413	LMG	O9-C10-C11-C12
40	N	624	LHG	O9-C7-C8-C9
31	b1	618	BCR	C21-C22-C23-C24
29	C	508	CLA	CBA-CGA-O2A-C1
38	S1	626	3PH	C32-C31-O31-C3
32	M1	101	SQD	C25-C26-C27-C28
29	G	612	CLA	C1A-C2A-CAA-CBA
29	b	617	CLA	C1A-C2A-CAA-CBA
29	B1	615	CLA	C1A-C2A-CAA-CBA
29	N1	612	CLA	C1A-C2A-CAA-CBA
29	b1	603	CLA	C1A-C2A-CAA-CBA
29	d1	402	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	g1	613	CLA	C1A-C2A-CAA-CBA
29	s1	609	CLA	C1A-C2A-CAA-CBA
48	G	607	CHL	C1A-C2A-CAA-CBA
48	Y	605	CHL	C1A-C2A-CAA-CBA
48	n	607	CHL	C1A-C2A-CAA-CBA
48	g	601	CHL	C1A-C2A-CAA-CBA
48	y	607	CHL	C1A-C2A-CAA-CBA
48	n1	607	CHL	C1A-C2A-CAA-CBA
48	g1	601	CHL	C1A-C2A-CAA-CBA
48	g1	606	CHL	C1A-C2A-CAA-CBA
48	g1	608	CHL	C1A-C2A-CAA-CBA
32	a	412	SQD	C7-C8-C9-C10
38	B1	624	3PH	C38-C39-C3A-C3B
40	Y1	624	LHG	C9-C10-C11-C12
29	B	608	CLA	CAA-CBA-CGA-O1A
29	R	612	CLA	CAA-CBA-CGA-O1A
29	R1	604	CLA	CAA-CBA-CGA-O1A
29	r1	604	CLA	CAA-CBA-CGA-O1A
38	B	624	3PH	O32-C31-C32-C33
38	S	626	3PH	O22-C21-C22-C23
38	s	626	3PH	O22-C21-C22-C23
39	j1	101	DGA	OB1-CB1-CB2-CB3
40	c	525	LHG	O9-C7-C8-C9
48	n1	605	CHL	CAA-CBA-CGA-O1A
48	g1	605	CHL	CAA-CBA-CGA-O1A
29	N1	614	CLA	CAA-CBA-CGA-O2A
29	c1	502	CLA	C8-C10-C11-C12
48	G	607	CHL	C15-C16-C17-C18
47	K1	101	4RF	C03-C04-C05-C06
29	b	604	CLA	C2-C1-O2A-CGA
40	d1	409	LHG	C15-C16-C17-C18
33	W1	201	LMG	C4-C5-C6-O5
29	y1	604	CLA	C10-C11-C12-C13
29	G	613	CLA	CAA-CBA-CGA-O1A
29	c	503	CLA	CAA-CBA-CGA-O1A
29	B1	609	CLA	CAA-CBA-CGA-O1A
29	C1	502	CLA	CAA-CBA-CGA-O1A
29	Y1	613	CLA	CAA-CBA-CGA-O1A
29	c1	512	CLA	CAA-CBA-CGA-O1A
29	y1	613	CLA	CAA-CBA-CGA-O1A
30	A	409	PHO	CAA-CBA-CGA-O1A
37	C	518	DGD	O1B-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
37	b	623	DGD	O1A-C1A-C2A-C3A
39	c	524	DGA	OB1-CB1-CB2-CB3
39	b1	625	DGA	OB1-CB1-CB2-CB3
40	D1	409	LHG	O9-C7-C8-C9
39	J1	101	DGA	CBB-CAB-CB9-CB8
39	j1	101	DGA	OG1-CG1-CG2-CG3
40	d1	409	LHG	C4-C5-C6-O8
47	i1	101	4RF	O18-C19-C20-C39
37	c1	518	DGD	O1G-C1A-C2A-C3A
29	B1	610	CLA	C10-C11-C12-C13
30	a1	409	PHO	C8-C10-C11-C12
29	B	608	CLA	C2A-CAA-CBA-CGA
29	N1	603	CLA	C2A-CAA-CBA-CGA
32	B	626	SQD	C30-C31-C32-C33
32	b	626	SQD	C10-C11-C12-C13
33	h	102	LMG	C18-C19-C20-C21
38	S	626	3PH	C2F-C2G-C2H-C2I
54	s1	625	LPX	C7-C8-C9-C10
29	b1	617	CLA	C16-C17-C18-C19
29	y1	602	CLA	C16-C17-C18-C19
29	c	505	CLA	CAA-CBA-CGA-O1A
29	y	613	CLA	CAA-CBA-CGA-O1A
39	C1	524	DGA	OB1-CB1-CB2-CB3
39	c1	524	DGA	OA1-CA1-CA2-CA3
40	D	408	LHG	O9-C7-C8-C9
54	s1	625	LPX	O7-C6-C7-C8
29	n	610	CLA	C13-C15-C16-C17
29	G1	603	CLA	C5-C6-C7-C8
33	B	622	LMG	C21-C22-C23-C24
29	A	405	CLA	C4-C3-C5-C6
29	A	405	CLA	CAA-CBA-CGA-O2A
29	b	607	CLA	CAA-CBA-CGA-O2A
29	C1	503	CLA	CAA-CBA-CGA-O2A
29	r1	612	CLA	CAA-CBA-CGA-O2A
33	c1	523	LMG	O7-C10-C11-C12
39	J	101	DGA	OG2-CB1-CB2-CB3
48	n	605	CHL	CAA-CBA-CGA-O2A
32	A1	412	SQD	O49-C7-O47-C45
55	Y	627	PTY	C6-C5-O14-P1
38	b	624	3PH	C2C-C2D-C2E-C2F
29	B	603	CLA	CAA-CBA-CGA-O1A
29	c1	502	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
40	N1	624	LHG	O9-C7-C8-C9
29	B	605	CLA	C2-C3-C5-C6
29	R	608	CLA	C2-C3-C5-C6
29	c1	513	CLA	C2-C3-C5-C6
29	g1	613	CLA	C2-C3-C5-C6
48	y1	605	CHL	CAA-CBA-CGA-O2A
29	B	609	CLA	C13-C15-C16-C17
29	N	610	CLA	C5-C6-C7-C8
29	B1	602	CLA	C8-C10-C11-C12
48	g1	601	CHL	C13-C15-C16-C17
29	c1	509	CLA	C2C-C3C-CAC-CBC
33	C	523	LMG	C14-C15-C16-C17
47	k1	101	4RF	C06-C07-C08-C09
29	B1	602	CLA	C4B-C3B-CAB-CBB
29	G1	612	CLA	C4B-C3B-CAB-CBB
29	b1	613	CLA	C4B-C3B-CAB-CBB
29	g1	612	CLA	C4B-C3B-CAB-CBB
40	D	410	LHG	C4-O6-P-O4
40	g	624	LHG	C3-O3-P-O5
40	C1	525	LHG	C3-O3-P-O4
40	n1	624	LHG	C3-O3-P-O5
48	N	605	CHL	C4B-C3B-CAB-CBB
48	s	607	CHL	C4B-C3B-CAB-CBB
48	N1	601	CHL	C4B-C3B-CAB-CBB
48	G1	605	CHL	C4B-C3B-CAB-CBB
48	S1	607	CHL	C4B-C3B-CAB-CBB
48	n1	606	CHL	C4B-C3B-CAB-CBB
48	r1	607	CHL	C4B-C3B-CAB-CBB
54	s	625	LPX	C3-O1-P1-O3
54	s1	625	LPX	C1-O2-P1-O4
55	Y	627	PTY	C3-O11-P1-O13
55	Y1	626	PTY	C5-O14-P1-O13
41	c1	527	LMK	O7-C8-C9-O8
37	B	623	DGD	C2B-C3B-C4B-C5B
37	C1	520	DGD	CDB-CEB-CFB-CGB
39	j	101	DGA	CB5-CB6-CB7-CB8
29	N	604	CLA	CAA-CBA-CGA-O1A
29	c	513	CLA	CAA-CBA-CGA-O1A
29	r	612	CLA	CAA-CBA-CGA-O1A
29	B1	608	CLA	CAA-CBA-CGA-O1A
30	A1	409	PHO	CAA-CBA-CGA-O1A
32	c1	526	SQD	O49-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	d	411	LMG	O9-C10-C11-C12
39	C	524	DGA	OA1-CA1-CA2-CA3
39	j1	101	DGA	OA1-CA1-CA2-CA3
40	d	408	LHG	O10-C23-C24-C25
40	y	624	LHG	O10-C23-C24-C25
48	y	606	CHL	CAA-CBA-CGA-O1A
55	y	626	PTY	O30-C30-C31-C32
29	B1	602	CLA	CAA-CBA-CGA-O2A
29	B1	602	CLA	C15-C16-C17-C18
29	g1	610	CLA	C13-C15-C16-C17
48	G	607	CHL	C13-C15-C16-C17
33	C	523	LMG	C37-C38-C39-C40
33	h	102	LMG	C39-C40-C41-C42
37	C	520	DGD	C9B-CAB-CBB-CCB
31	c	517	BCR	C23-C24-C25-C26
31	A1	411	BCR	C23-C24-C25-C26
31	C1	517	BCR	C1-C6-C7-C8
49	Y	621	LUT	C5-C6-C7-C8
49	Y1	620	LUT	C5-C6-C7-C8
43	d	405	PL9	C24-C26-C27-C28
41	C	527	LMK	C10-C11-C12-C13
29	r	608	CLA	C10-C11-C12-C13
55	y1	626	PTY	N1-C2-C3-O11
29	B	615	CLA	CAA-CBA-CGA-O1A
29	C	503	CLA	CAA-CBA-CGA-O1A
29	G	614	CLA	CAA-CBA-CGA-O1A
29	S	610	CLA	CAA-CBA-CGA-O1A
29	b	603	CLA	CAA-CBA-CGA-O1A
29	b	609	CLA	CAA-CBA-CGA-O1A
29	B1	603	CLA	CAA-CBA-CGA-O1A
29	n1	604	CLA	CAA-CBA-CGA-O1A
29	n1	614	CLA	CAA-CBA-CGA-O1A
33	W1	201	LMG	O9-C10-C11-C12
33	h1	102	LMG	O10-C28-C29-C30
40	d1	408	LHG	O9-C7-C8-C9
47	K	101	4RF	C14-C15-C16-O17
38	S1	626	3PH	O32-C31-O31-C3
29	C1	501	CLA	CAA-CBA-CGA-O2A
29	G1	603	CLA	CAA-CBA-CGA-O2A
33	a1	413	LMG	O7-C10-C11-C12
40	n	624	LHG	O7-C7-C8-C9
32	A	412	SQD	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
40	N1	624	LHG	C17-C18-C19-C20
29	N	613	CLA	CBA-CGA-O2A-C1
53	r	626	ERG	C21-C20-C22-C23
51	n	623	NEX	C30-C31-C32-C33
33	c	523	LMG	O9-C10-C11-C12
39	b1	625	DGA	OA1-CA1-CA2-CA3
40	Y	624	LHG	O10-C23-C24-C25
40	D1	410	LHG	C34-C35-C36-C37
38	b1	624	3PH	C38-C39-C3A-C3B
29	S1	612	CLA	CAA-CBA-CGA-O1A
29	G	603	CLA	CAA-CBA-CGA-O2A
37	C	519	DGD	O2G-C1B-C2B-C3B
37	c1	519	DGD	O2G-C1B-C2B-C3B
40	S1	624	LHG	O8-C23-C24-C25
29	S	610	CLA	C5-C6-C7-C8
29	Y1	612	CLA	C15-C16-C17-C18
38	s	626	3PH	C2E-C2F-C2G-C2H
39	B1	625	DGA	CBB-CAB-CB9-CB8
40	L	101	LHG	C17-C18-C19-C20
55	Y	626	PTY	C41-C42-C43-C44
32	A	412	SQD	O49-C7-C8-C9
38	b1	624	3PH	O22-C21-C22-C23
29	c	509	CLA	C4-C3-C5-C6
29	A1	410	CLA	C4-C3-C5-C6
48	S	608	CHL	C4-C3-C5-C6
32	b	626	SQD	C9-C10-C11-C12
43	D1	405	PL9	C26-C27-C28-C29
29	y	612	CLA	C2-C3-C5-C6
29	b1	607	CLA	C15-C16-C17-C18
47	k1	101	4RF	C50-C51-C52-C53
29	A	410	CLA	CAD-CBD-CGD-O1D
29	B	614	CLA	CAD-CBD-CGD-O1D
29	B	615	CLA	CAD-CBD-CGD-O1D
29	N	603	CLA	CAD-CBD-CGD-O1D
29	n	603	CLA	CAD-CBD-CGD-O1D
29	s	604	CLA	CAD-CBD-CGD-O1D
29	s	610	CLA	CAD-CBD-CGD-O1D
29	A1	406	CLA	CAD-CBD-CGD-O1D
29	N1	603	CLA	CAD-CBD-CGD-O1D
29	G1	611	CLA	CAD-CBD-CGD-O1D
29	Y1	603	CLA	CAD-CBD-CGD-O1D
29	c1	510	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	n1	611	CLA	CAD-CBD-CGD-O1D
29	g1	613	CLA	CAD-CBD-CGD-O1D
29	s1	609	CLA	CAD-CBD-CGD-O1D
32	B	626	SQD	O5-C5-C6-S
32	M	101	SQD	O5-C5-C6-S
32	c	526	SQD	O5-C5-C6-S
32	m	101	SQD	O5-C5-C6-S
32	b1	626	SQD	O5-C5-C6-S
32	b1	626	SQD	C5-C6-S-O9
48	S	607	CHL	CAD-CBD-CGD-O1D
48	n1	606	CHL	CAD-CBD-CGD-O1D
55	Y	627	PTY	C2-C3-O11-P1
55	y	627	PTY	C2-C3-O11-P1
55	Y1	627	PTY	C2-C3-O11-P1
33	b	622	LMG	C10-C11-C12-C13
29	N	613	CLA	O1A-CGA-O2A-C1
29	B	609	CLA	CAA-CBA-CGA-O1A
29	b	608	CLA	CAA-CBA-CGA-O1A
29	B1	615	CLA	CAA-CBA-CGA-O1A
29	g1	603	CLA	CAA-CBA-CGA-O1A
38	t	101	3PH	O32-C31-C32-C33
40	S	624	LHG	O10-C23-C24-C25
37	c1	519	DGD	C5B-C6B-C7B-C8B
55	Y	626	PTY	C13-C14-C15-C16
33	w	201	LMG	O7-C10-C11-C12
48	N	605	CHL	CAA-CBA-CGA-O2A
54	S1	625	LPX	O6-C6-C7-C8
29	A1	410	CLA	C5-C6-C7-C8
29	n1	610	CLA	C13-C15-C16-C17
29	B	606	CLA	C11-C12-C13-C14
29	B	614	CLA	C11-C10-C8-C9
29	C	508	CLA	C11-C10-C8-C9
29	D	403	CLA	C14-C13-C15-C16
29	G	610	CLA	C11-C10-C8-C9
29	g	610	CLA	C6-C7-C8-C9
29	g	610	CLA	C11-C12-C13-C14
29	y	604	CLA	C14-C13-C15-C16
29	A1	406	CLA	C11-C10-C8-C9
29	B1	613	CLA	C11-C12-C13-C14
29	C1	507	CLA	C14-C13-C15-C16
29	C1	512	CLA	C11-C10-C8-C9
29	G1	603	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	b1	605	CLA	C11-C10-C8-C9
29	b1	612	CLA	C6-C7-C8-C9
29	c1	513	CLA	C11-C12-C13-C14
29	d1	402	CLA	C11-C12-C13-C14
29	n1	613	CLA	C11-C10-C8-C9
37	C	518	DGD	CCB-CDB-CEB-CFB
29	S	605	CLA	C4C-C3C-CAC-CBC
37	C	520	DGD	C6A-C7A-C8A-C9A
40	c1	525	LHG	C35-C36-C37-C38
29	A	406	CLA	CAA-CBA-CGA-O1A
33	D	411	LMG	O9-C10-C11-C12
40	L1	101	LHG	O9-C7-C8-C9
40	c1	525	LHG	O9-C7-C8-C9
29	r1	602	CLA	C11-C12-C13-C14
29	C	505	CLA	CAA-CBA-CGA-O2A
29	a	406	CLA	CAA-CBA-CGA-O2A
29	C1	513	CLA	CAA-CBA-CGA-O2A
29	r1	609	CLA	CAA-CBA-CGA-O2A
32	c1	526	SQD	O48-C23-C24-C25
37	C1	519	DGD	O2G-C1B-C2B-C3B
39	j	101	DGA	OG1-CA1-CA2-CA3
39	B1	625	DGA	OG2-CB1-CB2-CB3
29	b	606	CLA	C5-C6-C7-C8
55	Y1	626	PTY	C35-C36-C37-C38
29	s1	610	CLA	C2A-CAA-CBA-CGA
40	Y	624	LHG	C17-C18-C19-C20
29	c	508	CLA	CAA-CBA-CGA-O2A
29	B1	613	CLA	CAA-CBA-CGA-O2A
29	C1	508	CLA	CAA-CBA-CGA-O2A
29	R1	612	CLA	CAA-CBA-CGA-O2A
29	c1	508	CLA	CAA-CBA-CGA-O2A
32	M1	101	SQD	O48-C23-C24-C25
32	b1	621	SQD	O48-C23-C24-C25
33	W	201	LMG	O7-C10-C11-C12
37	C1	520	DGD	O1G-C1A-C2A-C3A
39	b	625	DGA	OG1-CA1-CA2-CA3
48	G1	601	CHL	CAA-CBA-CGA-O2A
48	y1	606	CHL	CAA-CBA-CGA-O2A
32	b	621	SQD	C14-C15-C16-C17
29	B	610	CLA	CAA-CBA-CGA-O1A
29	R	604	CLA	CAA-CBA-CGA-O1A
32	a1	412	SQD	O49-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	a	413	LMG	O9-C10-C11-C12
40	y1	624	LHG	O10-C23-C24-C25
47	K1	101	4RF	O42-C41-C43-C44
33	c	521	LMG	C4-C5-C6-O5
40	d1	410	LHG	C10-C11-C12-C13
29	b	615	CLA	C16-C17-C18-C20
40	n	624	LHG	C2-C3-O3-P
29	s	604	CLA	C4-C3-C5-C6
29	Y1	604	CLA	C4-C3-C5-C6
48	G1	601	CHL	C4-C3-C5-C6
29	g	611	CLA	C8-C10-C11-C12
31	C	514	BCR	C11-C12-C13-C35
33	d1	411	LMG	C31-C32-C33-C34
38	B1	624	3PH	C3F-C3G-C3H-C3I
29	B	606	CLA	C11-C12-C13-C15
29	B	611	CLA	C12-C13-C15-C16
29	C	503	CLA	C12-C13-C15-C16
29	C	508	CLA	C11-C10-C8-C7
29	C	513	CLA	C11-C10-C8-C7
29	N	610	CLA	C11-C10-C8-C7
29	G	610	CLA	C11-C10-C8-C7
29	S	605	CLA	C3A-C2A-CAA-CBA
29	c	505	CLA	C11-C10-C8-C7
29	c	513	CLA	C12-C13-C15-C16
29	n	614	CLA	C3A-C2A-CAA-CBA
29	g	610	CLA	C6-C7-C8-C10
29	g	610	CLA	C11-C12-C13-C15
29	r	610	CLA	C6-C7-C8-C10
29	y	612	CLA	C11-C12-C13-C15
29	B1	603	CLA	C11-C12-C13-C15
29	C1	506	CLA	C12-C13-C15-C16
29	C1	507	CLA	C11-C10-C8-C7
29	C1	507	CLA	C12-C13-C15-C16
29	C1	512	CLA	C11-C10-C8-C7
29	N1	613	CLA	C12-C13-C15-C16
29	G1	603	CLA	C11-C10-C8-C7
29	b1	612	CLA	C6-C7-C8-C10
29	c1	507	CLA	C11-C10-C8-C7
29	c1	511	CLA	C11-C10-C8-C7
29	d1	402	CLA	C12-C13-C15-C16
29	n1	613	CLA	C11-C10-C8-C7
29	s1	611	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
29	y1	611	CLA	C3A-C2A-CAA-CBA
29	y1	612	CLA	C11-C12-C13-C15
29	y1	614	CLA	C11-C12-C13-C15
37	B	623	DGD	C1B-C2B-C3B-C4B
38	B1	624	3PH	O11-C1-C2-O21
48	N	601	CHL	C11-C12-C13-C15
48	n	605	CHL	C6-C7-C8-C10
48	G1	601	CHL	C12-C13-C15-C16
48	Y1	606	CHL	C11-C12-C13-C15
48	g1	609	CHL	C11-C12-C13-C15
29	a	405	CLA	CAA-CBA-CGA-O1A
29	b	613	CLA	CAA-CBA-CGA-O1A
29	b1	607	CLA	CAA-CBA-CGA-O1A
37	c	519	DGD	O1B-C1B-C2B-C3B
47	K1	101	4RF	O23-C22-C24-C25
55	Y	626	PTY	C20-C21-C22-C23
29	b	613	CLA	CAA-CBA-CGA-O2A
29	s	603	CLA	CAA-CBA-CGA-O2A
29	A1	406	CLA	CAA-CBA-CGA-O2A
29	B1	606	CLA	CAA-CBA-CGA-O2A
29	C1	505	CLA	CAA-CBA-CGA-O2A
29	G1	614	CLA	CAA-CBA-CGA-O2A
29	c1	503	CLA	CAA-CBA-CGA-O2A
29	c1	513	CLA	CAA-CBA-CGA-O2A
33	B1	622	LMG	O7-C10-C11-C12
39	j	101	DGA	OG2-CB1-CB2-CB3
55	y1	626	PTY	C12-C11-C8-O7
33	C1	521	LMG	C19-C20-C21-C22
33	C1	523	LMG	C21-C22-C23-C24
38	S1	626	3PH	C27-C28-C29-C2A
29	G	604	CLA	O2A-C1-C2-C3
29	r	609	CLA	C3-C5-C6-C7
48	g	609	CHL	C3-C5-C6-C7
47	i	101	4RF	C01-C02-C03-C04
41	c1	527	LMK	N4-C3-C4-O2
31	A	411	BCR	C21-C22-C23-C24
45	H1	101	RRX	C17-C18-C19-C20
50	Y	622	XAT	C27-C28-C29-C30
50	r1	621	XAT	C27-C28-C29-C30
50	y1	622	XAT	C27-C28-C29-C30
51	g	623	NEX	C11-C12-C13-C14
29	g	603	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
29	G1	603	CLA	CAA-CBA-CGA-O1A
29	g1	613	CLA	CAA-CBA-CGA-O1A
33	B1	622	LMG	O9-C10-C11-C12
37	C	519	DGD	O1B-C1B-C2B-C3B
39	J	101	DGA	OB1-CB1-CB2-CB3
39	j	101	DGA	OA1-CA1-CA2-CA3
55	Y	626	PTY	O30-C30-C31-C32
45	h	101	RRX	C15-C16-C17-C18
49	g	620	LUT	C9-C10-C11-C12
49	G1	620	LUT	C33-C34-C35-C15
51	y1	623	NEX	C29-C30-C31-C32
40	C	525	LHG	C15-C16-C17-C18
52	r	625	LMT	O1'-C1-C2-C3
41	c1	527	LMK	C2-C1-O1-C7
32	A	412	SQD	O48-C23-C24-C25
32	c	526	SQD	O47-C7-C8-C9
33	d1	411	LMG	O7-C10-C11-C12
37	b1	623	DGD	O1G-C1A-C2A-C3A
40	G1	624	LHG	O8-C23-C24-C25
47	i1	101	4RF	C14-C15-C16-O18
48	n1	606	CHL	CAA-CBA-CGA-O2A
29	y	611	CLA	C13-C15-C16-C17
29	C1	507	CLA	C8-C10-C11-C12
29	Y1	610	CLA	C13-C15-C16-C17
29	r1	603	CLA	C5-C6-C7-C8
29	r1	612	CLA	C10-C11-C12-C13
29	C	508	CLA	O1A-CGA-O2A-C1
29	b	616	CLA	O1A-CGA-O2A-C1
29	b1	614	CLA	O1A-CGA-O2A-C1
29	a	406	CLA	CAA-CBA-CGA-O1A
29	C1	503	CLA	CAA-CBA-CGA-O1A
29	N1	614	CLA	CAA-CBA-CGA-O1A
29	R1	612	CLA	CAA-CBA-CGA-O1A
29	c1	503	CLA	CAA-CBA-CGA-O1A
37	C1	519	DGD	O1B-C1B-C2B-C3B
39	b	625	DGA	OA1-CA1-CA2-CA3
48	n	605	CHL	CAA-CBA-CGA-O1A
48	G1	601	CHL	CAA-CBA-CGA-O1A
41	C1	527	LMK	C8-C7-O1-C1
29	B	605	CLA	CBA-CGA-O2A-C1
29	G1	611	CLA	C5-C6-C7-C8
48	G	609	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	N1	604	CLA	CAA-CBA-CGA-O2A
29	b1	606	CLA	CAA-CBA-CGA-O2A
37	c1	518	DGD	O2G-C1B-C2B-C3B
38	S	626	3PH	O31-C31-C32-C33
48	n	607	CHL	CAA-CBA-CGA-O2A
29	s	603	CLA	C10-C11-C12-C13
29	b	607	CLA	CAA-CBA-CGA-O1A
29	b	615	CLA	CAA-CBA-CGA-O1A
29	c	508	CLA	CAA-CBA-CGA-O1A
29	B1	613	CLA	CAA-CBA-CGA-O1A
29	c1	513	CLA	CAA-CBA-CGA-O1A
29	g1	614	CLA	CAA-CBA-CGA-O1A
33	c1	523	LMG	O9-C10-C11-C12
40	n	624	LHG	O9-C7-C8-C9
43	D1	405	PL9	C42-C43-C44-C45
29	S	613	CLA	C6-C7-C8-C10
33	B1	622	LMG	C11-C12-C13-C14
29	a	406	CLA	C8-C10-C11-C12
48	G1	609	CHL	C15-C16-C17-C18
40	G	624	LHG	C16-C17-C18-C19
40	G	624	LHG	C18-C19-C20-C21
29	C	505	CLA	CAA-CBA-CGA-O1A
29	B1	606	CLA	CAA-CBA-CGA-O1A
48	S1	608	CHL	CAA-CBA-CGA-O1A
29	C	513	CLA	C4-C3-C5-C6
32	c1	526	SQD	C31-C32-C33-C34
33	C	523	LMG	C34-C35-C36-C37
38	S	626	3PH	C2E-C2F-C2G-C2H
29	s	617	CLA	CAA-CBA-CGA-O2A
37	C	518	DGD	O1G-C1A-C2A-C3A
39	b	625	DGA	OG2-CB1-CB2-CB3
48	G	601	CHL	CAA-CBA-CGA-O2A
48	G	605	CHL	CAA-CBA-CGA-O2A
55	y1	626	PTY	O4-C30-C31-C32

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	N	623	NEX	C1-C2-C3-C4-C5-C6
51	n	623	NEX	C1-C2-C3-C4-C5-C6

662 monomers are involved in 2295 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	y	612	CLA	5	0
40	L1	101	LHG	6	0
29	C1	505	CLA	4	0
29	S1	602	CLA	6	0
49	y	621	LUT	3	0
39	J1	101	DGA	4	0
49	y1	620	LUT	6	0
29	B	617	CLA	5	0
29	c	507	CLA	6	0
48	n1	608	CHL	5	0
29	c	501	CLA	5	0
29	y	610	CLA	1	0
34	y	625	SPH	4	0
50	g1	622	XAT	6	0
40	D	408	LHG	3	0
55	y1	626	PTY	9	0
29	B	603	CLA	8	0
29	b	602	CLA	1	0
29	g	614	CLA	2	0
29	a	406	CLA	5	0
29	d1	402	CLA	9	0
29	C1	508	CLA	7	0
33	d	411	LMG	2	0
29	B1	609	CLA	9	0
31	C	515	BCR	3	0
48	s	606	CHL	3	0
29	b1	613	CLA	6	0
49	R	620	LUT	6	0
29	N	610	CLA	4	0
29	c	504	CLA	4	0
29	A1	406	CLA	4	0
29	Y1	611	CLA	8	0
29	r	603	CLA	3	0
38	s	626	3PH	6	0
50	G	622	XAT	6	0
31	B1	619	BCR	1	0
32	b1	626	SQD	4	0
53	r	626	ERG	7	0
48	G1	601	CHL	3	0
40	g1	624	LHG	7	0
48	g1	609	CHL	4	0
29	r	608	CLA	4	0
29	B1	610	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	r	625	LMT	4	0
29	g1	610	CLA	4	0
32	m	101	SQD	6	0
29	C1	512	CLA	8	0
48	G1	605	CHL	1	0
33	b1	622	LMG	5	0
44	f1	101	HEM	3	0
48	Y1	609	CHL	7	0
29	y1	604	CLA	2	0
29	s	604	CLA	2	0
47	K	101	4RF	2	0
40	d1	408	LHG	4	0
29	b	616	CLA	8	0
31	d1	404	BCR	3	0
29	b1	614	CLA	7	0
29	C1	501	CLA	8	0
29	G	602	CLA	8	0
29	y	608	CLA	3	0
47	I1	102	4RF	9	0
29	a	410	CLA	6	0
29	g1	612	CLA	1	0
29	N	611	CLA	4	0
48	y1	607	CHL	8	0
29	n1	611	CLA	2	0
49	G1	620	LUT	6	0
37	C1	518	DGD	11	0
51	S1	623	NEX	4	0
34	a1	414	SPH	1	0
29	N1	603	CLA	7	0
31	C	517	BCR	1	0
29	g1	602	CLA	12	0
50	Y1	622	XAT	4	0
29	A	407	CLA	1	0
31	c1	515	BCR	7	0
37	c	520	DGD	2	0
39	j	101	DGA	3	0
47	i1	101	4RF	2	0
49	S	621	LUT	5	0
48	y	606	CHL	2	0
29	s	603	CLA	2	0
48	g	606	CHL	3	0
50	n1	622	XAT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	F	101	HEM	3	0
48	G1	609	CHL	6	0
29	A1	410	CLA	7	0
50	r1	621	XAT	5	0
37	C	520	DGD	2	0
51	s	623	NEX	3	0
52	R1	625	LMT	7	0
49	S1	621	LUT	6	0
47	i	101	4RF	6	0
48	N	608	CHL	1	0
31	b	619	BCR	1	0
29	c	513	CLA	3	0
29	B	604	CLA	4	0
29	R1	609	CLA	4	0
29	y1	614	CLA	6	0
33	B	622	LMG	2	0
29	Y1	610	CLA	4	0
38	t	101	3PH	2	0
54	s1	625	LPX	3	0
48	N	601	CHL	4	0
29	S1	609	CLA	2	0
29	C	506	CLA	7	0
29	C	512	CLA	3	0
40	N1	624	LHG	5	0
29	y1	603	CLA	6	0
29	G1	602	CLA	8	0
30	a	408	PHO	5	0
37	c1	519	DGD	9	0
48	N	605	CHL	3	0
48	g1	608	CHL	2	0
33	C1	523	LMG	4	0
43	d	405	PL9	7	0
29	s1	602	CLA	4	0
48	N	607	CHL	3	0
29	r	602	CLA	2	0
48	N1	601	CHL	8	0
29	R	608	CLA	4	0
30	a1	409	PHO	11	0
29	g1	604	CLA	3	0
51	N1	623	NEX	6	0
49	Y	621	LUT	6	0
37	C	519	DGD	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	y	603	CLA	3	0
47	k1	101	4RF	2	0
49	G	621	LUT	7	0
39	c	524	DGA	9	0
29	c1	505	CLA	9	0
29	y	602	CLA	9	0
33	B1	622	LMG	5	0
48	r1	607	CHL	2	0
29	c	506	CLA	6	0
30	A	408	PHO	5	0
29	c1	506	CLA	3	0
49	n	620	LUT	3	0
33	b	622	LMG	5	0
37	C1	520	DGD	12	0
40	D	410	LHG	2	0
29	B	612	CLA	8	0
51	r1	622	NEX	5	0
29	N	612	CLA	3	0
38	B1	624	3PH	6	0
29	C1	503	CLA	2	0
29	B1	613	CLA	3	0
29	S1	614	CLA	1	0
48	Y	607	CHL	1	0
53	R	626	ERG	7	0
31	a1	411	BCR	4	0
29	b1	605	CLA	9	0
48	S	606	CHL	3	0
29	B	615	CLA	2	0
32	B	621	SQD	2	0
31	c1	517	BCR	8	0
29	B	610	CLA	7	0
31	C1	515	BCR	5	0
29	Y1	614	CLA	3	0
33	c	521	LMG	4	0
39	C1	524	DGA	6	0
37	c1	518	DGD	11	0
29	y1	611	CLA	4	0
29	c1	513	CLA	8	0
29	C	502	CLA	2	0
40	c1	525	LHG	11	0
48	g	607	CHL	2	0
48	y1	606	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	R	610	CLA	5	0
40	d1	409	LHG	6	0
32	B	626	SQD	4	0
49	N	620	LUT	6	0
40	s	624	LHG	4	0
49	n1	620	LUT	4	0
48	g1	605	CHL	2	0
29	c	509	CLA	4	0
29	g	612	CLA	1	0
40	y	624	LHG	5	0
29	c1	509	CLA	4	0
40	C	525	LHG	7	0
29	Y	602	CLA	15	0
29	s1	614	CLA	2	0
26	a1	401	OEX	1	0
29	B1	607	CLA	4	0
29	b	617	CLA	5	0
48	n1	601	CHL	6	0
29	b	614	CLA	4	0
29	G	614	CLA	1	0
54	S	625	LPX	4	0
29	b1	608	CLA	4	0
50	r	621	XAT	2	0
31	b1	618	BCR	2	0
29	N	614	CLA	1	0
48	r	607	CHL	1	0
29	C	508	CLA	3	0
29	n1	614	CLA	1	0
48	s	607	CHL	2	0
29	A1	405	CLA	6	0
29	c1	503	CLA	5	0
48	r1	606	CHL	4	0
29	C	509	CLA	3	0
29	b	615	CLA	6	0
29	C1	510	CLA	2	0
29	N1	612	CLA	3	0
40	d	409	LHG	7	0
33	A	413	LMG	3	0
48	n	605	CHL	4	0
54	S1	625	LPX	2	0
29	R1	610	CLA	7	0
49	s1	620	LUT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	B1	625	DGA	1	0
29	g	611	CLA	3	0
30	a	409	PHO	2	0
49	G1	621	LUT	10	0
48	S	607	CHL	1	0
29	S1	613	CLA	2	0
49	y1	621	LUT	7	0
29	N1	610	CLA	8	0
33	c1	523	LMG	4	0
29	a1	407	CLA	3	0
43	d1	405	PL9	8	0
50	n	622	XAT	6	0
29	G1	603	CLA	9	0
52	R	625	LMT	4	0
31	c	517	BCR	1	0
52	r1	625	LMT	2	0
29	C1	504	CLA	6	0
29	a1	405	CLA	9	0
44	f	101	HEM	1	0
48	N1	606	CHL	7	0
29	B1	616	CLA	11	0
29	C1	507	CLA	8	0
48	g1	601	CHL	7	0
53	R1	626	ERG	9	0
29	Y1	608	CLA	5	0
29	s	602	CLA	1	0
29	R1	612	CLA	2	0
29	g1	611	CLA	3	0
29	s1	611	CLA	7	0
26	A	401	OEX	1	0
32	M	101	SQD	4	0
29	N	602	CLA	6	0
33	w	201	LMG	6	0
48	g	609	CHL	4	0
29	n1	602	CLA	7	0
54	s	625	LPX	3	0
29	C	501	CLA	8	0
29	G1	610	CLA	2	0
31	c1	514	BCR	9	0
48	n1	607	CHL	6	0
29	s	613	CLA	2	0
49	r1	620	LUT	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	R1	621	XAT	5	0
29	Y	604	CLA	4	0
48	y1	609	CHL	6	0
48	R1	607	CHL	2	0
31	C1	517	BCR	5	0
47	I	102	4RF	2	0
45	h	101	RRX	3	0
29	y1	610	CLA	7	0
48	y	607	CHL	3	0
32	b	621	SQD	5	0
29	b1	606	CLA	8	0
29	S	617	CLA	1	0
40	C1	525	LHG	8	0
34	A1	414	SPH	4	0
29	C	511	CLA	1	0
29	S1	611	CLA	4	0
48	R	607	CHL	2	0
29	b	611	CLA	5	0
40	D1	408	LHG	3	0
48	g	605	CHL	1	0
29	B	613	CLA	5	0
40	S	624	LHG	5	0
29	N	613	CLA	4	0
29	n1	612	CLA	1	0
29	b	605	CLA	4	0
32	a1	412	SQD	3	0
55	y	626	PTY	9	0
49	Y	620	LUT	2	0
49	G	620	LUT	6	0
29	Y	603	CLA	4	0
29	c1	501	CLA	8	0
29	y1	612	CLA	6	0
40	l	101	LHG	4	0
49	n1	621	LUT	10	0
49	g	620	LUT	4	0
34	Y	625	SPH	4	0
29	G1	611	CLA	6	0
40	S1	624	LHG	5	0
45	H	101	RRX	1	0
29	c	508	CLA	4	0
48	S1	601	CHL	2	0
29	c	503	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	b1	615	CLA	3	0
48	G	601	CHL	4	0
48	y	605	CHL	1	0
49	g1	621	LUT	13	0
29	C	505	CLA	6	0
31	C	514	BCR	10	0
39	c1	524	DGA	4	0
31	b	618	BCR	5	0
29	b	604	CLA	3	0
29	B	602	CLA	2	0
48	Y1	601	CHL	4	0
29	C1	509	CLA	3	0
29	b1	609	CLA	8	0
32	B1	626	SQD	3	0
49	g1	620	LUT	9	0
29	N	604	CLA	2	0
29	R	612	CLA	1	0
29	n1	604	CLA	6	0
29	B1	606	CLA	5	0
29	s	612	CLA	2	0
29	B	608	CLA	4	0
29	A	410	CLA	6	0
29	Y	613	CLA	9	0
29	G	613	CLA	2	0
29	n	610	CLA	3	0
29	C1	502	CLA	2	0
31	D1	404	BCR	4	0
29	N1	611	CLA	3	0
29	N1	602	CLA	8	0
29	B1	614	CLA	8	0
48	G1	608	CHL	2	0
55	Y	626	PTY	5	0
33	w1	201	LMG	4	0
29	N1	613	CLA	10	0
48	Y	609	CHL	3	0
40	G	624	LHG	4	0
30	A1	409	PHO	8	0
43	D	405	PL9	4	0
48	Y	601	CHL	1	0
47	k	101	4RF	2	0
29	g	603	CLA	4	0
29	g	604	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	Y1	612	CLA	6	0
48	Y	605	CHL	2	0
48	G	605	CHL	1	0
29	d	402	CLA	5	0
31	D	404	BCR	3	0
50	G1	622	XAT	10	0
29	R1	608	CLA	2	0
51	Y	623	NEX	2	0
29	G1	613	CLA	6	0
34	a	414	SPH	3	0
40	c	525	LHG	4	0
29	b	612	CLA	2	0
48	G1	607	CHL	6	0
33	W1	201	LMG	8	0
48	n	607	CHL	7	0
29	b	606	CLA	5	0
29	S	609	CLA	3	0
33	h	102	LMG	5	0
34	A	414	SPH	1	0
38	b1	624	3PH	8	0
29	c1	511	CLA	9	0
29	s1	603	CLA	3	0
48	n1	606	CHL	7	0
29	B1	602	CLA	5	0
43	D1	405	PL9	11	0
48	n	609	CHL	2	0
48	R1	606	CHL	2	0
29	S	604	CLA	3	0
29	b1	617	CLA	7	0
29	y1	602	CLA	17	0
38	T1	101	3PH	8	0
48	g1	607	CHL	3	0
29	n1	603	CLA	8	0
29	Y	612	CLA	2	0
29	G	612	CLA	1	0
29	B1	617	CLA	7	0
32	b	626	SQD	2	0
40	d1	410	LHG	7	0
29	S	613	CLA	1	0
29	D1	402	CLA	8	0
40	Y	624	LHG	6	0
55	Y1	626	PTY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	y1	625	SPH	2	0
49	N	621	LUT	2	0
48	Y1	605	CHL	2	0
49	n	621	LUT	2	0
29	R1	602	CLA	4	0
31	A1	411	BCR	4	0
51	Y1	623	NEX	3	0
29	c	510	CLA	2	0
29	R	603	CLA	2	0
29	y1	608	CLA	2	0
48	G1	606	CHL	1	0
32	B1	621	SQD	3	0
29	B	605	CLA	5	0
29	b	608	CLA	7	0
29	b1	611	CLA	7	0
40	y1	624	LHG	6	0
48	G	609	CHL	4	0
29	s1	610	CLA	6	0
29	C	504	CLA	7	0
33	D1	411	LMG	2	0
29	S	603	CLA	3	0
32	A	412	SQD	5	0
29	R	602	CLA	4	0
48	Y1	607	CHL	4	0
29	y1	613	CLA	5	0
29	b1	607	CLA	5	0
29	C	507	CLA	4	0
29	b	610	CLA	6	0
29	r1	602	CLA	4	0
32	C	526	SQD	4	0
33	c	523	LMG	8	0
40	L	101	LHG	5	0
32	b1	621	SQD	4	0
33	A1	413	LMG	10	0
40	d	410	LHG	3	0
29	C	513	CLA	10	0
37	B	623	DGD	3	0
29	C1	511	CLA	7	0
29	s1	617	CLA	1	0
37	b	623	DGD	3	0
49	g	621	LUT	9	0
29	c1	502	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	611	CLA	2	0
29	g1	613	CLA	7	0
31	C1	516	BCR	3	0
48	s1	601	CHL	4	0
29	Y	614	CLA	9	0
48	s1	607	CHL	3	0
51	s1	623	NEX	6	0
31	B1	618	BCR	2	0
29	B1	604	CLA	5	0
39	B	625	DGA	1	0
29	A	405	CLA	4	0
29	R1	603	CLA	6	0
51	y1	623	NEX	2	0
29	c1	507	CLA	8	0
29	Y1	602	CLA	10	0
29	b1	602	CLA	2	0
40	n1	624	LHG	10	0
48	y	609	CHL	2	0
29	B1	608	CLA	7	0
33	a	413	LMG	5	0
49	N1	620	LUT	5	0
32	C1	526	SQD	3	0
51	n1	623	NEX	6	0
48	g	601	CHL	4	0
29	B1	605	CLA	4	0
49	s1	621	LUT	6	0
31	C1	514	BCR	9	0
50	y1	622	XAT	9	0
29	n	604	CLA	1	0
29	S1	610	CLA	6	0
29	A	406	CLA	6	0
29	b1	616	CLA	3	0
29	a1	406	CLA	9	0
29	r1	609	CLA	4	0
32	M1	101	SQD	4	0
29	d1	403	CLA	4	0
33	W	201	LMG	2	0
29	G	604	CLA	2	0
29	a	405	CLA	3	0
29	Y1	613	CLA	4	0
37	C1	519	DGD	8	0
29	G	611	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	G1	624	LHG	6	0
47	K1	101	4RF	5	0
29	r1	604	CLA	1	0
29	s1	612	CLA	1	0
48	N	606	CHL	3	0
38	T	101	3PH	2	0
33	d1	411	LMG	2	0
29	s	614	CLA	1	0
29	S	610	CLA	6	0
29	b	603	CLA	5	0
31	a	411	BCR	3	0
29	S	611	CLA	3	0
34	Y1	625	SPH	7	0
29	S1	603	CLA	1	0
29	n	602	CLA	4	0
48	g	608	CHL	1	0
29	c	502	CLA	3	0
29	C1	506	CLA	5	0
48	g1	606	CHL	2	0
29	b1	610	CLA	9	0
29	S1	604	CLA	3	0
29	d	403	CLA	3	0
51	y	623	NEX	1	0
33	H1	102	LMG	15	0
29	B	607	CLA	5	0
37	c	518	DGD	7	0
53	r1	626	ERG	5	0
45	h1	101	RRX	4	0
29	Y1	604	CLA	7	0
48	S	601	CHL	2	0
48	N1	605	CHL	4	0
33	a1	413	LMG	8	0
50	g	622	XAT	9	0
48	N1	607	CHL	8	0
29	g	613	CLA	2	0
49	y	620	LUT	2	0
29	B	609	CLA	8	0
29	C1	513	CLA	14	0
48	S	608	CHL	3	0
33	c1	521	LMG	3	0
29	n	613	CLA	8	0
40	d	408	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	s	609	CLA	2	0
40	D1	410	LHG	4	0
30	A	409	PHO	6	0
29	B	606	CLA	8	0
29	s1	604	CLA	3	0
29	G	603	CLA	3	0
30	a1	408	PHO	9	0
29	c	512	CLA	1	0
48	s1	608	CHL	5	0
31	A	411	BCR	2	0
48	s1	606	CHL	2	0
29	s1	609	CLA	6	0
31	b1	619	BCR	4	0
29	N	603	CLA	4	0
29	n	603	CLA	5	0
33	C	521	LMG	3	0
38	t1	101	3PH	5	0
29	y	614	CLA	7	0
51	R	622	NEX	2	0
48	S1	608	CHL	5	0
39	b	625	DGA	5	0
29	s1	613	CLA	4	0
29	Y	611	CLA	3	0
29	c1	510	CLA	5	0
29	B1	611	CLA	6	0
29	r1	612	CLA	3	0
29	a	407	CLA	1	0
48	n	601	CHL	2	0
29	b	607	CLA	4	0
32	c1	526	SQD	4	0
48	y1	605	CHL	1	0
49	S	620	LUT	2	0
29	Y	610	CLA	4	0
29	G	610	CLA	6	0
51	n	623	NEX	3	0
37	b1	623	DGD	4	0
49	Y1	620	LUT	6	0
29	g1	603	CLA	8	0
29	B	616	CLA	7	0
29	C	510	CLA	2	0
48	Y1	606	CHL	4	0
29	b	609	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	R	609	CLA	3	0
29	B1	612	CLA	9	0
48	S1	607	CHL	1	0
33	h1	102	LMG	4	0
29	A1	407	CLA	2	0
31	c	514	BCR	3	0
29	Y1	603	CLA	5	0
50	R	621	XAT	4	0
37	c1	520	DGD	6	0
29	B1	615	CLA	5	0
29	N1	604	CLA	5	0
32	A1	412	SQD	6	0
33	H	102	LMG	2	0
50	N1	622	XAT	9	0
29	r1	610	CLA	6	0
40	g	624	LHG	7	0
49	S1	620	LUT	7	0
49	Y1	621	LUT	8	0
29	g	602	CLA	6	0
29	D	403	CLA	4	0
33	D	411	LMG	2	0
40	N	624	LHG	4	0
40	n	624	LHG	3	0
48	N	609	CHL	5	0
48	n1	609	CHL	4	0
48	r	606	CHL	2	0
48	R	606	CHL	2	0
29	c1	512	CLA	5	0
37	B1	623	DGD	2	0
38	B	624	3PH	7	0
32	a	412	SQD	2	0
32	m1	101	SQD	3	0
50	Y	622	XAT	6	0
31	c	516	BCR	5	0
31	B	618	BCR	3	0
51	N	623	NEX	3	0
29	n1	613	CLA	10	0
37	c	519	DGD	1	0
50	N	622	XAT	5	0
29	D1	403	CLA	2	0
40	s1	624	LHG	7	0
29	g1	614	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	s1	626	3PH	5	0
49	r	620	LUT	4	0
49	s	620	LUT	3	0
33	C1	521	LMG	9	0
31	d	404	BCR	3	0
51	r	622	NEX	3	0
29	c	505	CLA	5	0
31	C	516	BCR	2	0
29	G1	604	CLA	3	0
29	G1	614	CLA	3	0
29	b1	612	CLA	6	0
48	G	608	CHL	2	0
40	Y1	624	LHG	6	0
29	r	610	CLA	5	0
29	s	610	CLA	5	0
29	R1	604	CLA	2	0
44	F1	101	HEM	3	0
29	s	611	CLA	6	0
30	A1	408	PHO	5	0
29	y	604	CLA	1	0
39	j1	101	DGA	4	0
37	C	518	DGD	4	0
29	n1	610	CLA	4	0
48	N1	608	CHL	4	0
38	S	626	3PH	7	0
45	H1	101	RRX	3	0
29	y	611	CLA	6	0
29	c	511	CLA	4	0
49	N1	621	LUT	7	0
40	D1	409	LHG	5	0
29	a1	410	CLA	11	0
31	c1	516	BCR	7	0
39	C	524	DGA	3	0
29	y	613	CLA	6	0
48	G	607	CHL	6	0
48	S1	606	CHL	4	0
29	r	612	CLA	1	0
51	g	623	NEX	1	0
29	B1	603	CLA	13	0
49	s	621	LUT	1	0
48	N1	609	CHL	9	0
49	R1	620	LUT	4	0

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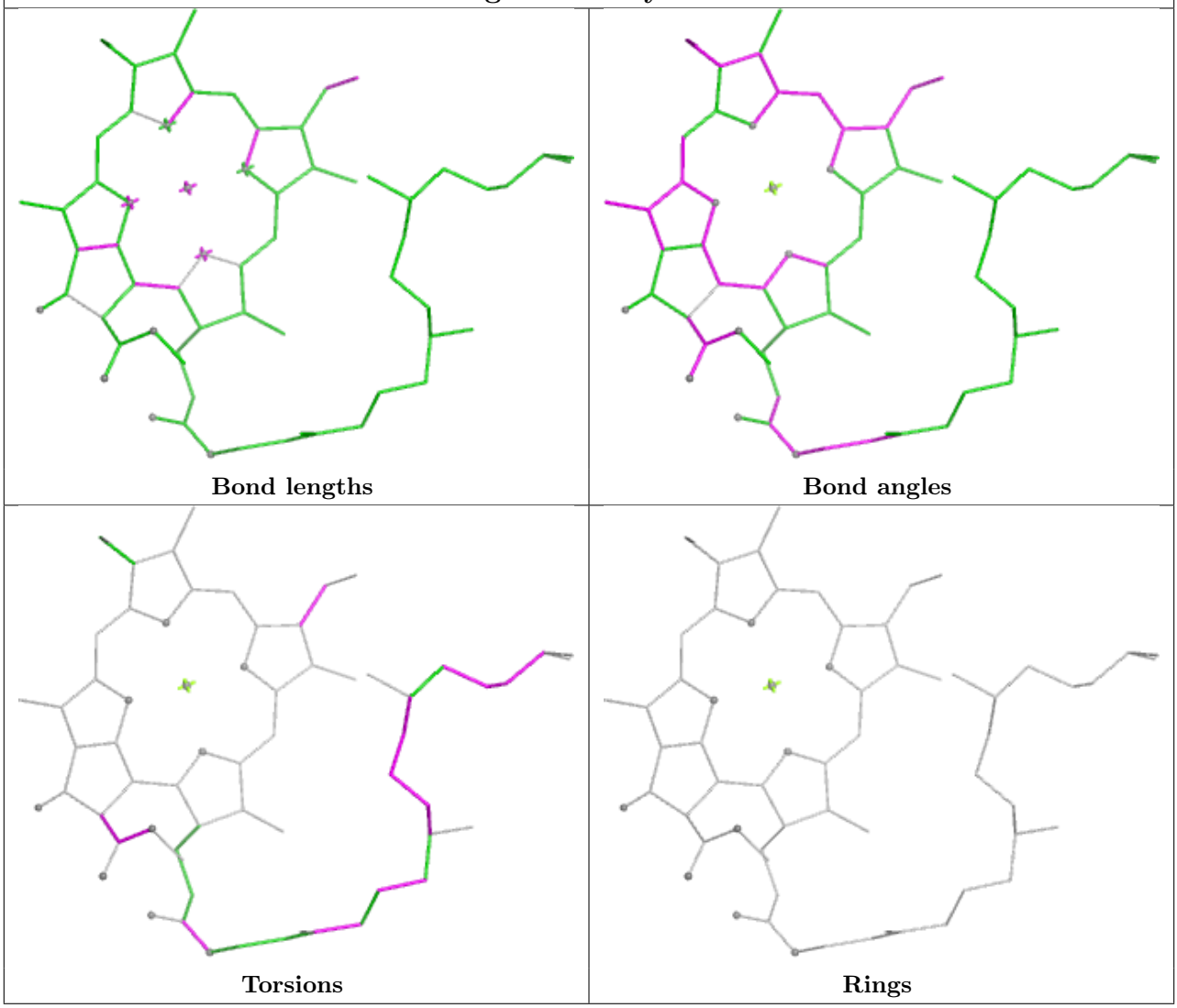
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	D	402	CLA	6	0
38	S1	626	3PH	4	0
51	R1	622	NEX	4	0
39	b1	625	DGA	4	0
48	y	601	CHL	1	0
40	D	409	LHG	6	0
39	J	101	DGA	2	0
29	g	610	CLA	3	0
48	s	608	CHL	5	0
29	r	609	CLA	2	0
29	n	612	CLA	1	0
29	Y	608	CLA	2	0
29	C	503	CLA	2	0
42	D1	401	BCT	1	0
29	b1	604	CLA	9	0
29	c1	508	CLA	8	0
31	c	515	BCR	3	0
29	c1	504	CLA	4	0
29	r	604	CLA	1	0
50	y	622	XAT	4	0
29	r1	603	CLA	2	0
48	n1	605	CHL	3	0
48	G	606	CHL	2	0
38	b	624	3PH	6	0
29	B	614	CLA	6	0
29	S	602	CLA	3	0
33	C	523	LMG	4	0
29	b	613	CLA	4	0
48	n	606	CHL	6	0
29	r1	608	CLA	3	0
29	b1	603	CLA	3	0

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

equivalents in the CSD to analyse the geometry.

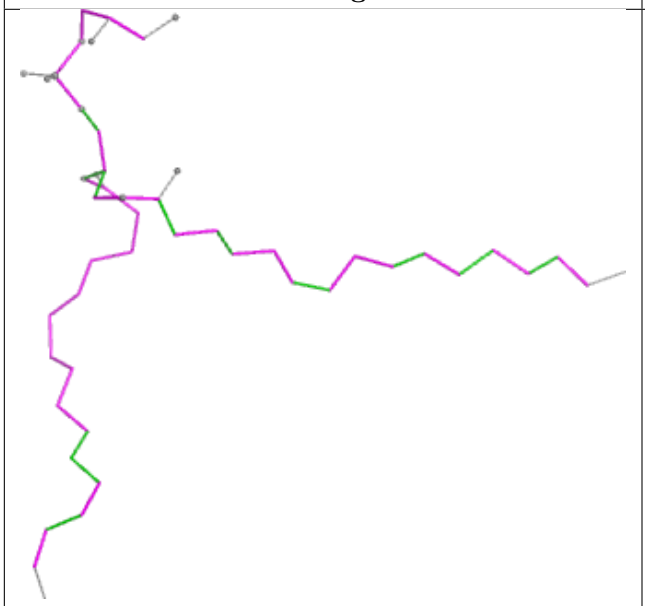
Ligand CLA y 612



Ligand LHG L1 101

Bond lengths

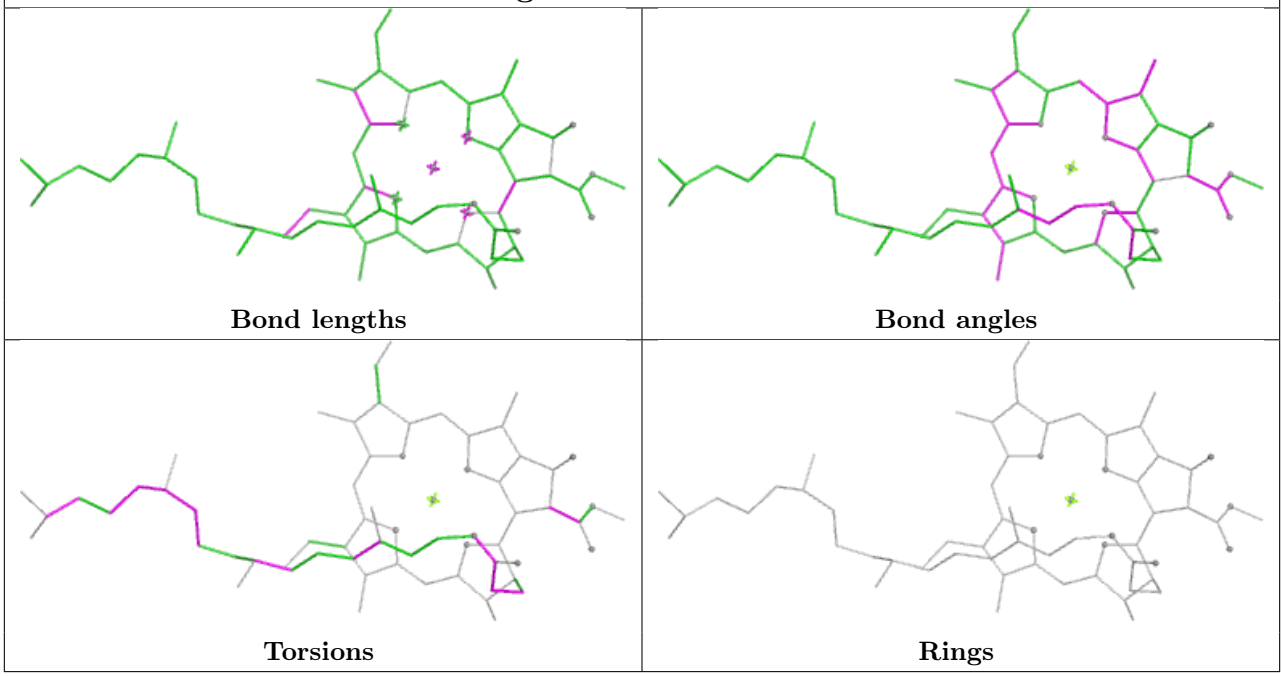
Bond angles



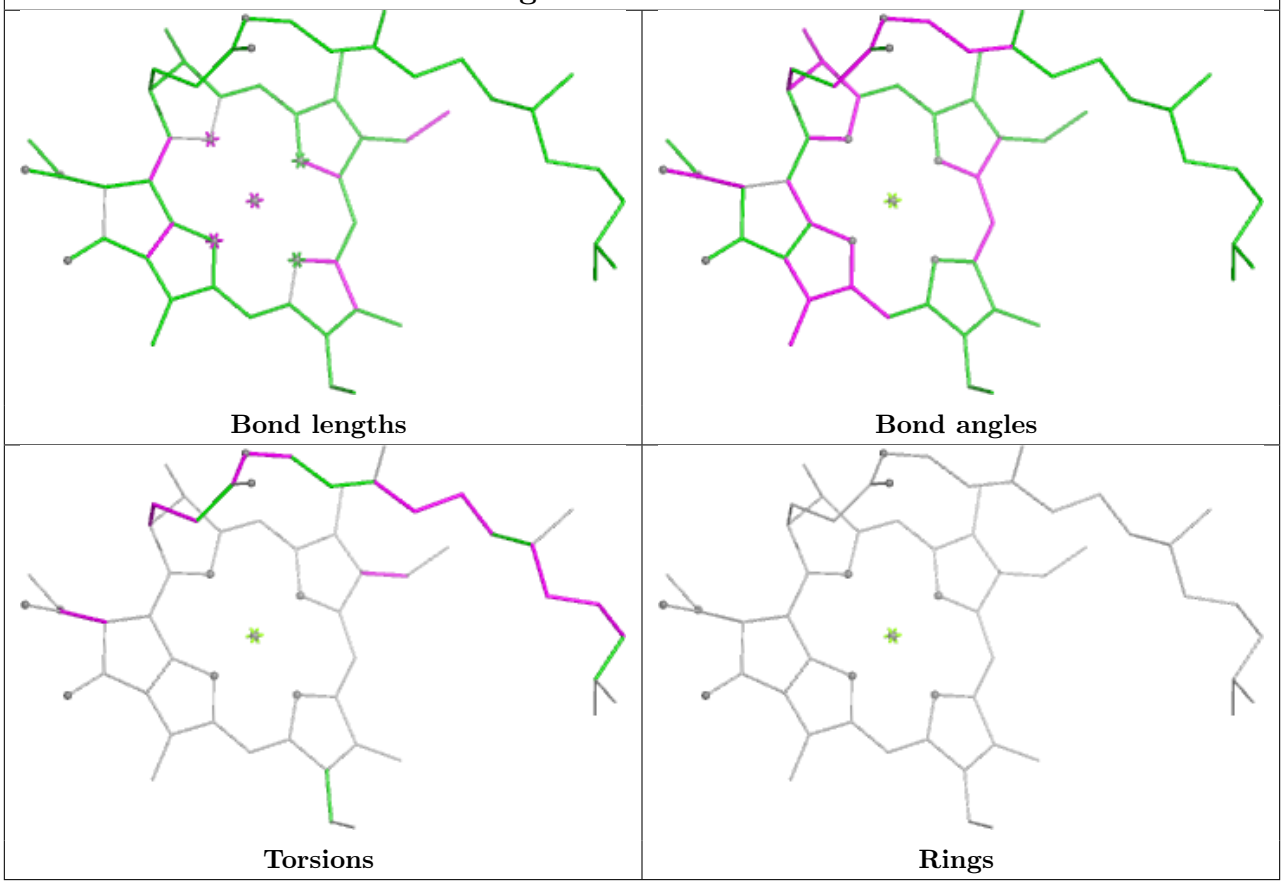
Torsions

Rings

Ligand CLA C1 505

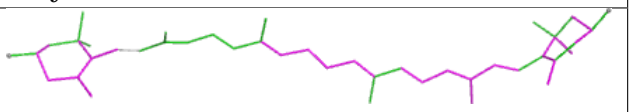


Ligand CLA S1 602

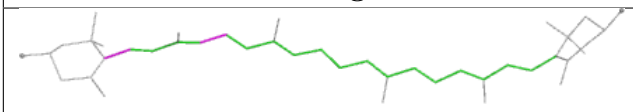


Ligand LUT y 621

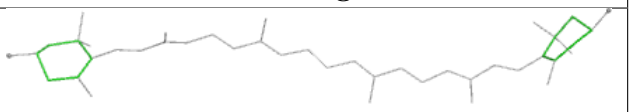
Bond lengths



Bond angles

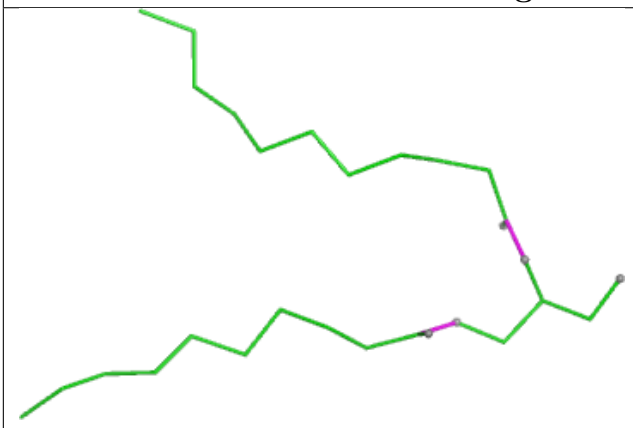


Torsions

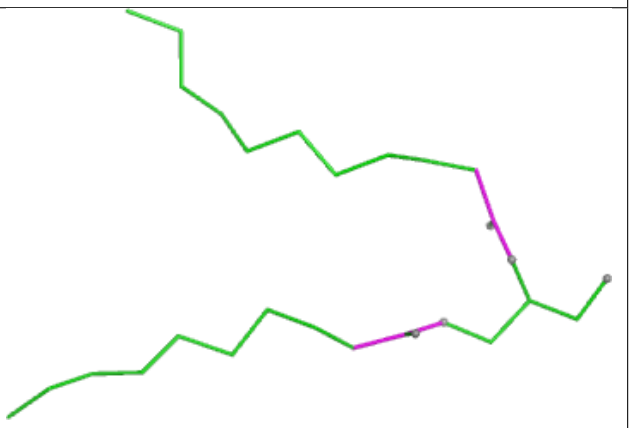


Rings

Ligand DGA J1 101



Bond lengths



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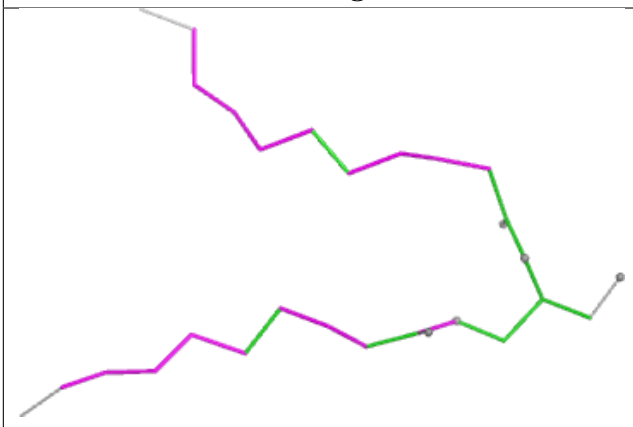
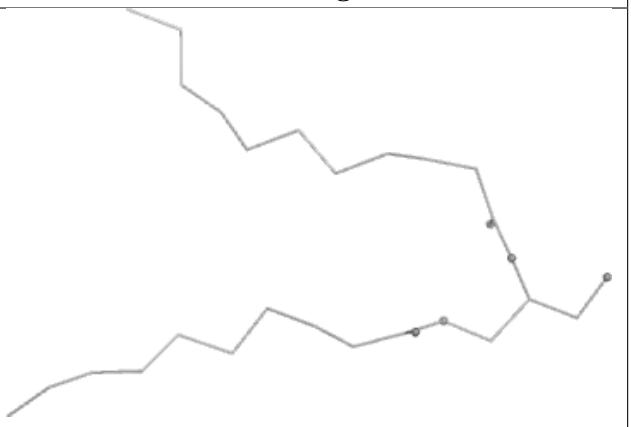


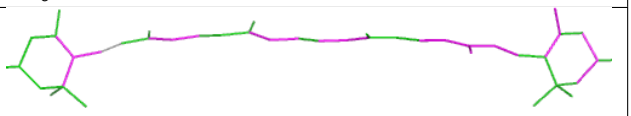
Torsions



Rings

Ligand LUT y1 620

Bond lengths



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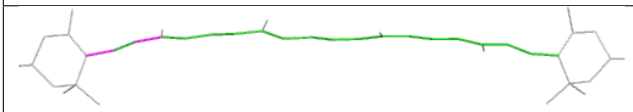

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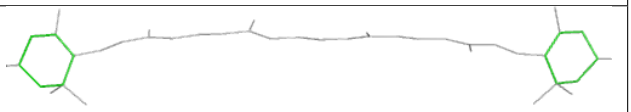
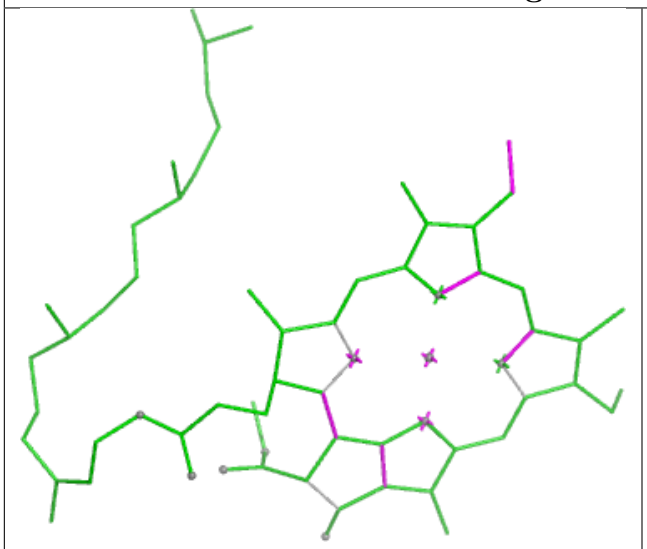


Rings

Ligand CLA B 617



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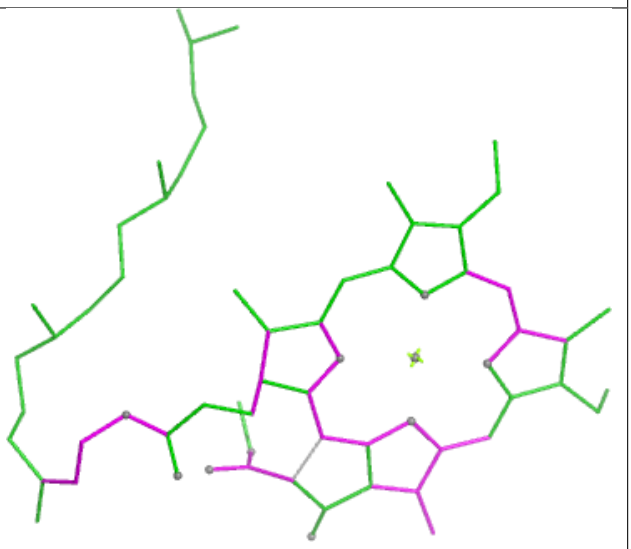

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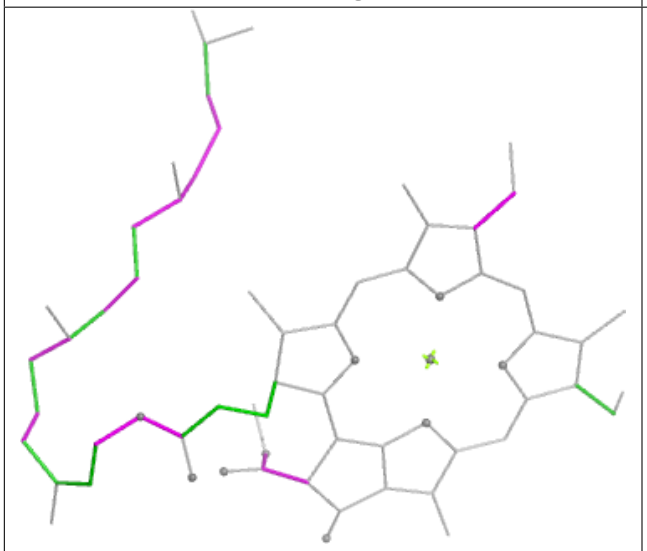

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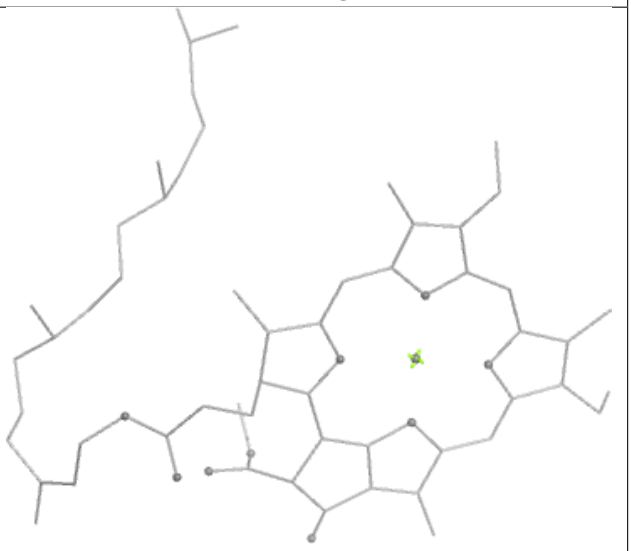

Rings

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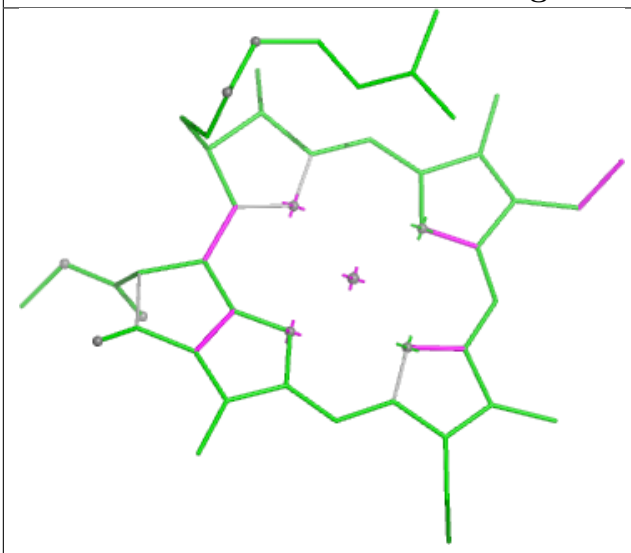
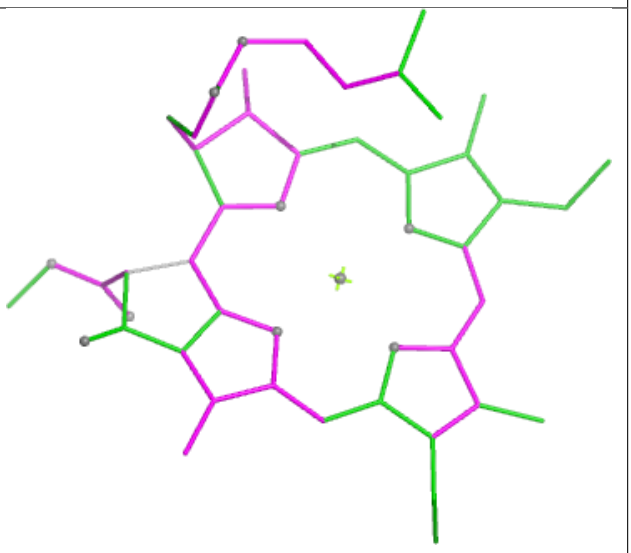
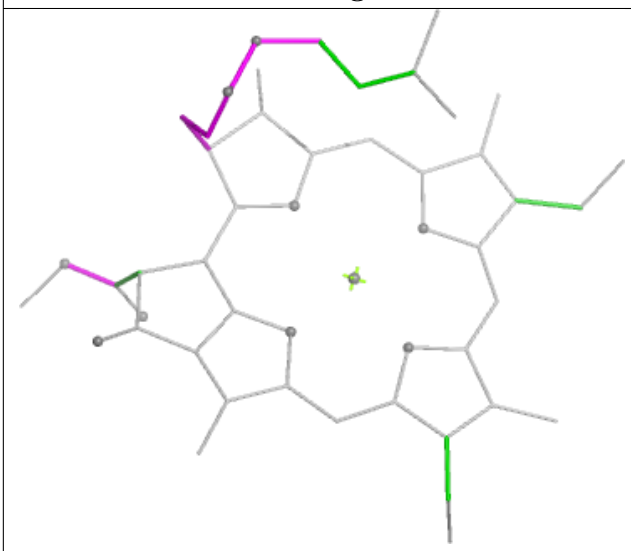
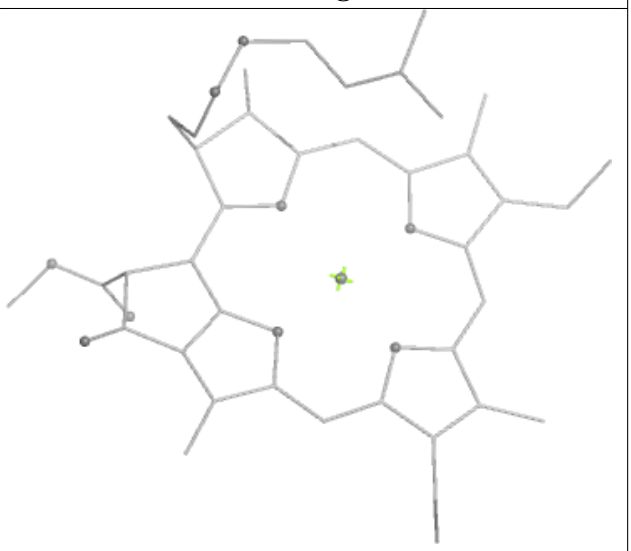
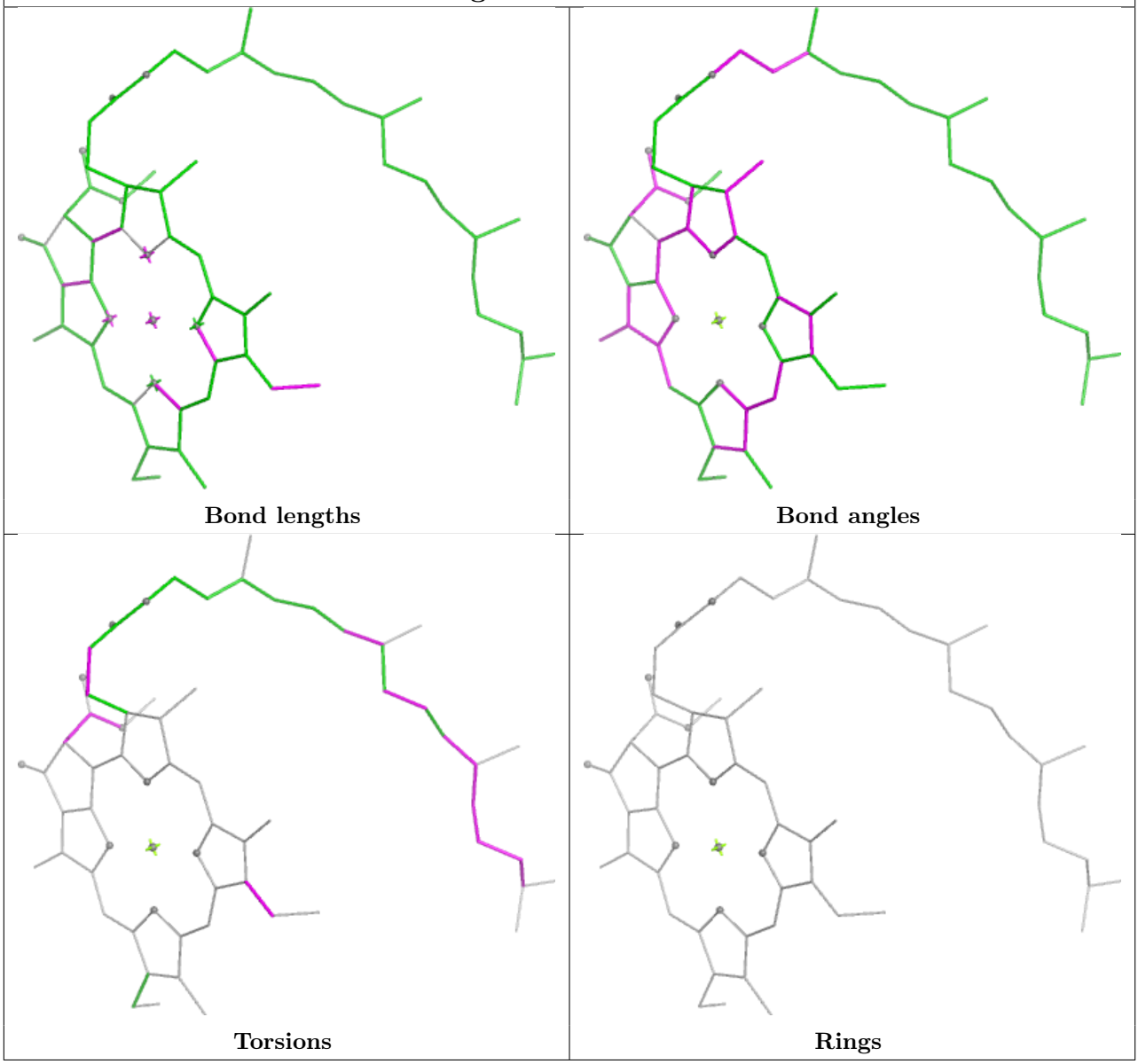
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 507



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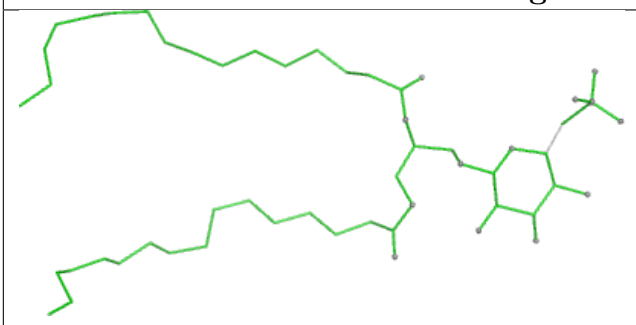
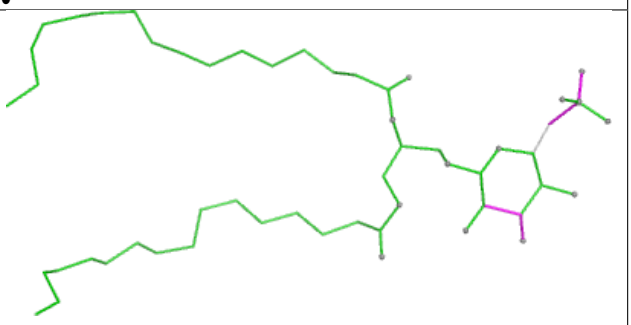
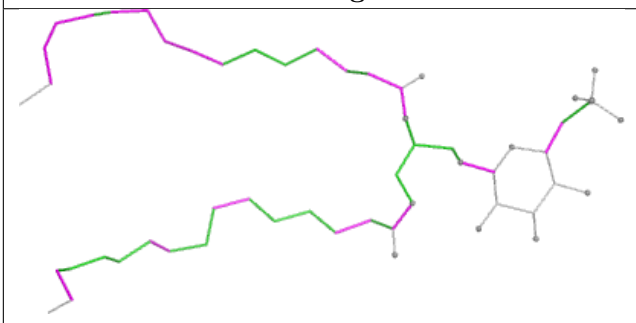
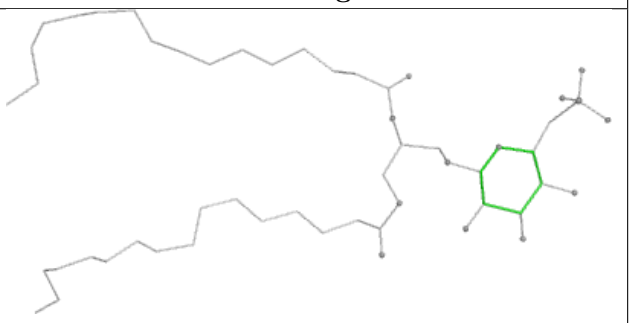
 Bond lengths	 Bond angles
 Torsions	 Rings

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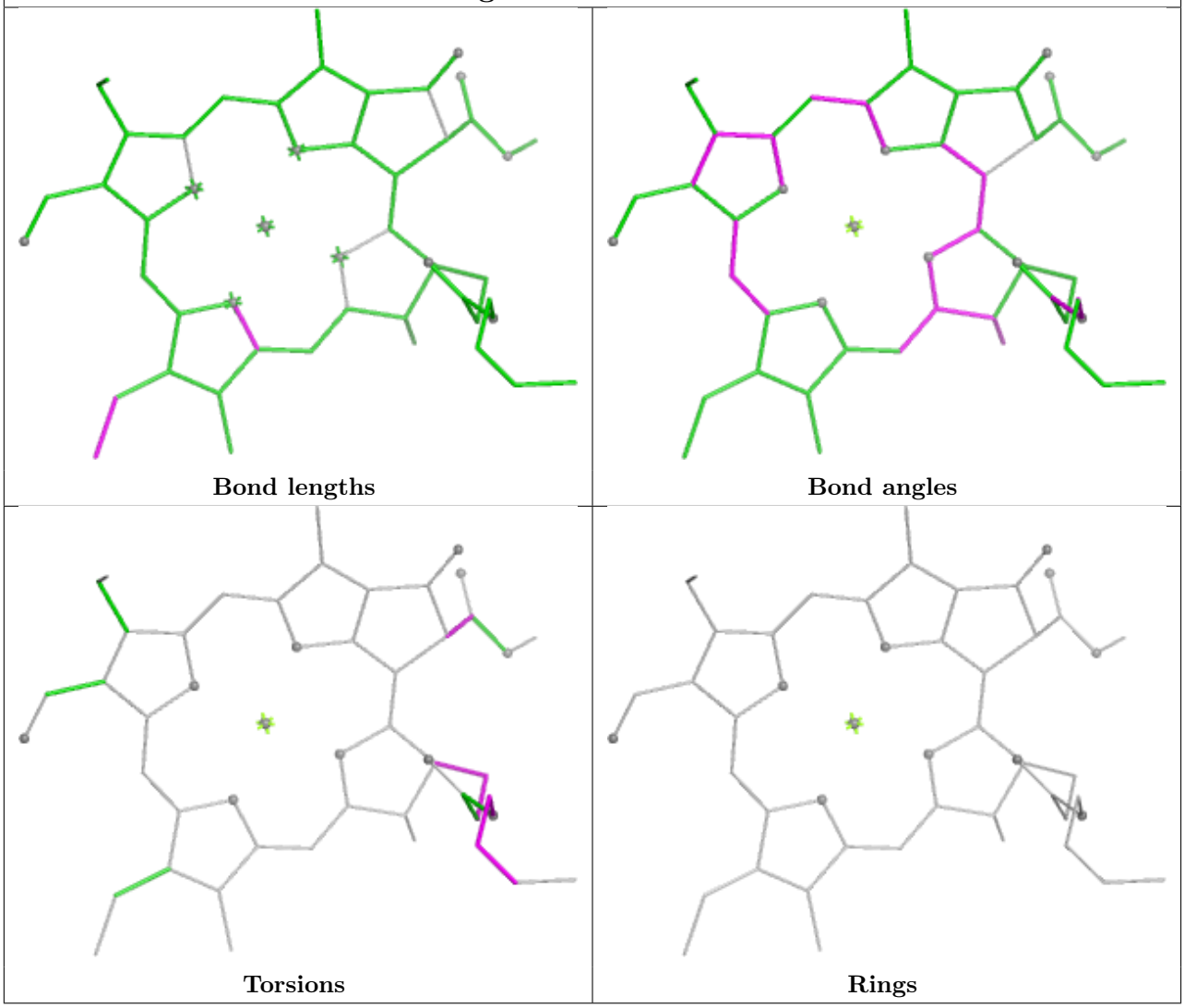

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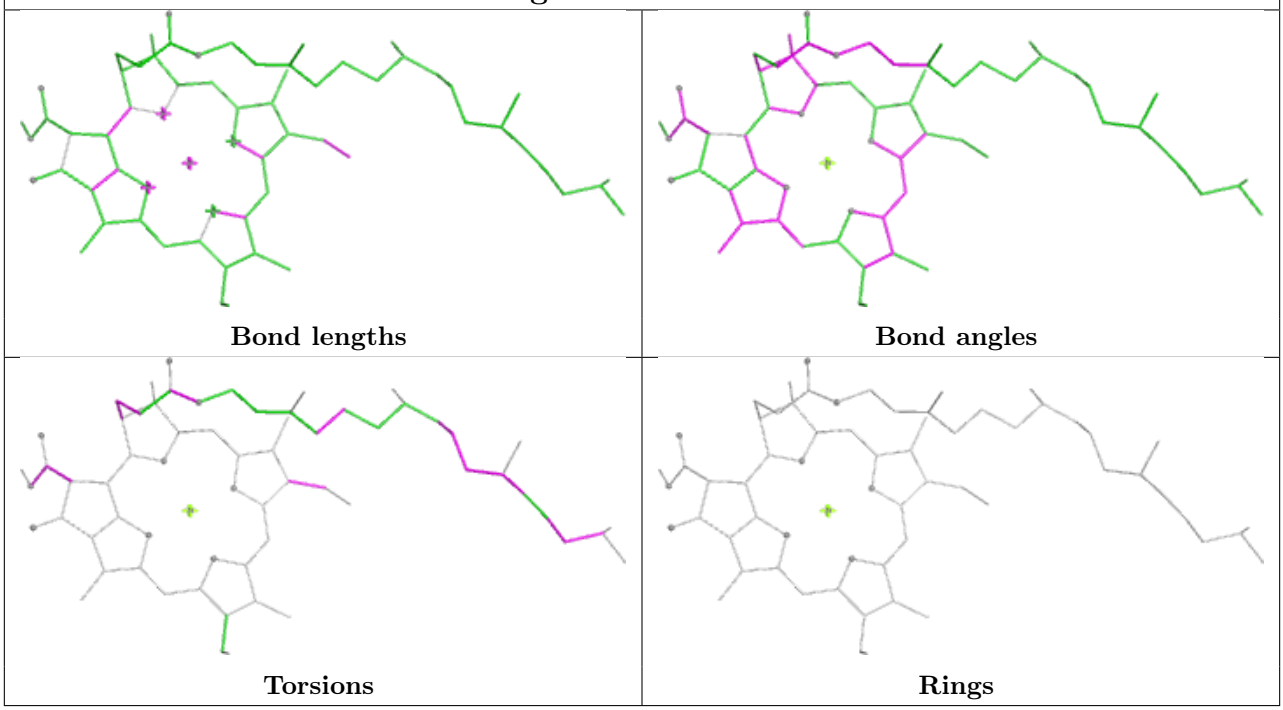
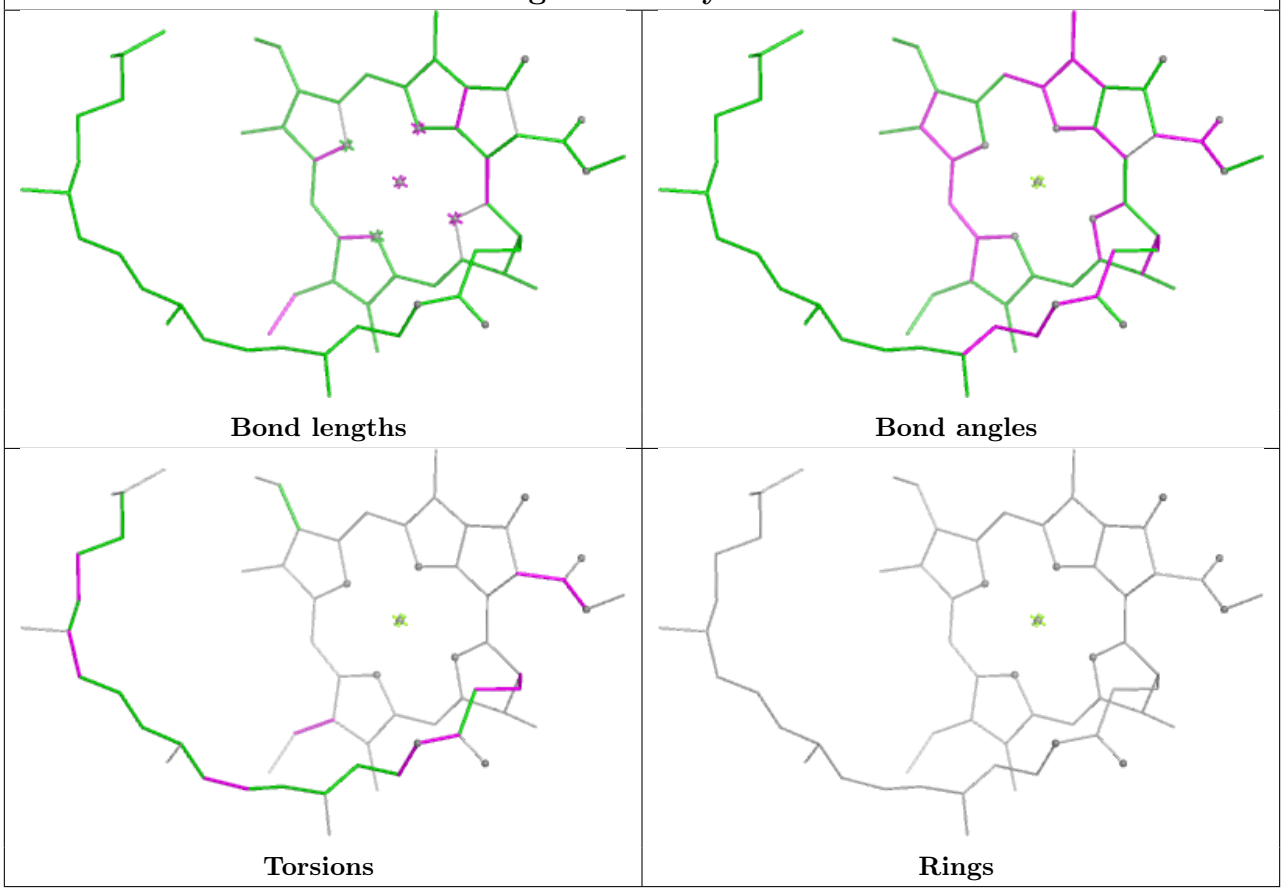


Ligand CLA y 610



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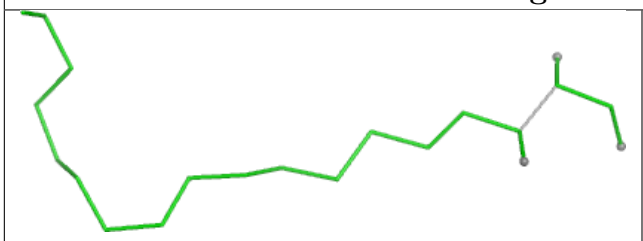
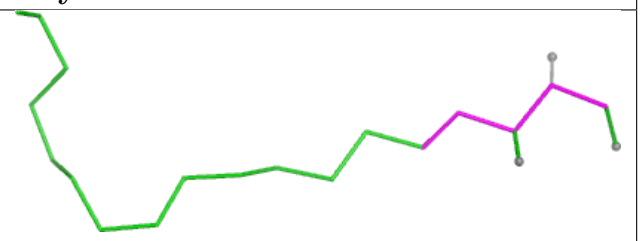
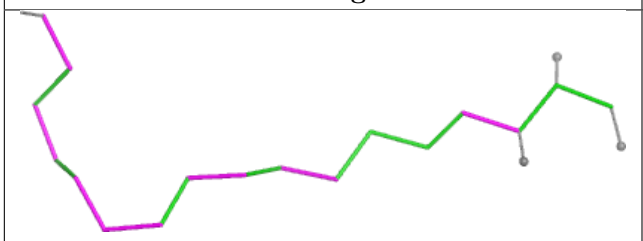
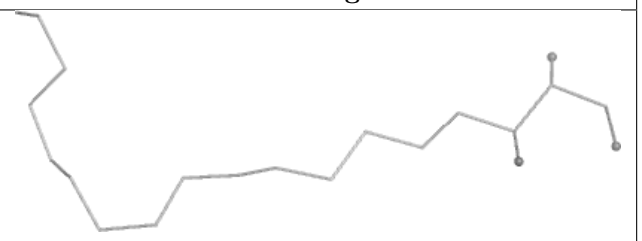
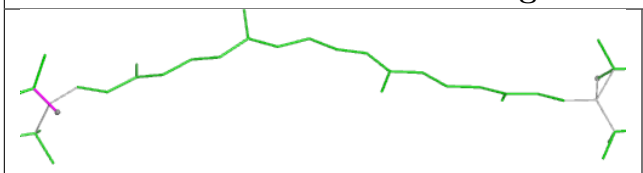
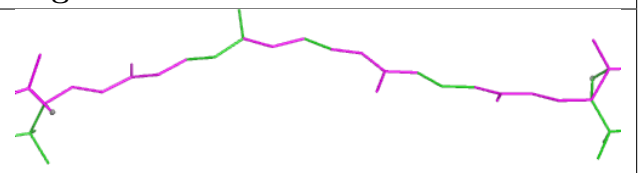
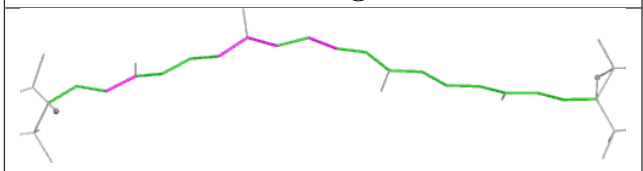
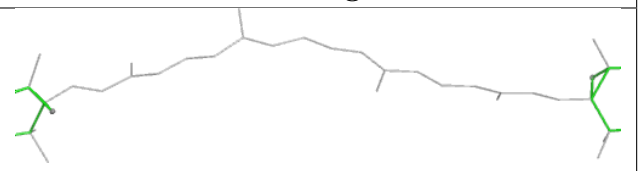
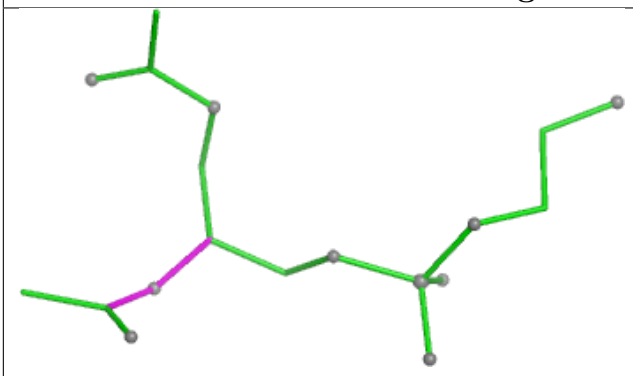
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT g1 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PTY y1 627



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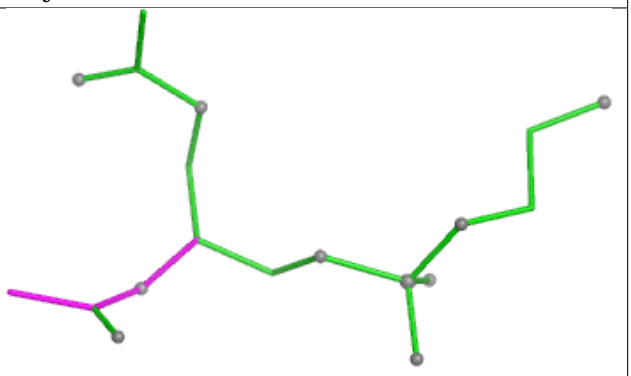
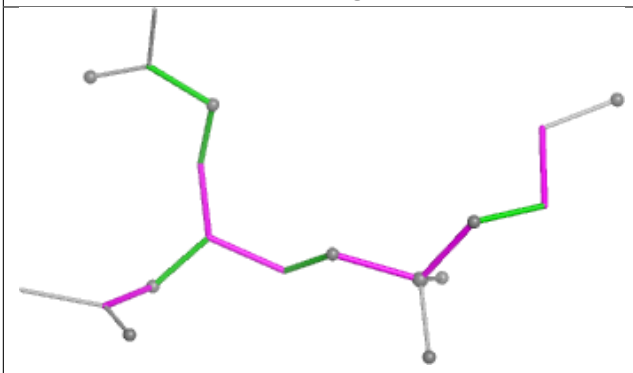
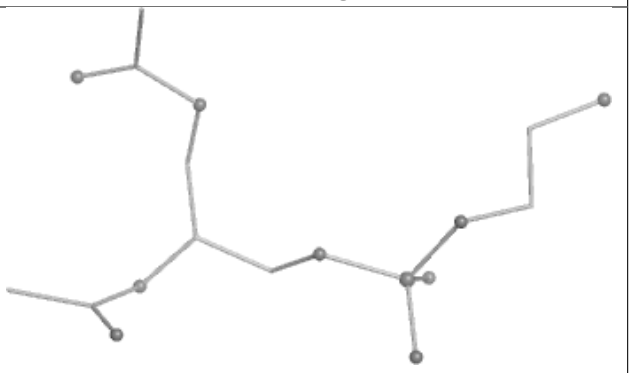


Bond angles

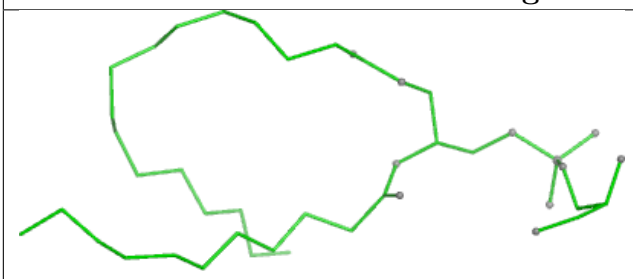


Torsions



Rings

Ligand LHG D 408



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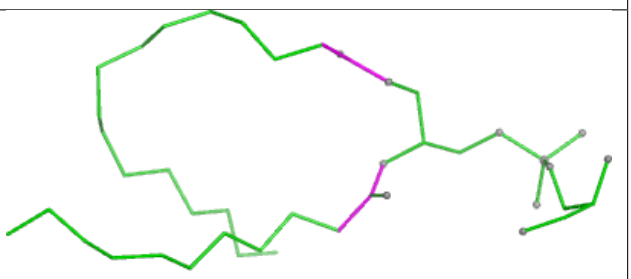
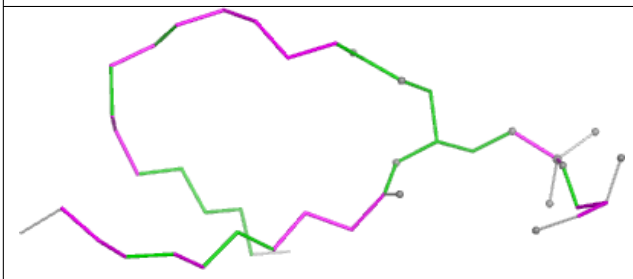
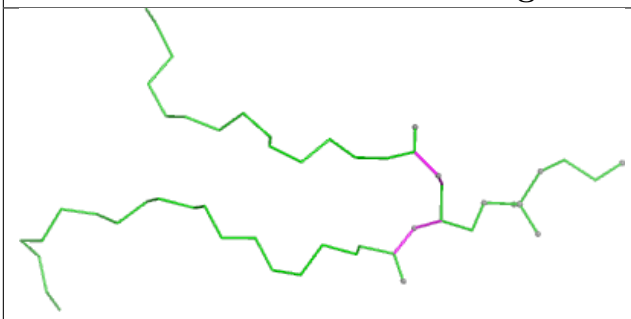
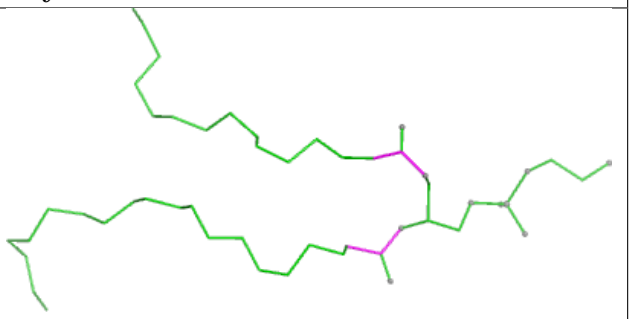
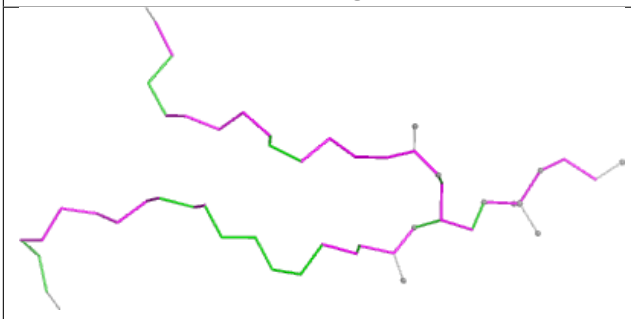
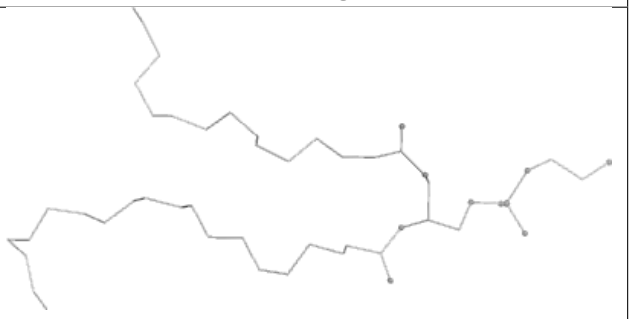


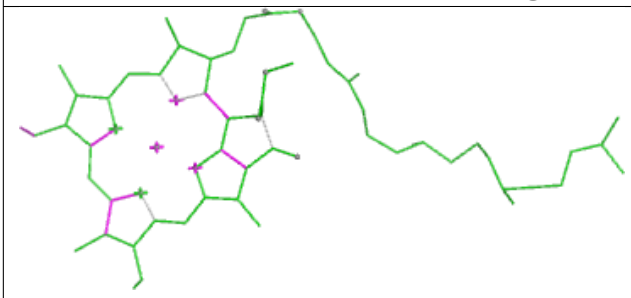
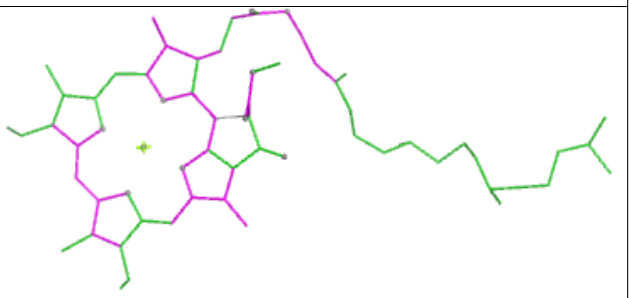
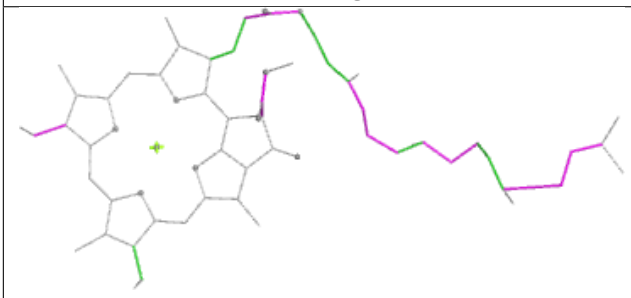
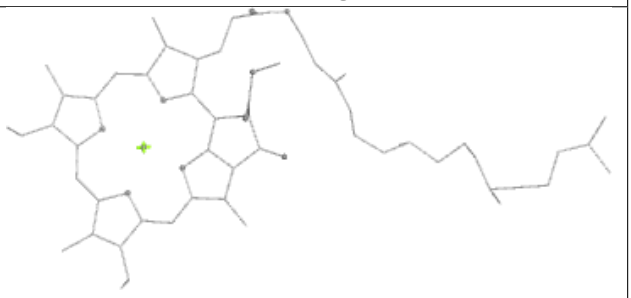
Bond angles

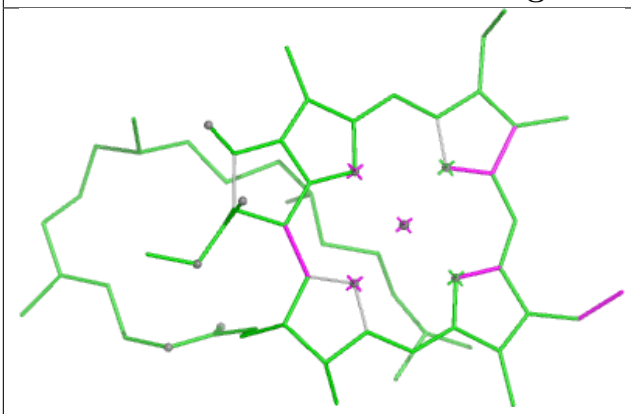
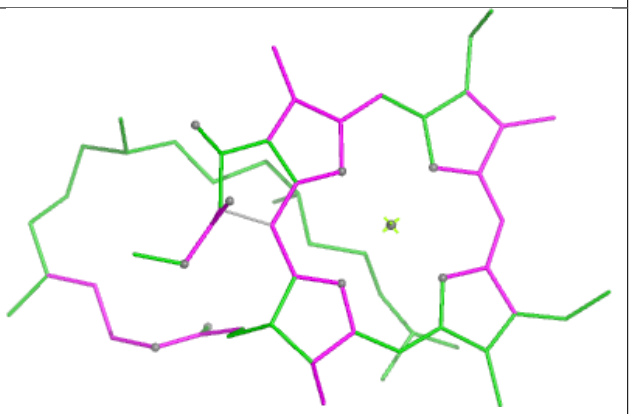
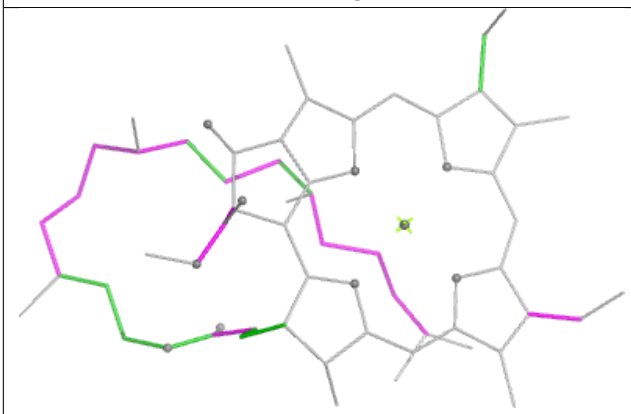
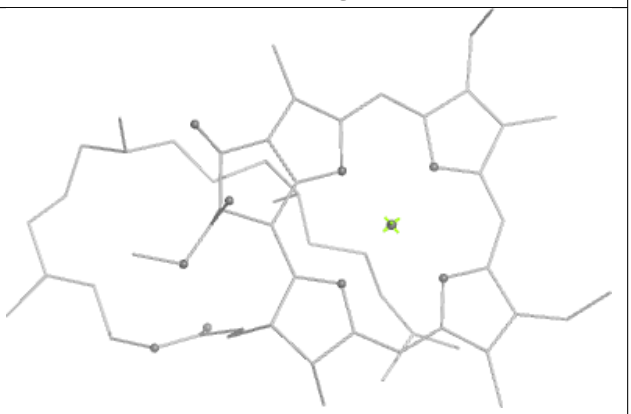


Torsions

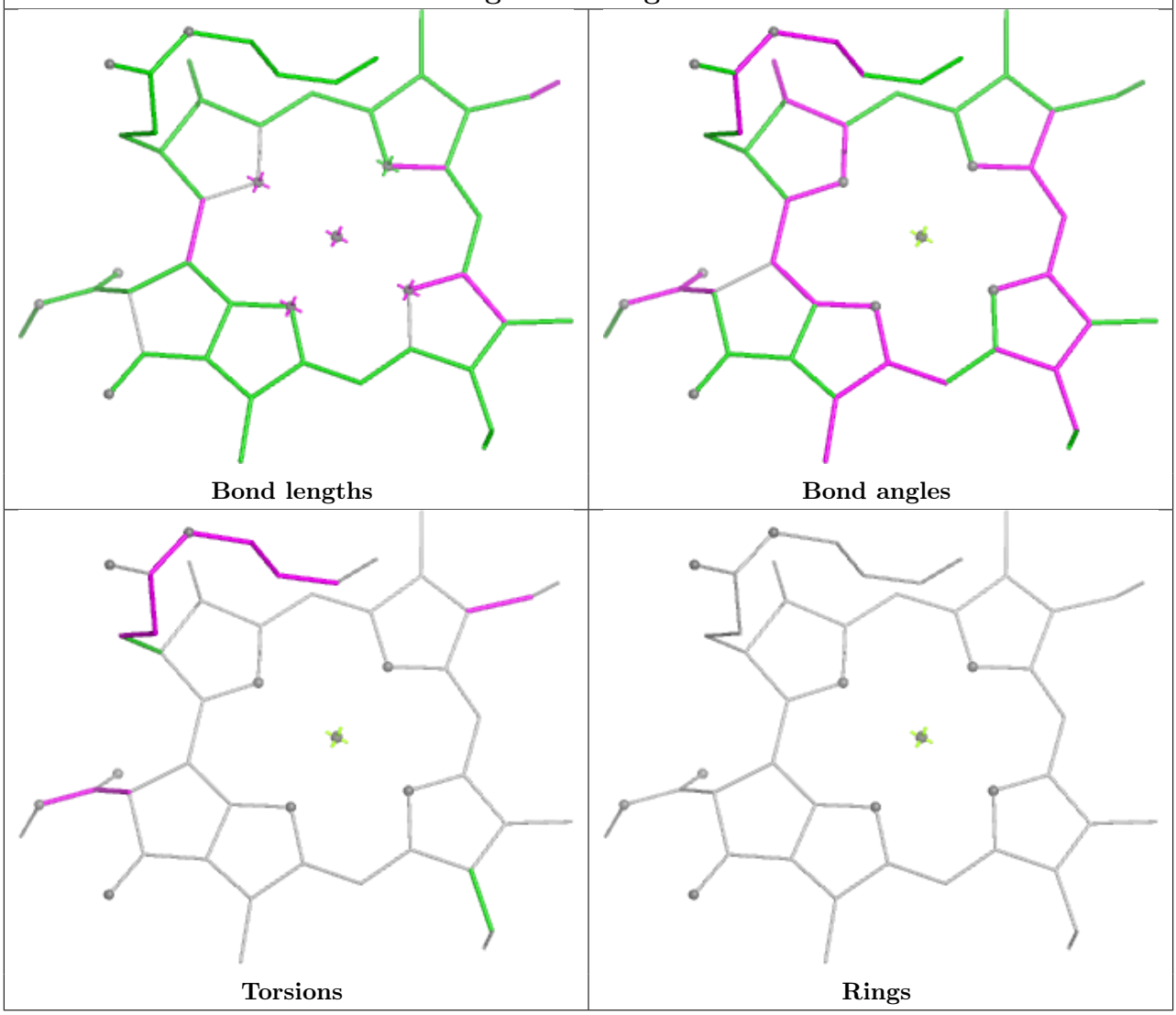
Rings

Ligand PTY y1 626	
 Bond lengths	 Bond angles
 Torsions	 Rings

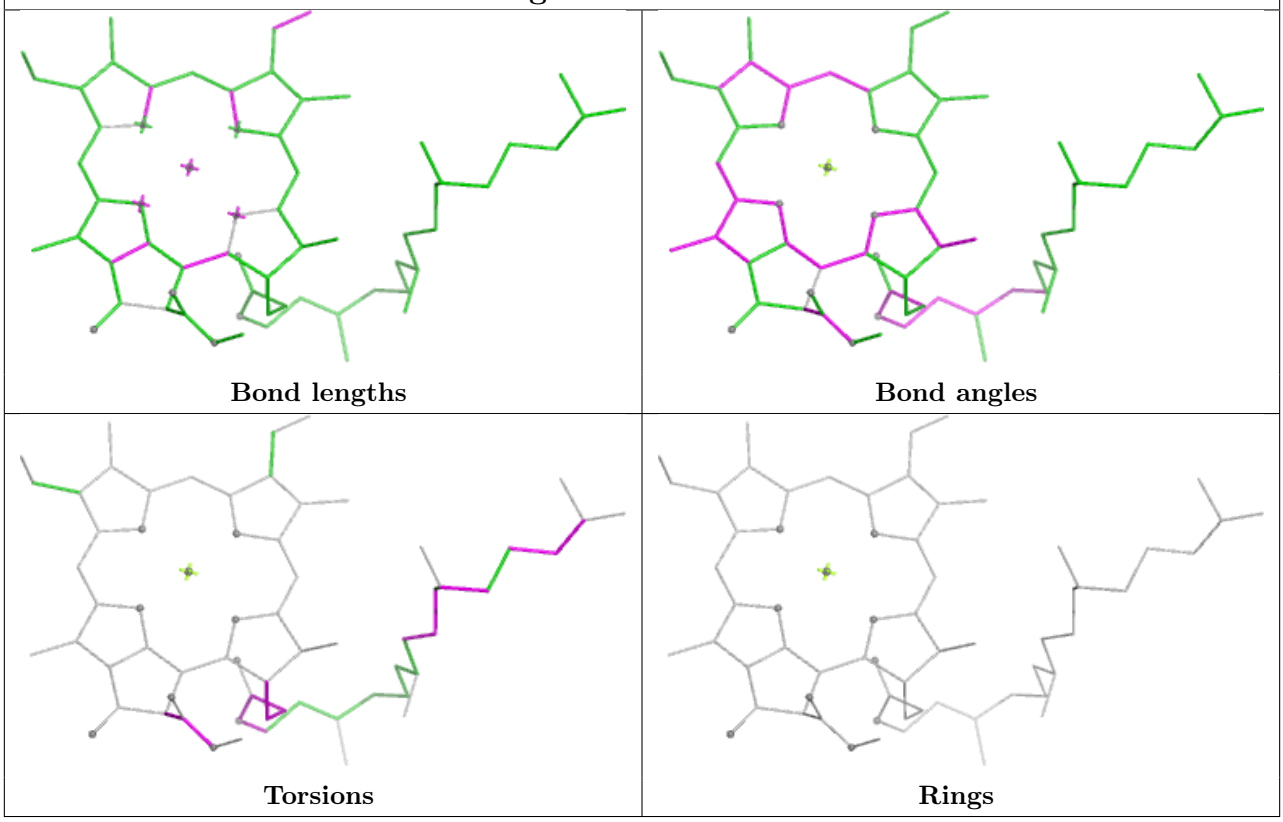
Ligand CLA B 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

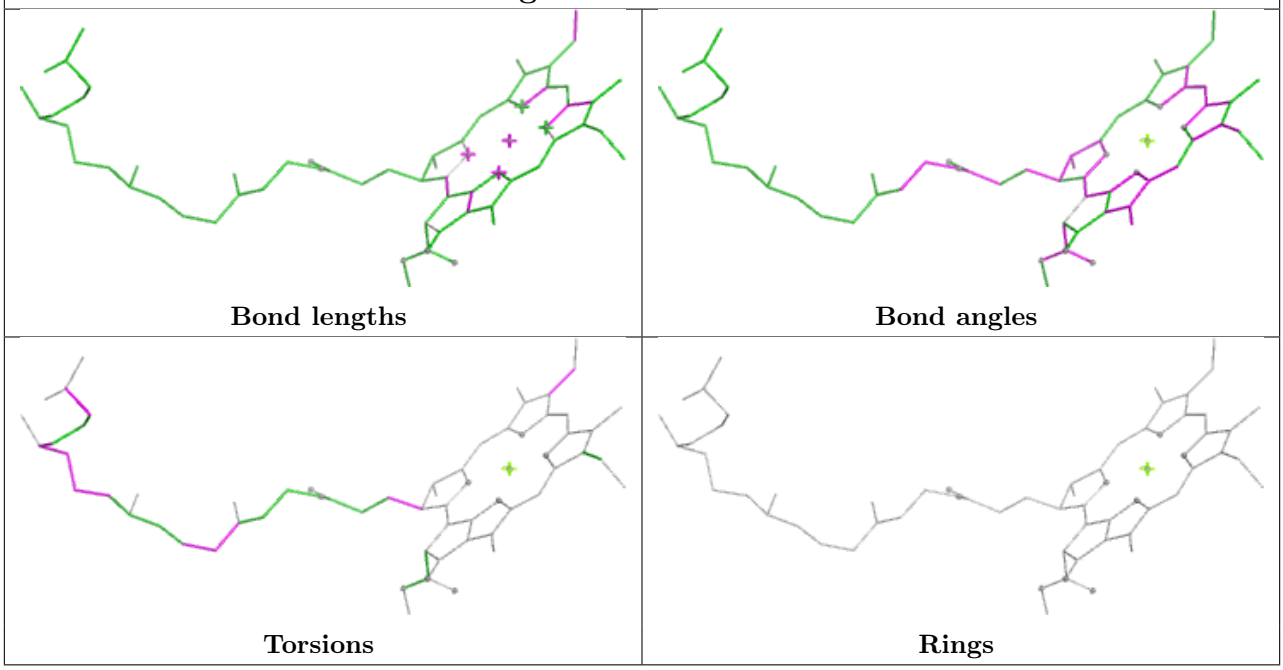
Ligand CLA g 614



Ligand CLA a 406



Ligand CLA d1 402



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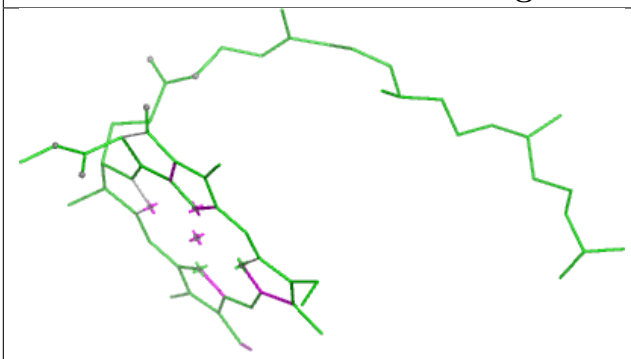
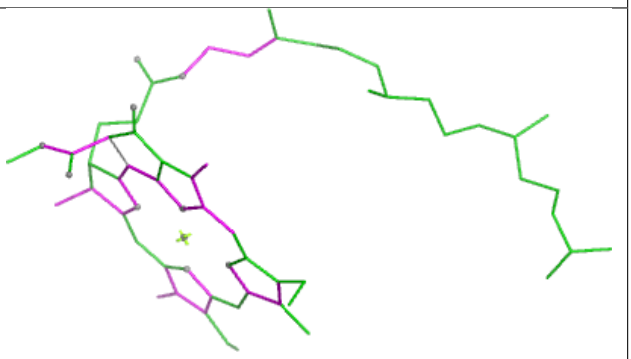
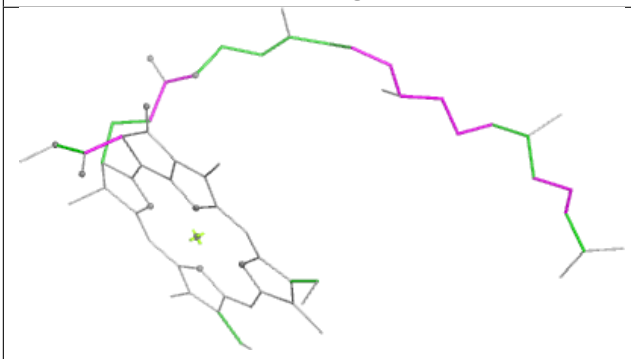
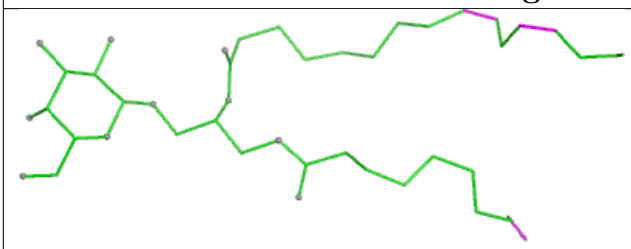
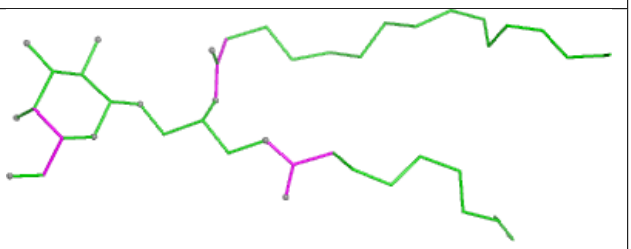
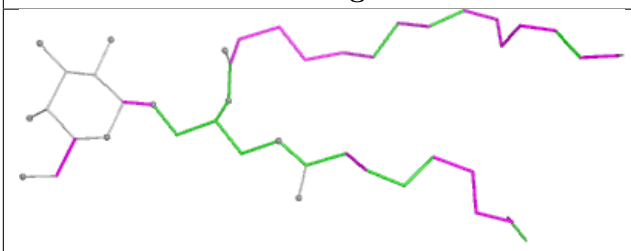
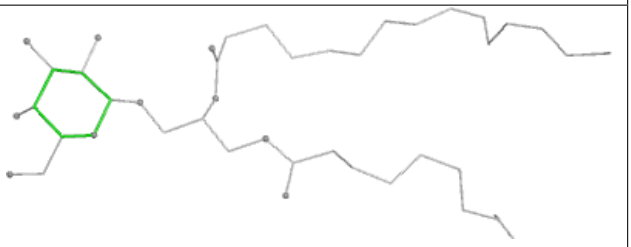
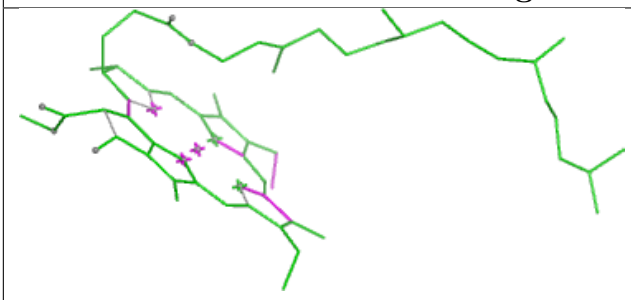
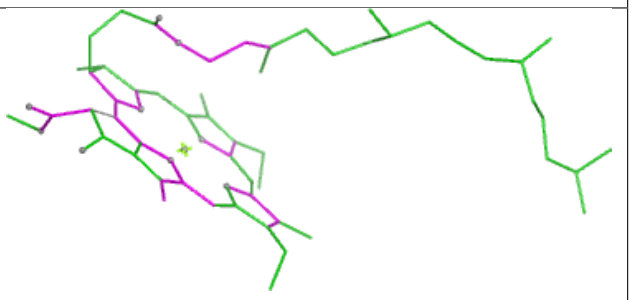
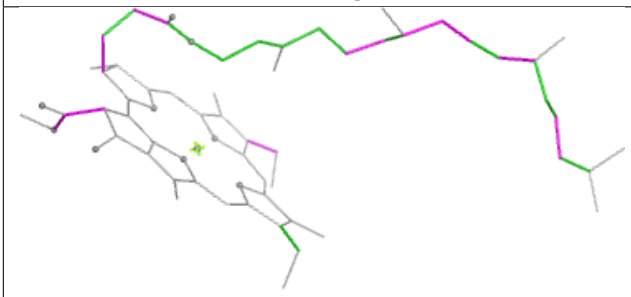
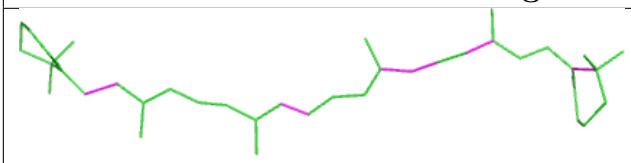
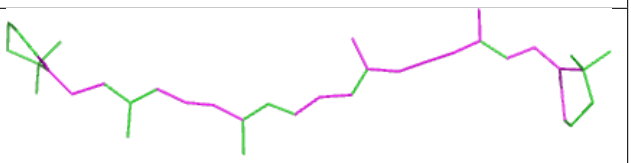
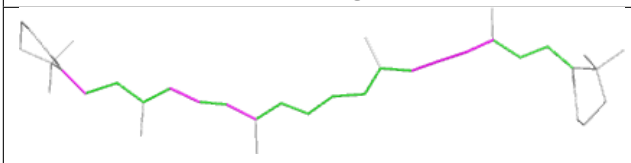
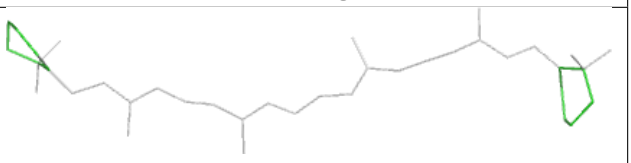
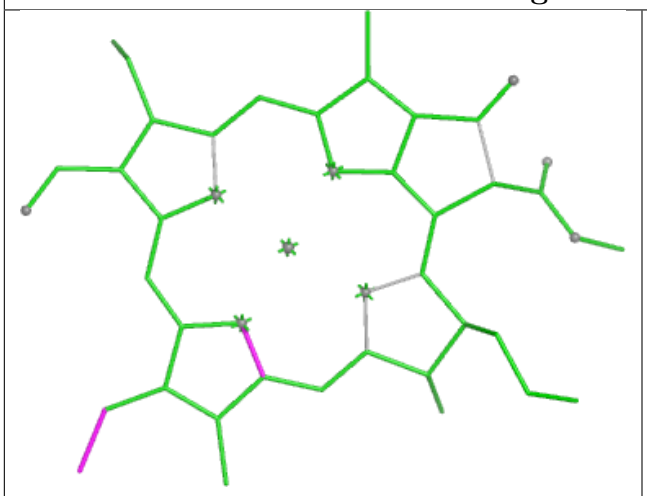
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand LMG d 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 609	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand BCR C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL s 606



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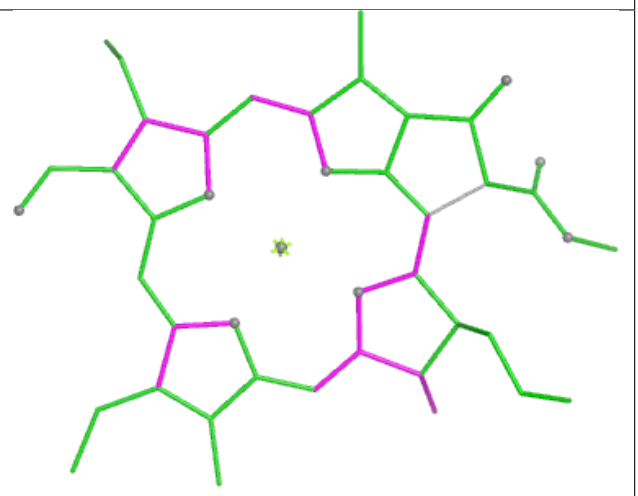
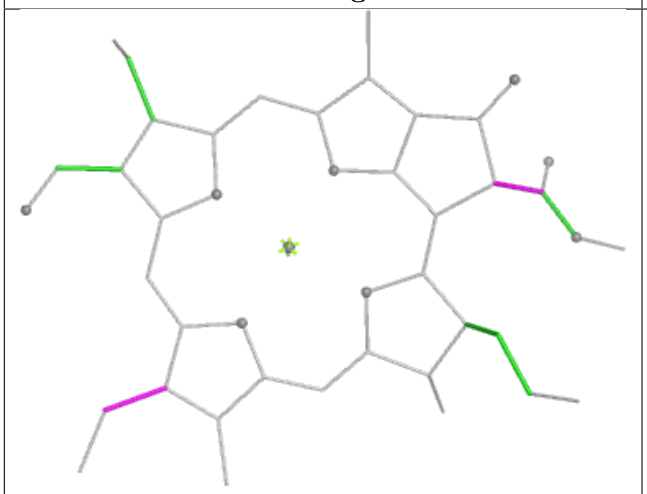


Bond angles



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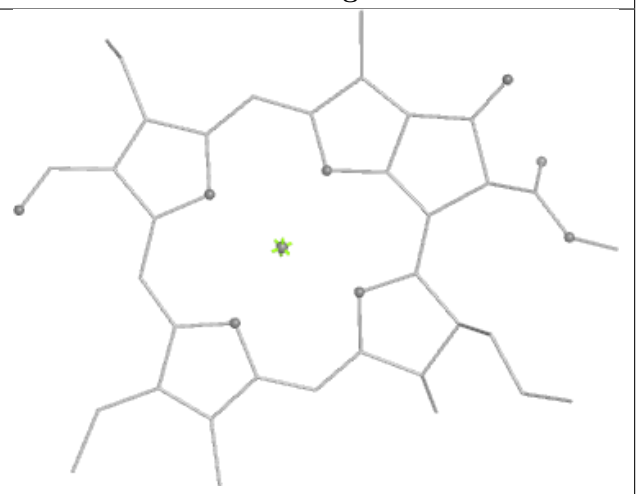
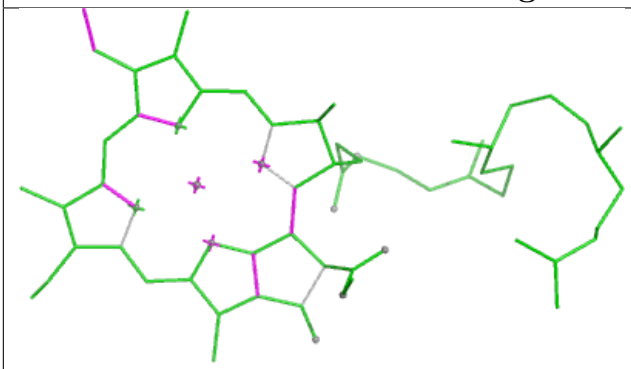
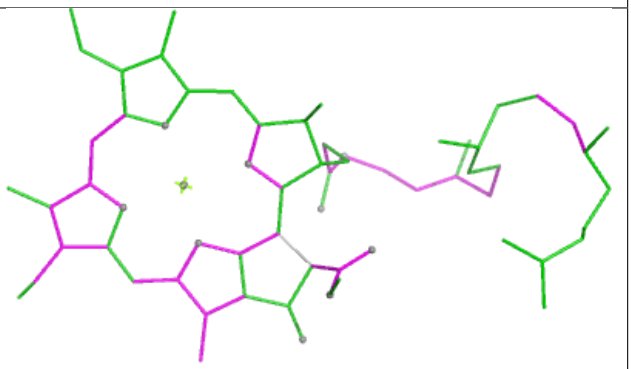
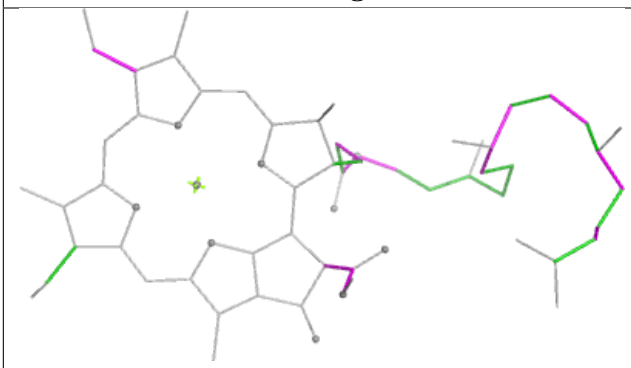
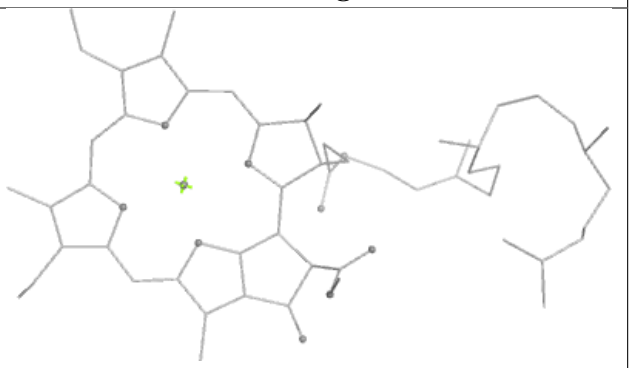


Rings

Ligand CLA b1 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

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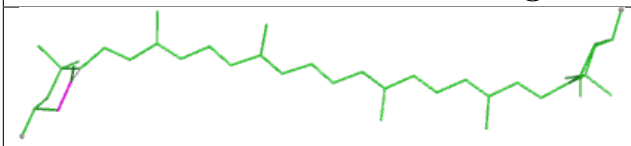
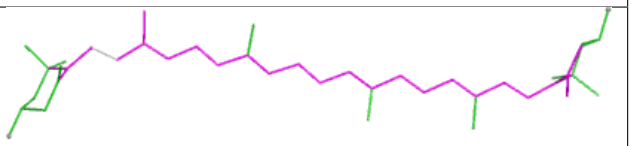
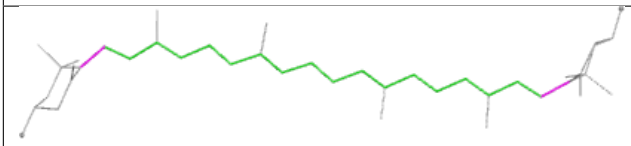
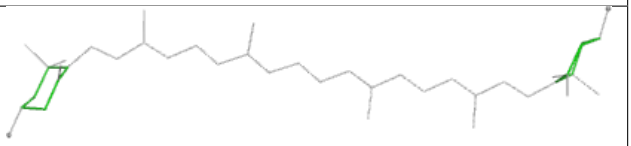
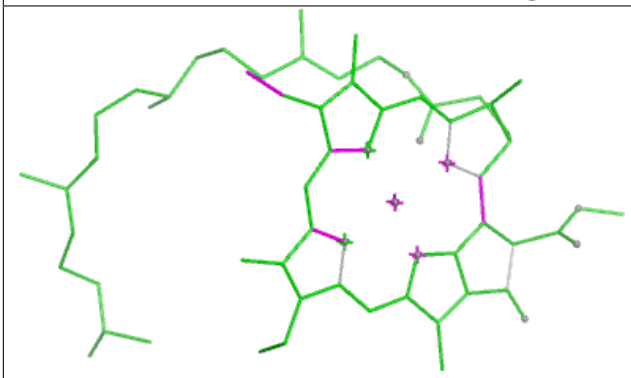
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA N 610



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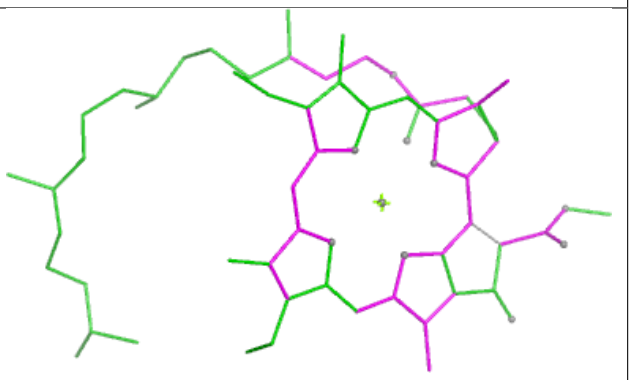
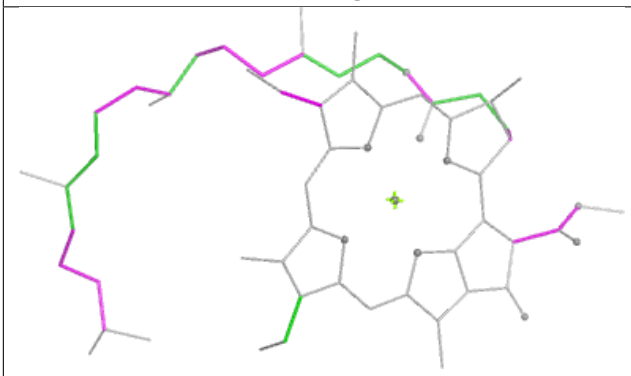
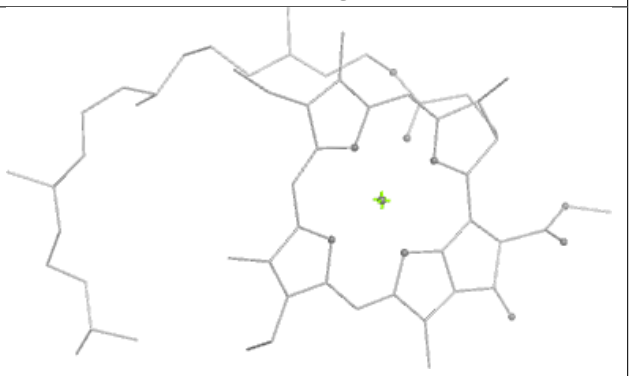


Bond angles

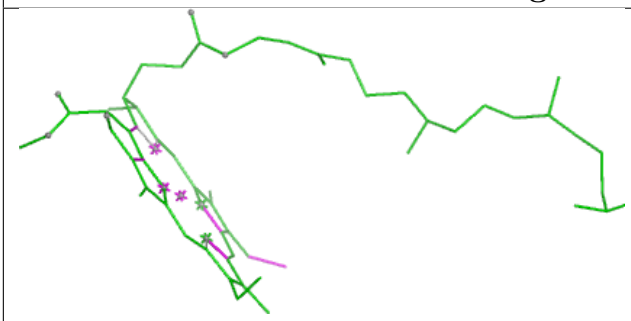


Torsions



Rings

Ligand CLA c 504



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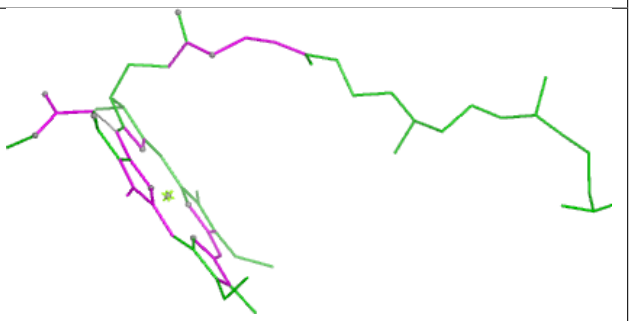

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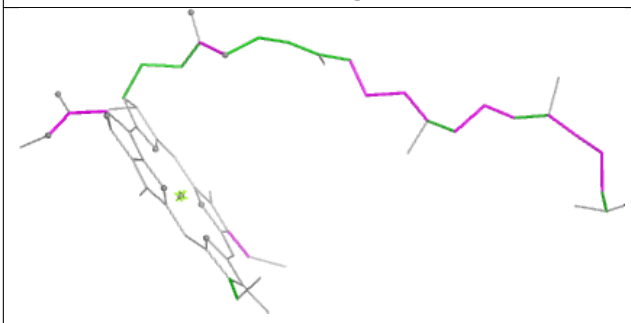
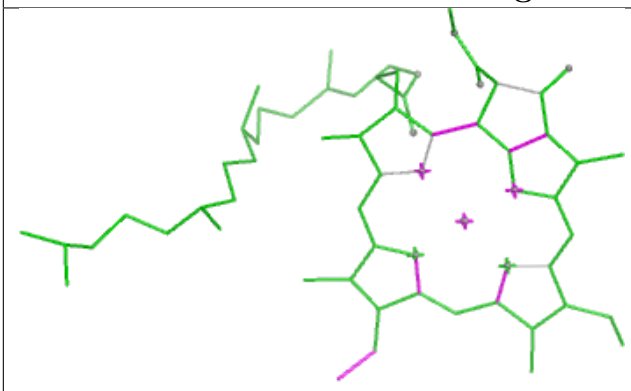


Torsions

Rings

Ligand CLA A1 406



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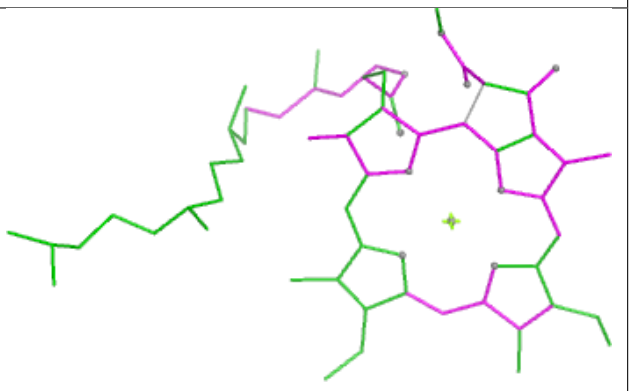

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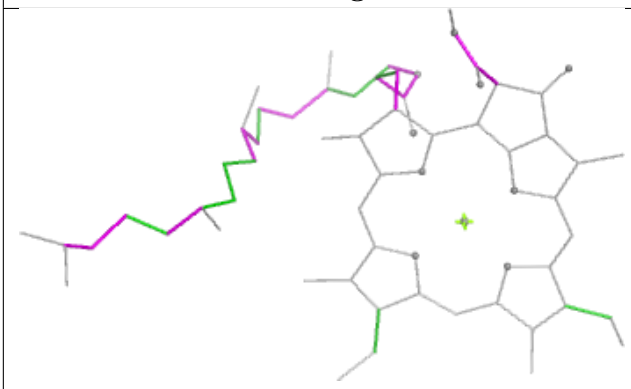

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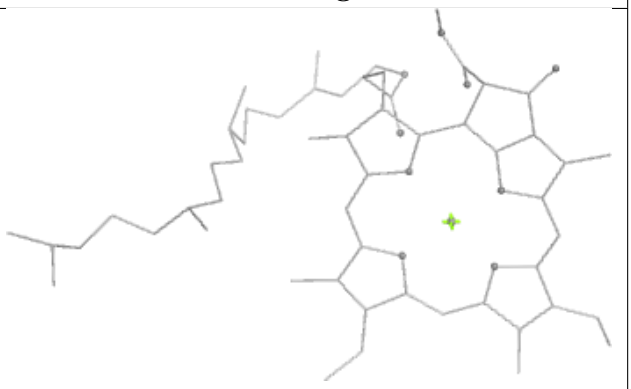
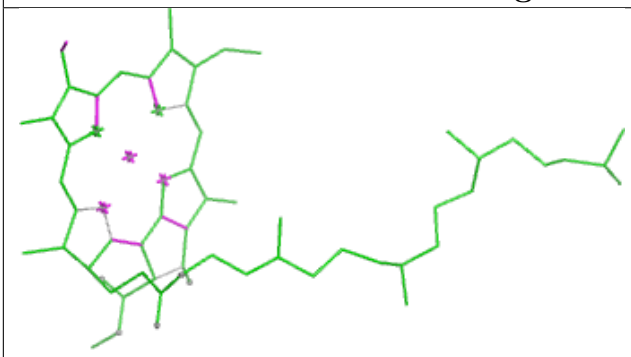


Rings

Ligand CLA Y1 611



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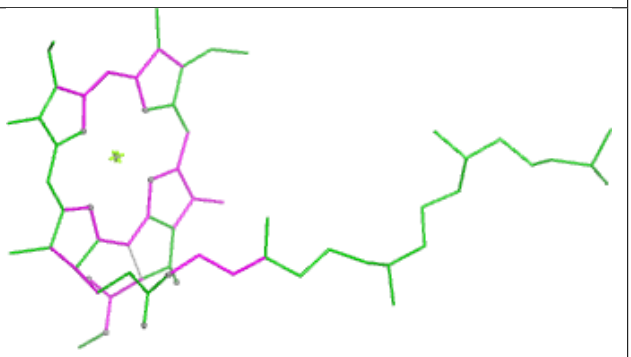

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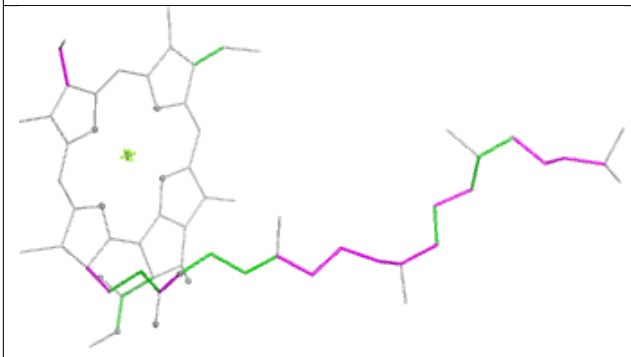

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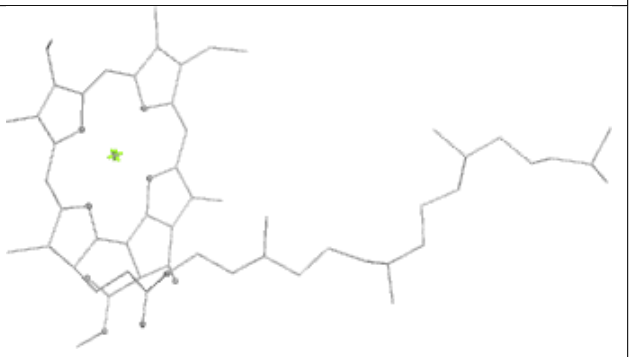
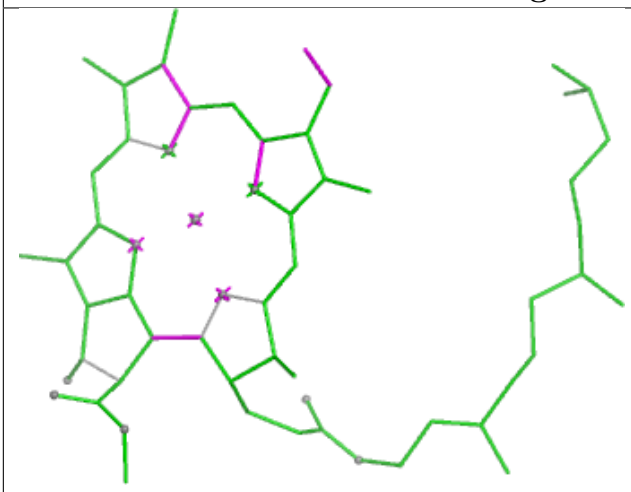


Rings

Ligand CLA r 603



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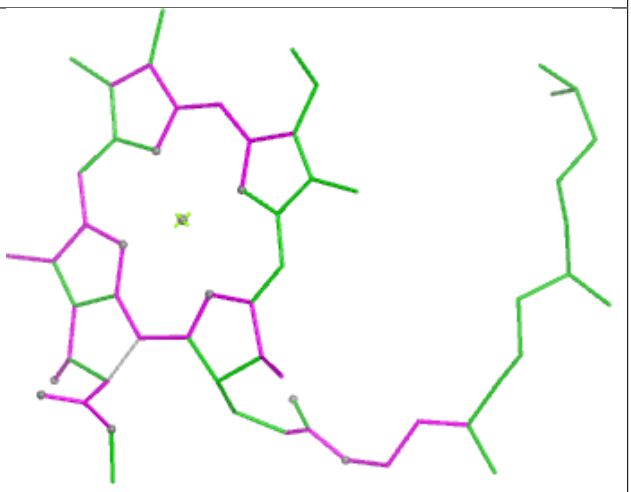

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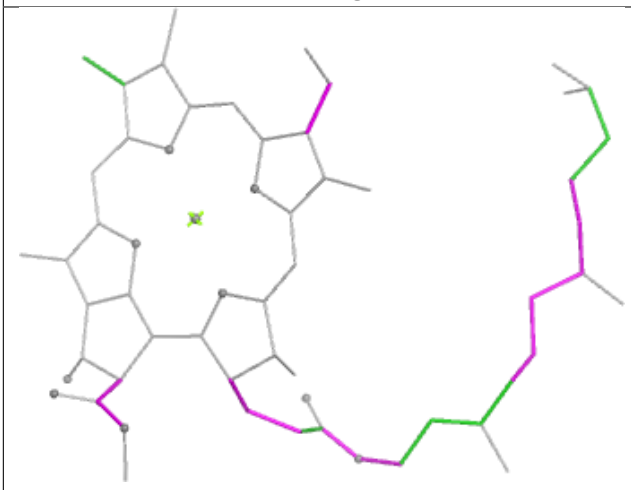

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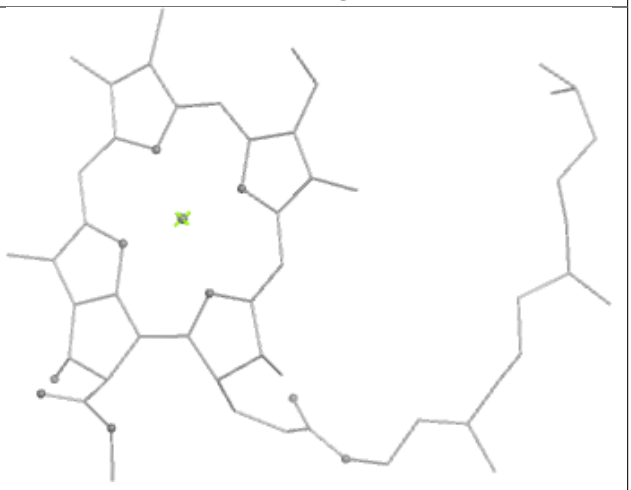
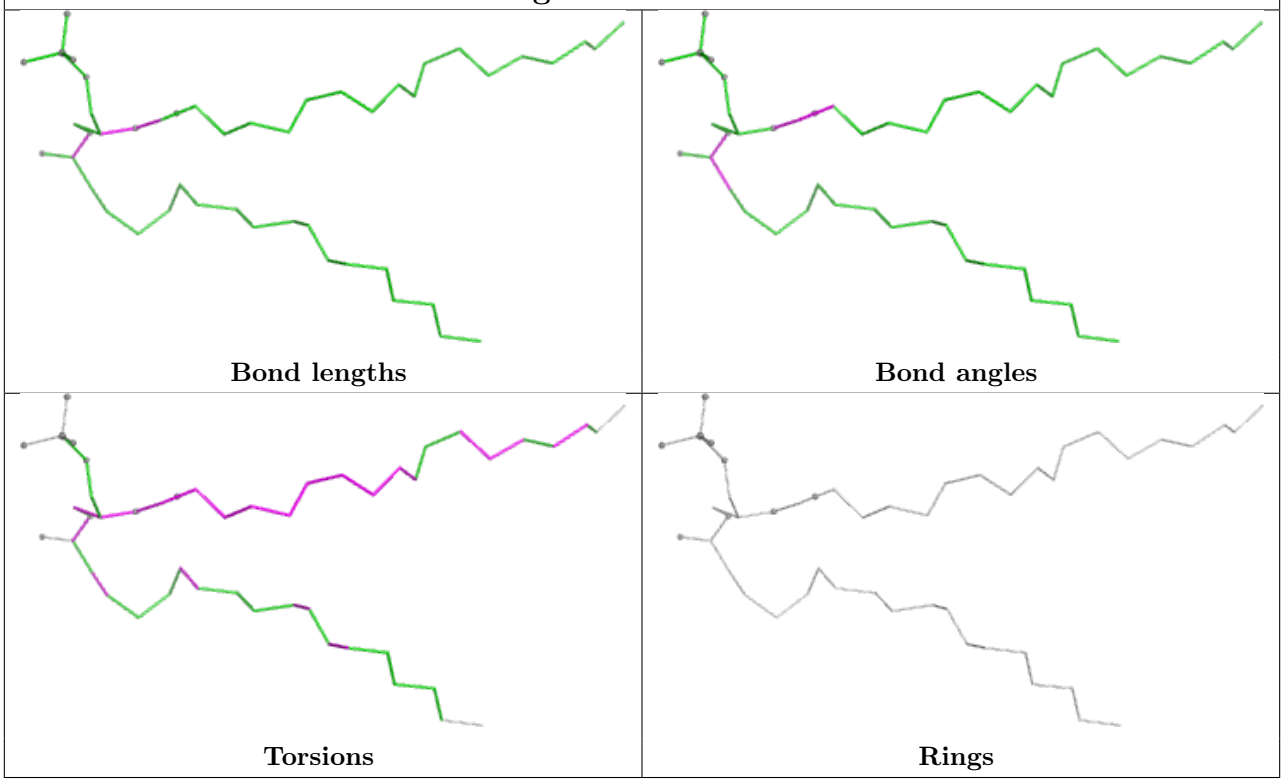
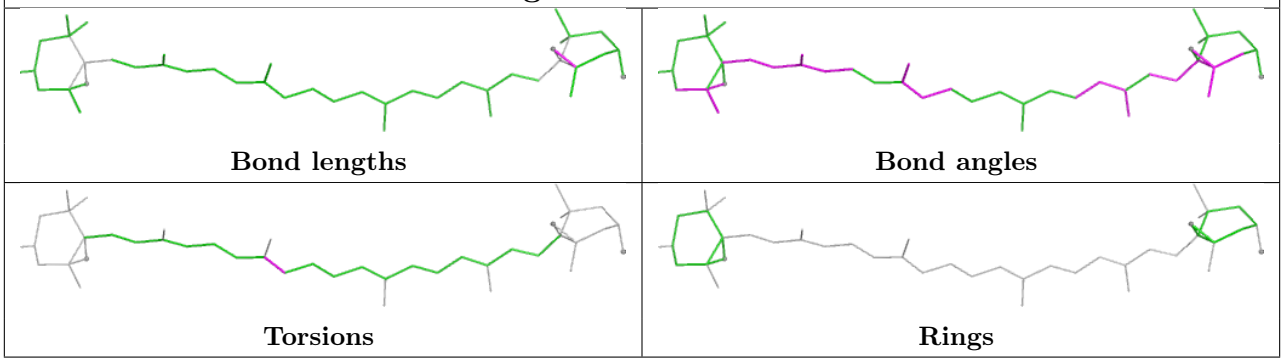


Rings

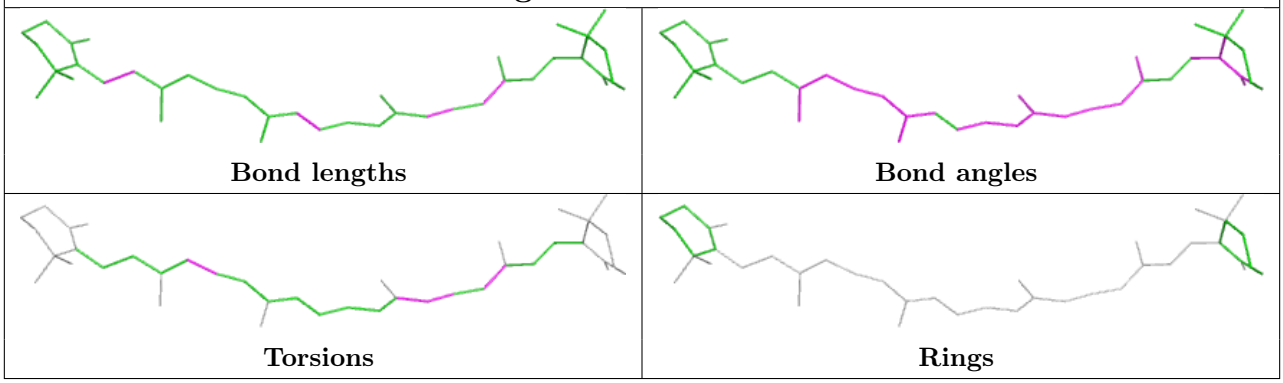
Ligand 3PH s 626



Ligand XAT G 622



Ligand BCR B1 619



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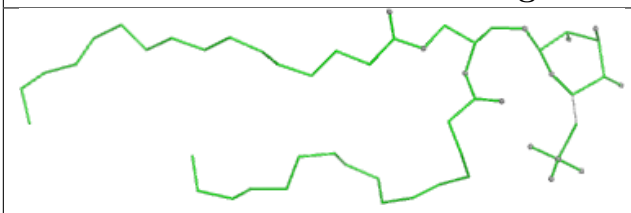
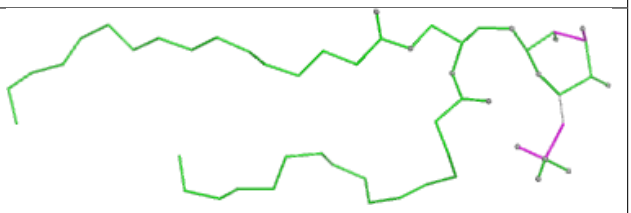
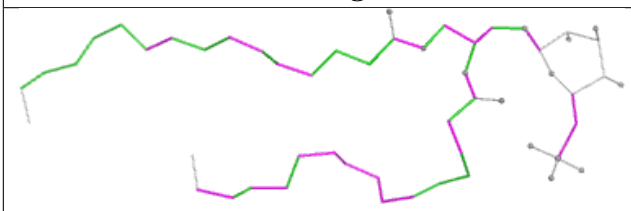


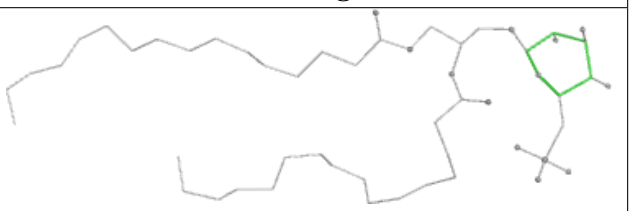
Bond lengths



Bond angles

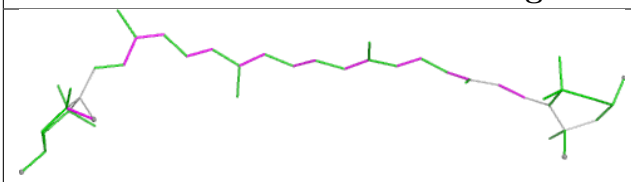


Torsions



Rings

Ligand NEX S 623



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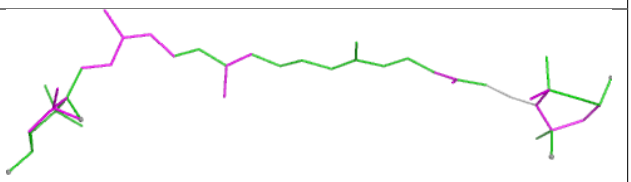
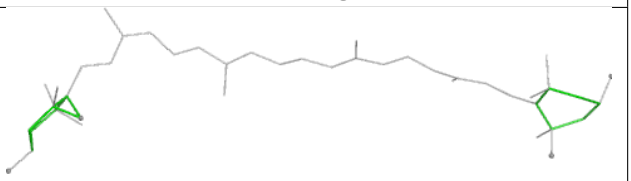


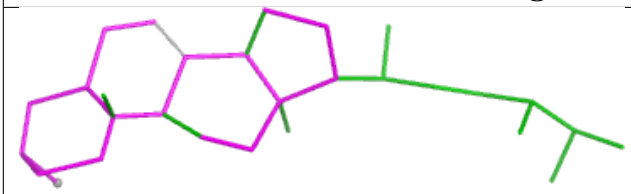
Bond angles

Torsions



Rings

Ligand ERG r 626



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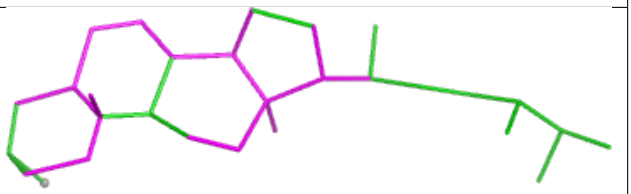
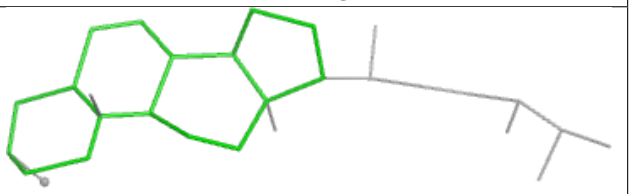
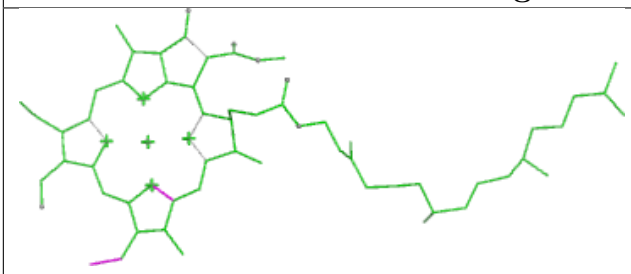
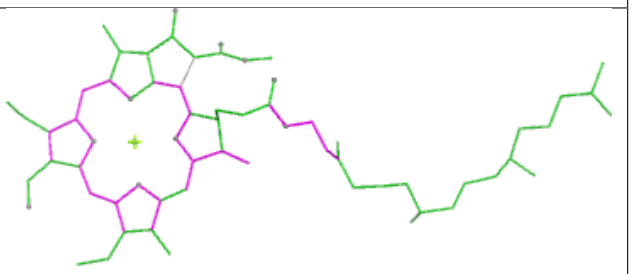
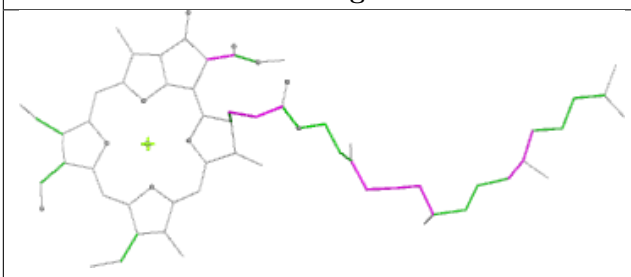
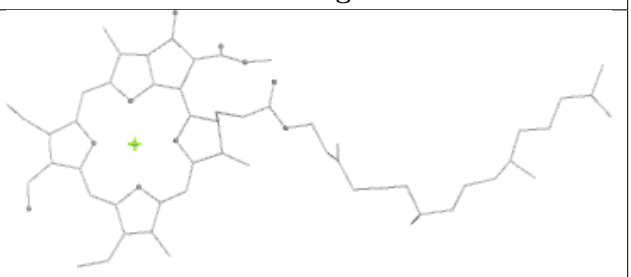


Bond angles

Torsions

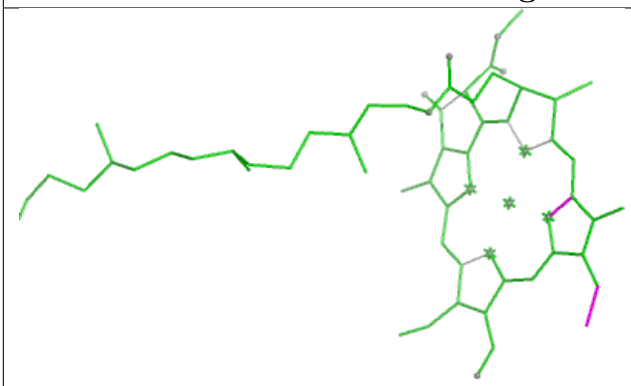


Rings

Ligand CHL G1 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG g1 624	
Bond lengths	Bond angles
Torsions	Rings

Ligand CHL g1 609



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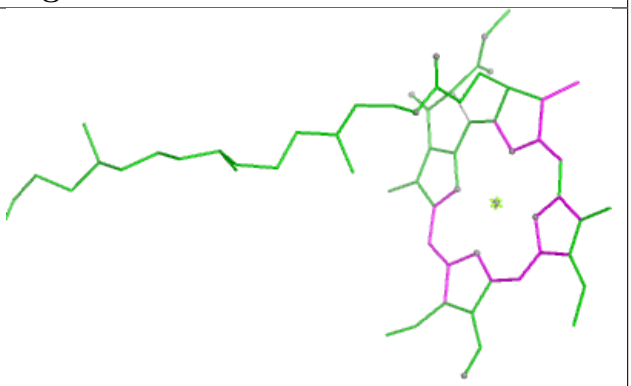

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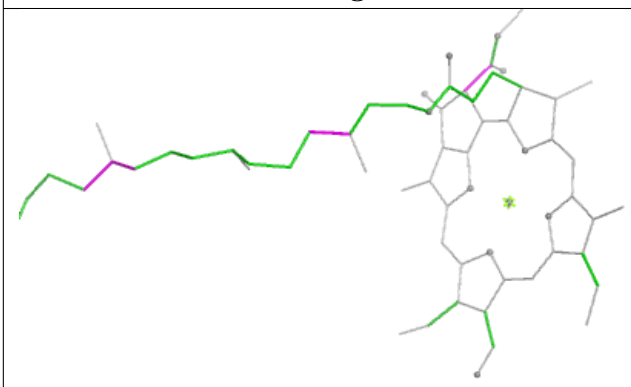
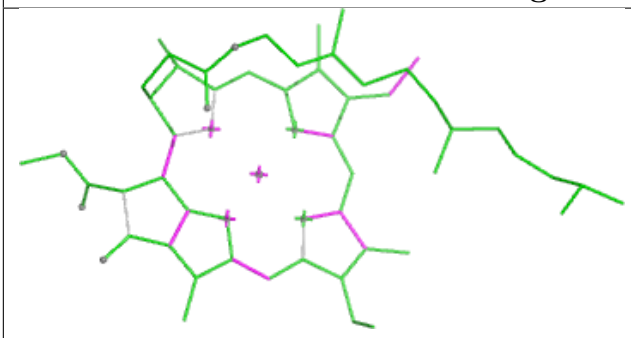


Torsions

Rings

Ligand CLA r 608



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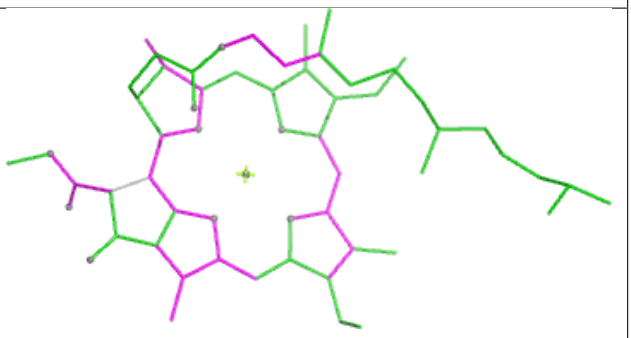

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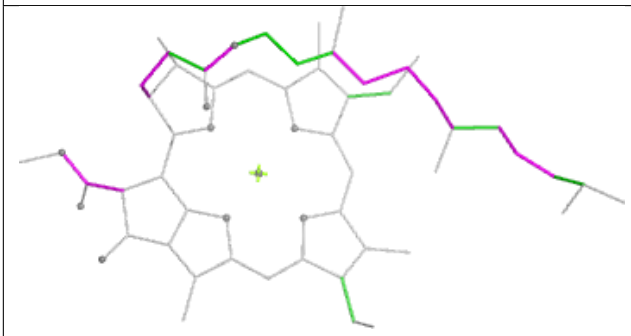

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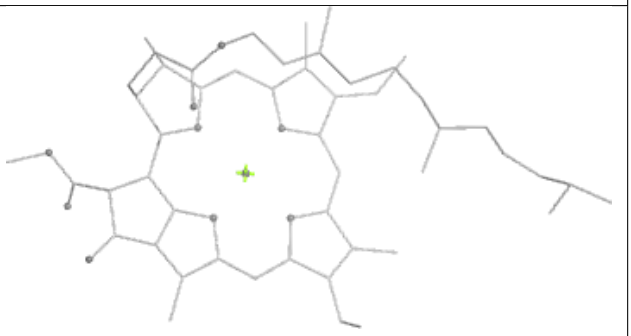

Rings

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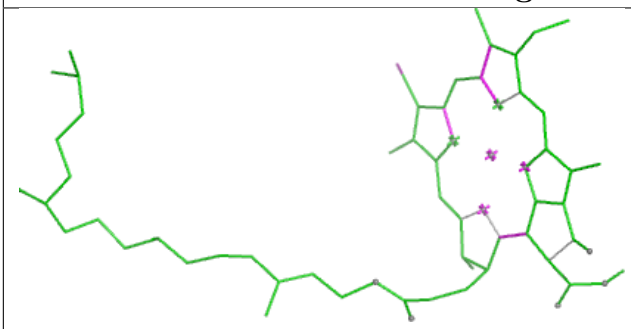
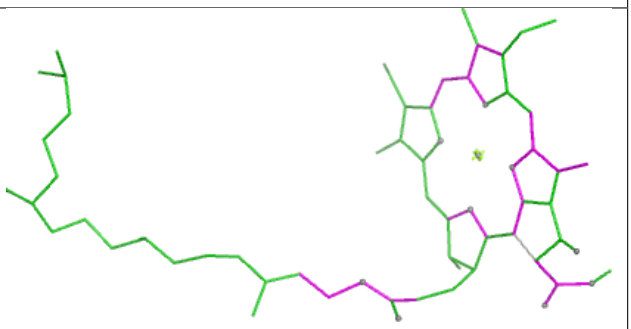
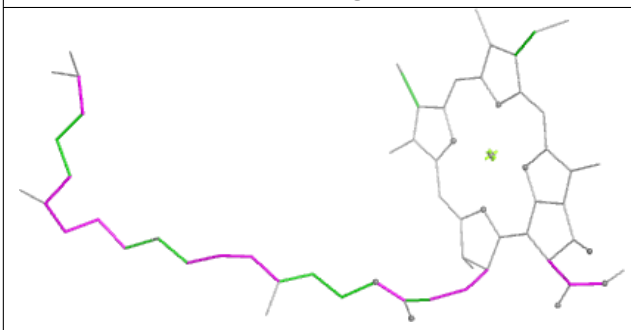
 Bond lengths	 Bond angles
 Torsions	Rings

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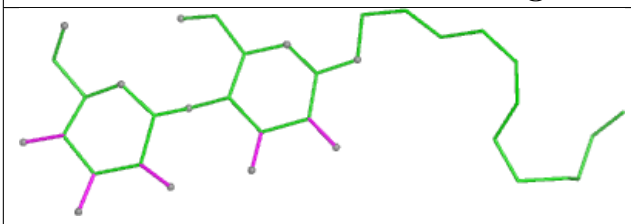
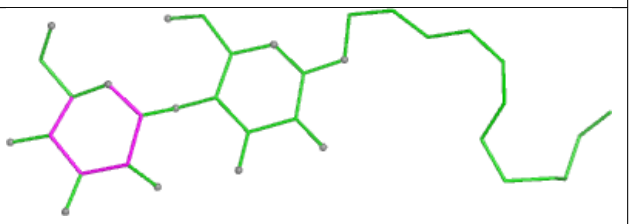
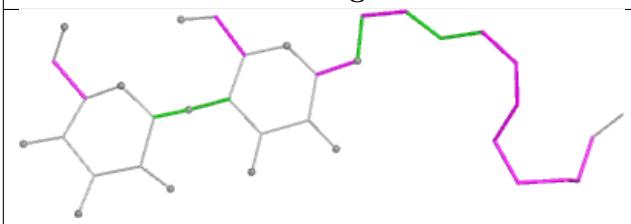
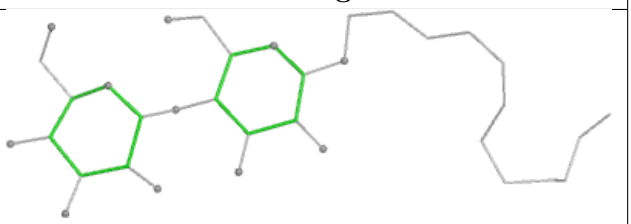
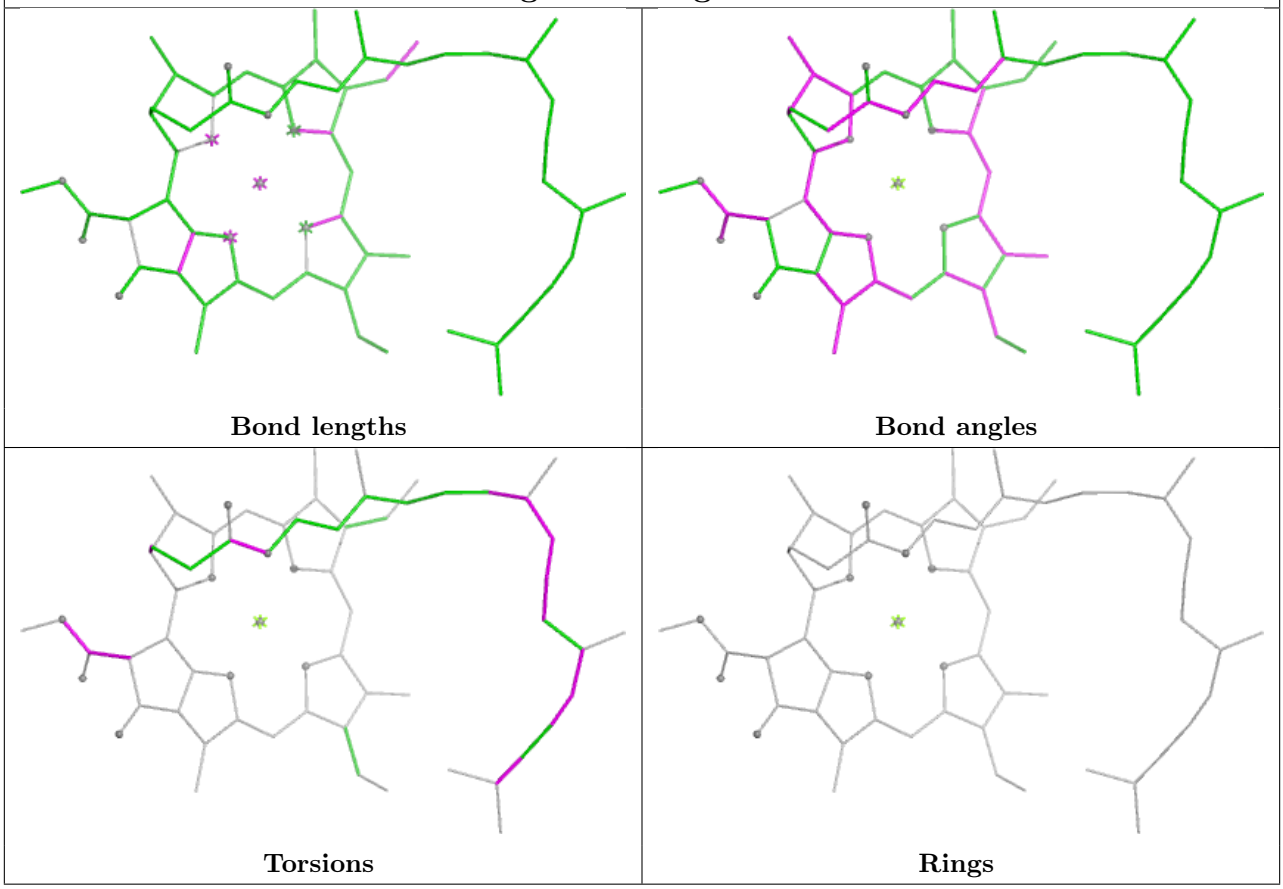
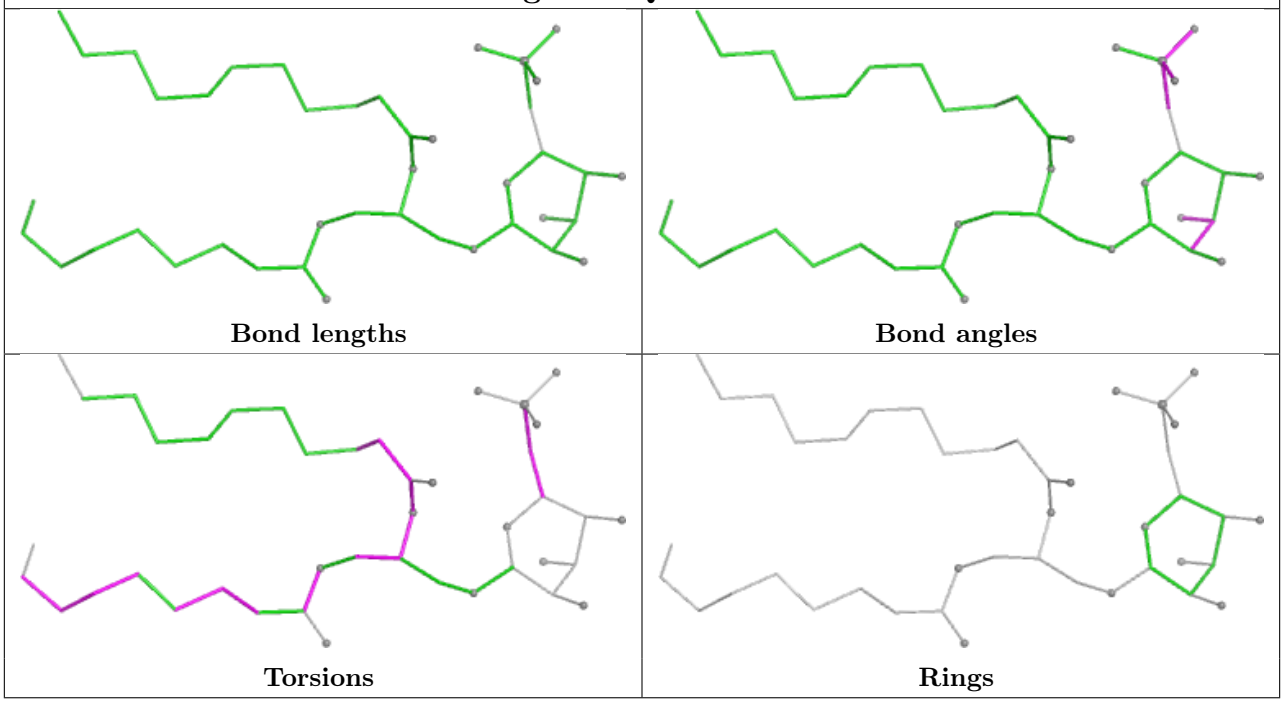
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g1 610



Ligand SQD m 101



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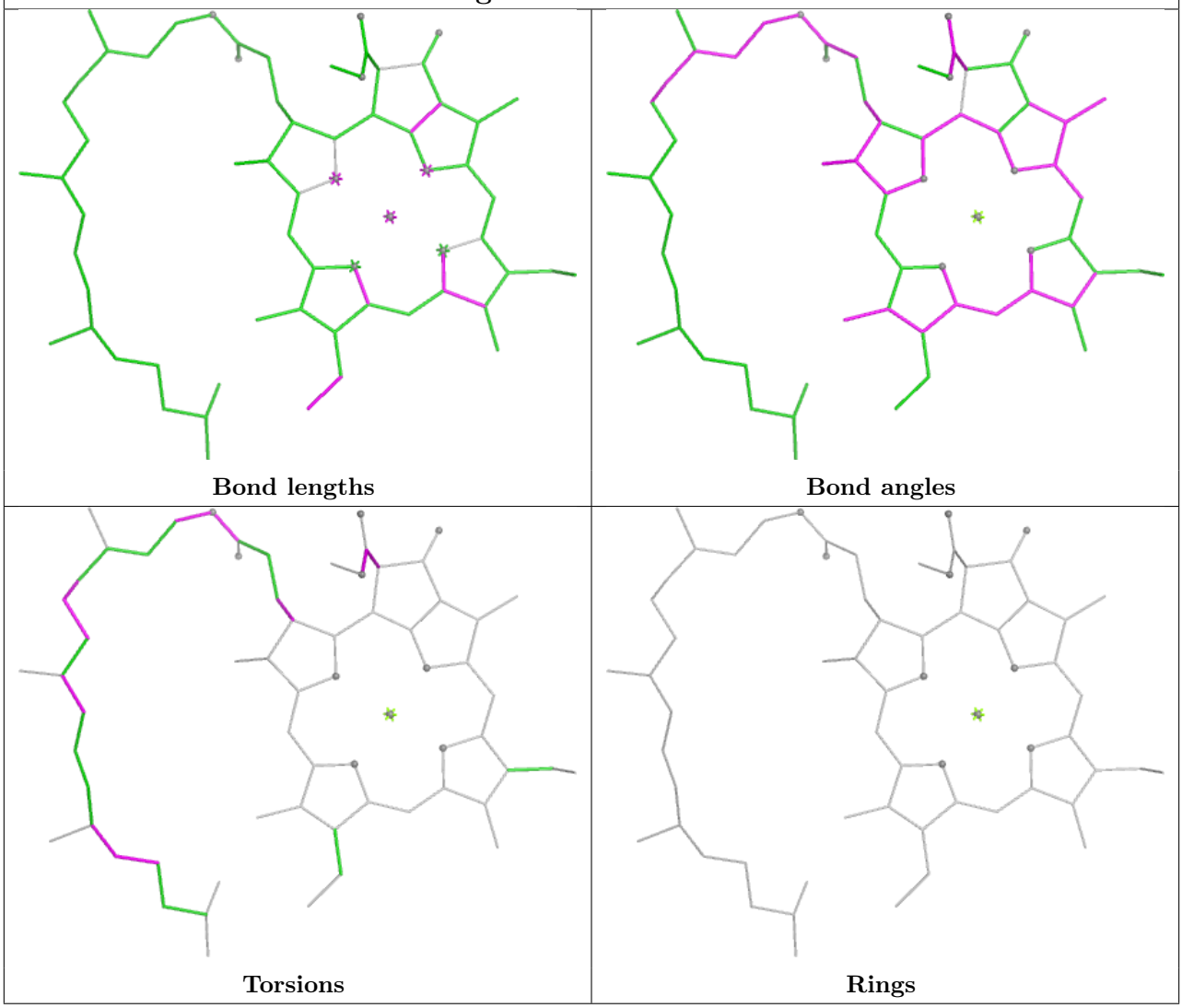

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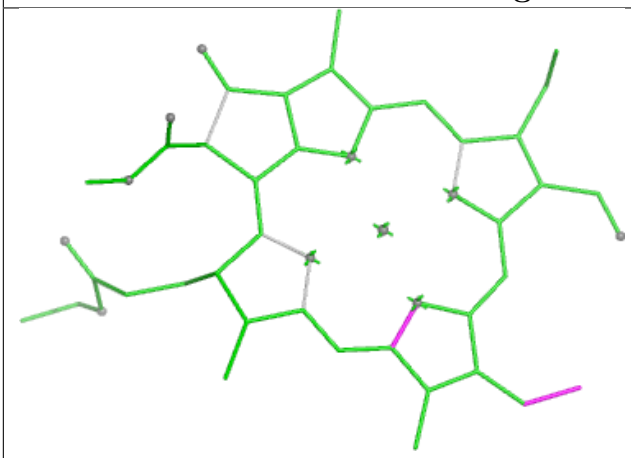
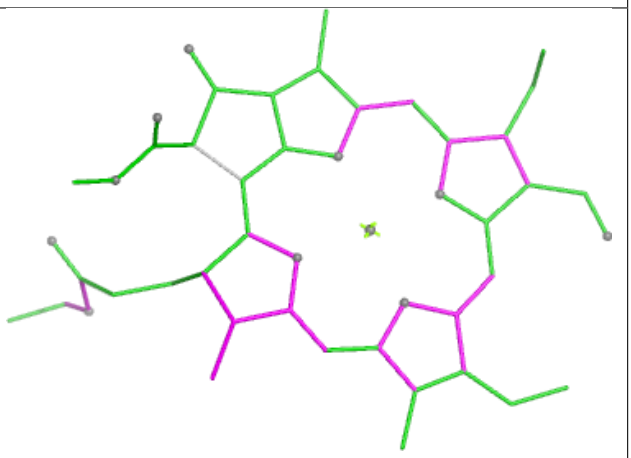
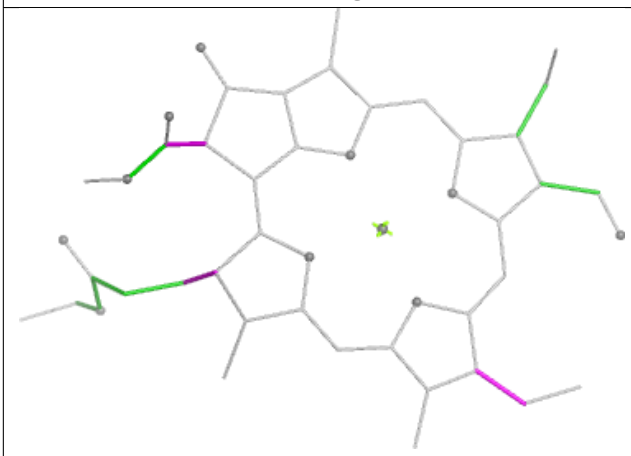
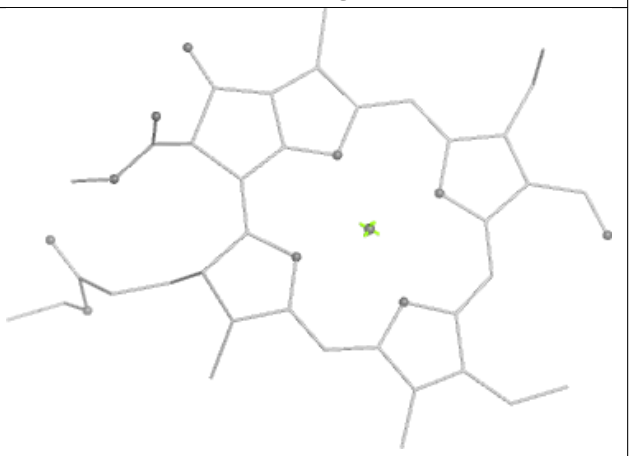
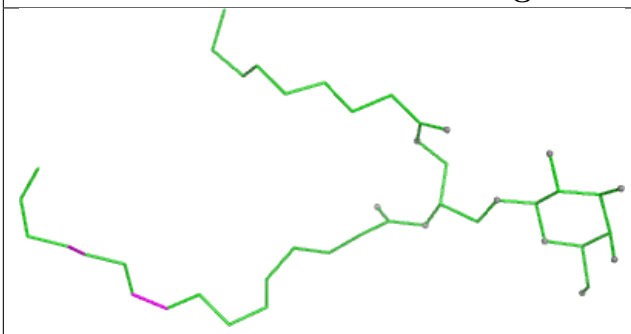
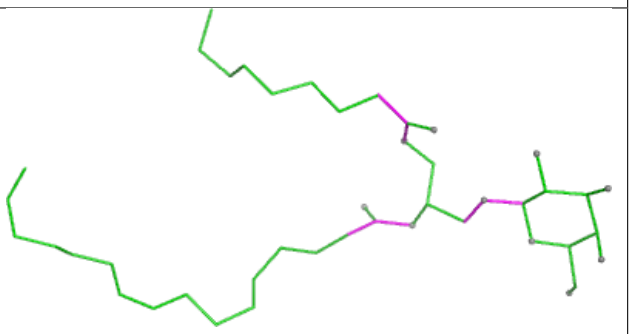
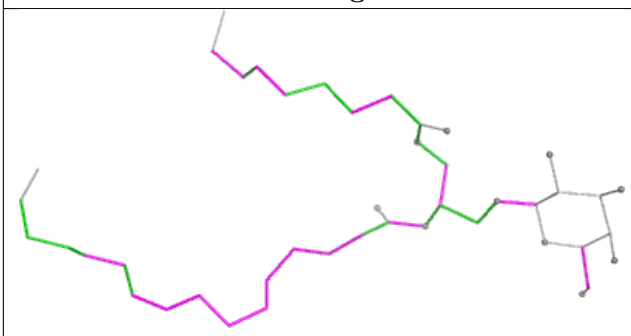
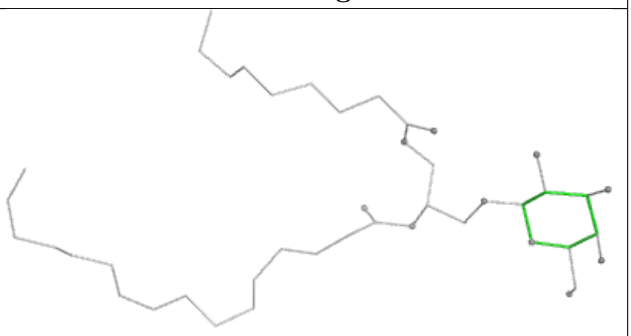
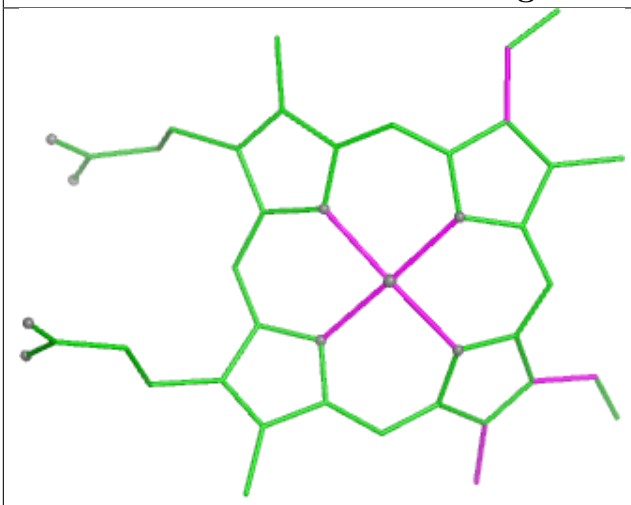
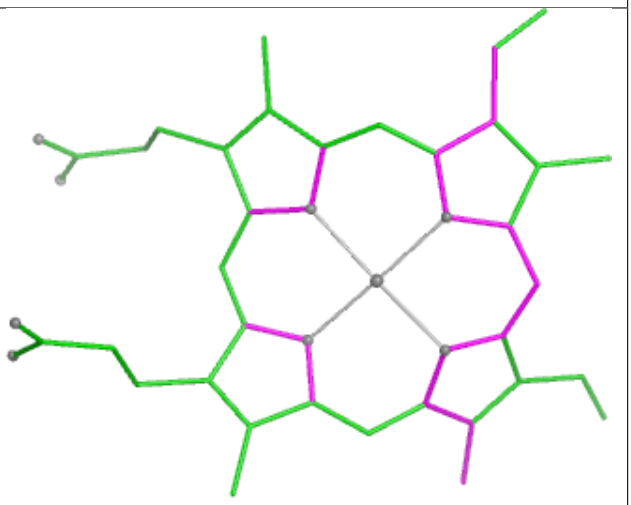
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG b1 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM f1 101



Bond lengths



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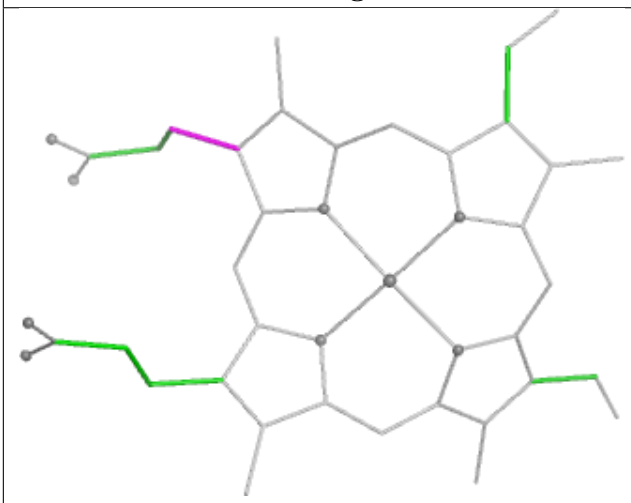
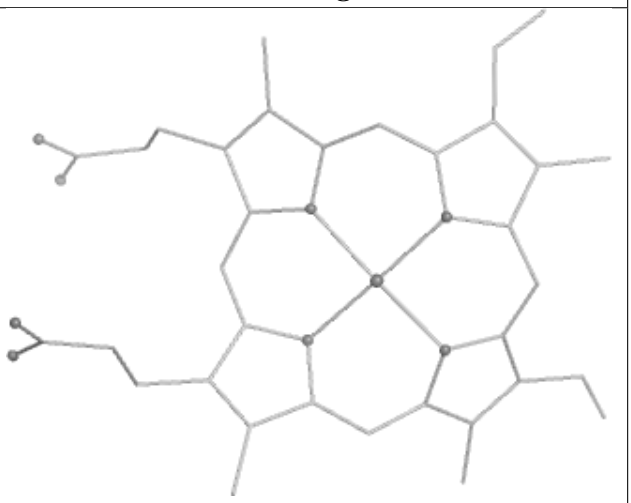
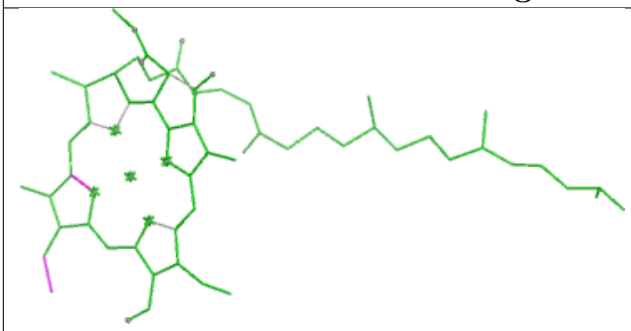
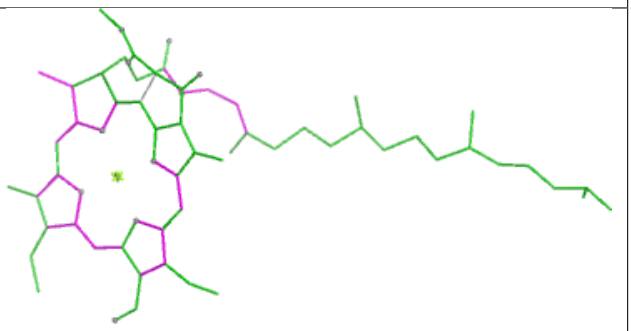
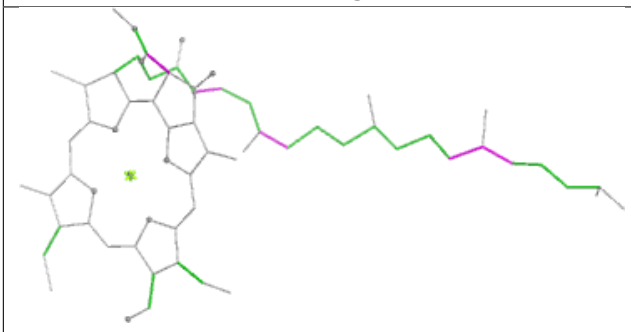
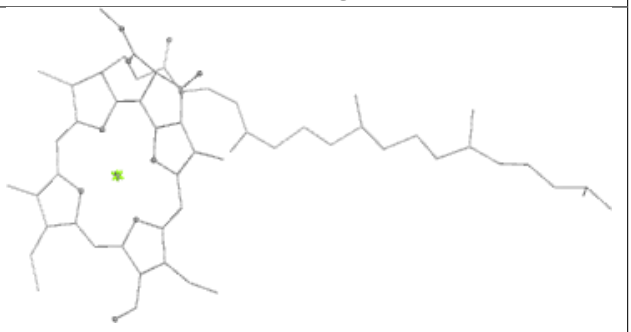
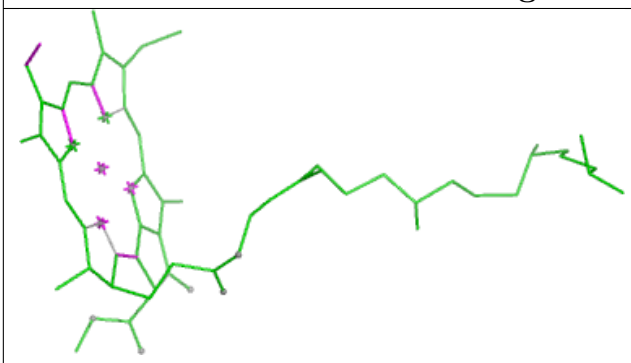
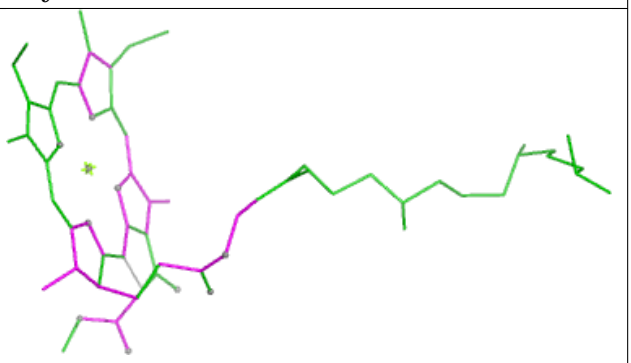
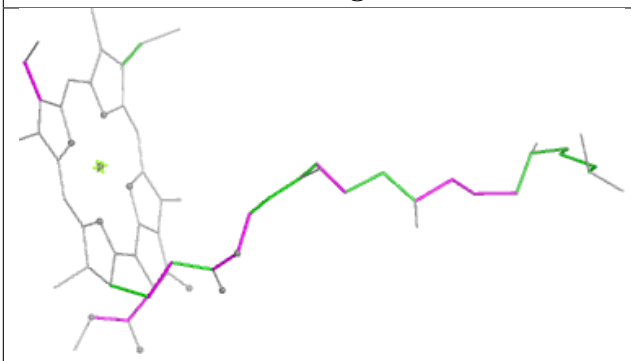
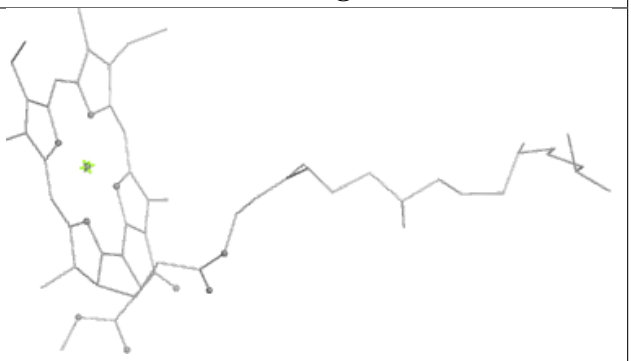


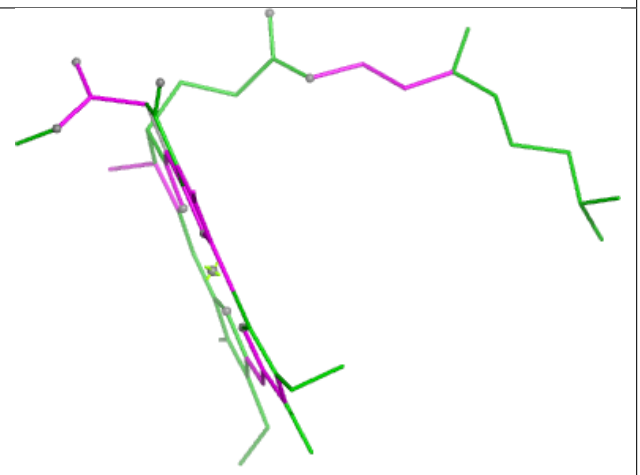
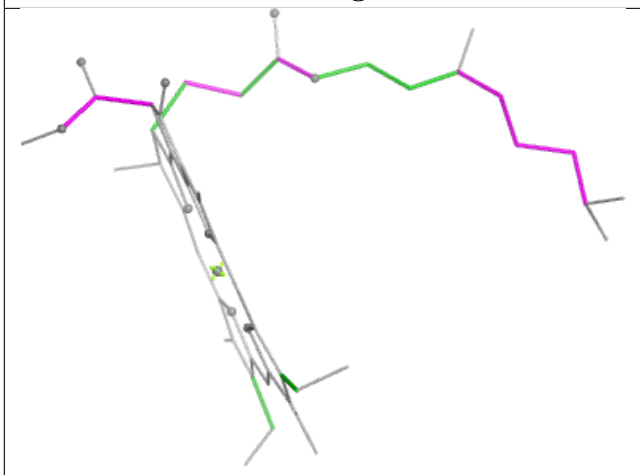
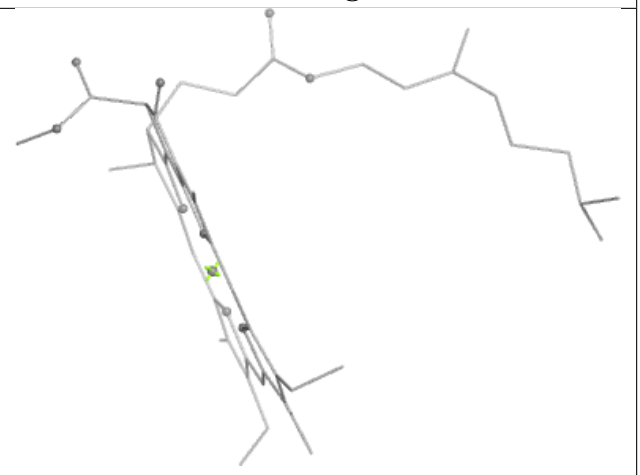
Torsions



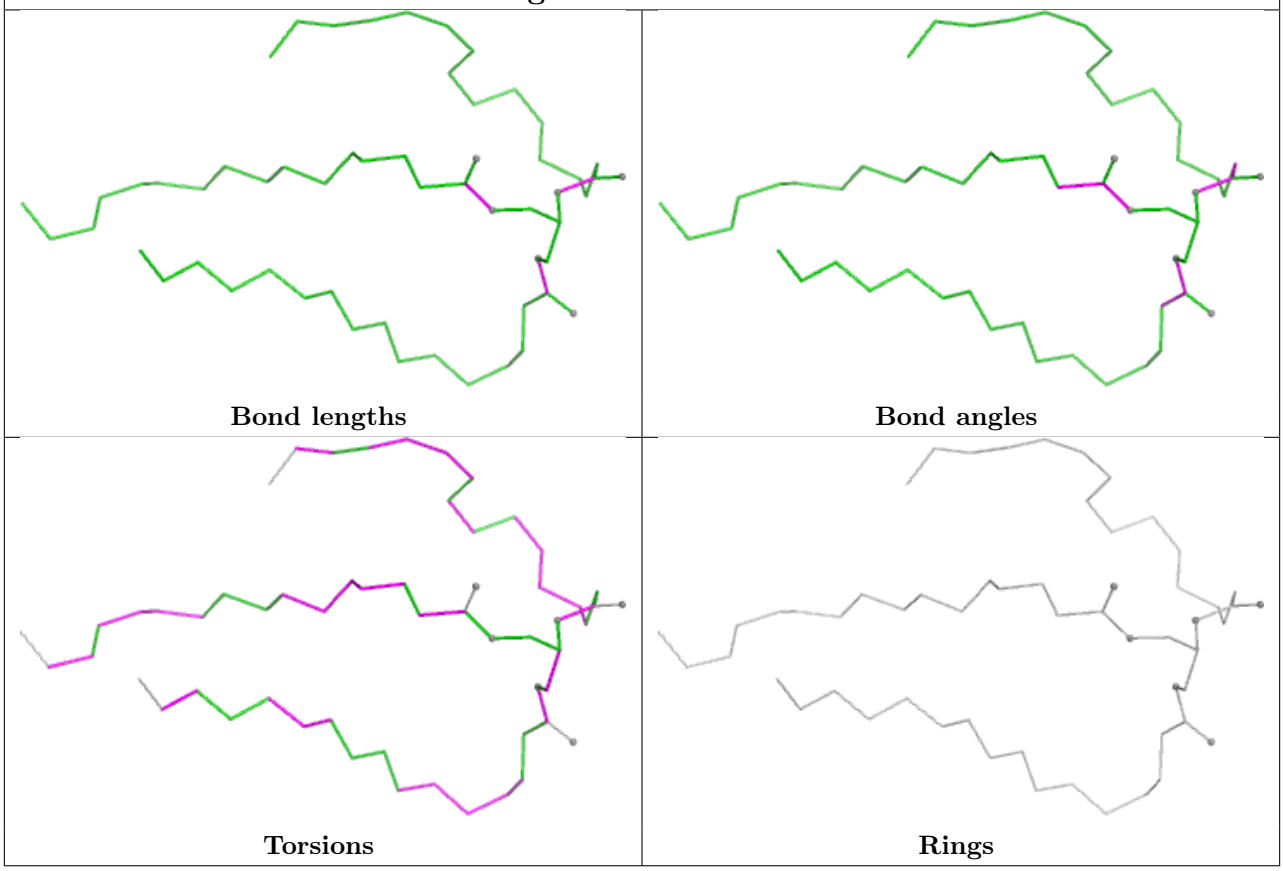
Rings

Ligand CHL Y1 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

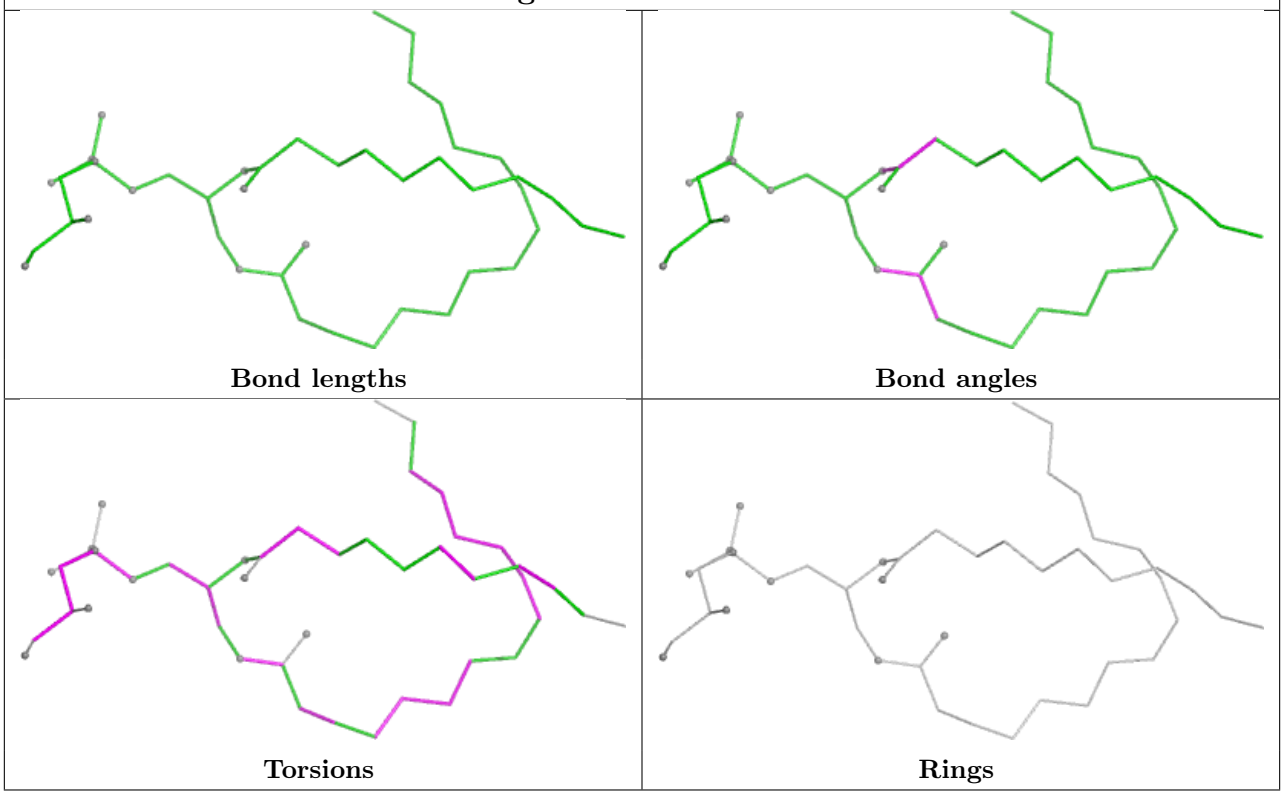
Ligand CLA y1 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 604	
Bond lengths	 Bond angles
 Torsions	 Rings

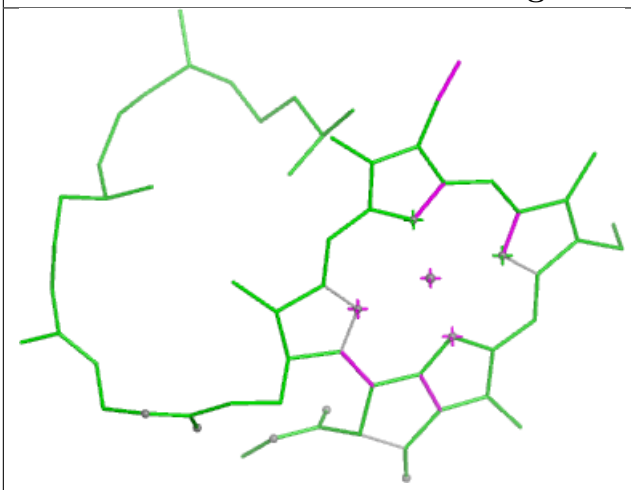
Ligand 4RF K 101



Ligand LHG d1 408



Ligand CLA b 616



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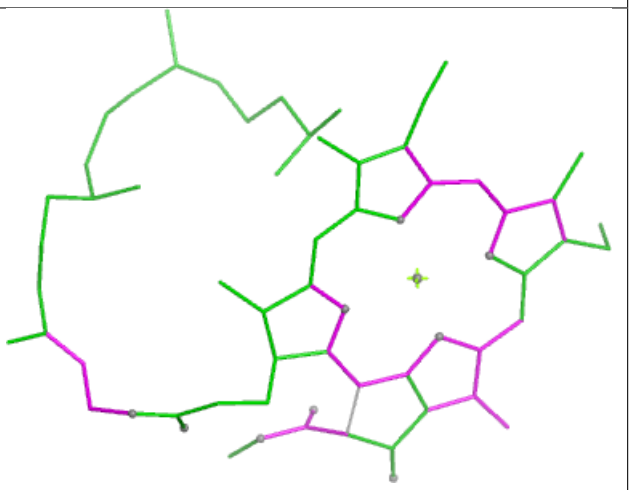
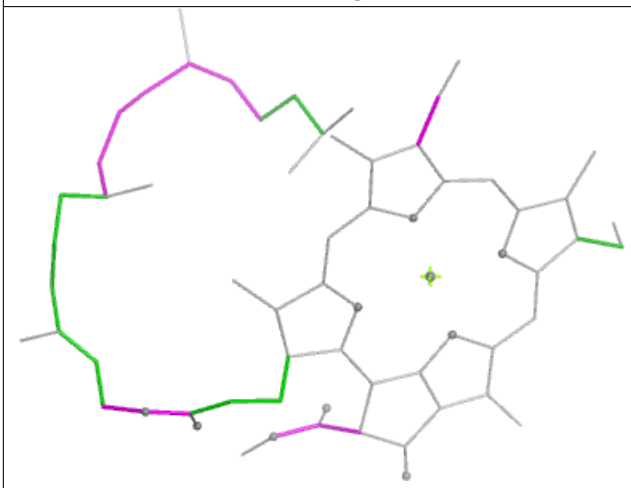


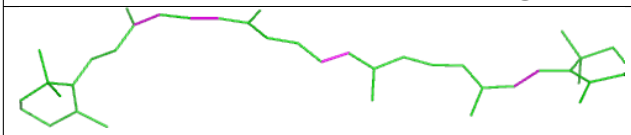
Bond angles



Torsions

Rings

Ligand BCR d1 404



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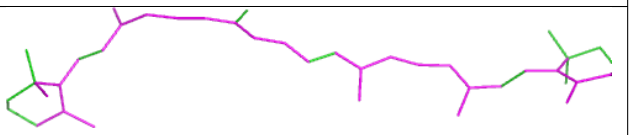
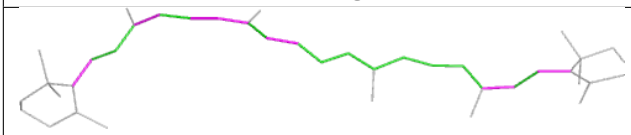


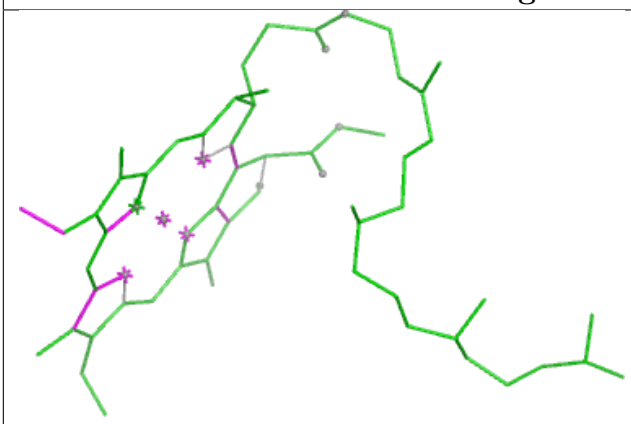
Bond angles



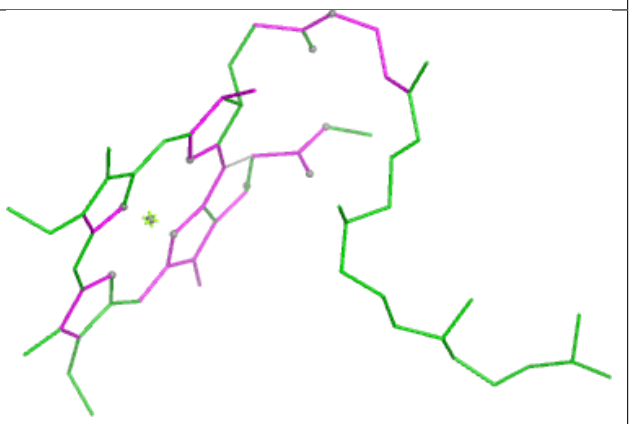
Torsions

Rings

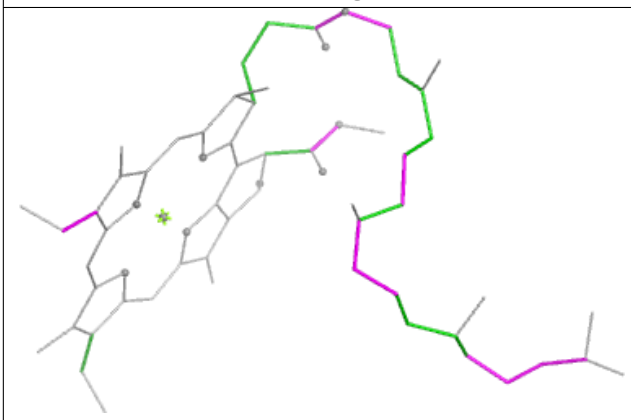
Ligand CLA b1 614



Bond lengths



Bond angles



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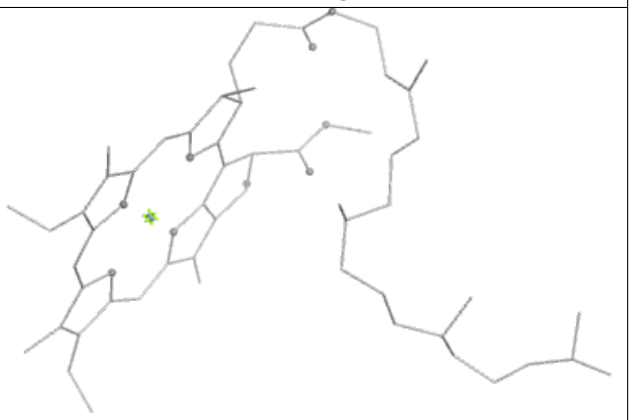
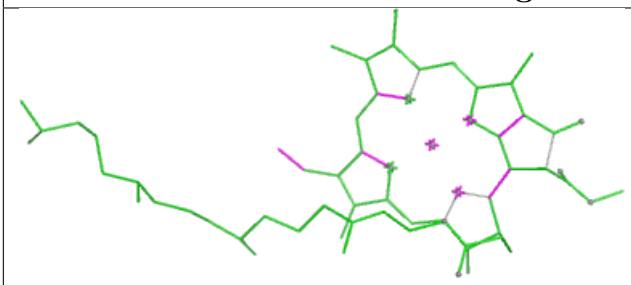
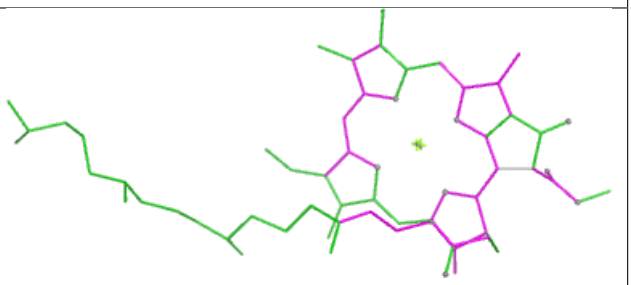


Rings

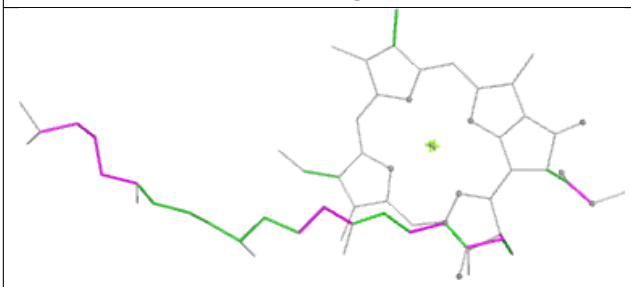
Ligand CLA C1 501



Bond lengths



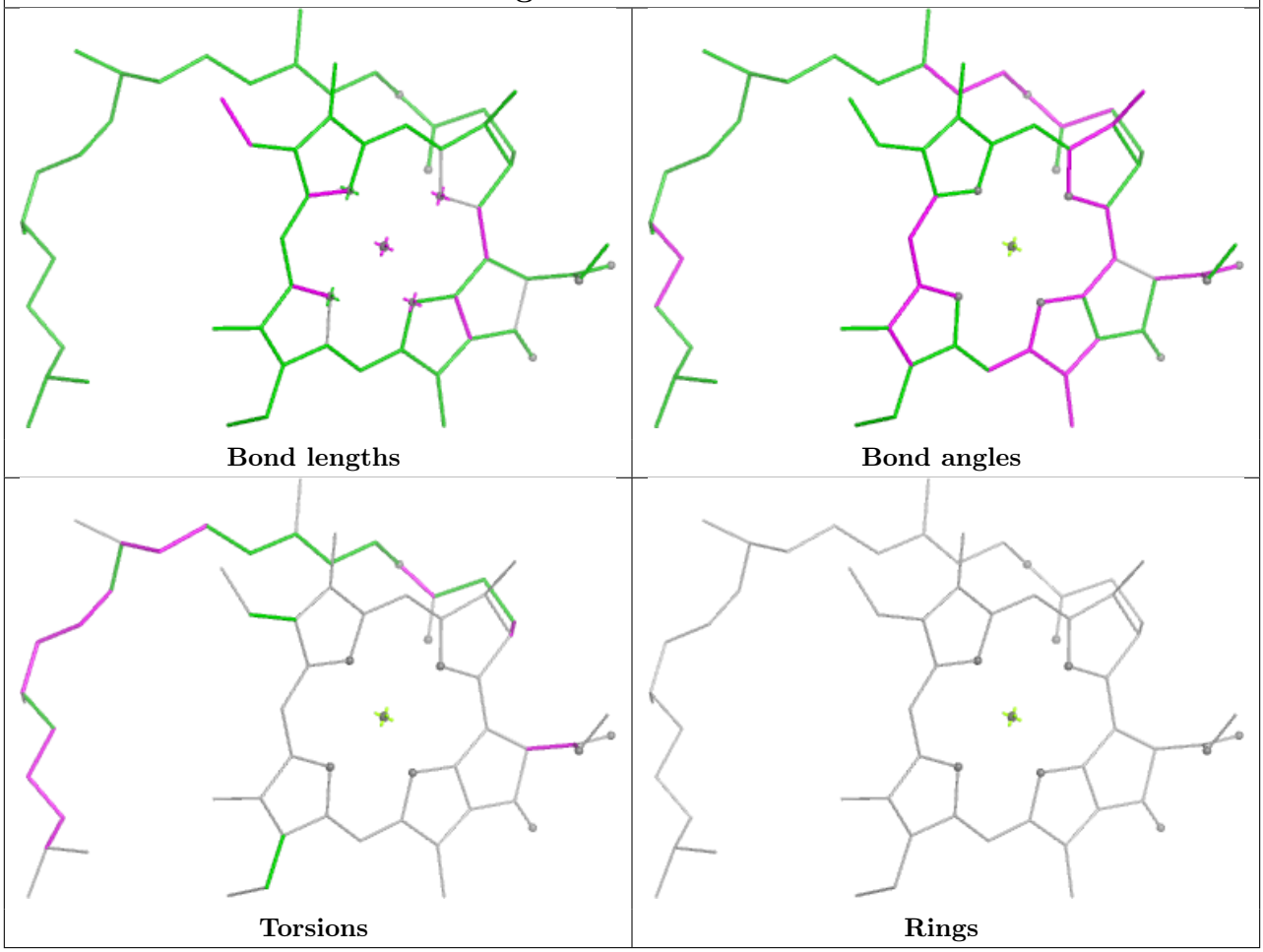
Bond angles

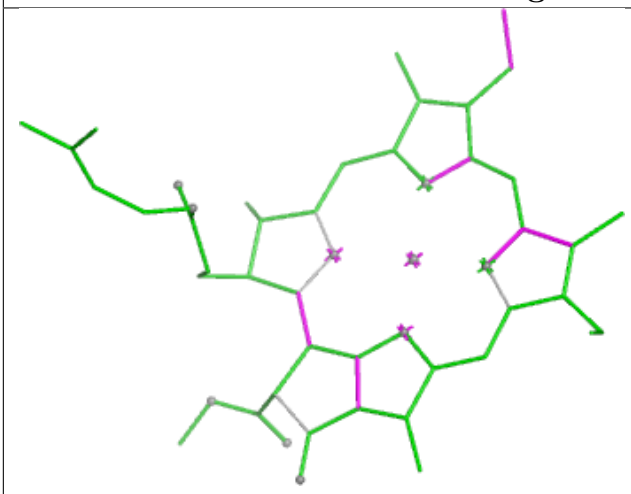
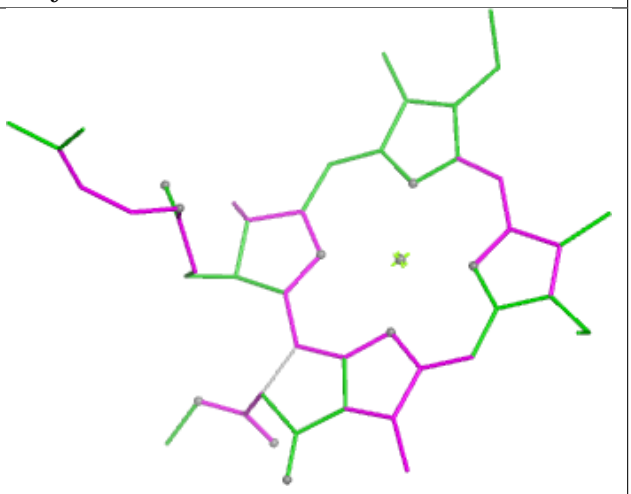
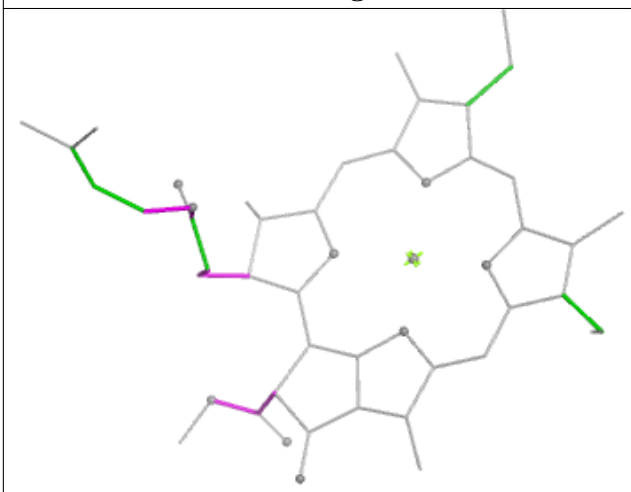
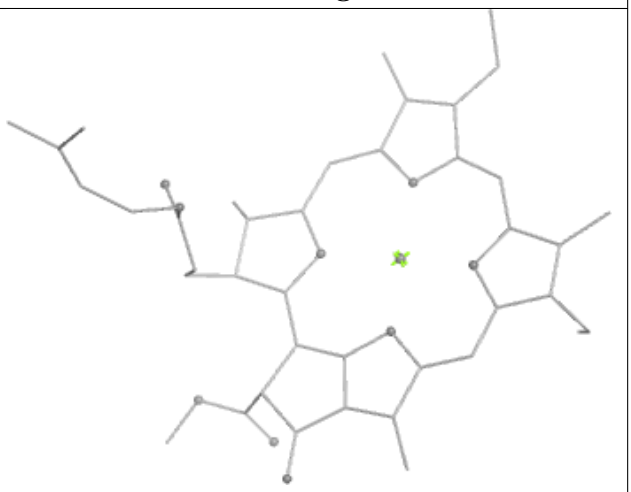


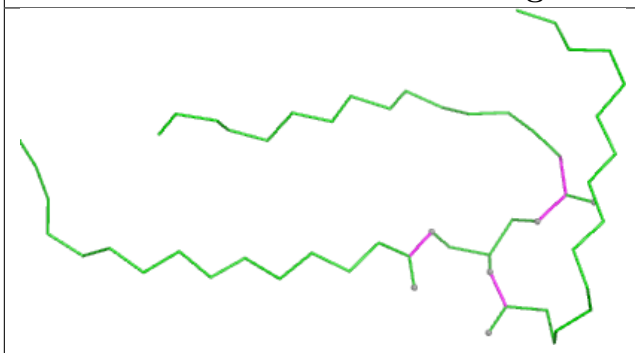
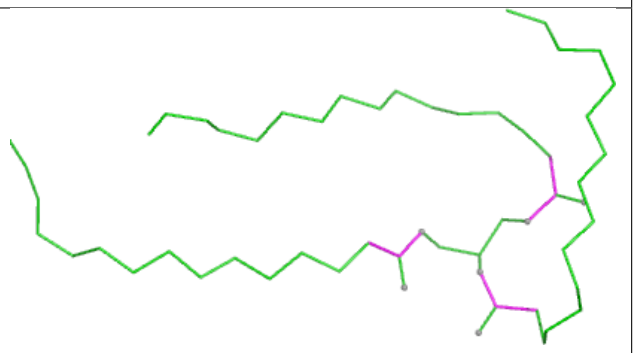
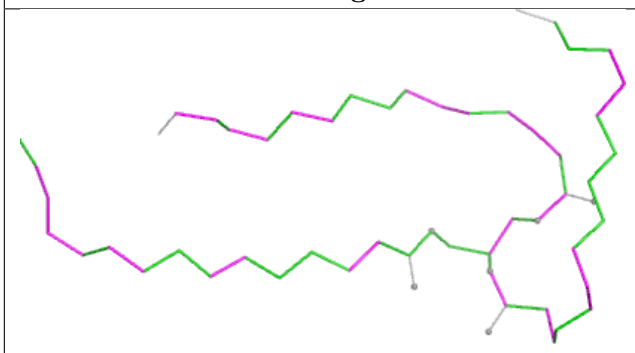
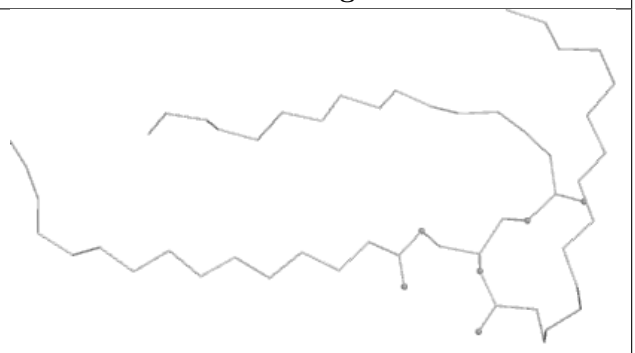
Torsions

Rings

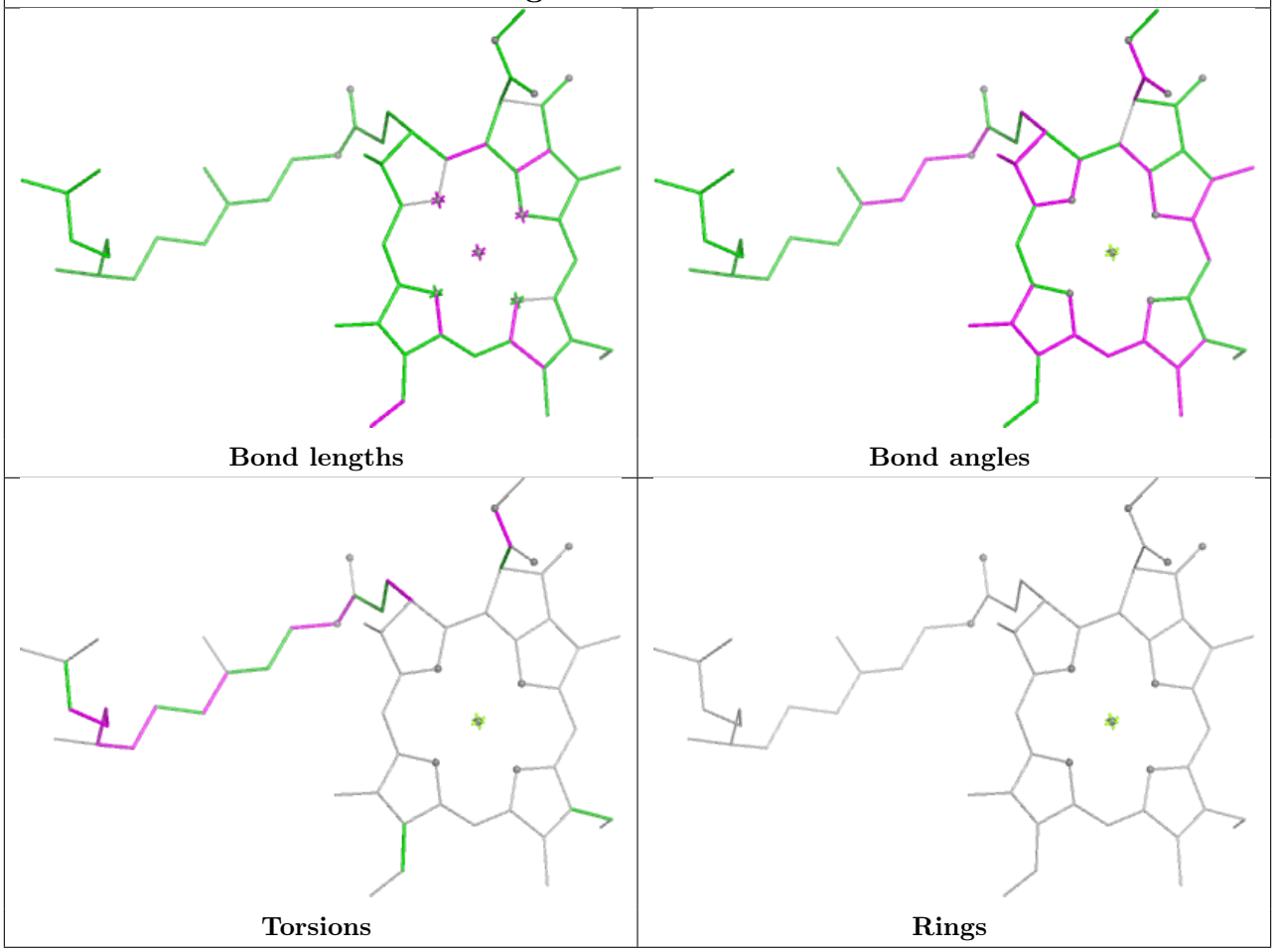
Ligand CLA G 602



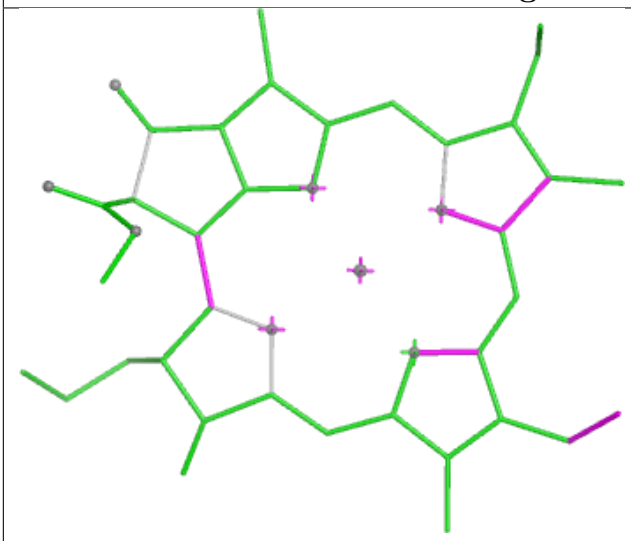
Ligand CLA y 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 4RF I1 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

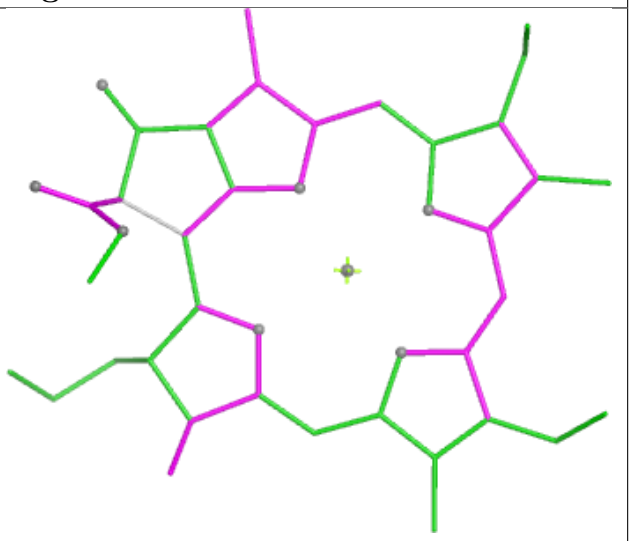
Ligand CLA a 410



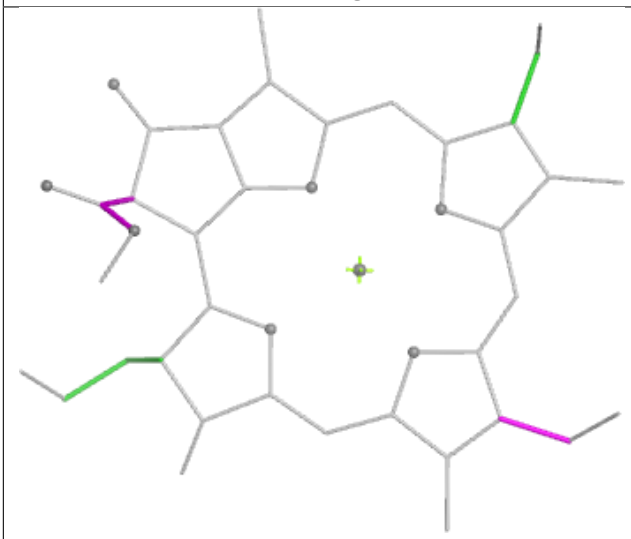
Ligand CLA g1 612



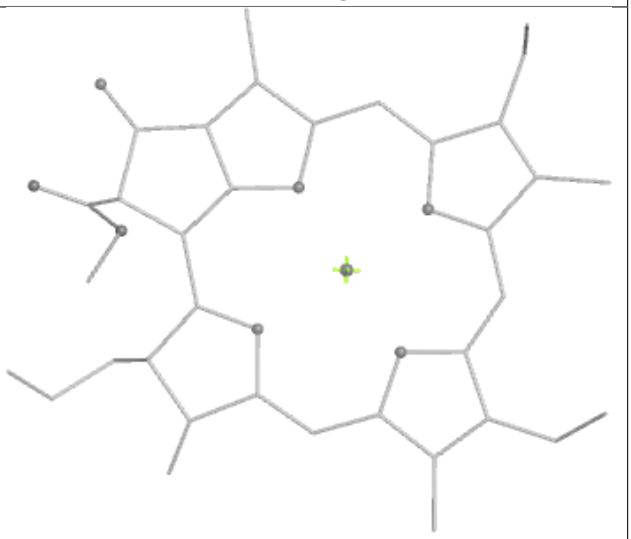
Bond lengths



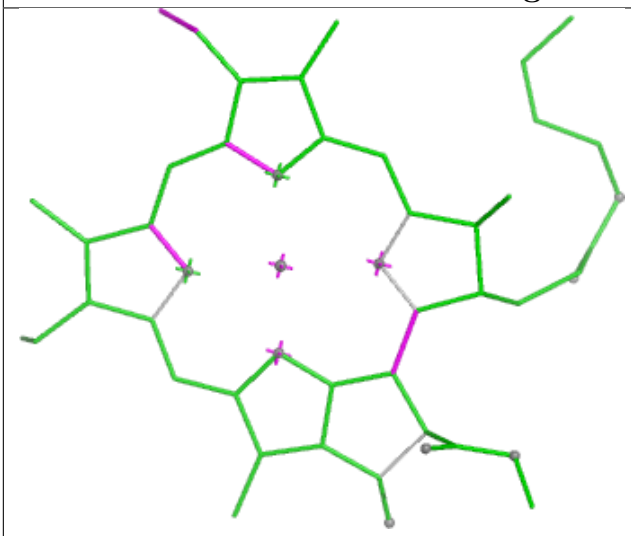
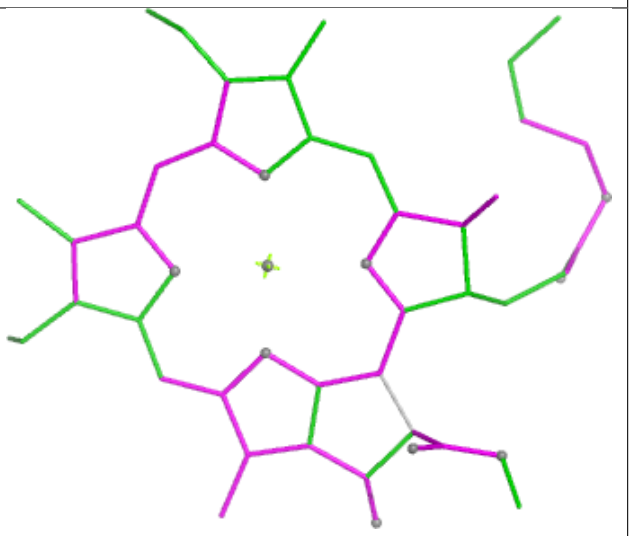
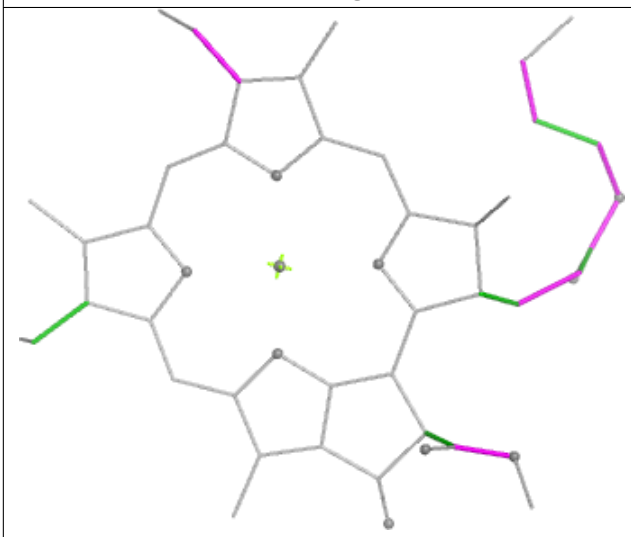
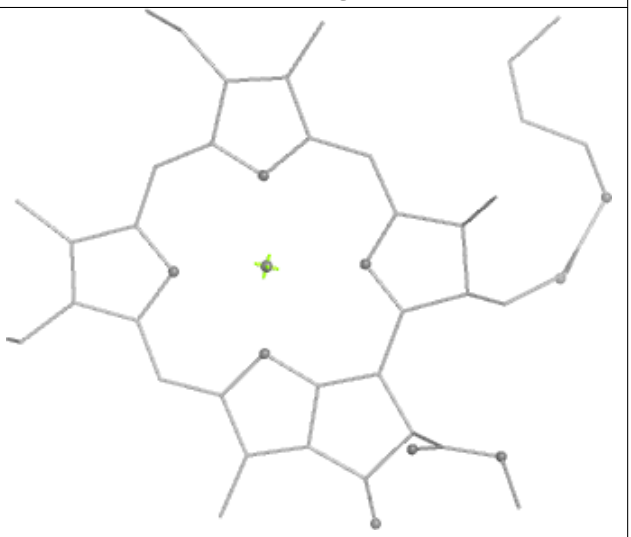
Bond angles



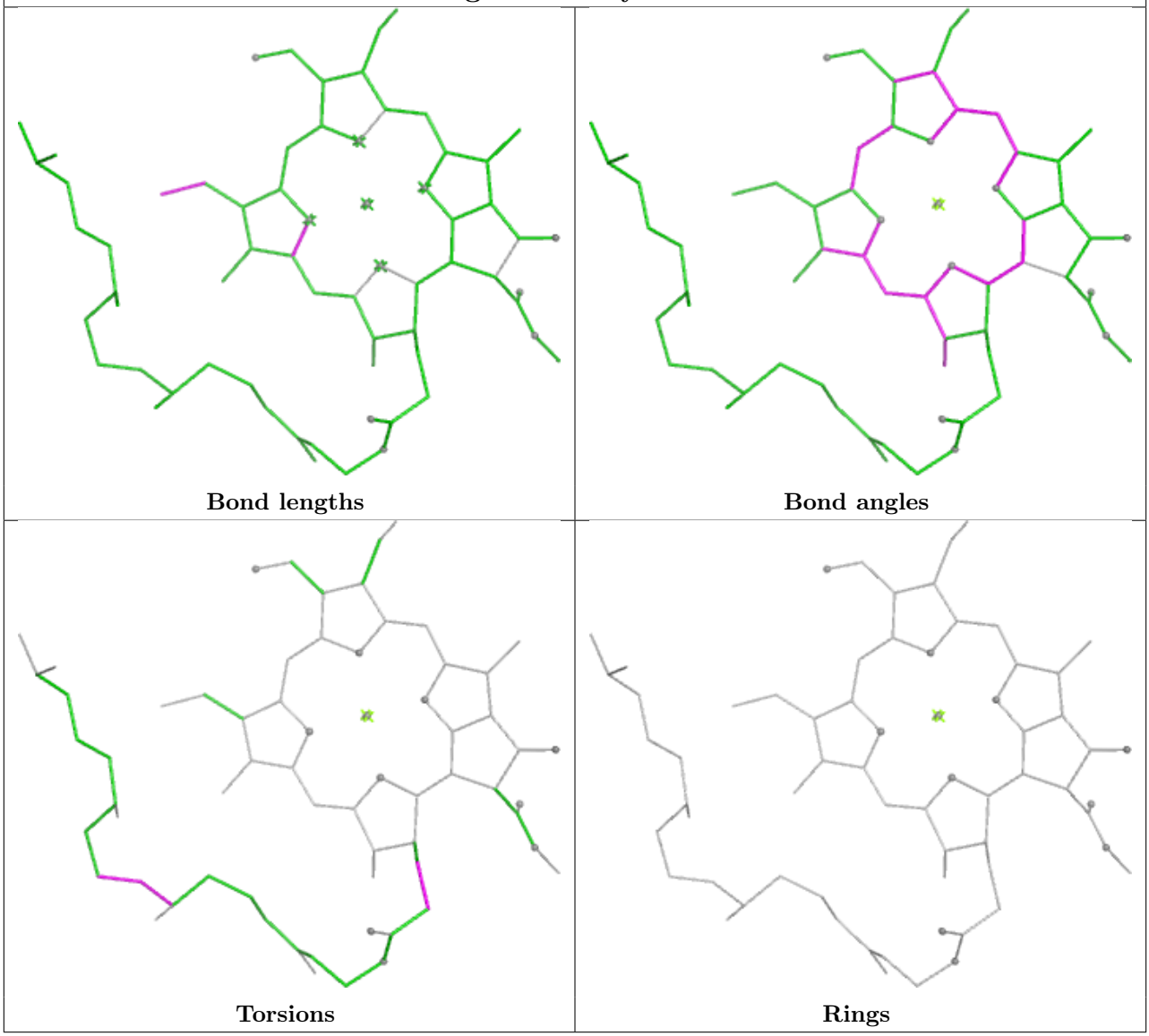
Torsions



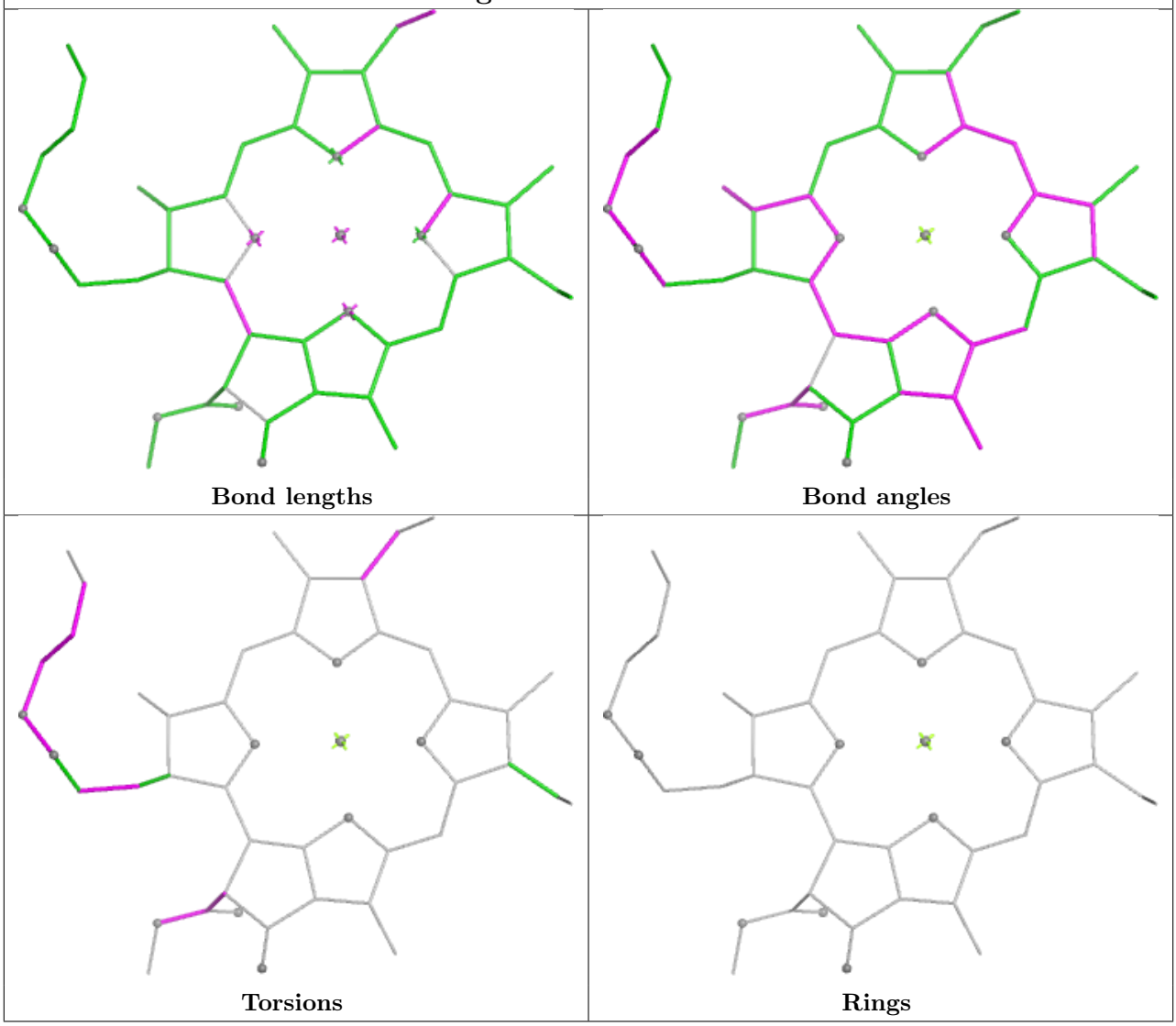
Rings

Ligand CLA N 611	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

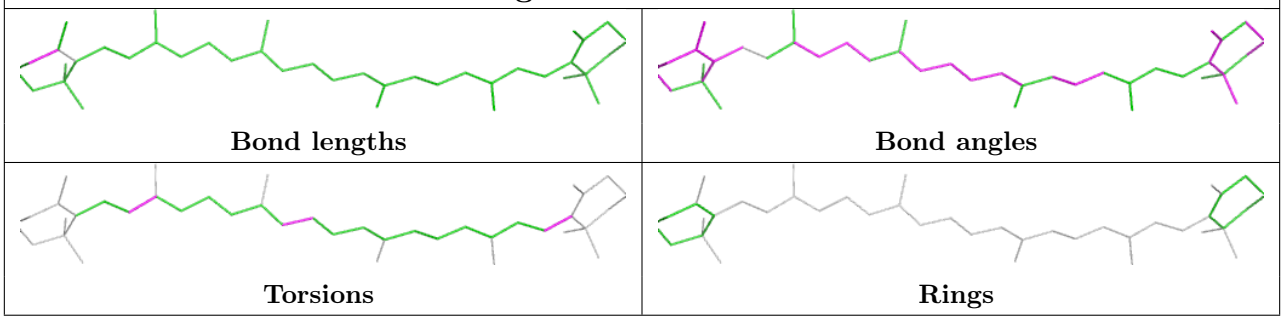
Ligand CHL y1 607



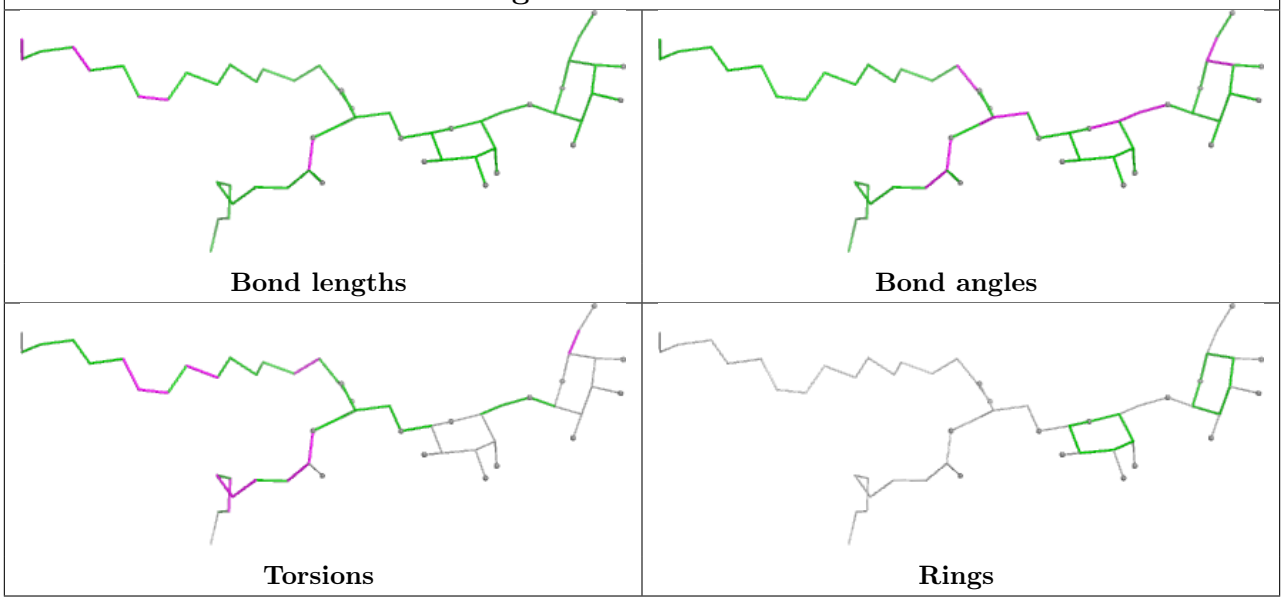
Ligand CLA n1 611



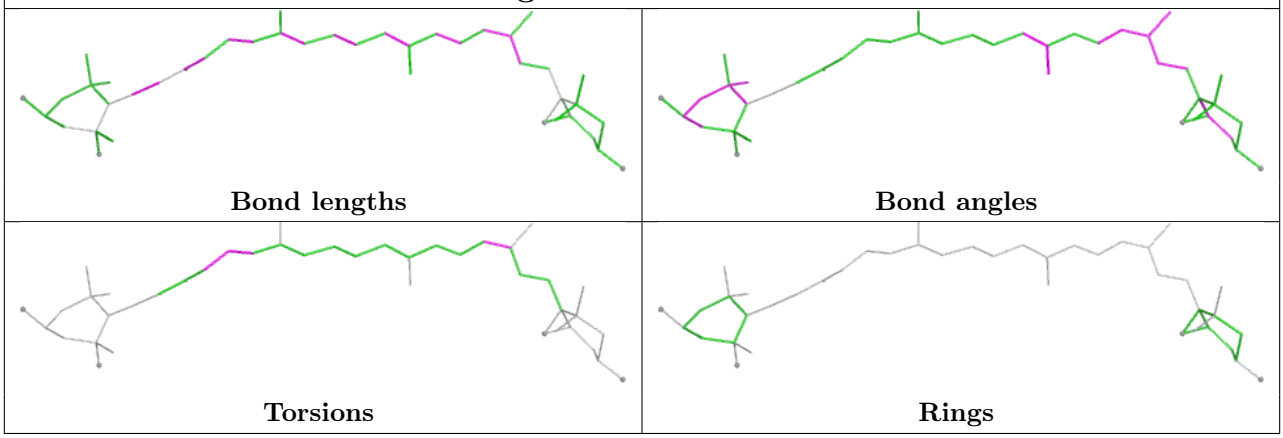
Ligand LUT G1 620



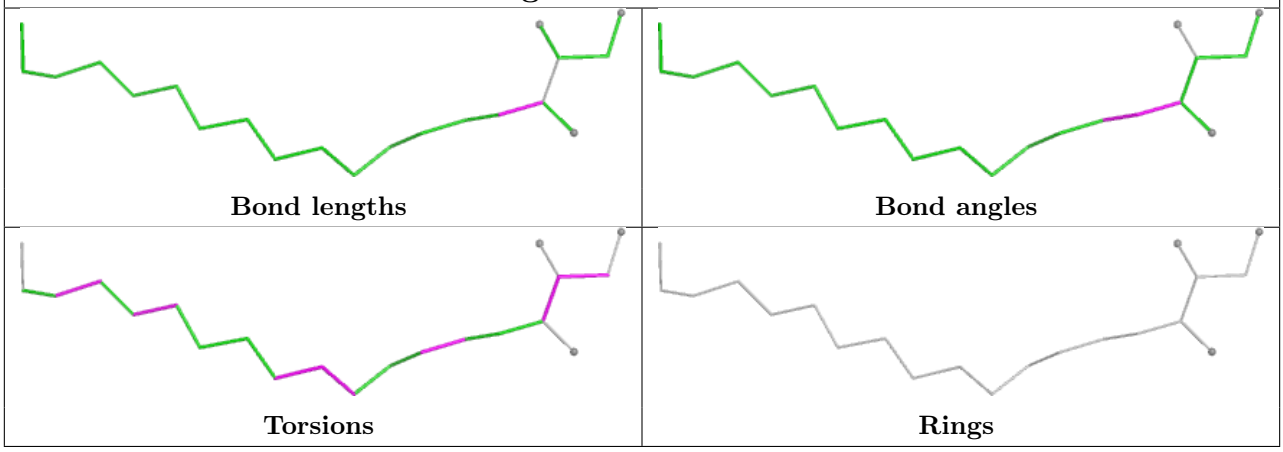
Ligand DGD C1 518



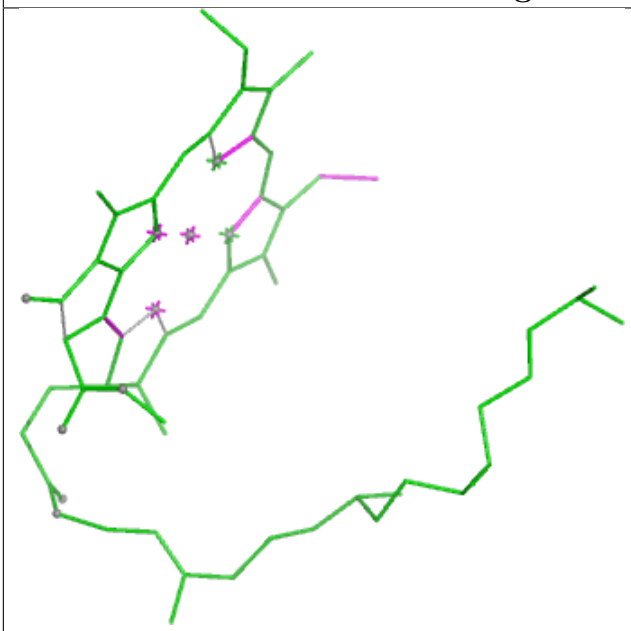
Ligand NEX S1 623



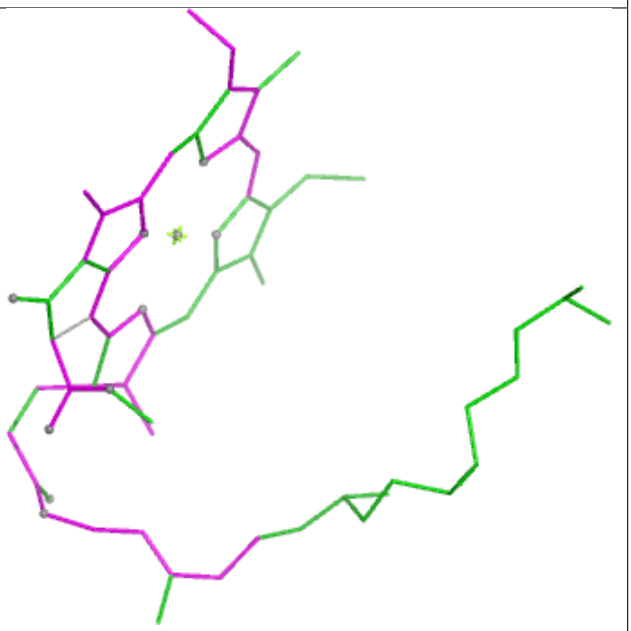
Ligand SPH a1 414



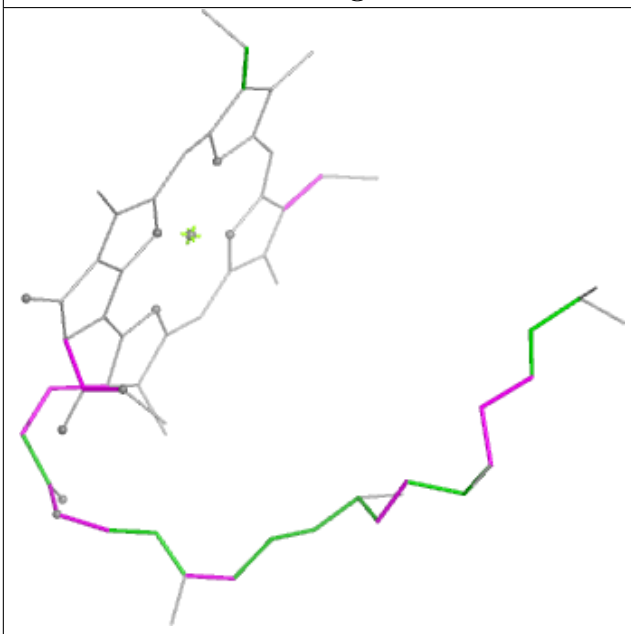
Ligand CLA N1 603



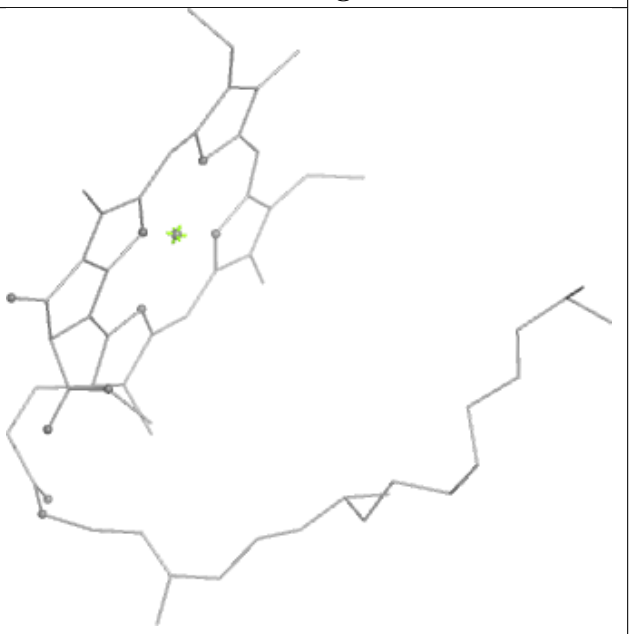
Bond lengths



Bond angles

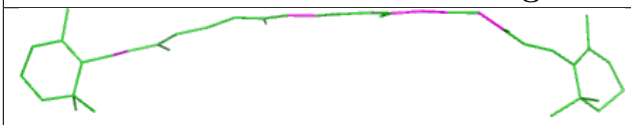


Torsions

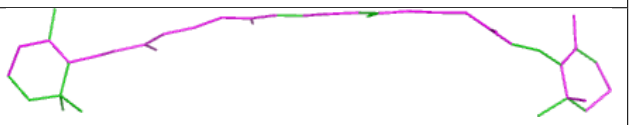


Rings

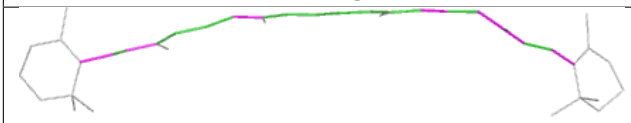
Ligand BCR C 517



Bond lengths

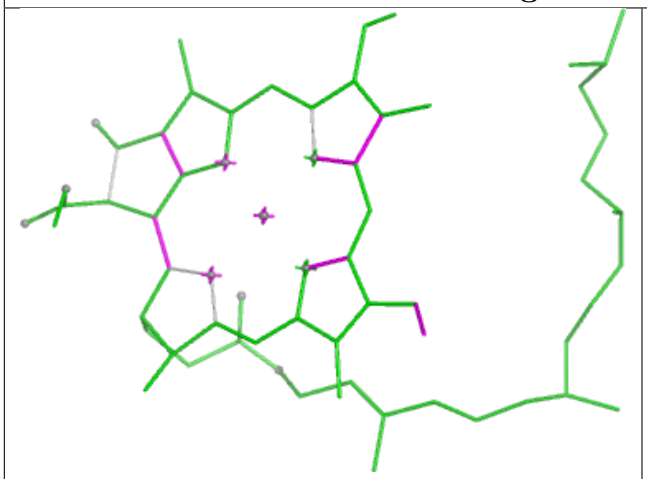
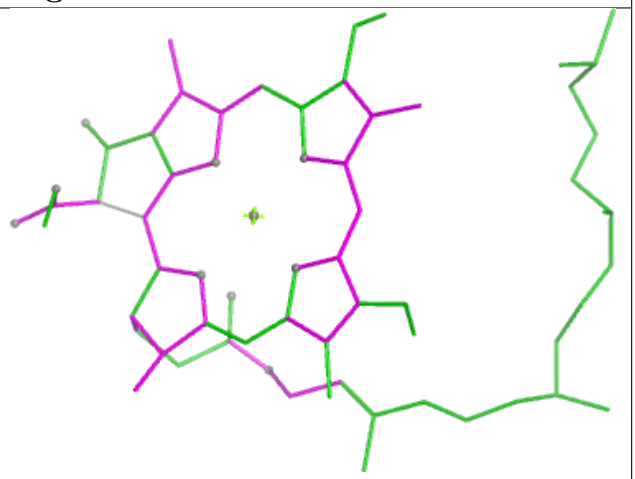
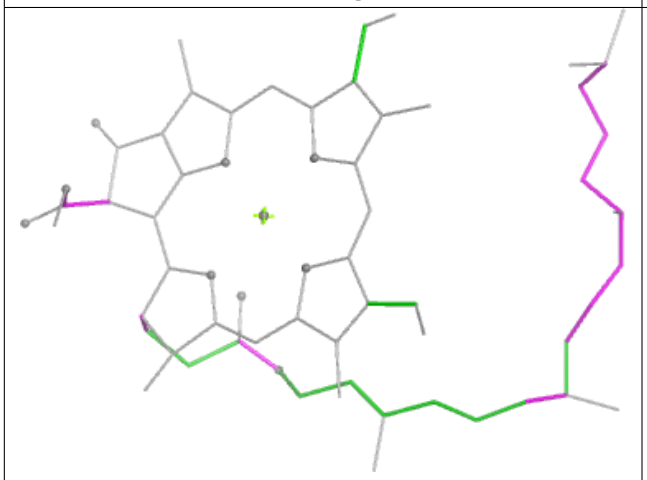
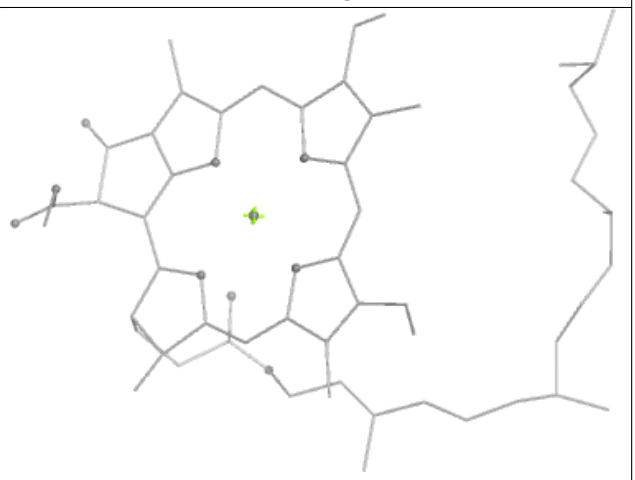


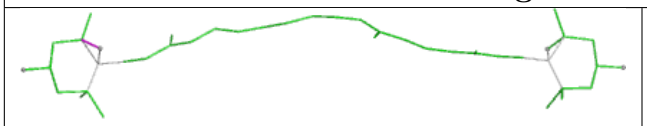
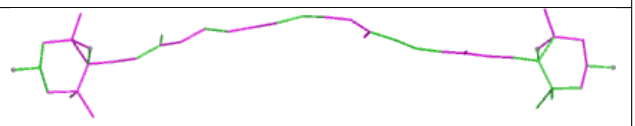
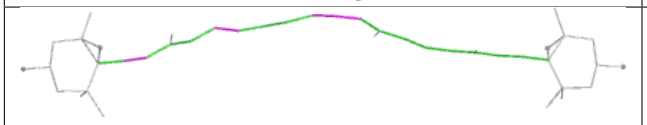
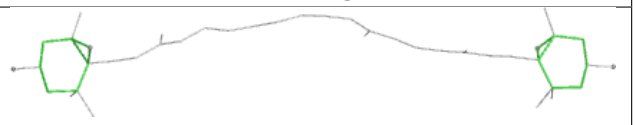
Bond angles



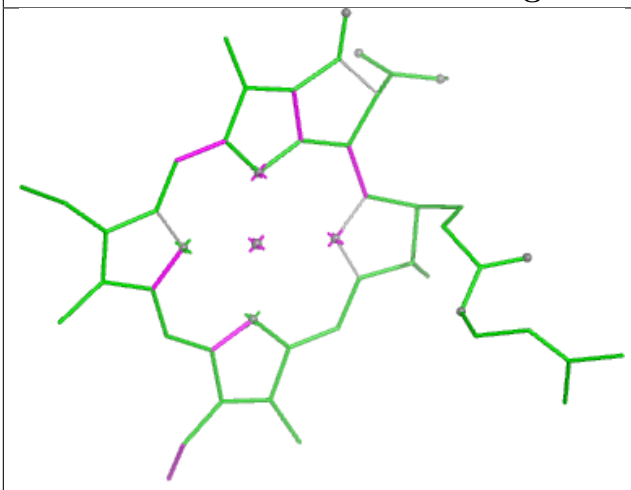
Torsions

Rings

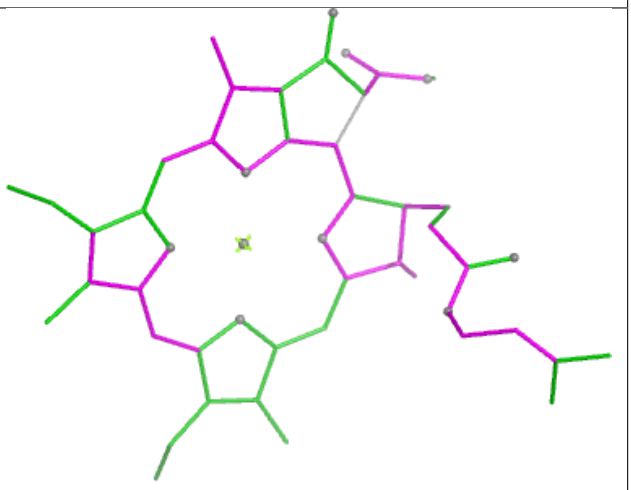
Ligand CLA g1 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT Y1 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

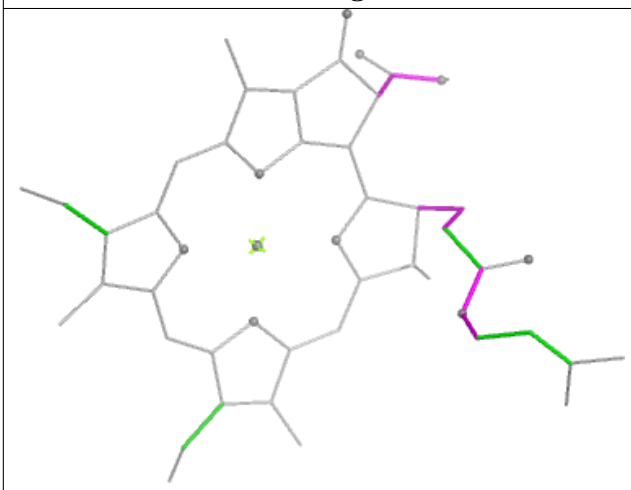
Ligand CLA A 407



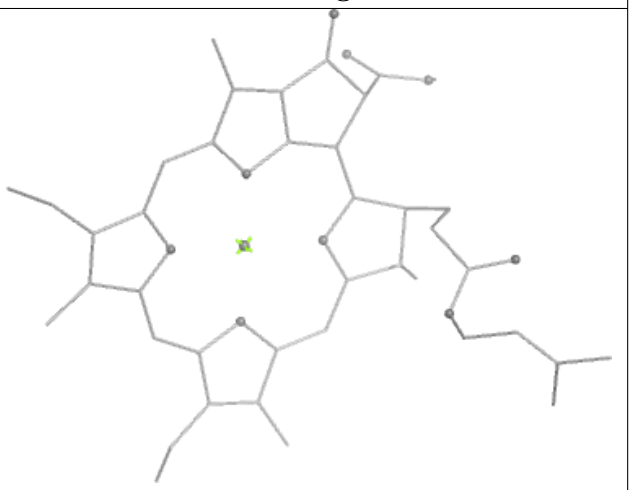
Bond lengths



Bond angles

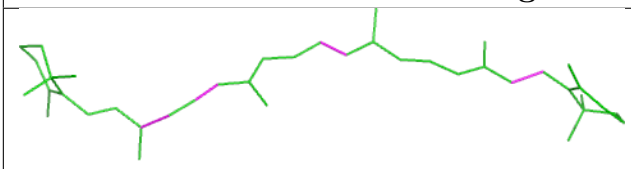


Torsions

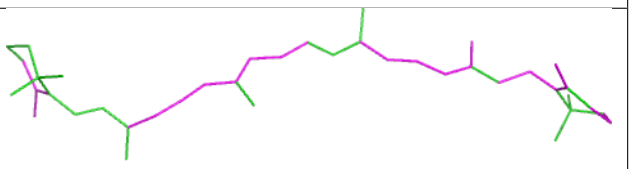


Rings

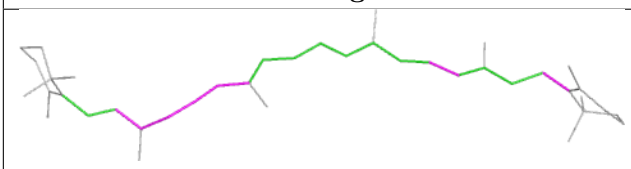
Ligand BCR c1 515



Bond lengths



Bond angles



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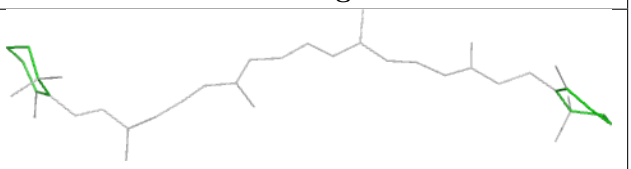
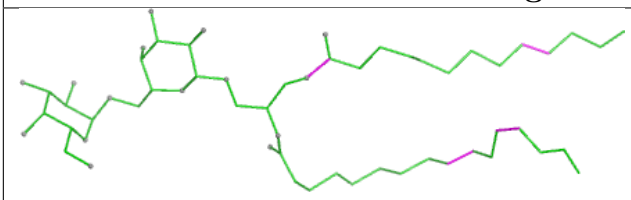
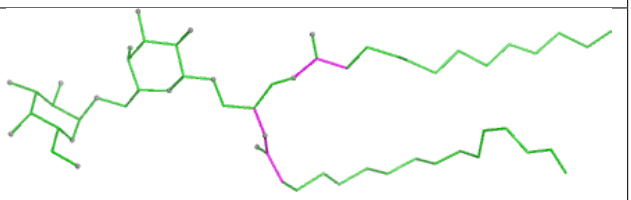
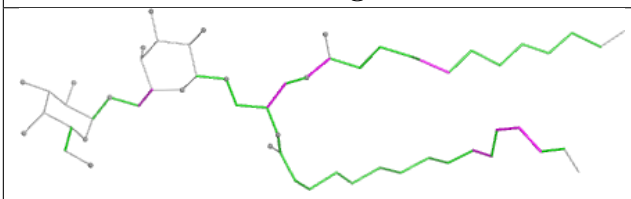
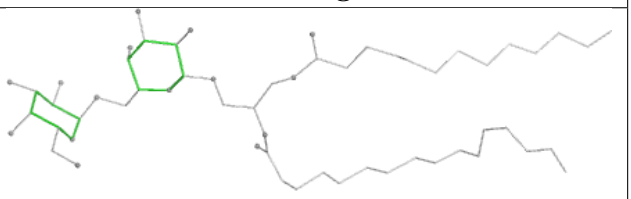
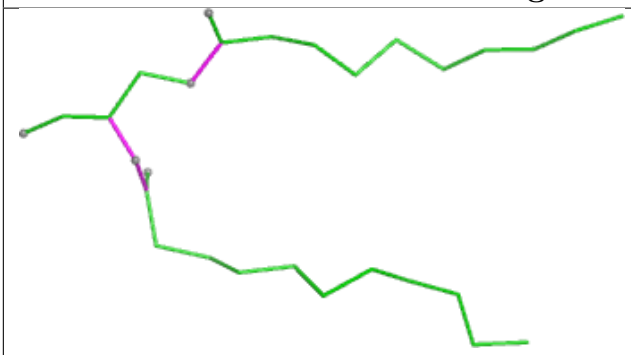
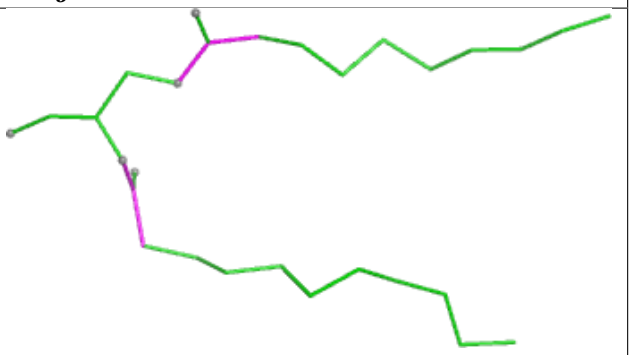
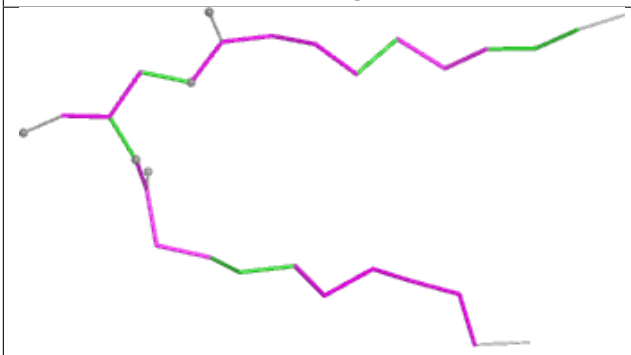
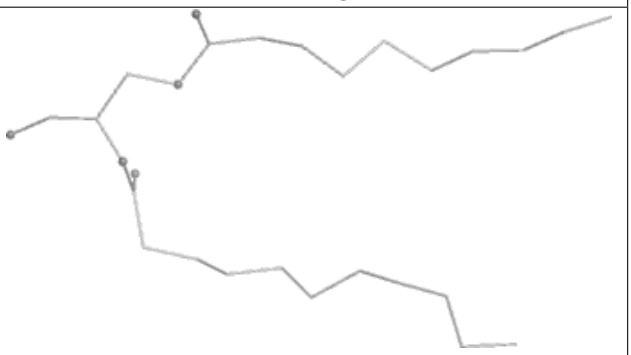
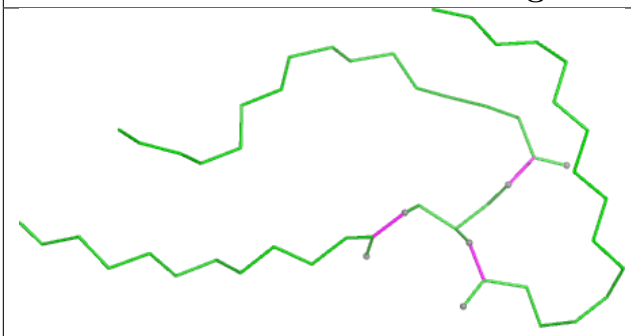
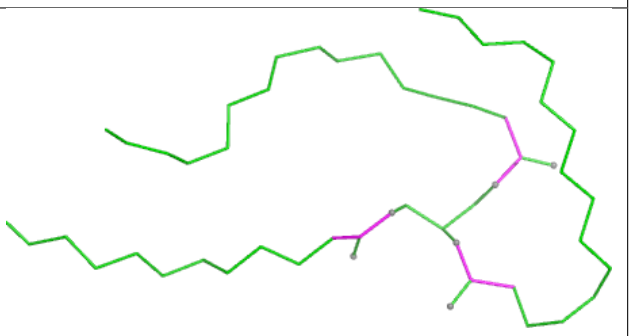
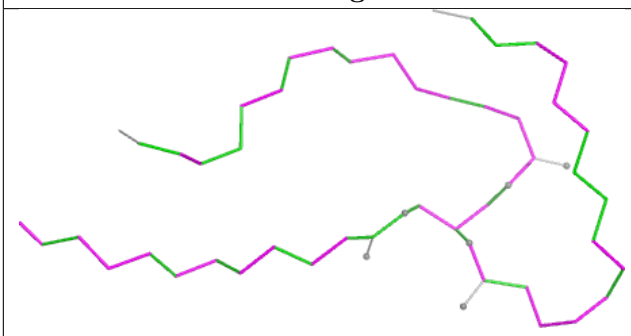
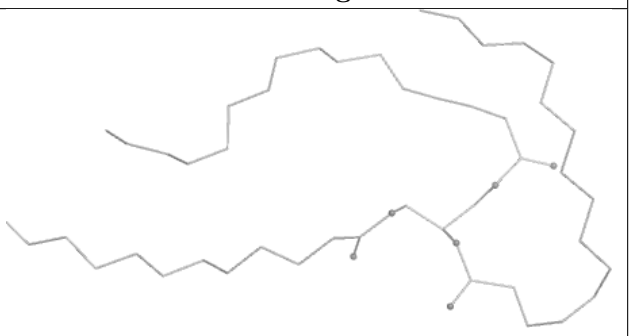
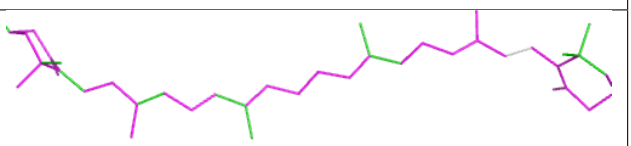
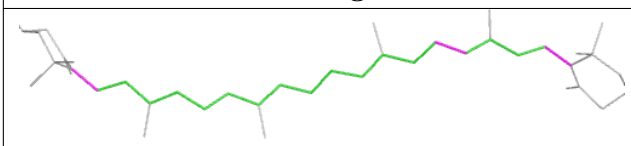
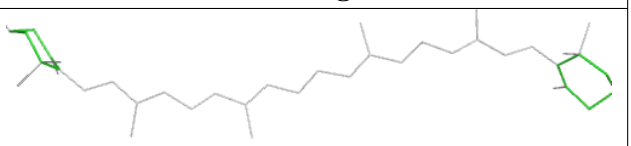


Rings

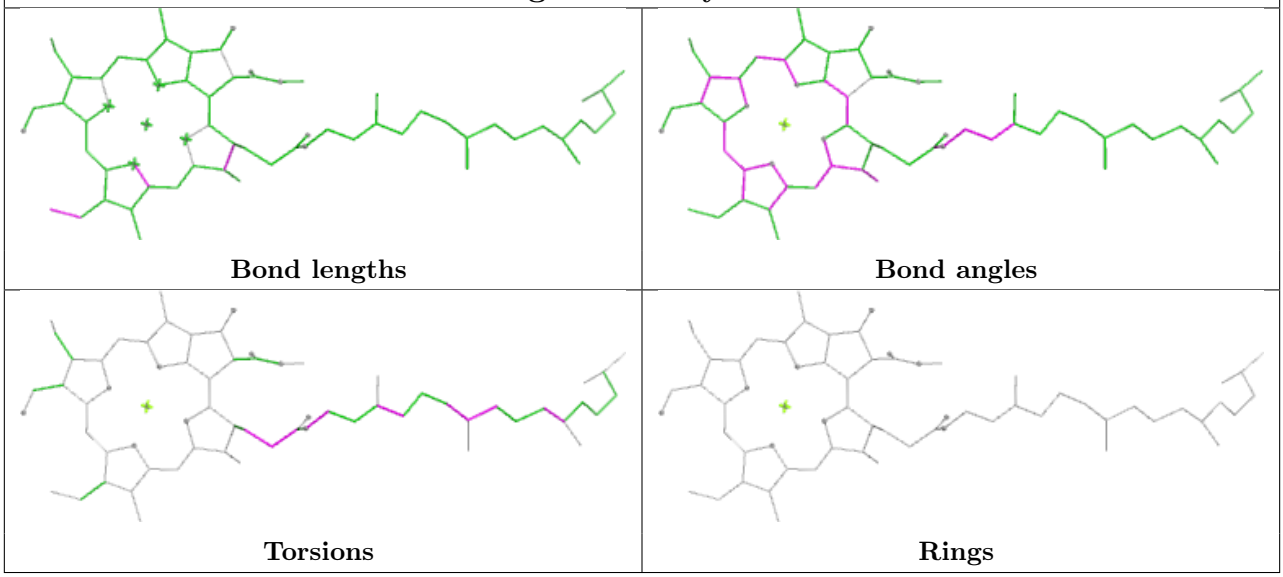
Ligand DGD c 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGA j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

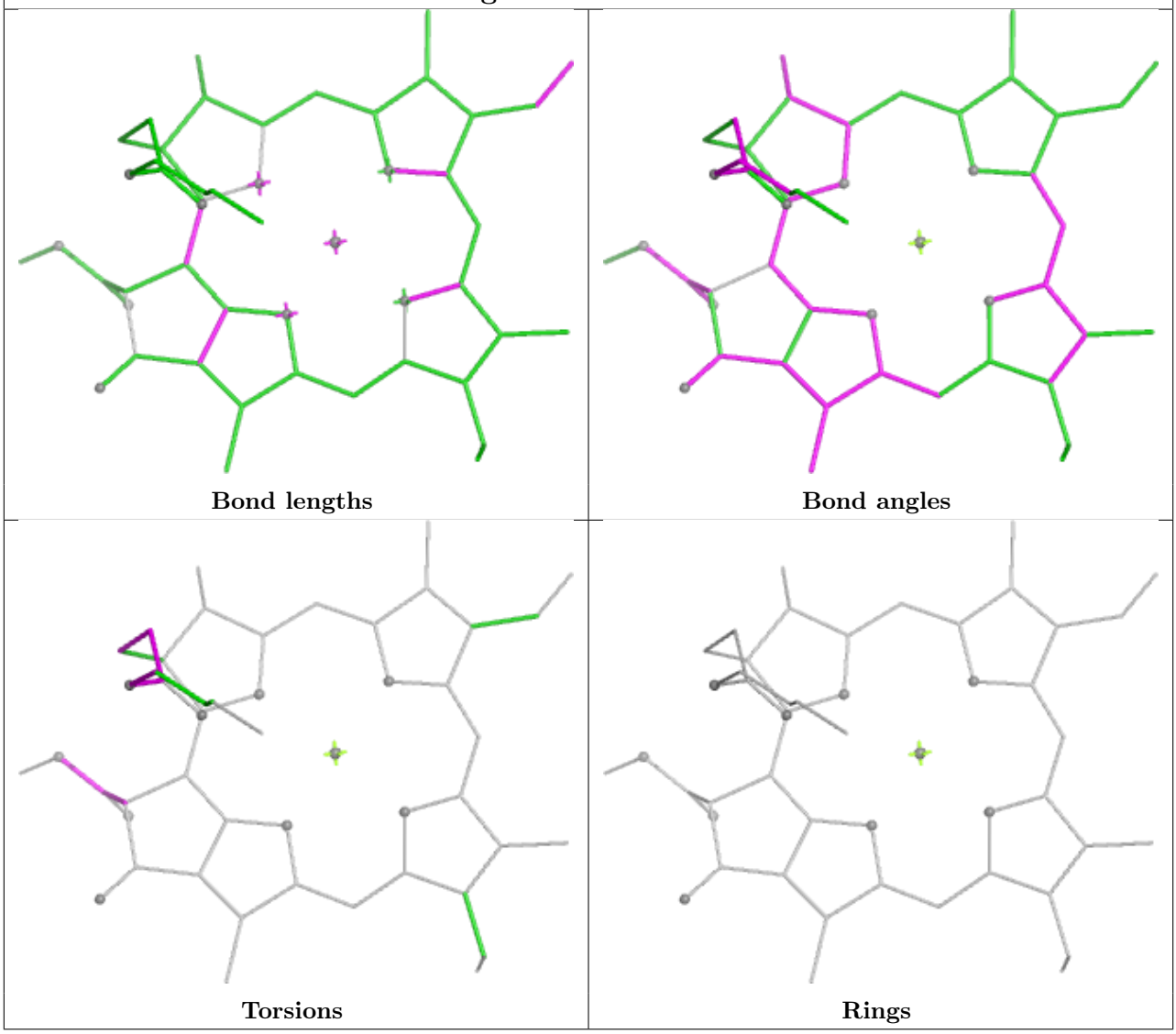
Ligand 4RF i1 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT S 621	
Bond lengths	 Bond angles
 Torsions	 Rings

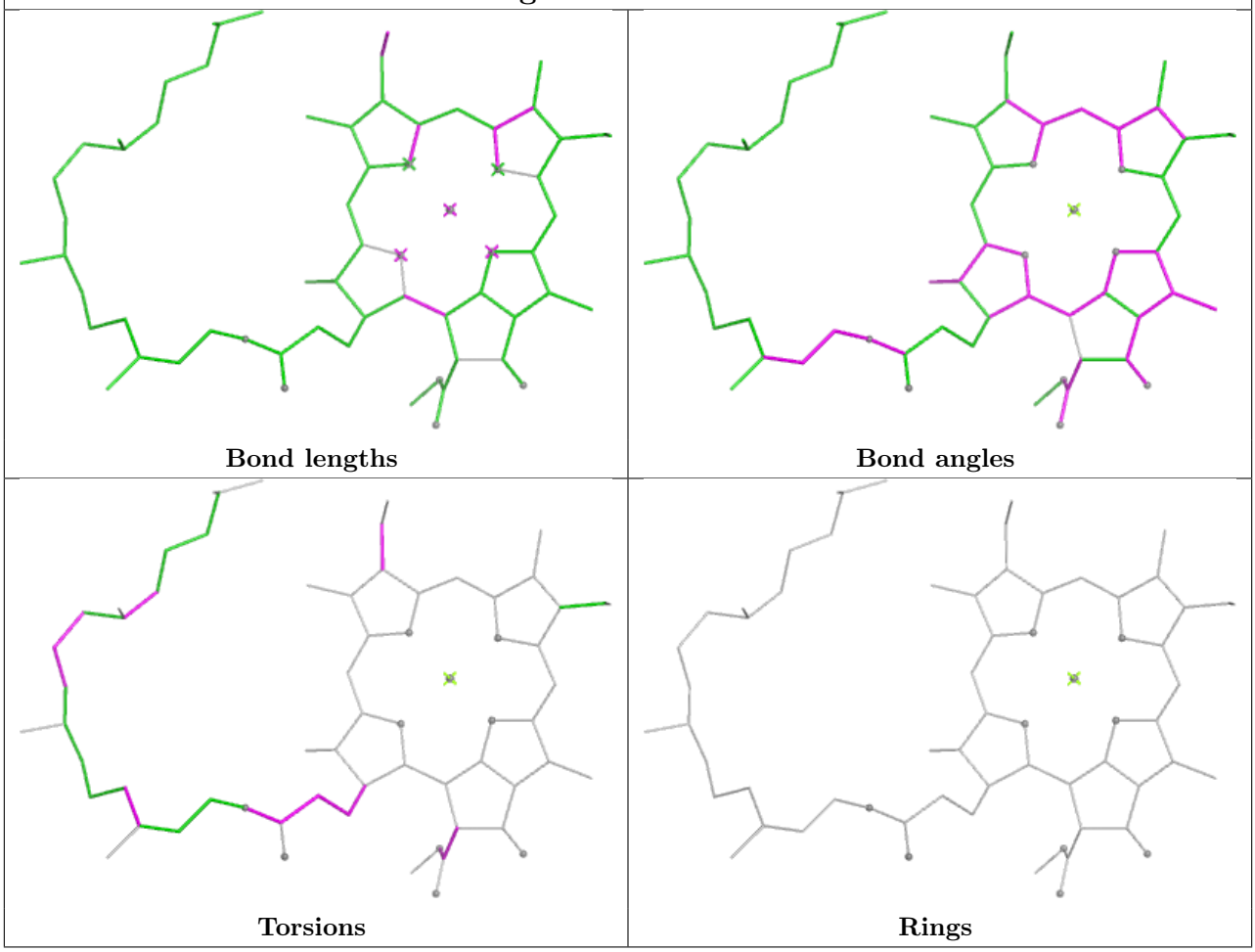
Ligand CHL y 606



Ligand CLA R 604



Ligand CLA s 603



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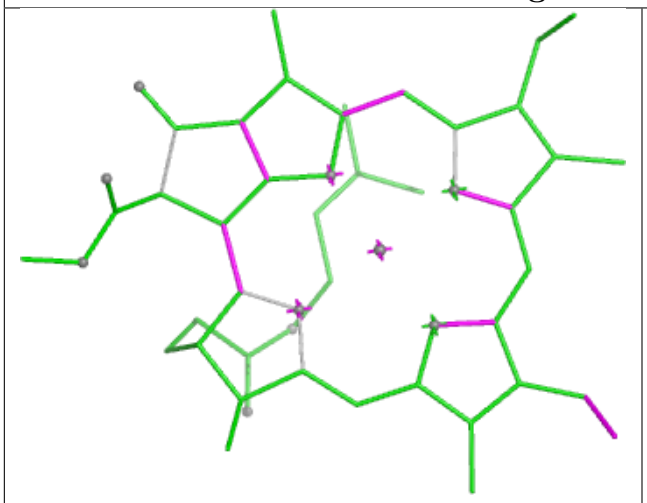
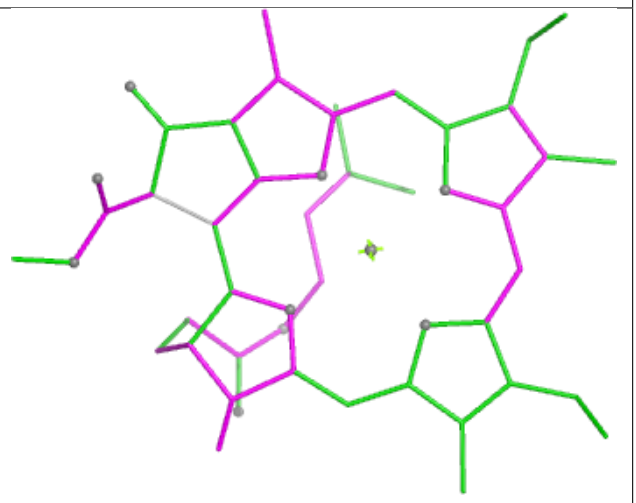
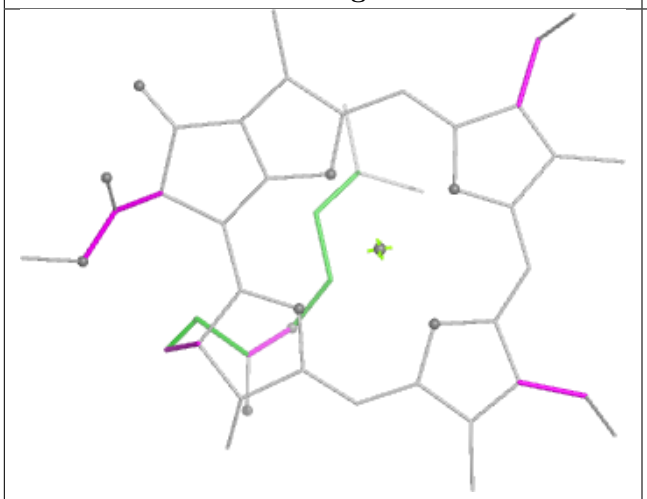


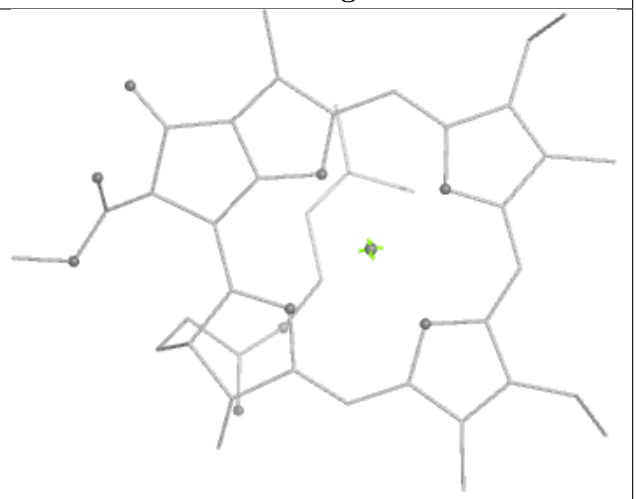
Bond lengths



Bond angles

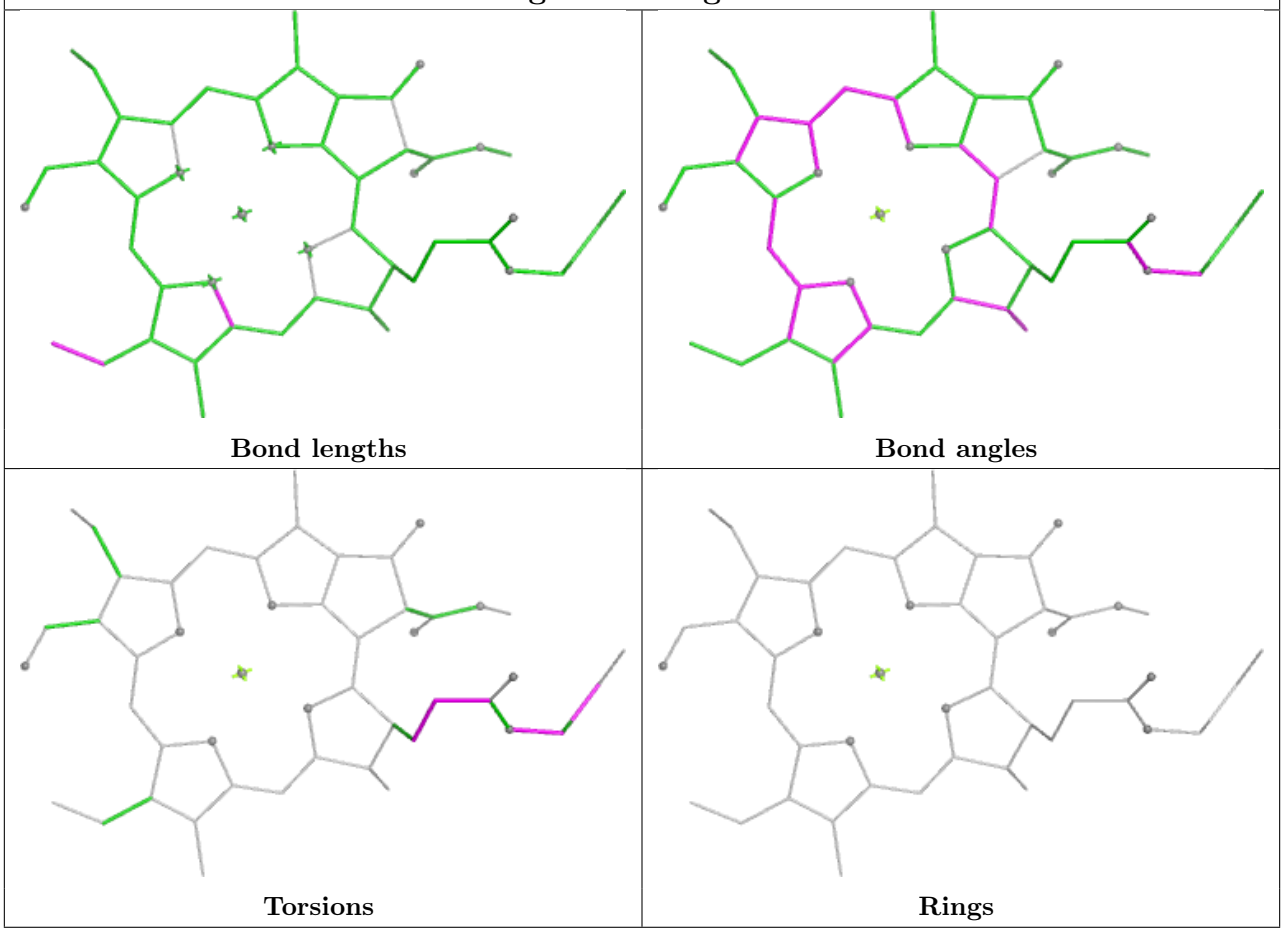


Torsions

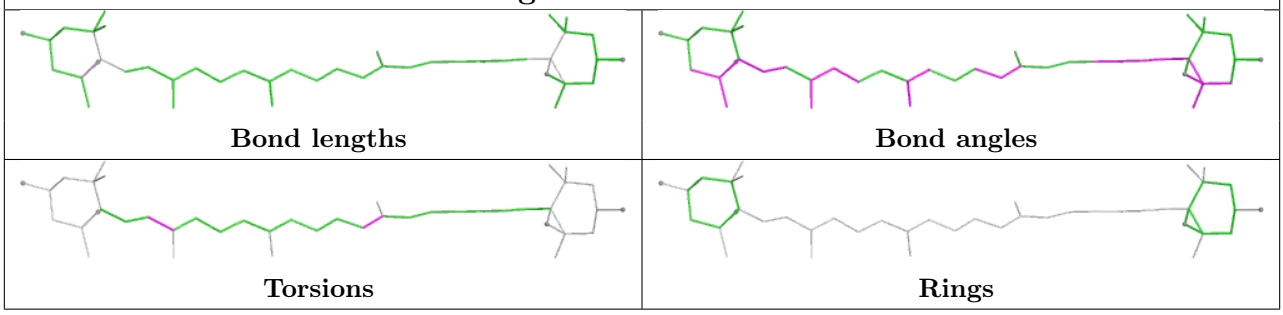


Rings

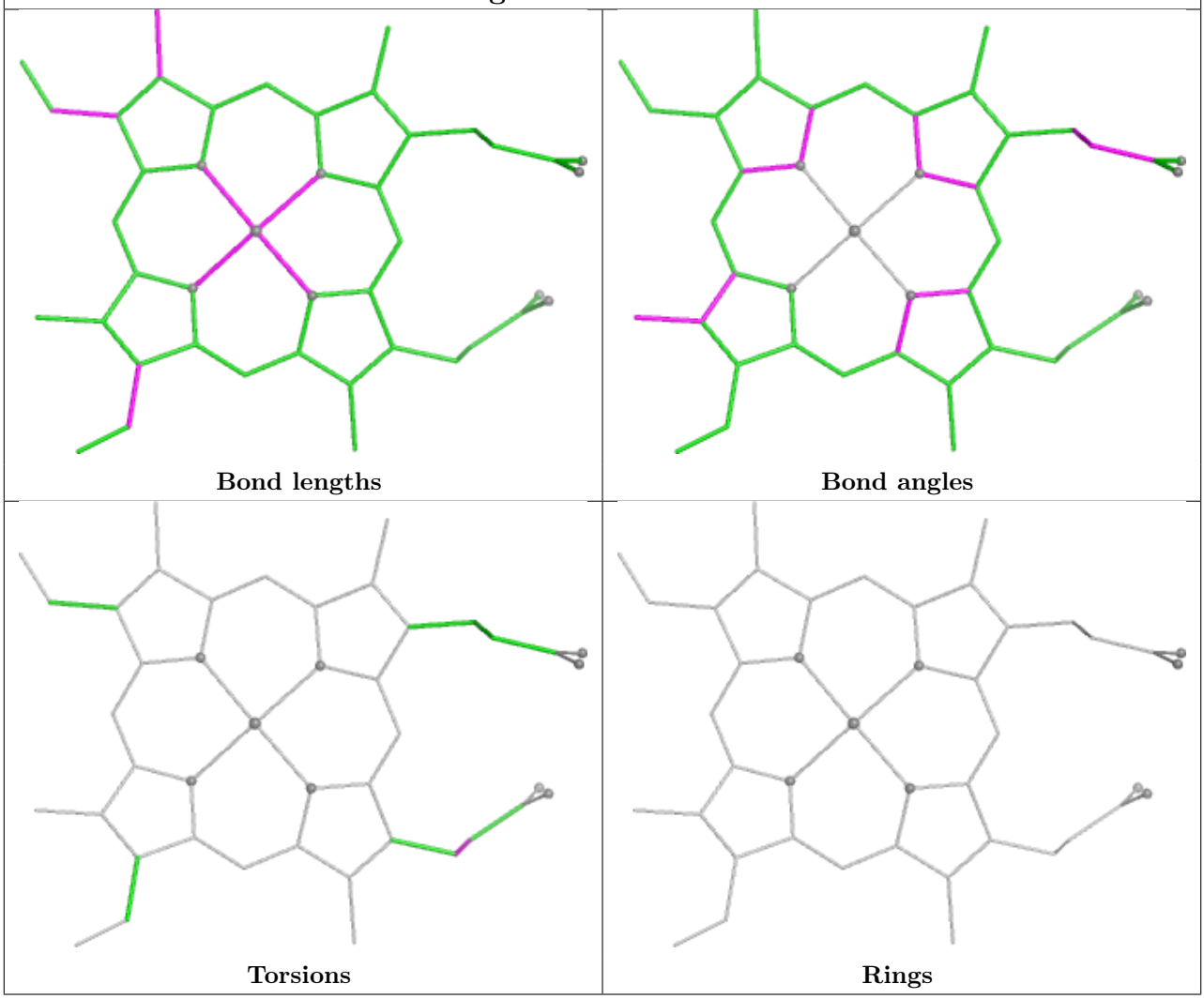
Ligand CHL g 606

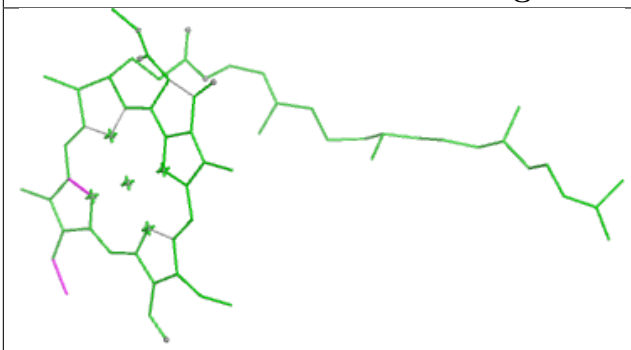
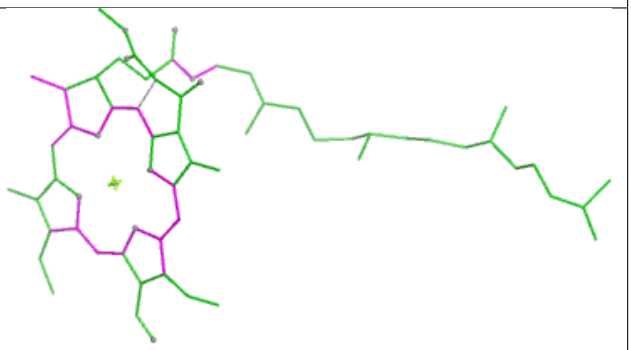
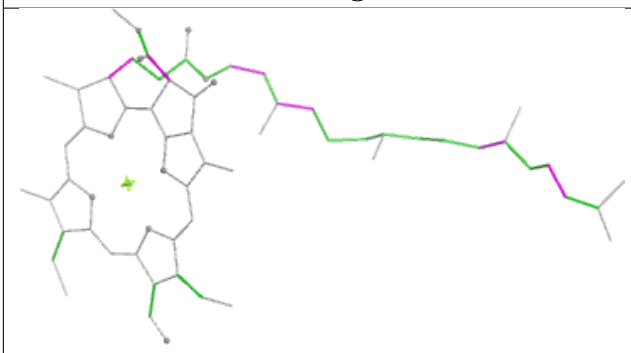
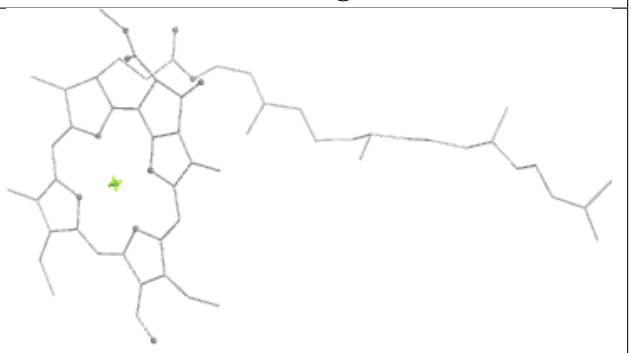


Ligand XAT n1 622

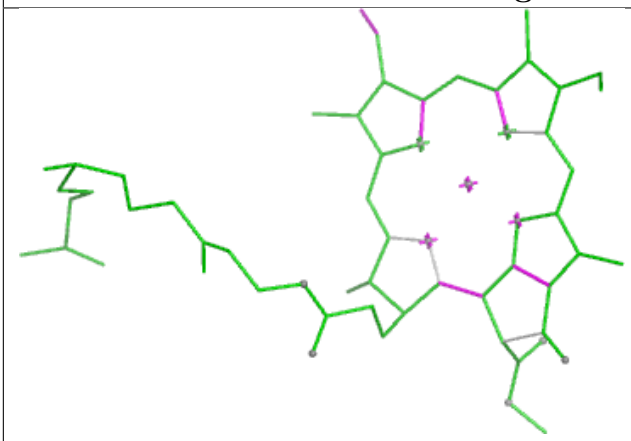


Ligand HEM F 101

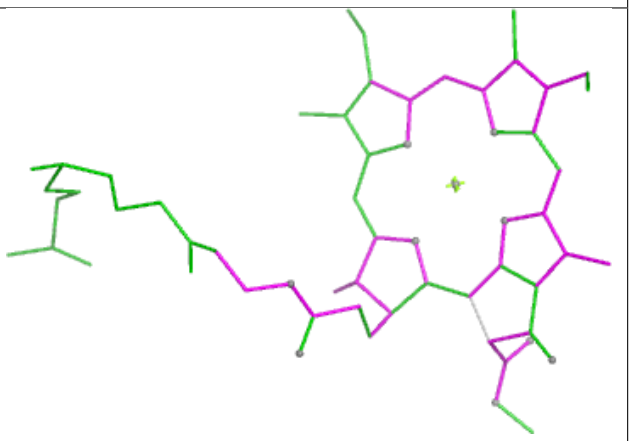


Ligand CHL G1 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

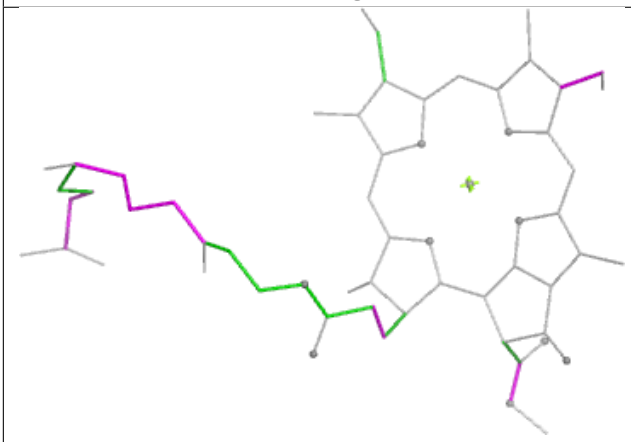
Ligand CLA A1 410



Bond lengths



Bond angles



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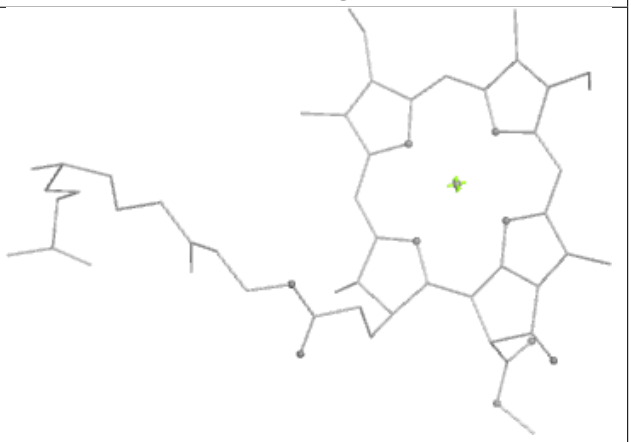
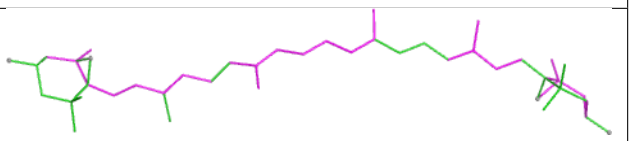


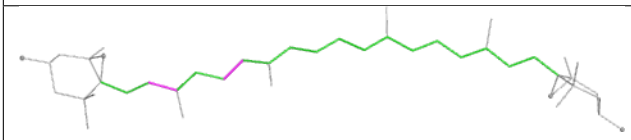
Rings

Ligand XAT r1 621

Bond lengths



Bond angles



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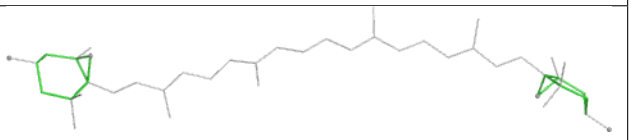
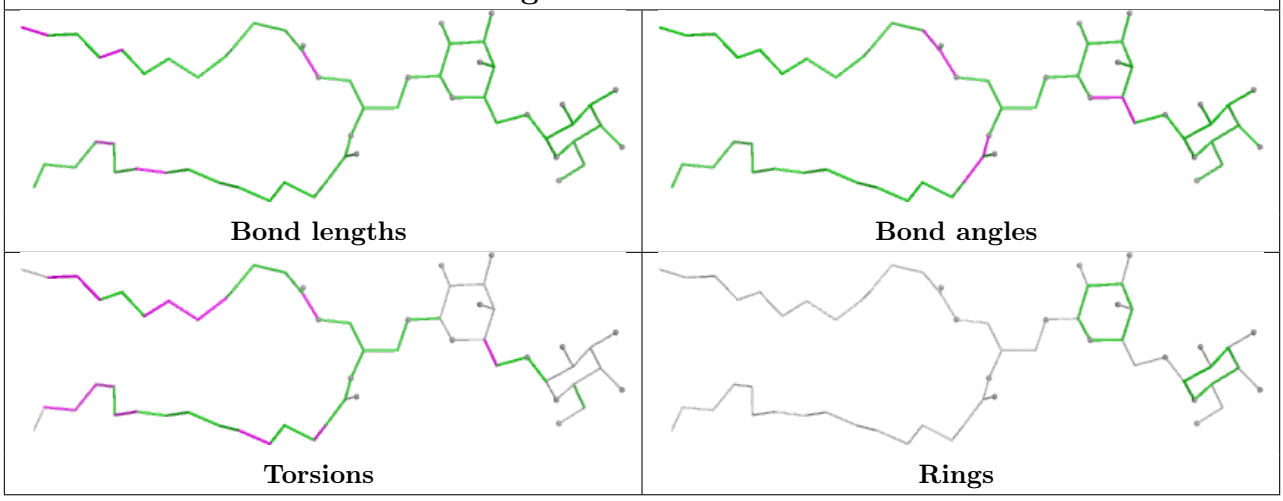
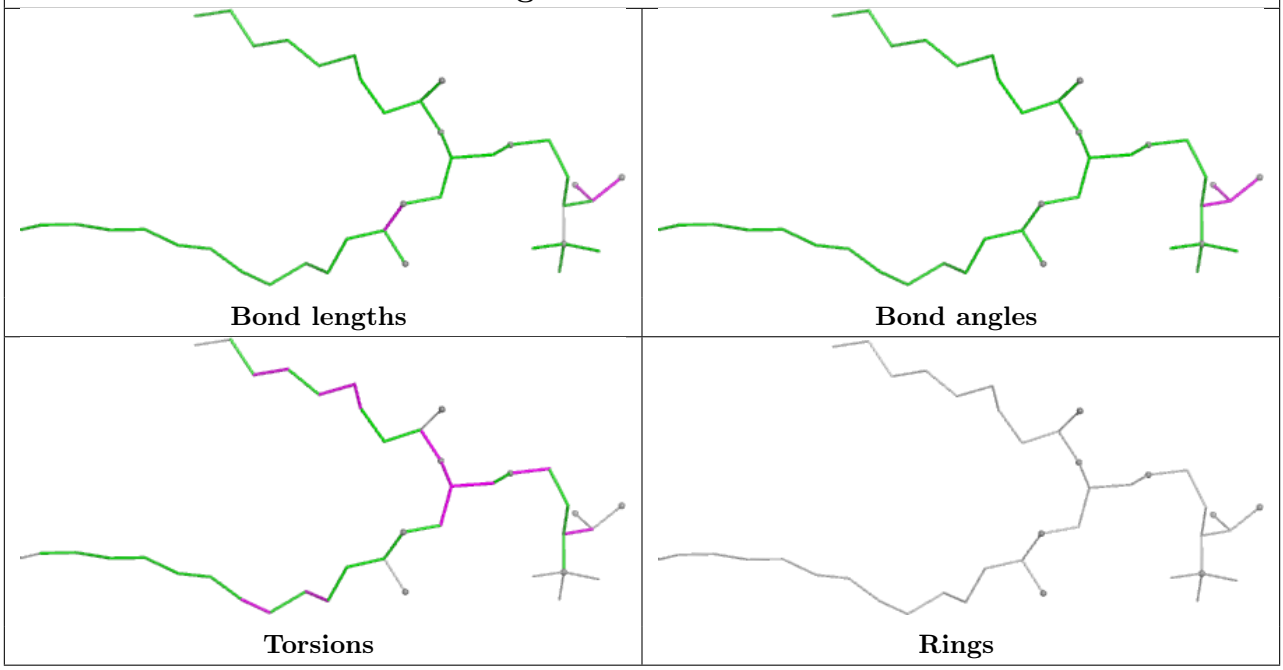


Rings

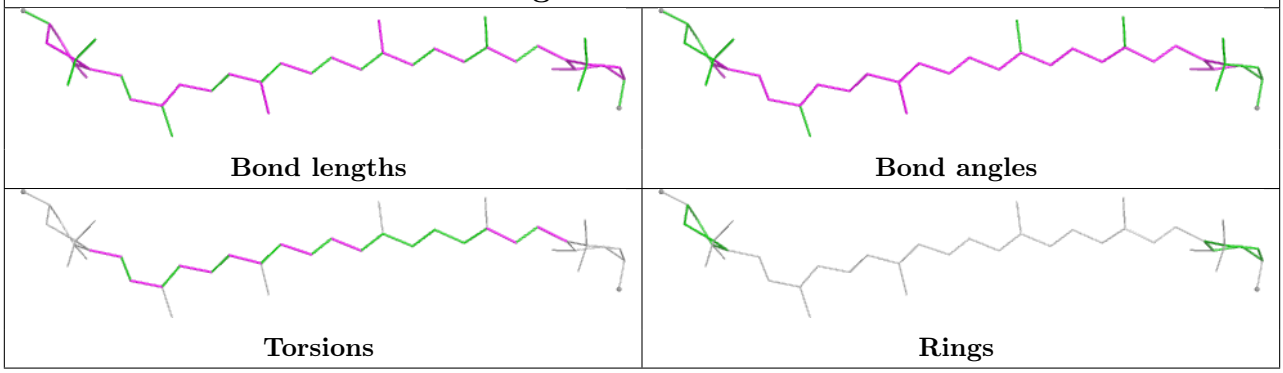
Ligand DGD C 520



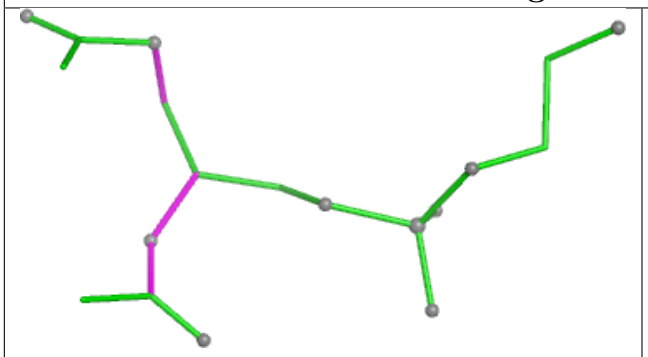
Ligand LMK c1 527



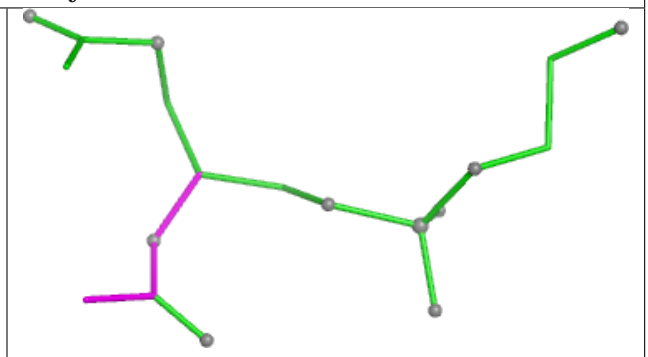
Ligand C7Z b 620



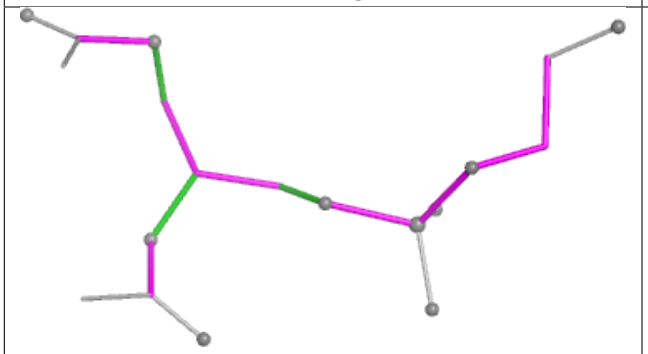
Ligand PTY y 627



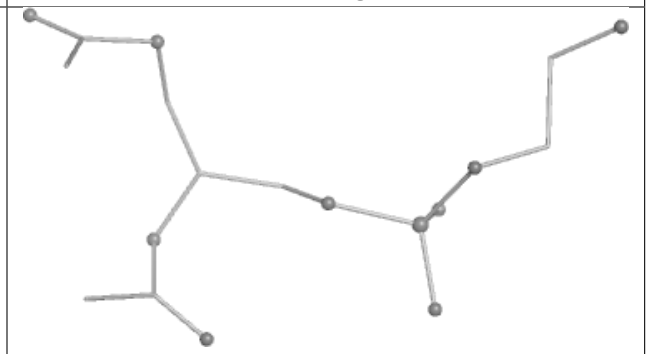
Bond lengths



Bond angles

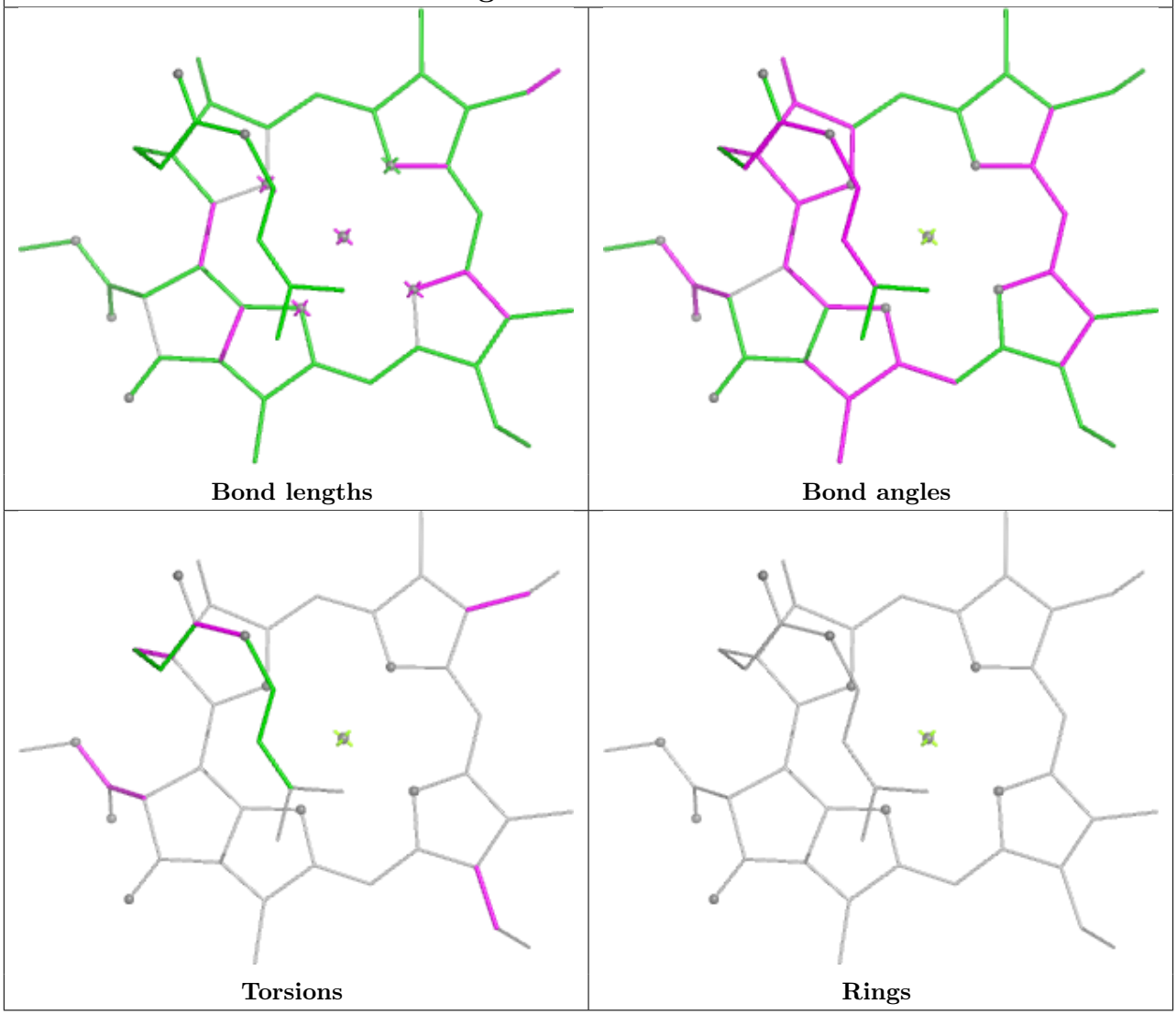


Torsions

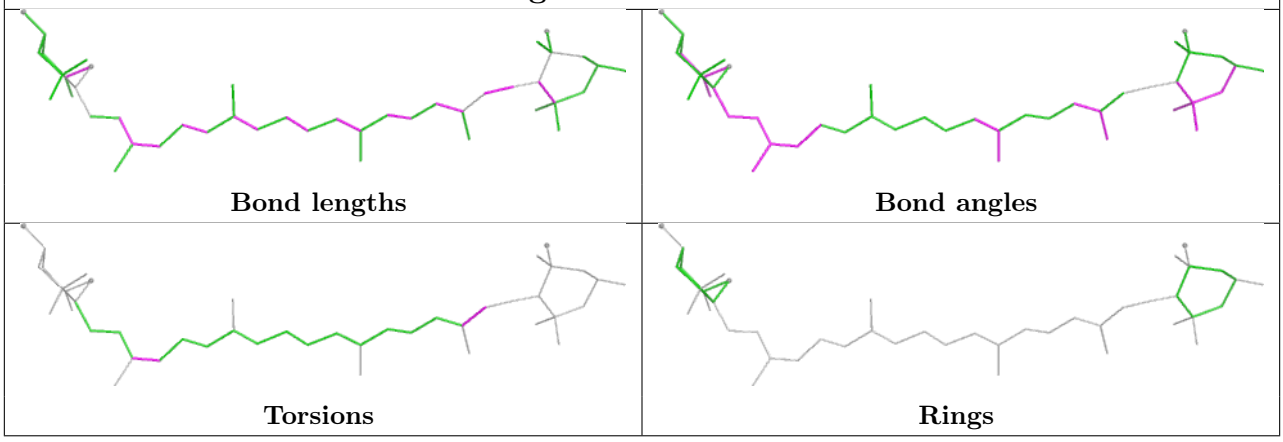


Rings

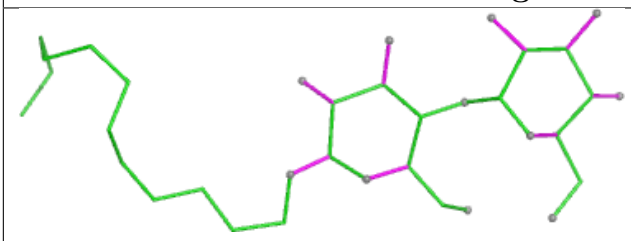
Ligand CLA s1 605



Ligand NEX s 623



Ligand LMT R1 625



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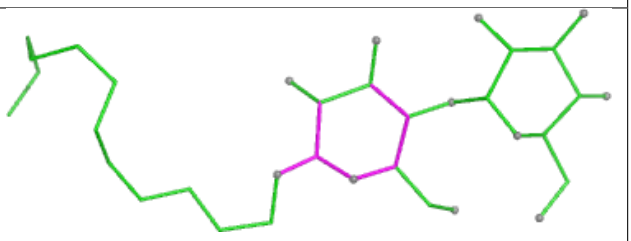
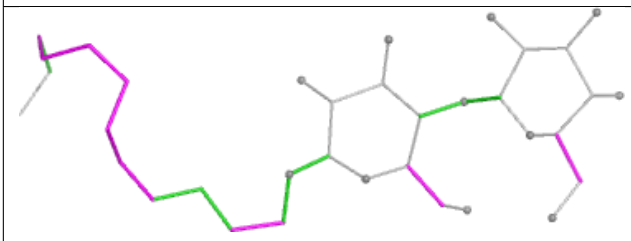


Bond angles



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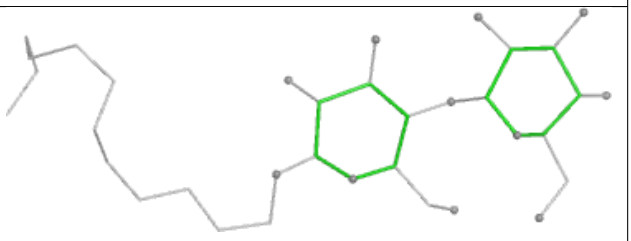
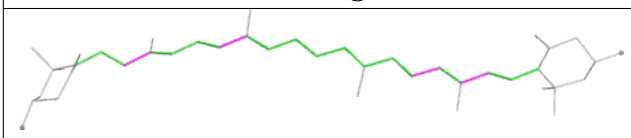


Rings

Ligand LUT S1 621

Bond lengths

Bond angles



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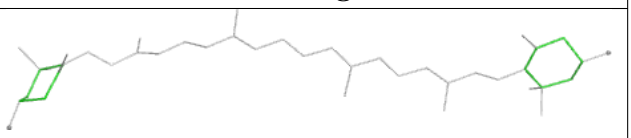
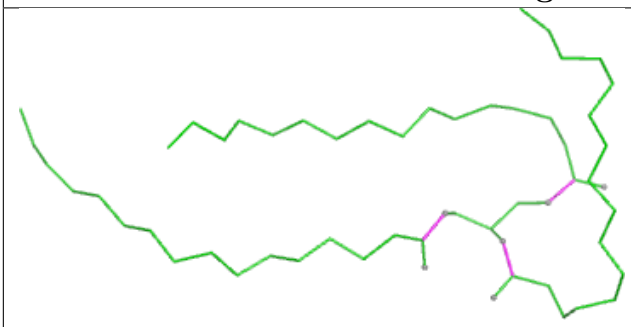
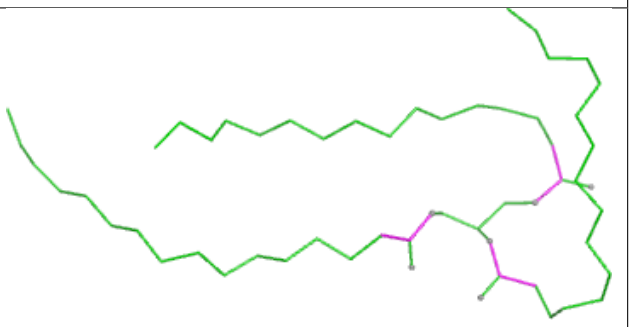


Rings

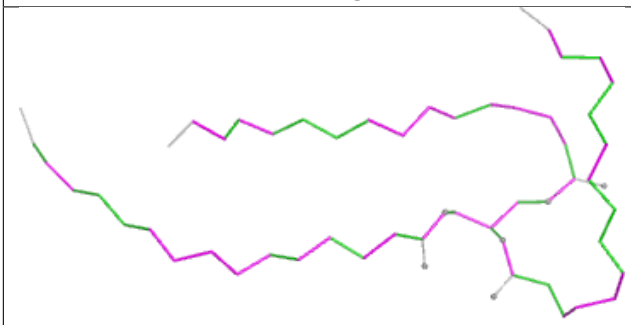
Ligand 4RF i 101



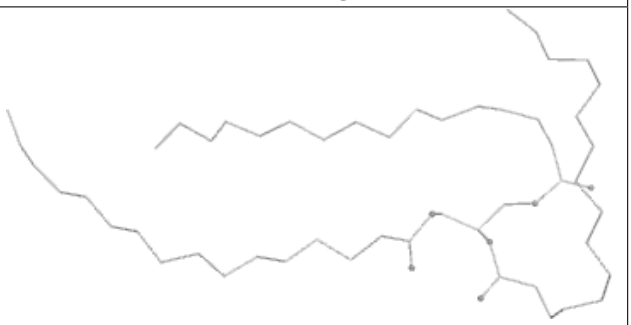
Bond lengths



Bond angles

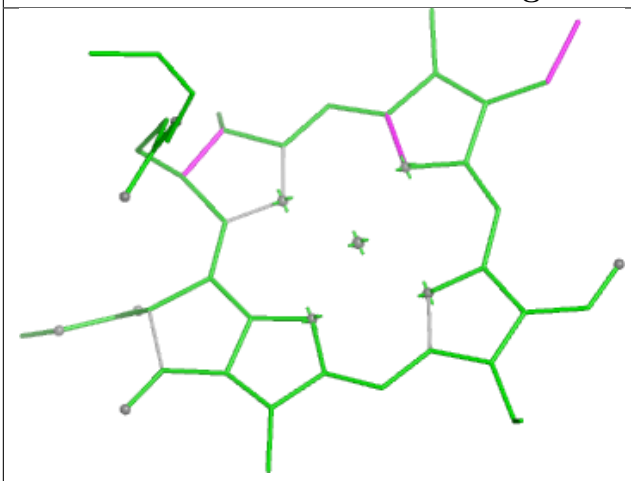


Torsions



Rings

Ligand CHL N 608



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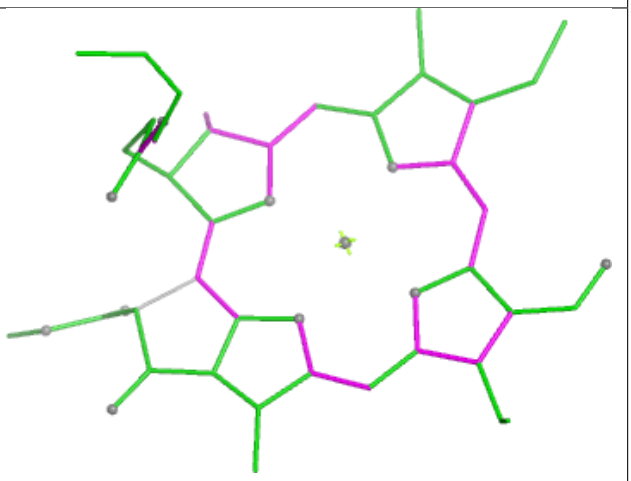
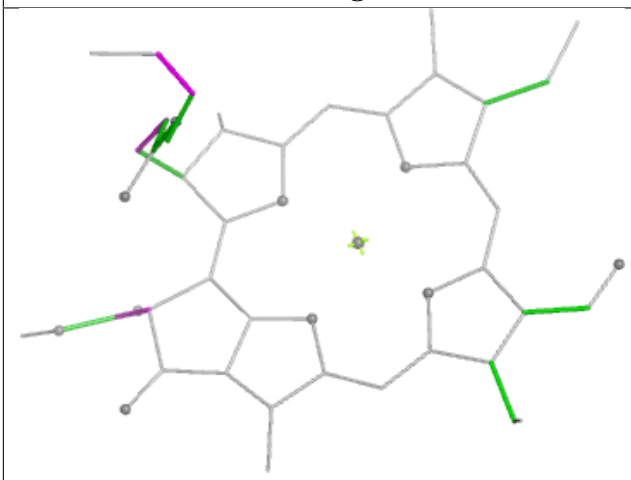


Bond angles



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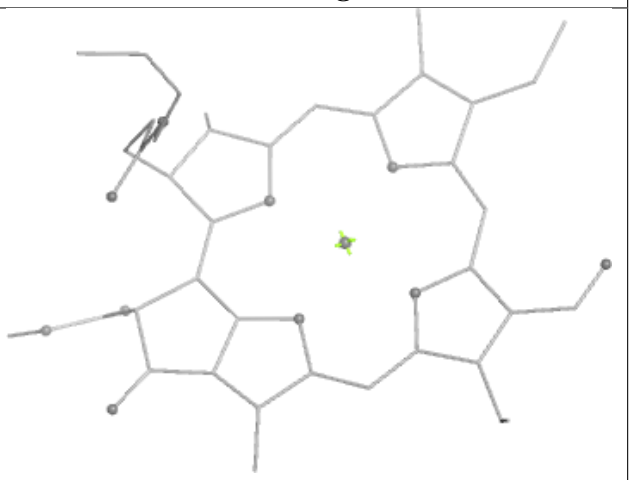
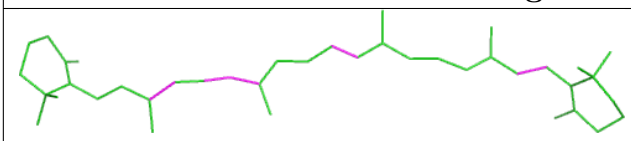


Rings

Ligand BCR b 619



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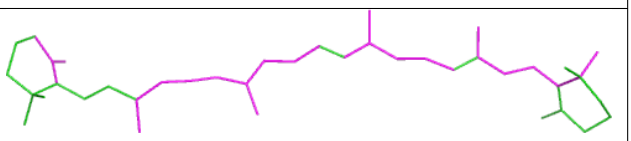
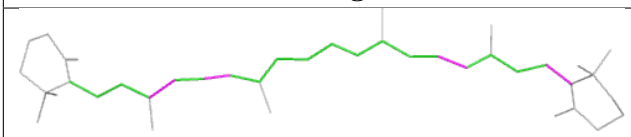


Bond angles



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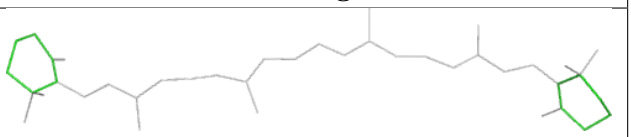
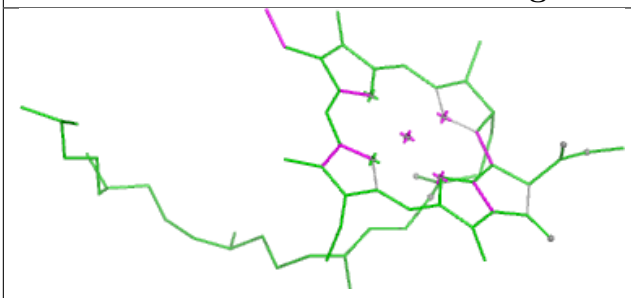
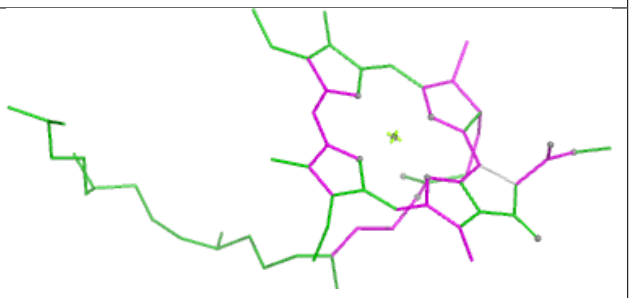
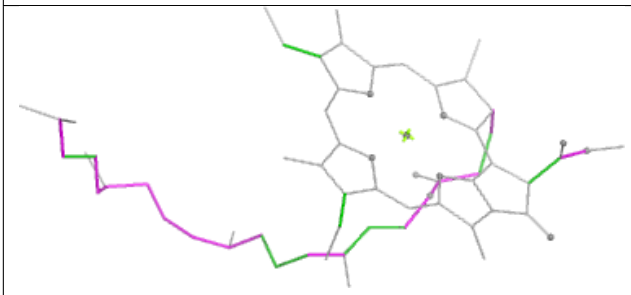
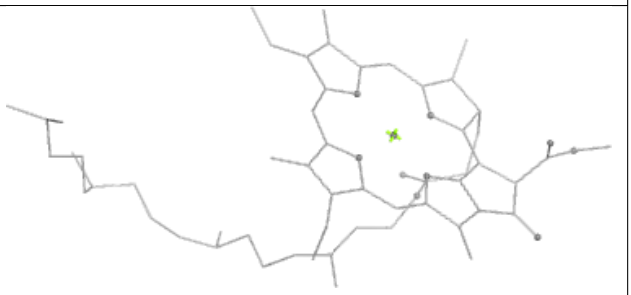


Rings

Ligand CLA c 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

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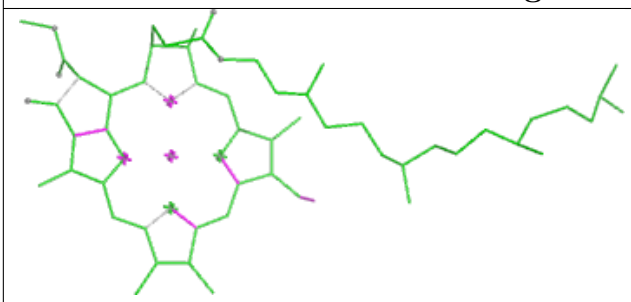
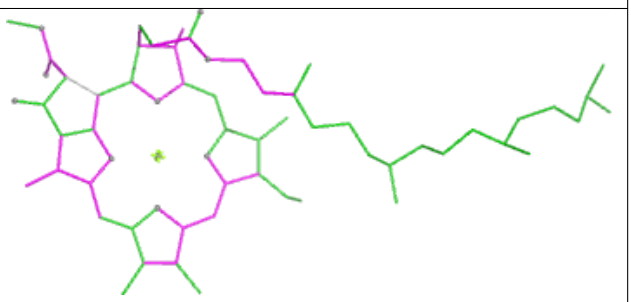
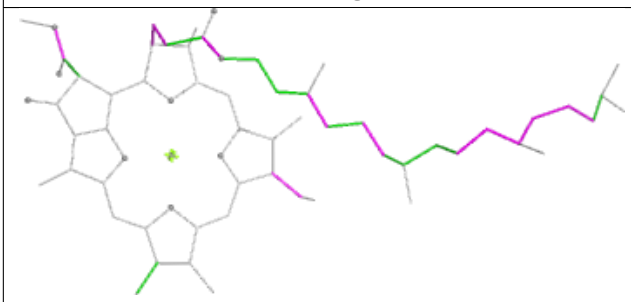
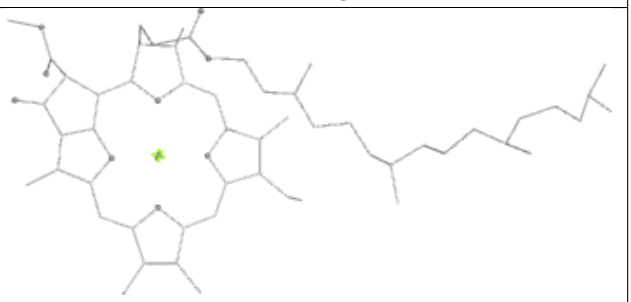
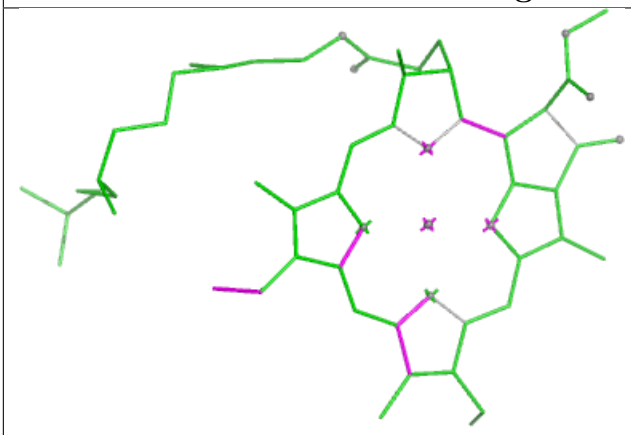
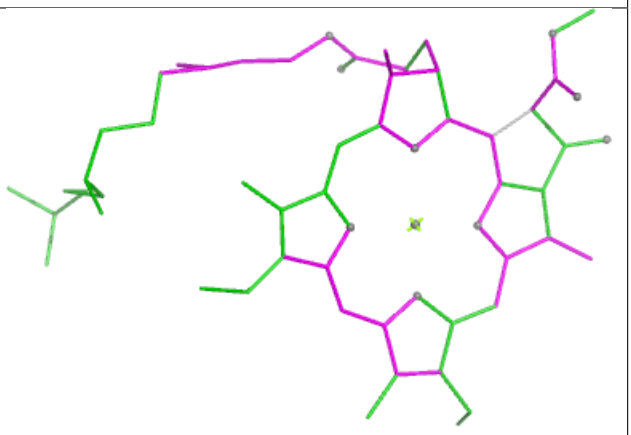
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R1 609



Bond lengths



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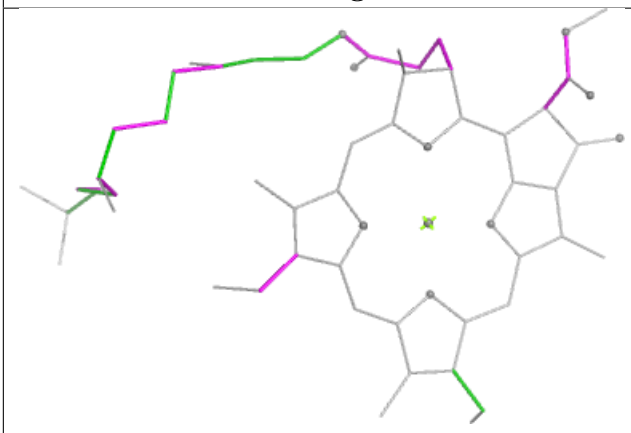
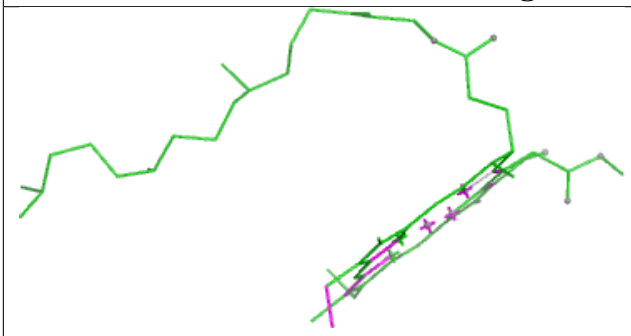


Torsions

Rings

Ligand CLA y1 614



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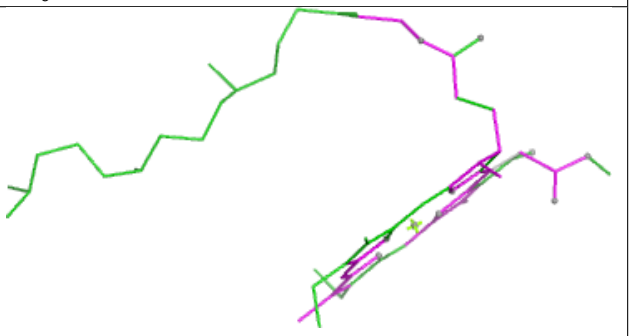
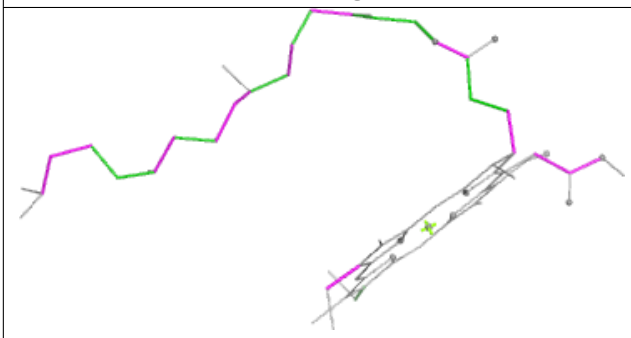


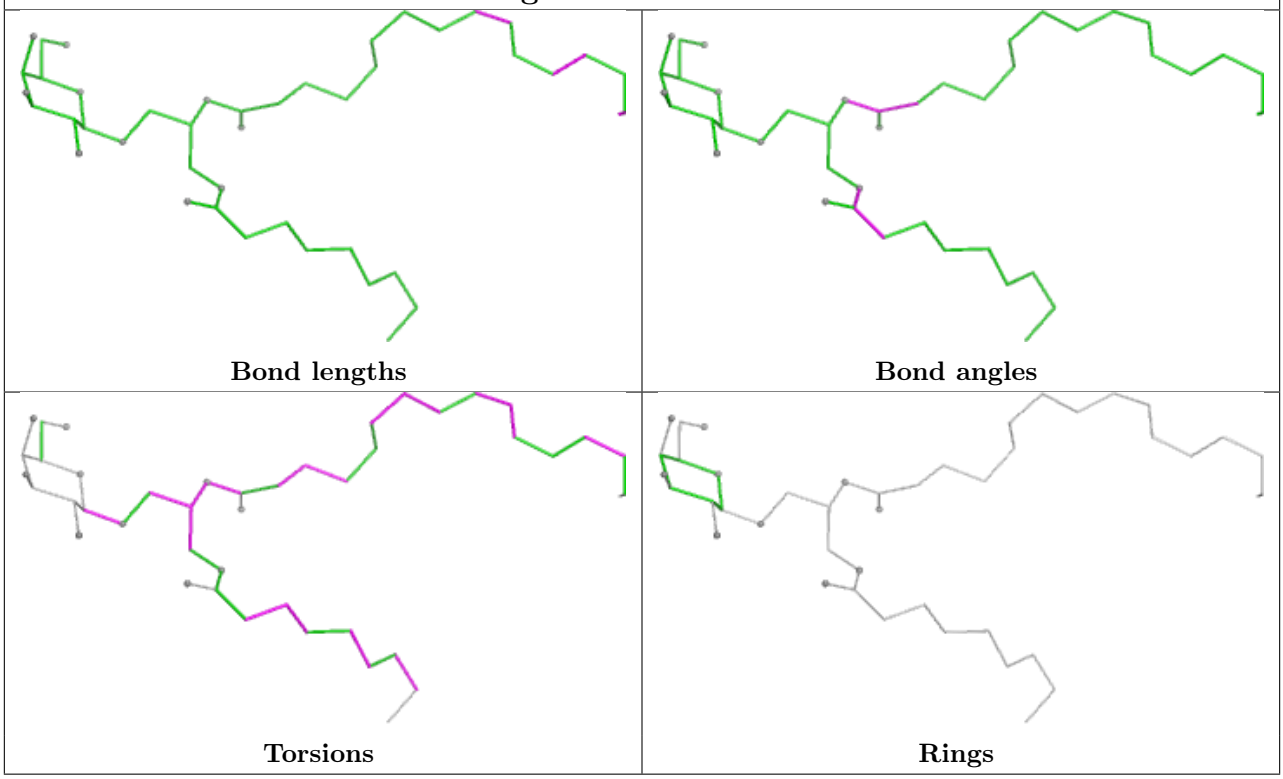
Bond angles



Torsions

Rings

Ligand LMG B 622



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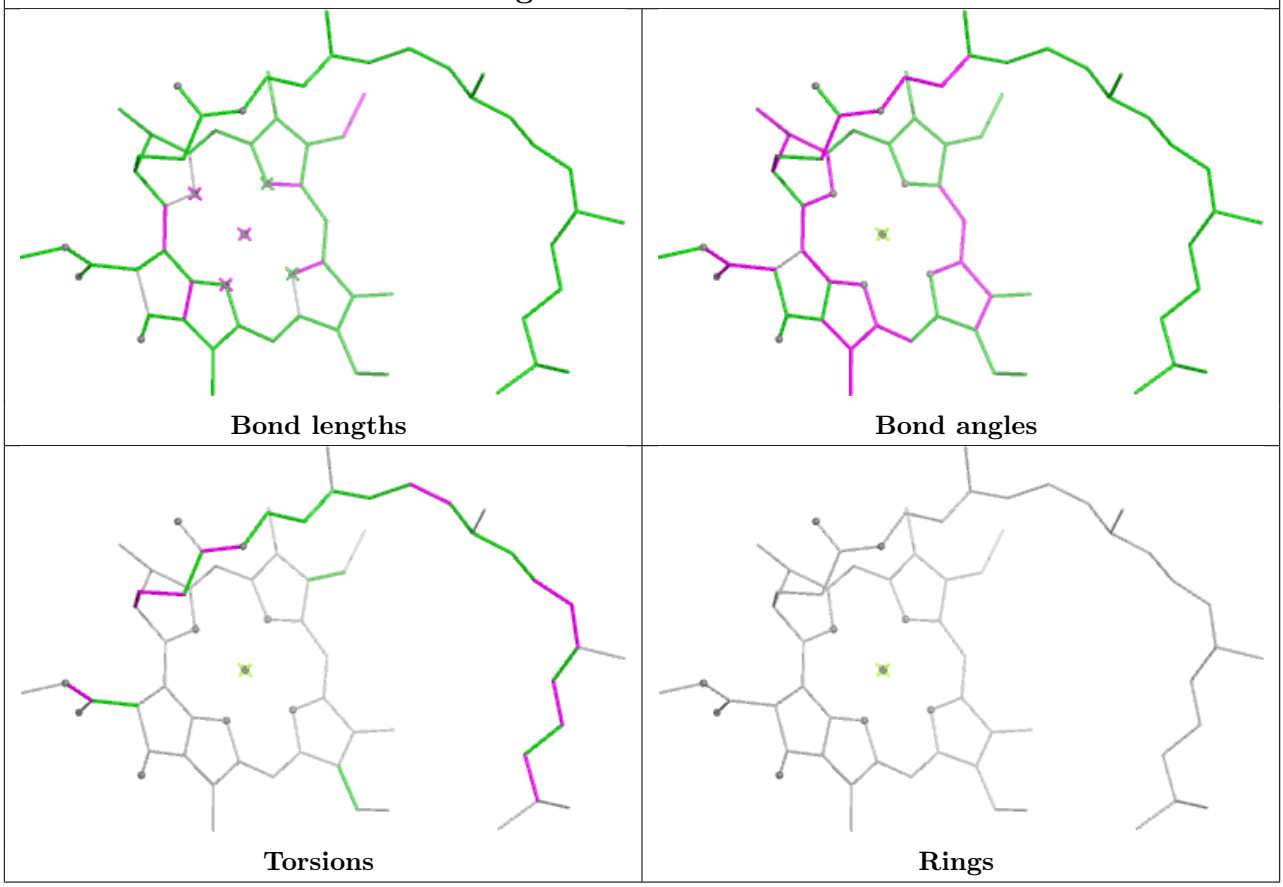
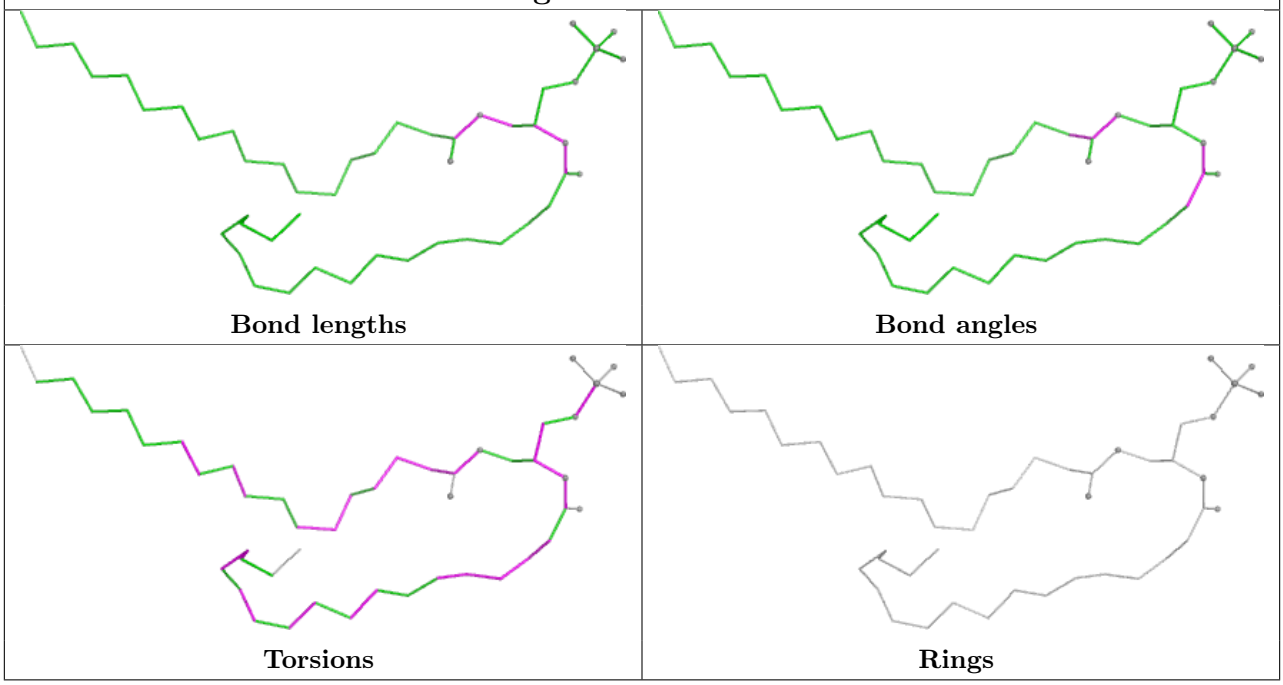


Ligand 3PH t 101



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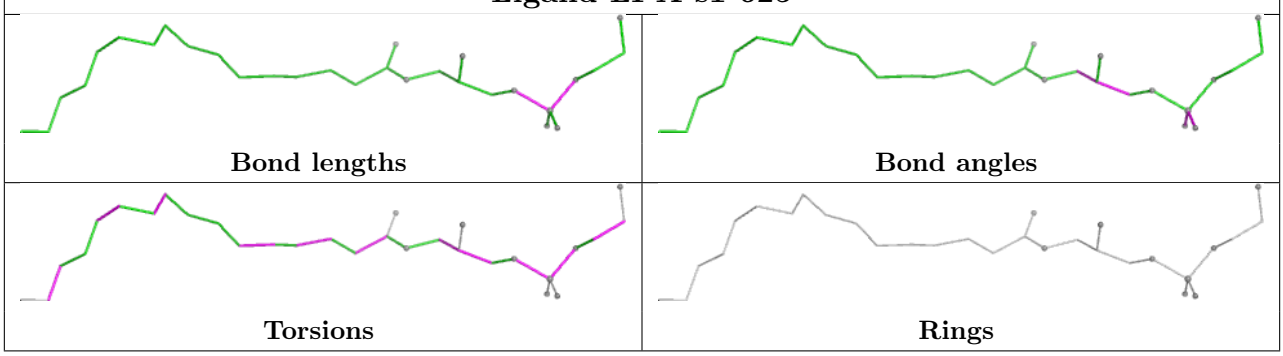
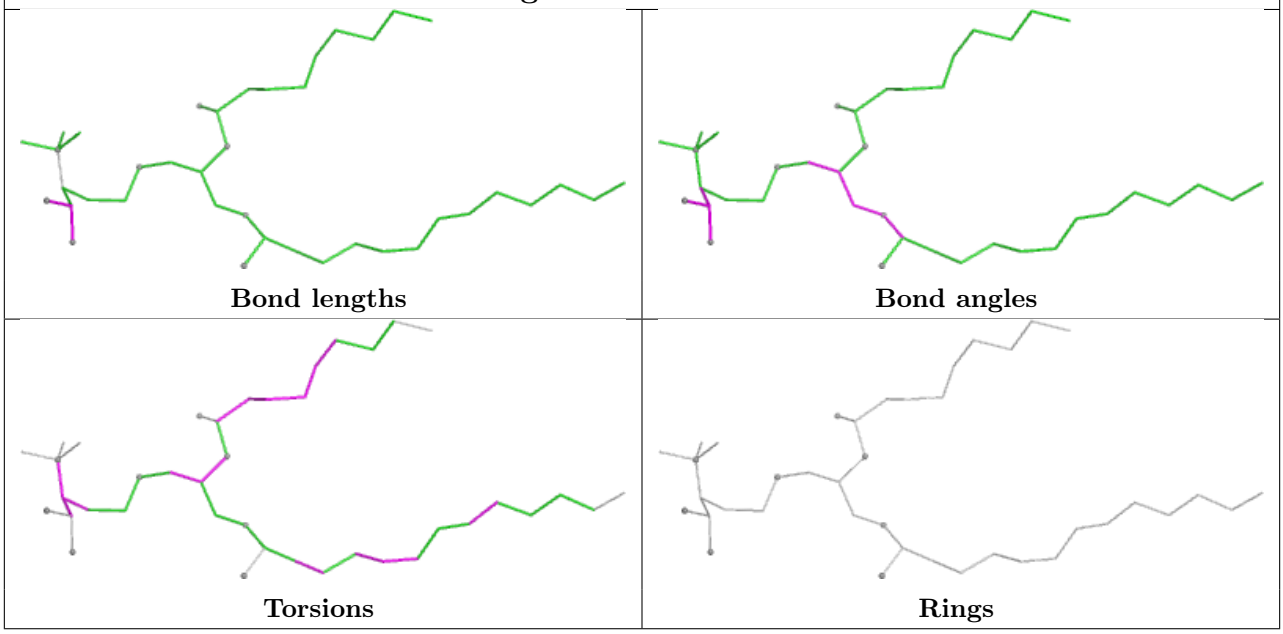
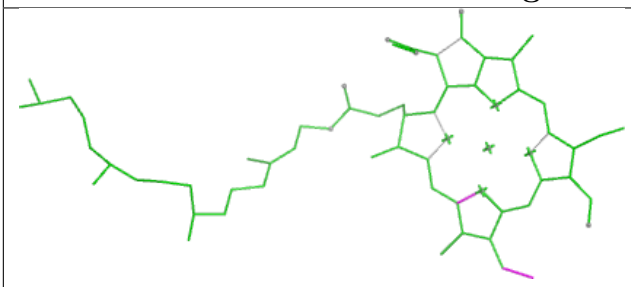


Ligand LMK C 527



Ligand CHL N 601



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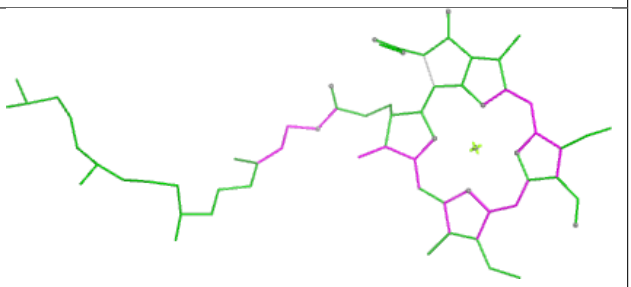
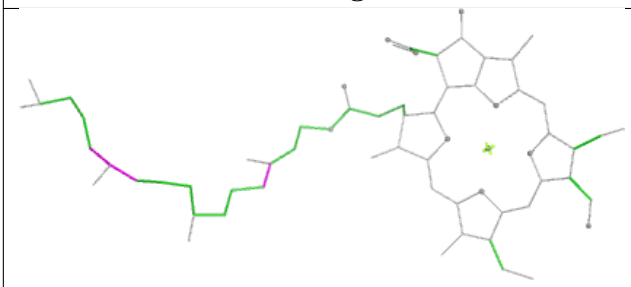


Bond angles



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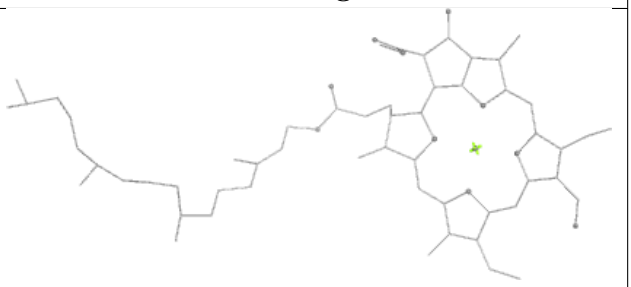

Rings

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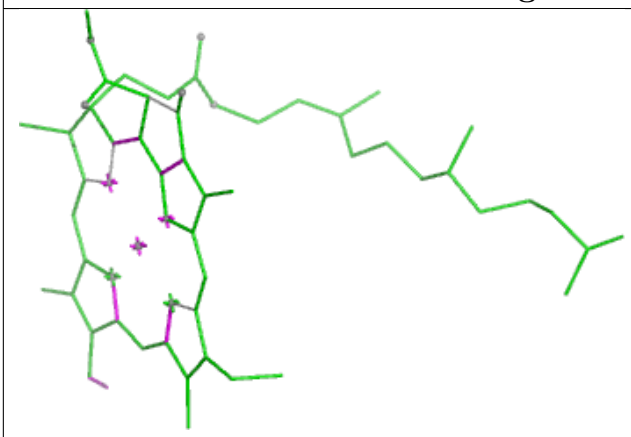

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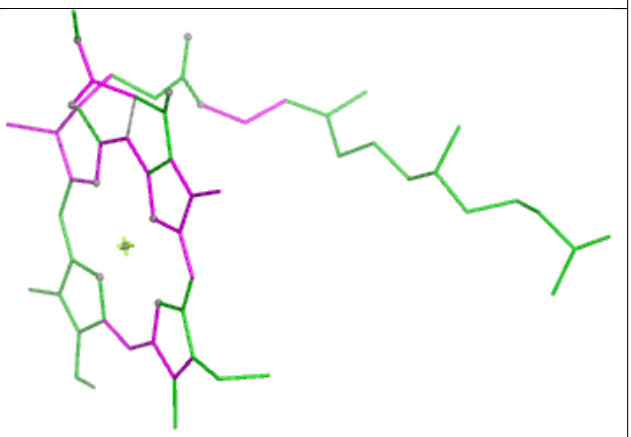

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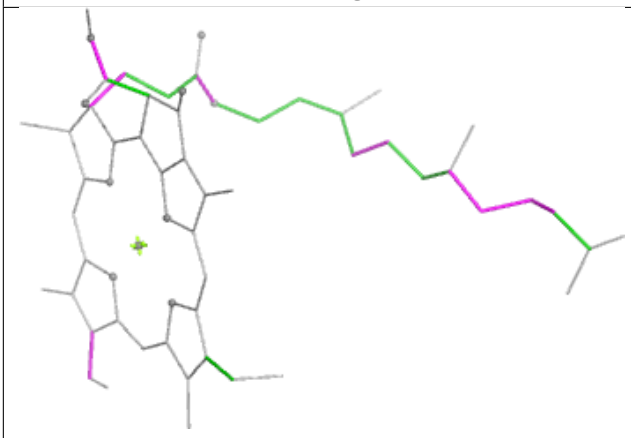

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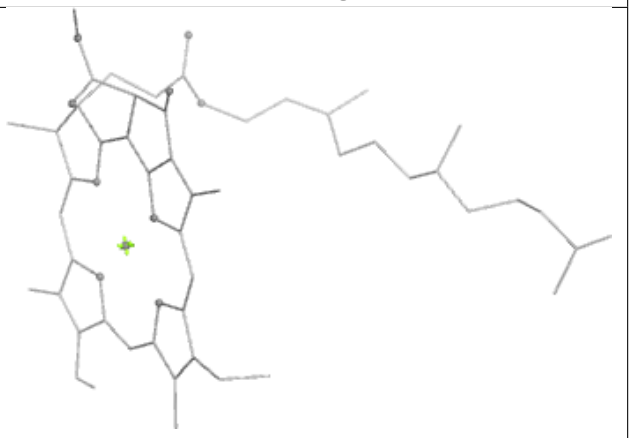
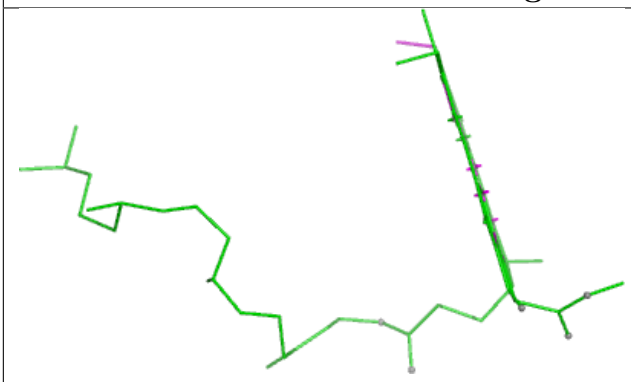
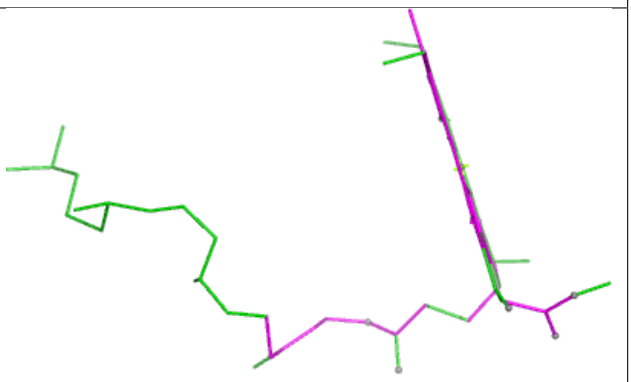
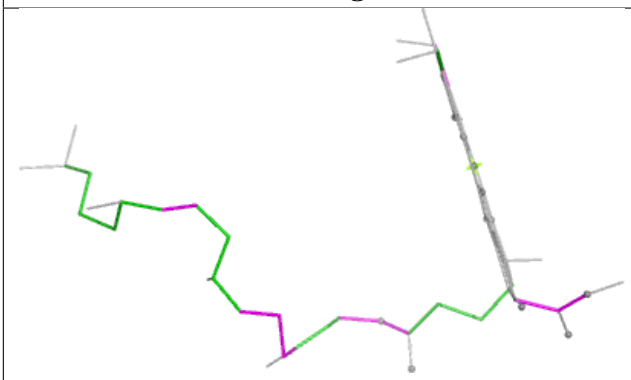
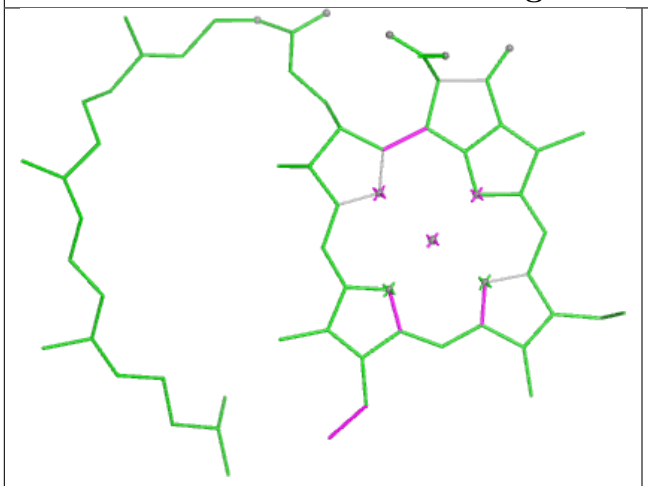


Rings

Ligand CLA C 506	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA C 512



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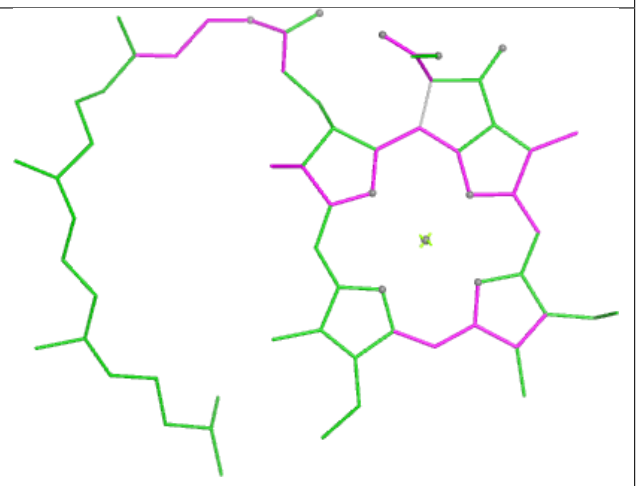
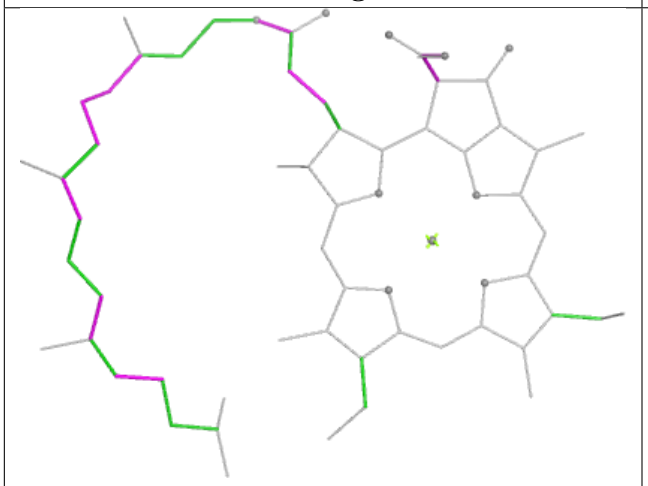
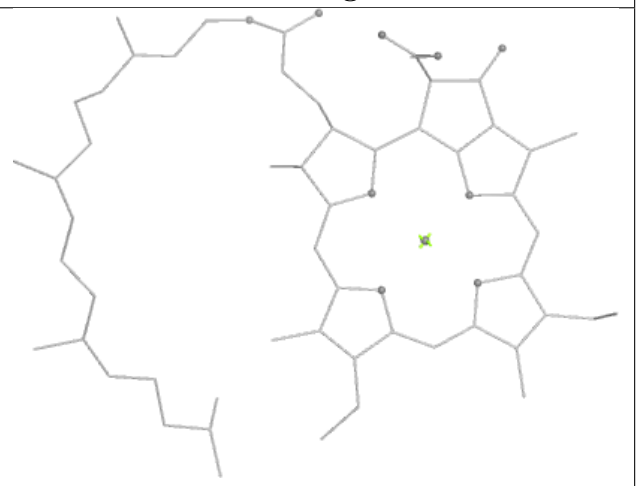


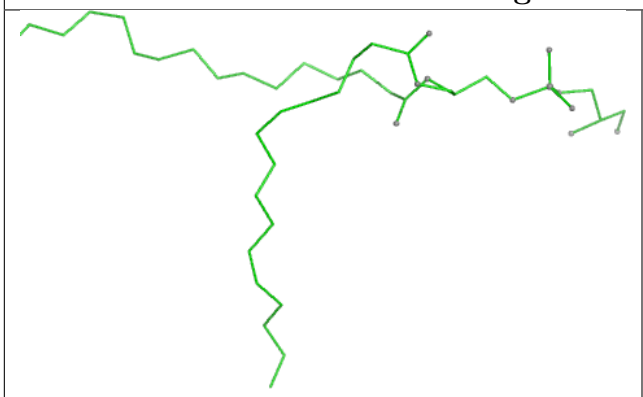
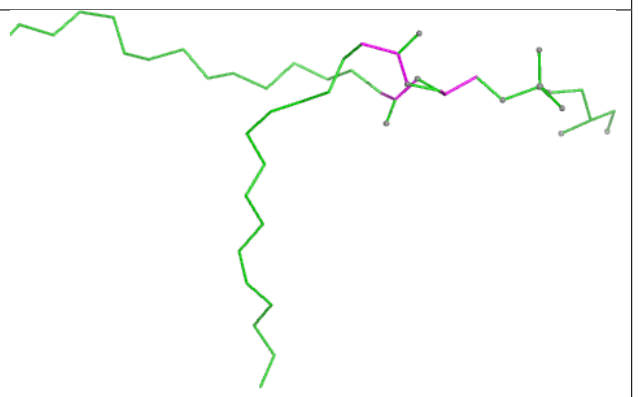
Bond angles



Torsions



Rings

Ligand LHG N1 624	
	
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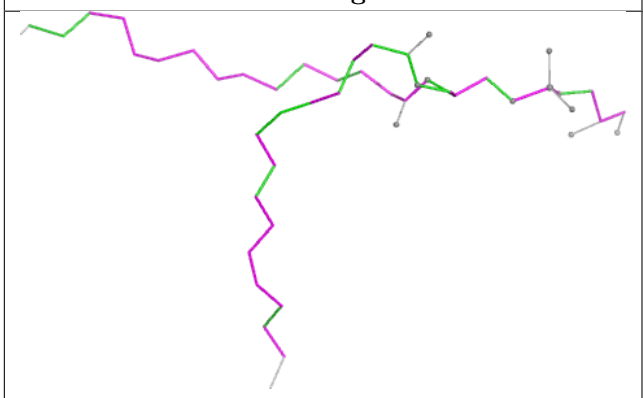
	
Torsions	**Rings**

Ligand CLA y1 603

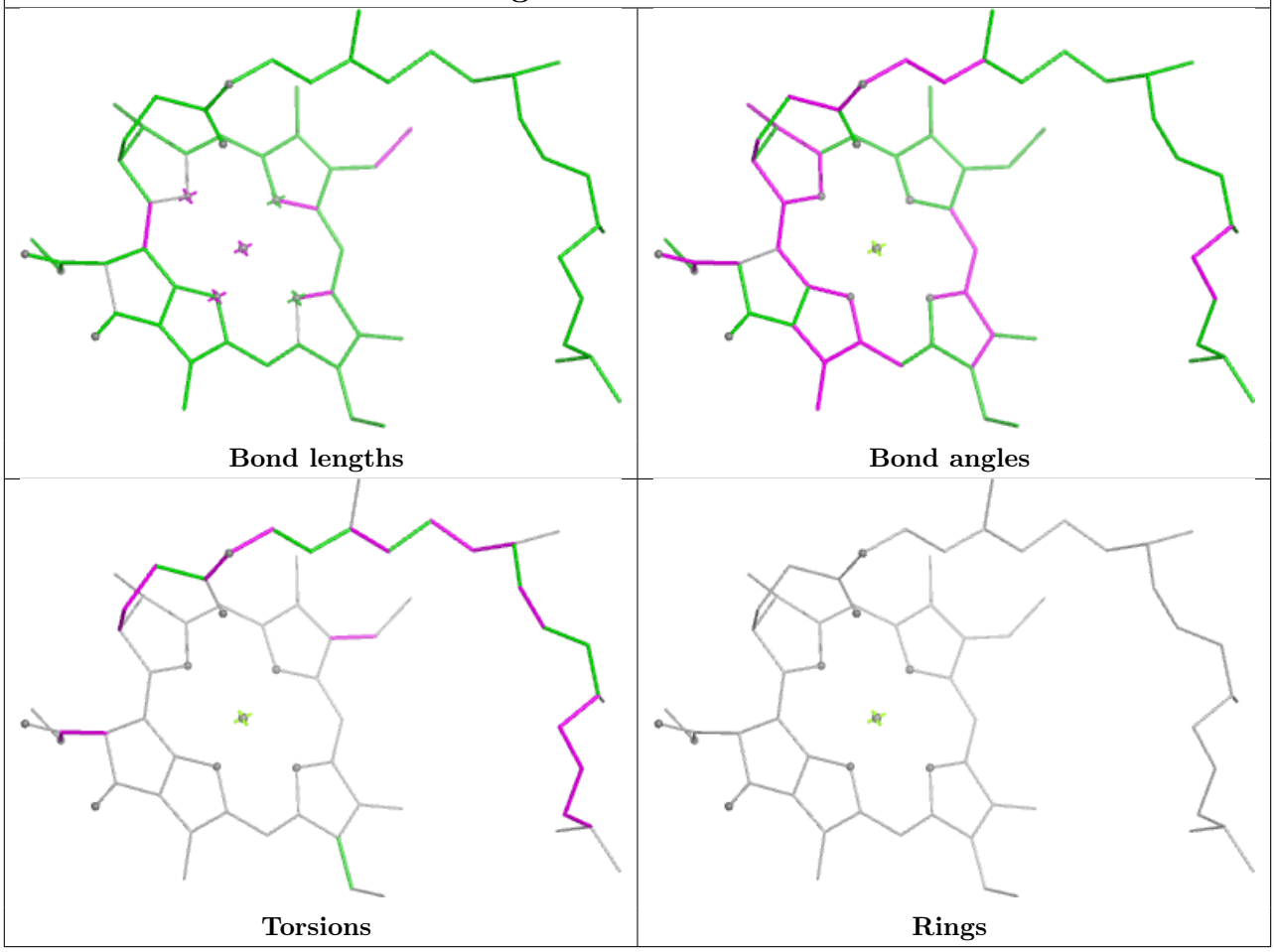
Bond lengths

Bond angles

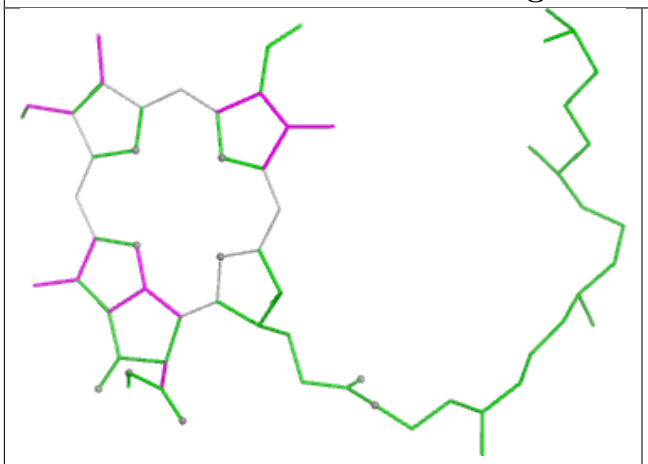
Torsions

Rings

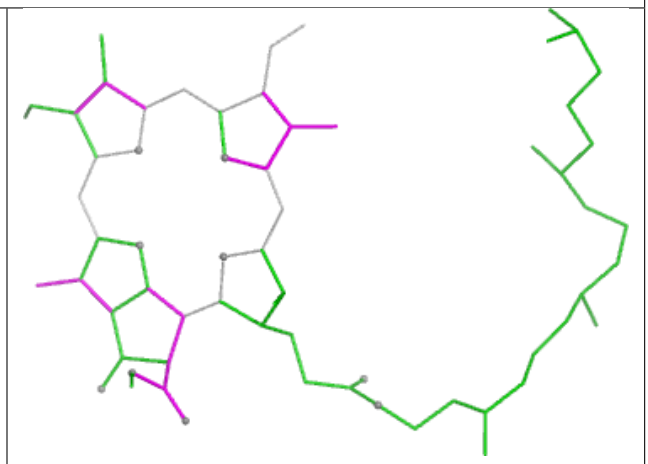
Ligand CLA G1 602



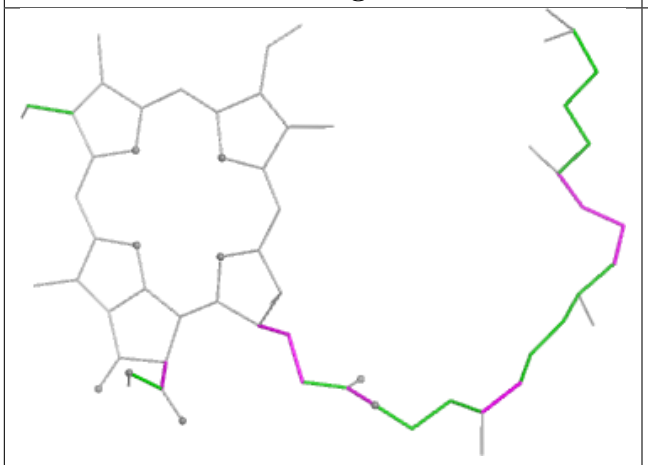
Ligand PHO a 408



Bond lengths



Bond angles



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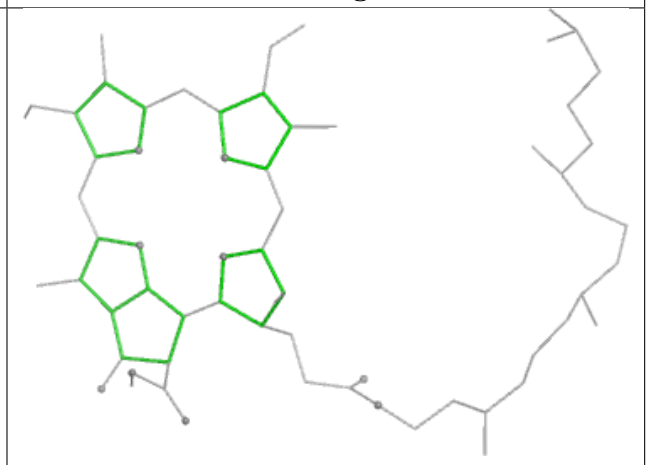
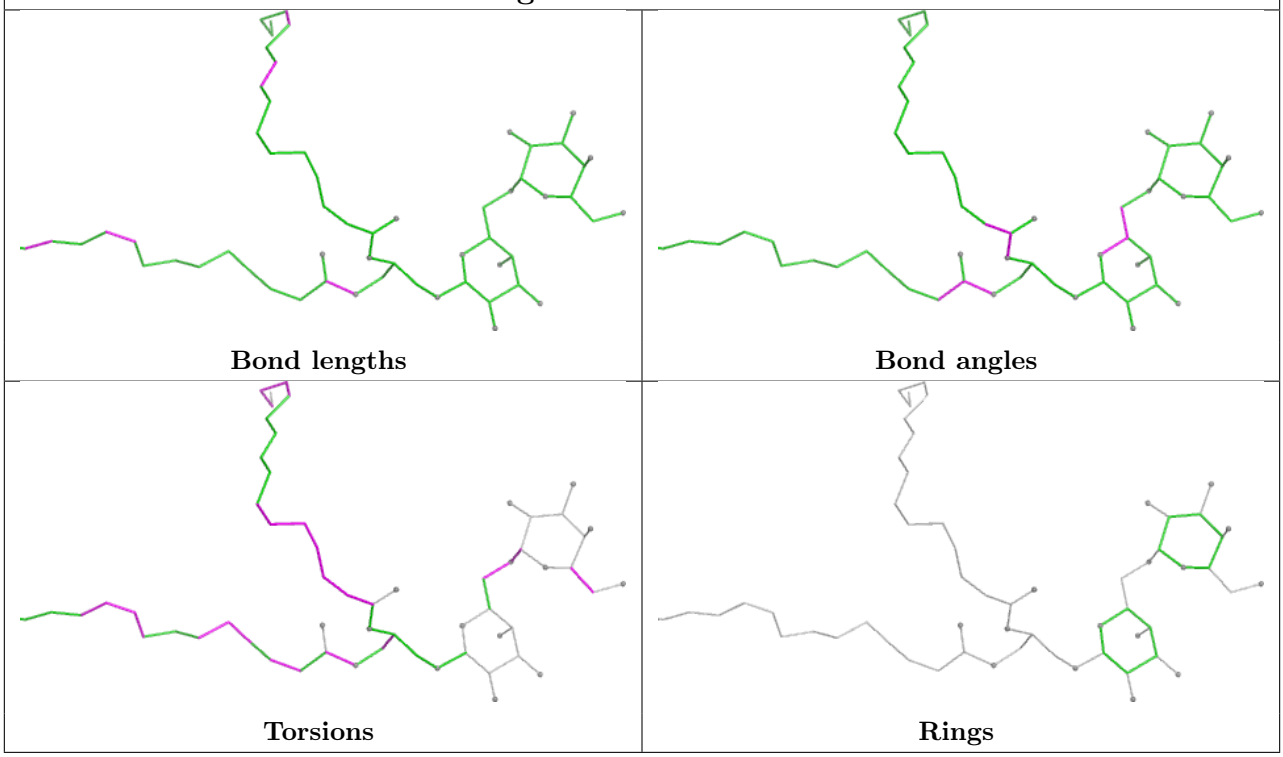


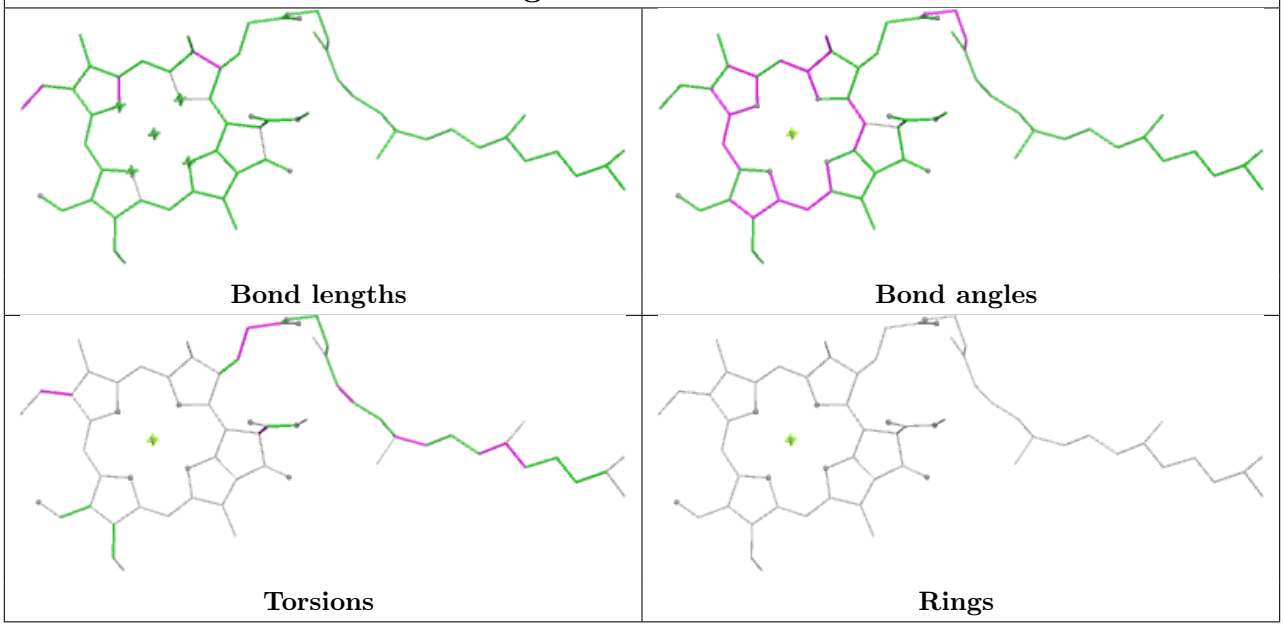
Rings

Ligand DGD c1 519



Ligand NEX G 623

Ligand CHL N 605



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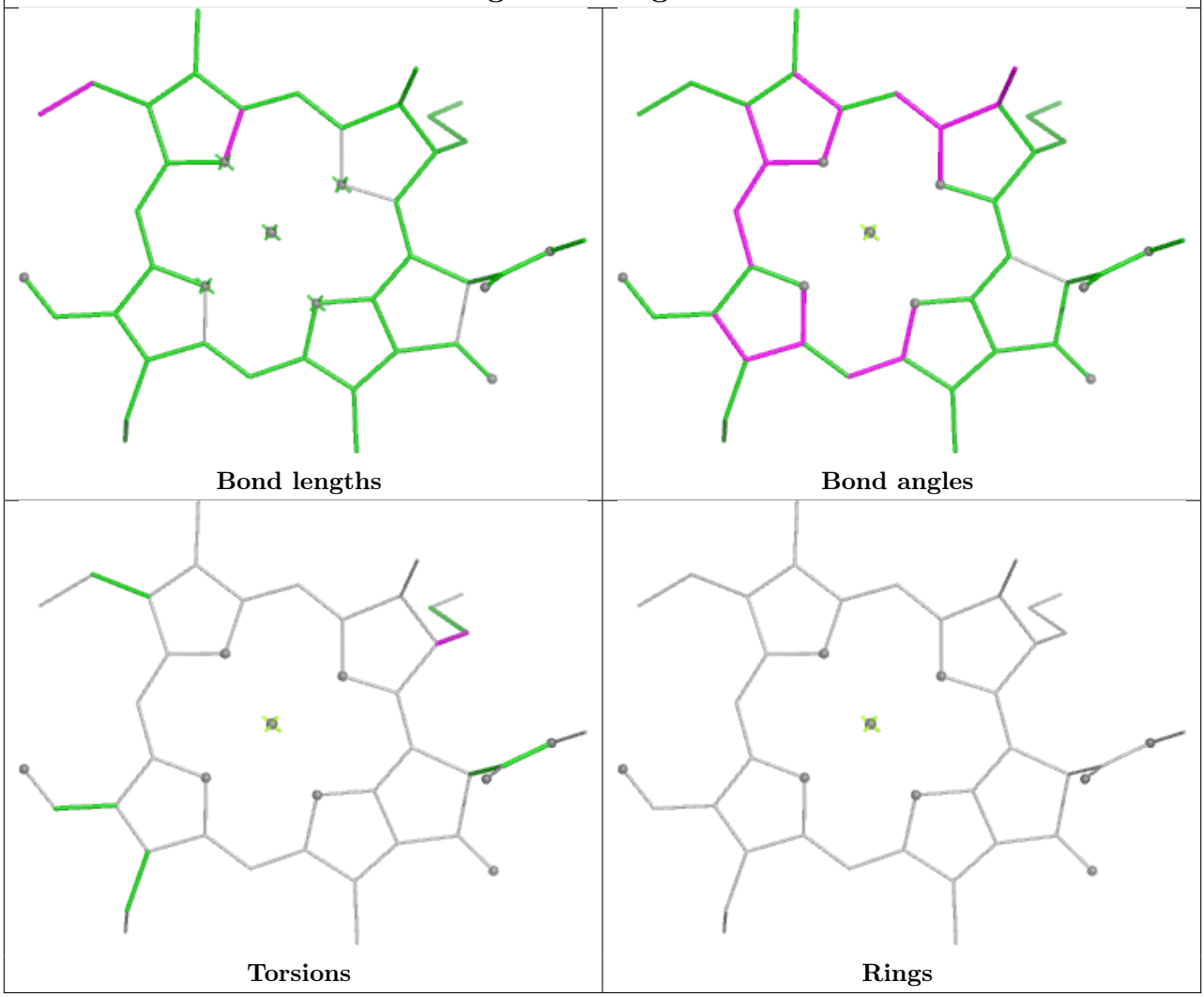
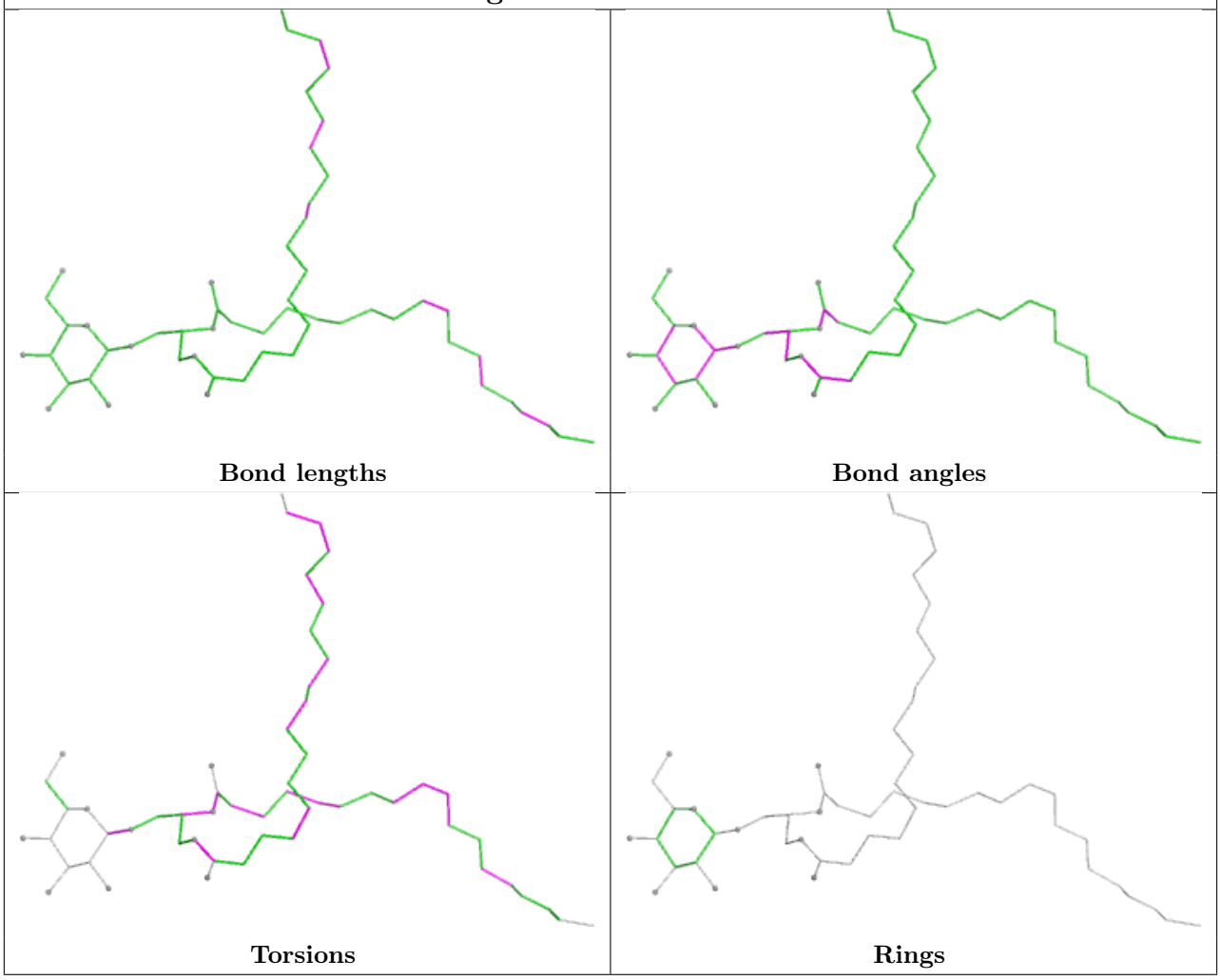


Ligand LMG C1 523



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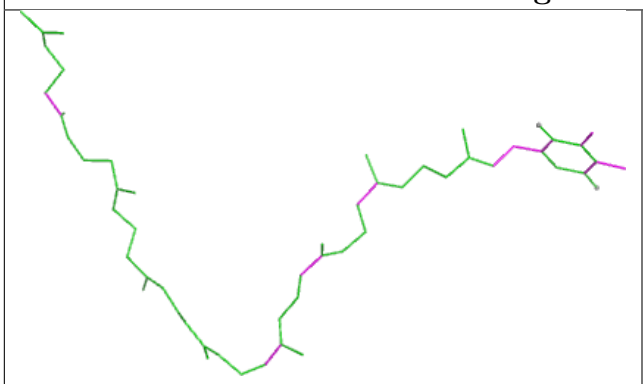
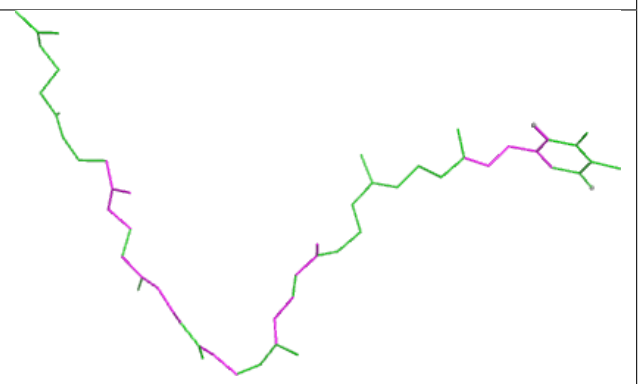
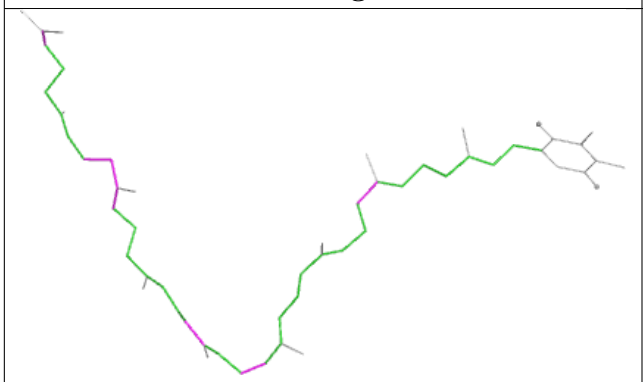
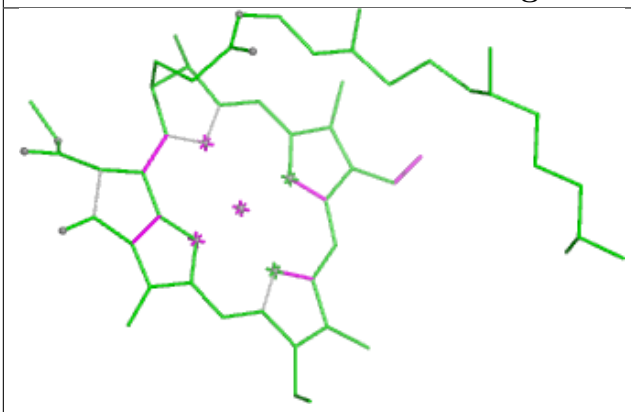
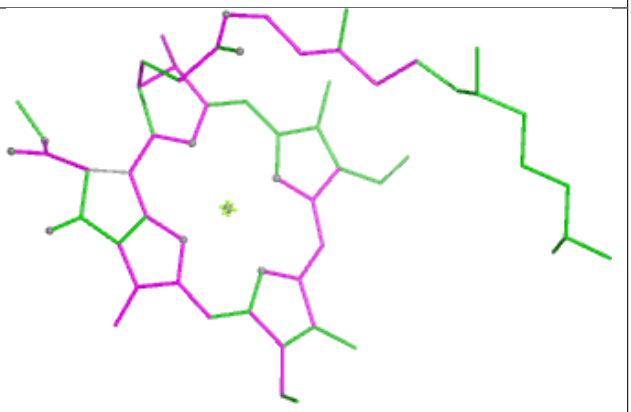
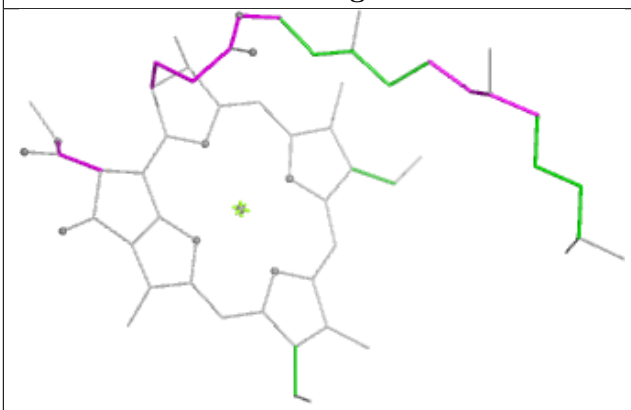
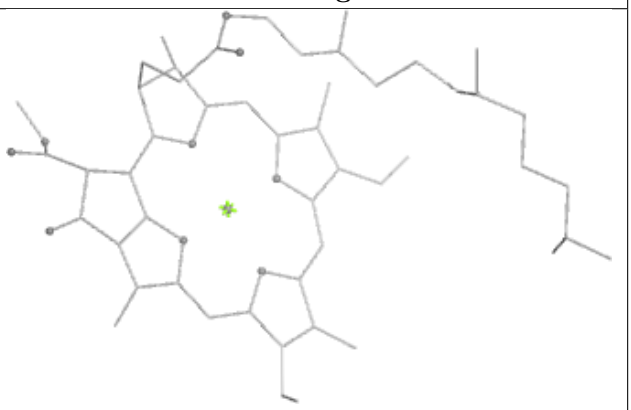
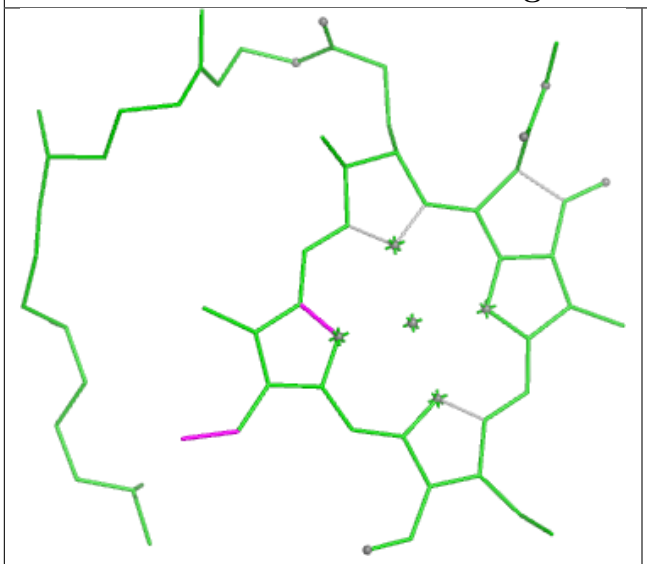
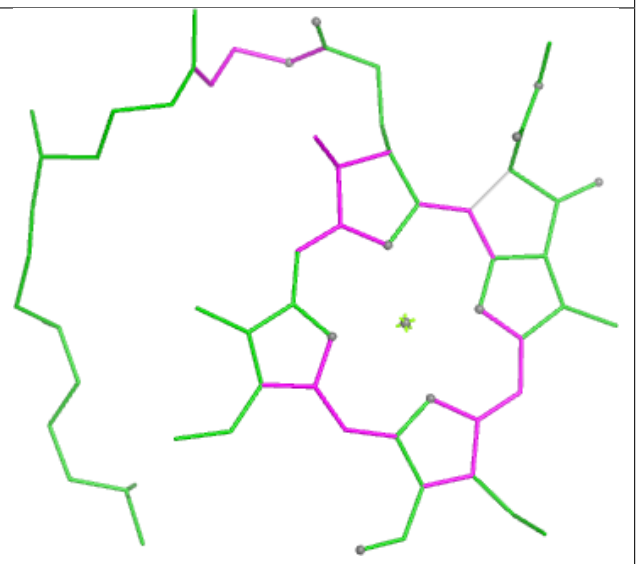
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA s1 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL N 607



Bond lengths



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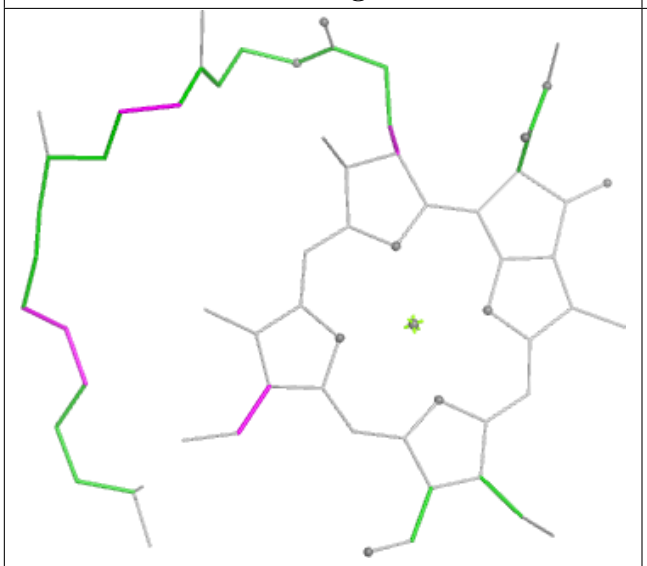
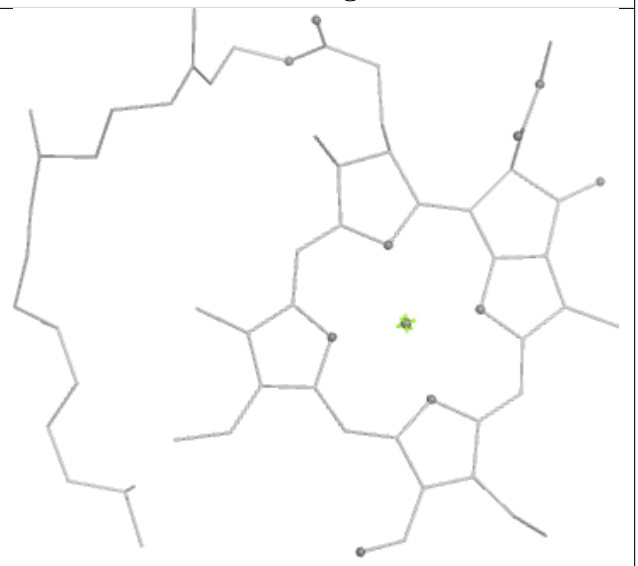
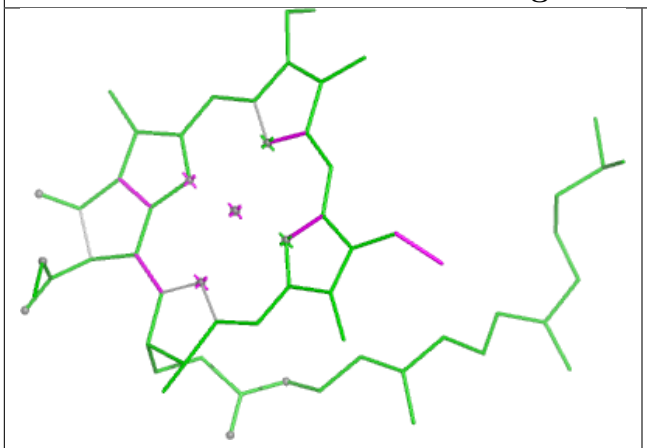


Torsions

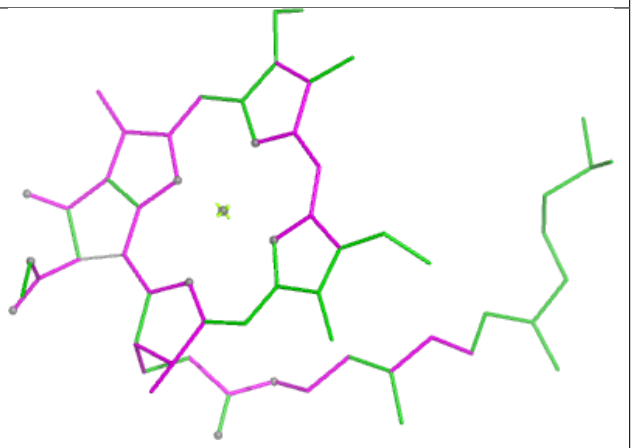


Rings

Ligand CLA r 602



Bond lengths



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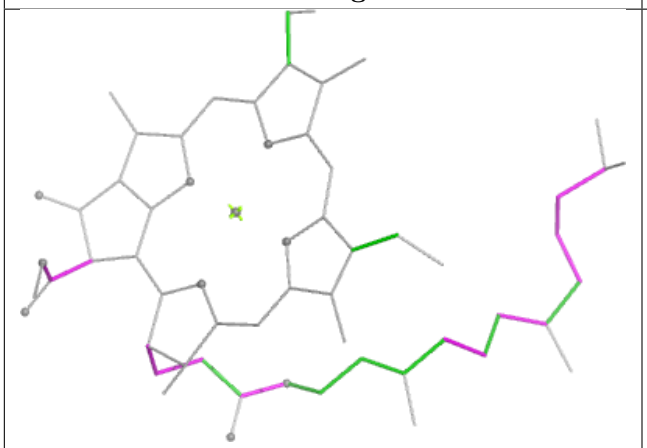
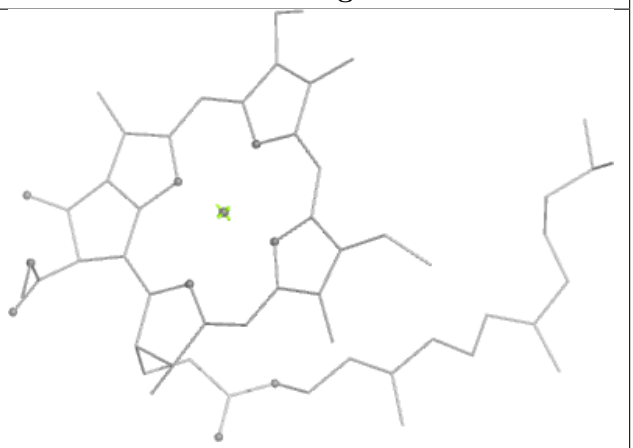
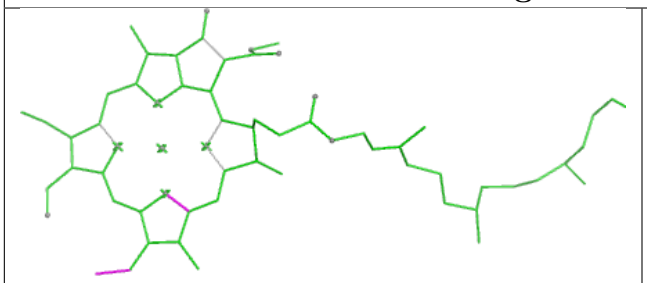


Torsions



Rings

Ligand CHL N1 601



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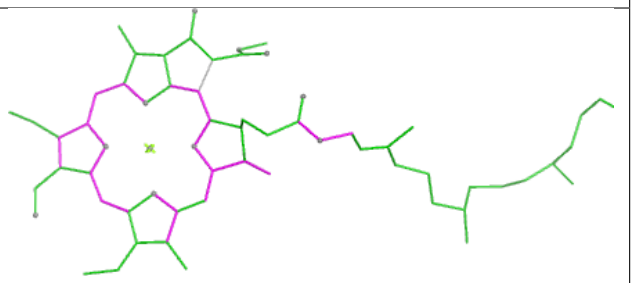

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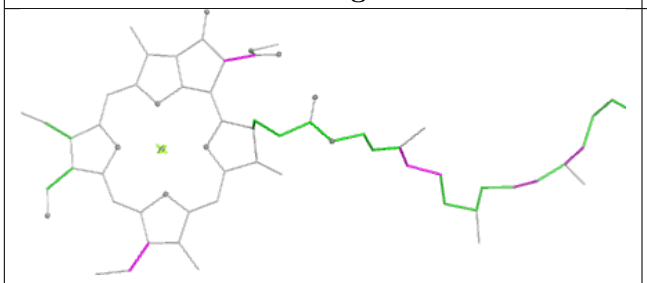

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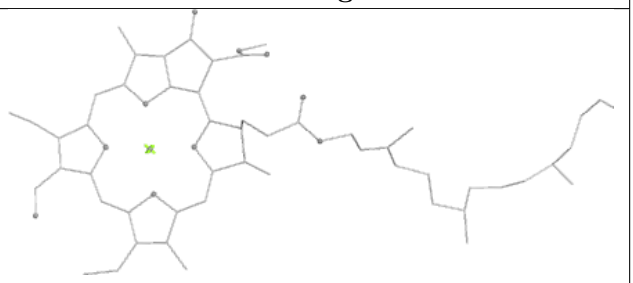
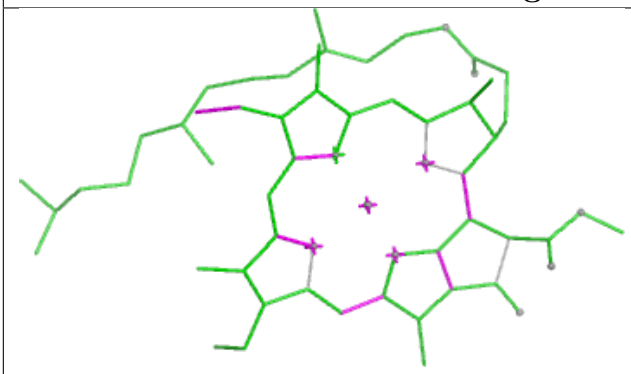
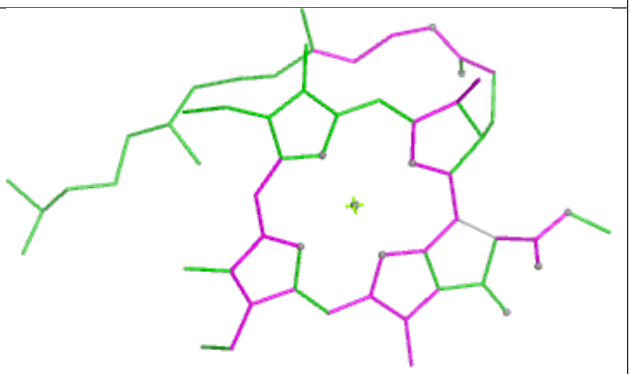
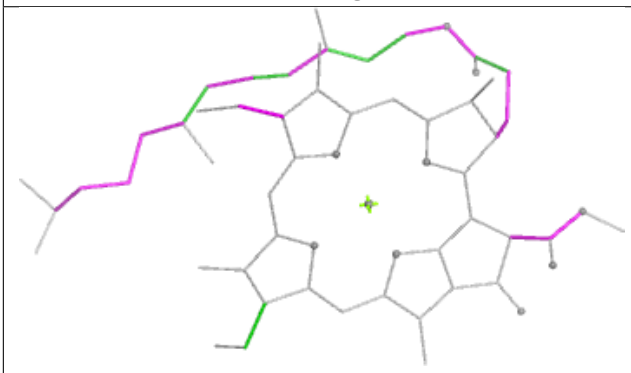
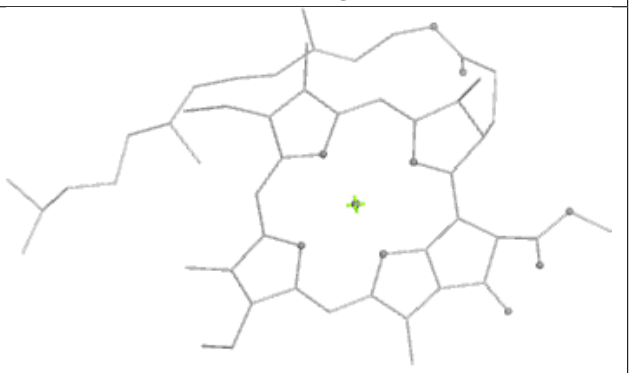
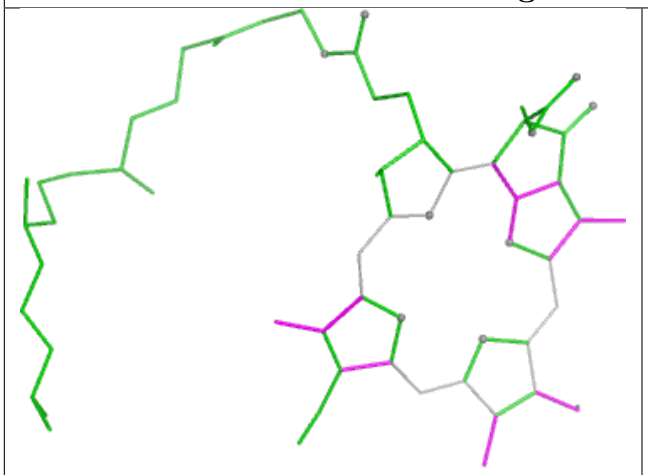


Rings

Ligand CLA R 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO a1 409



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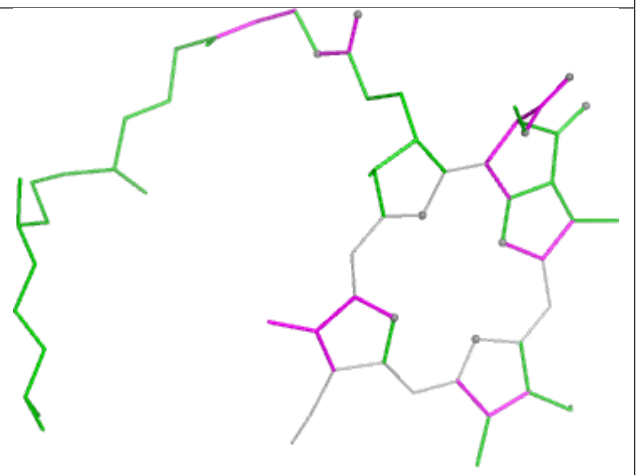

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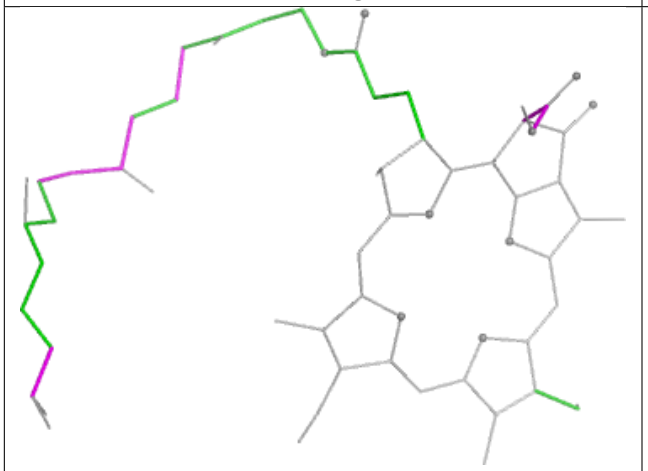

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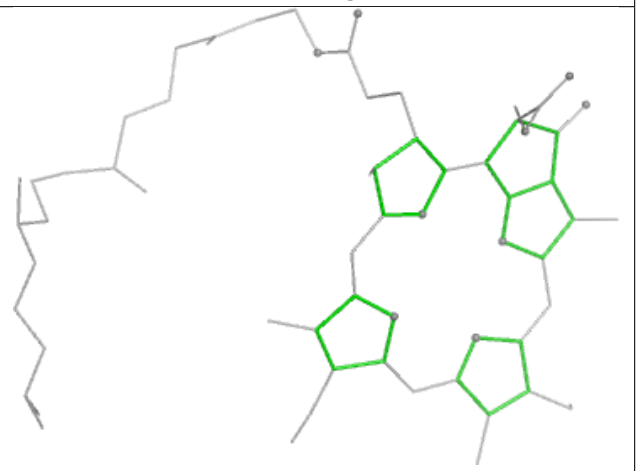
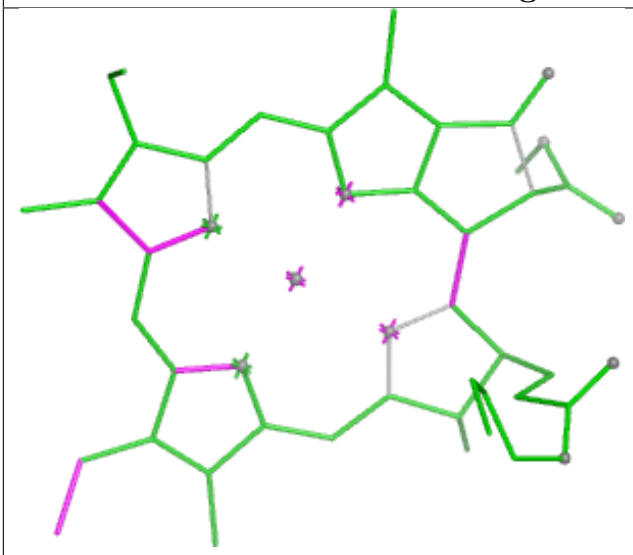


Rings

Ligand CLA g1 604



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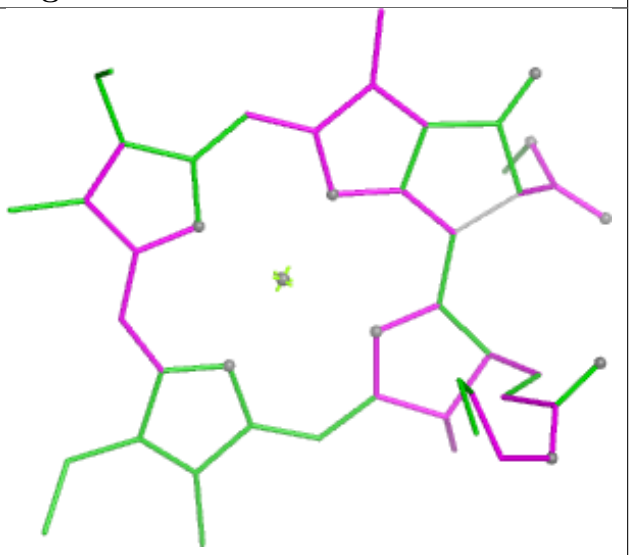

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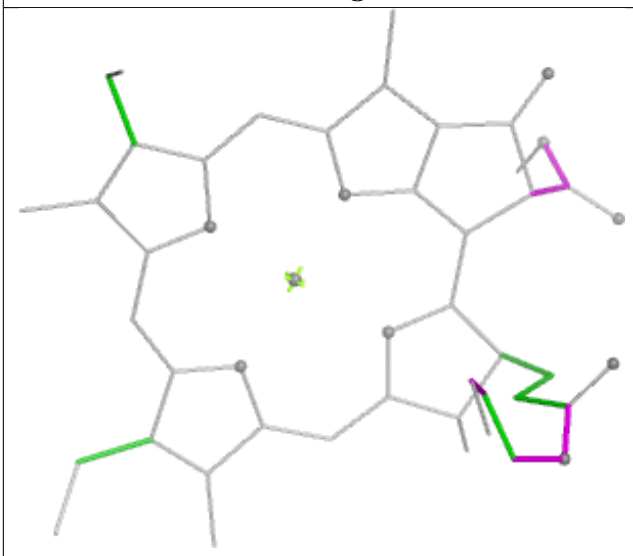

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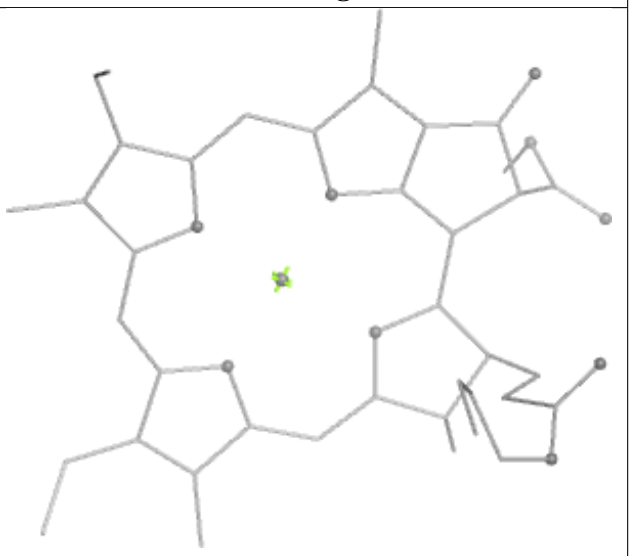
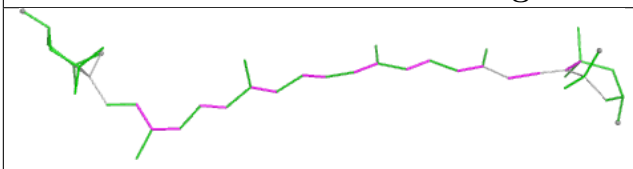


Rings

Ligand NEX N1 623



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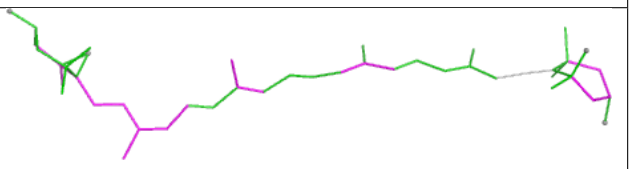

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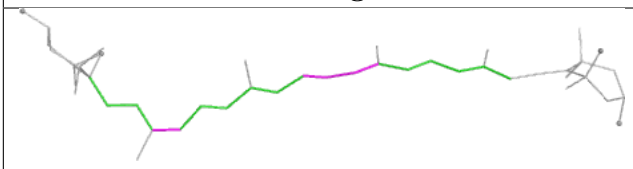

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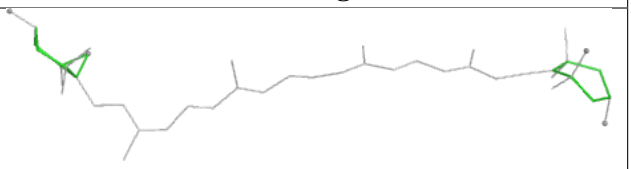
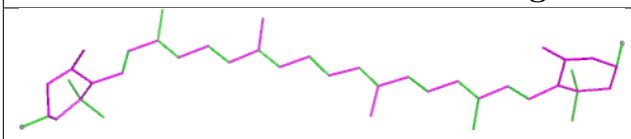


Rings

Ligand C7Z B 620



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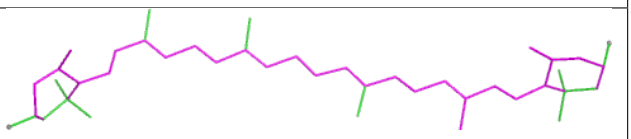

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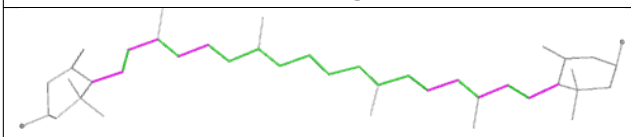

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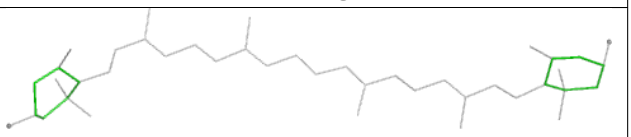
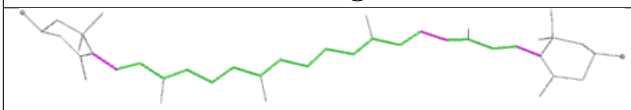


Rings

Ligand LUT Y 621

Bond lengths

Bond angles



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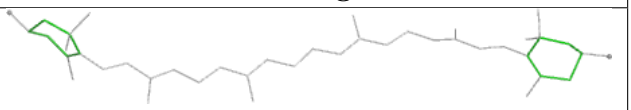
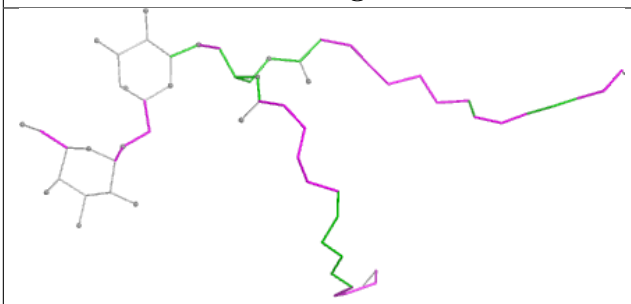


Rings

Ligand DGD C 519

Bond lengths

Bond angles



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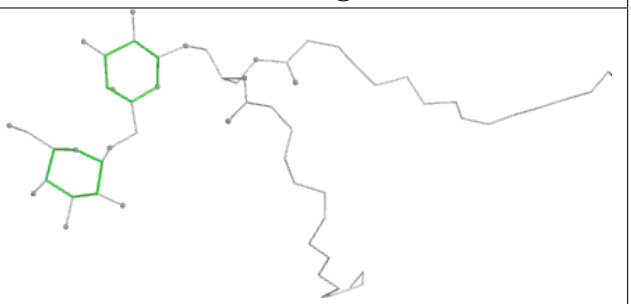
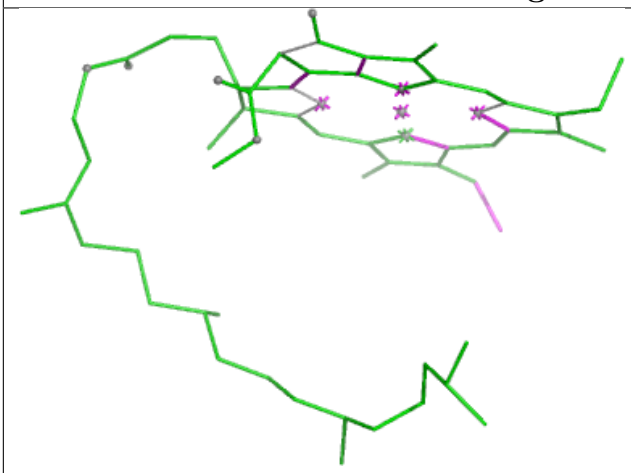
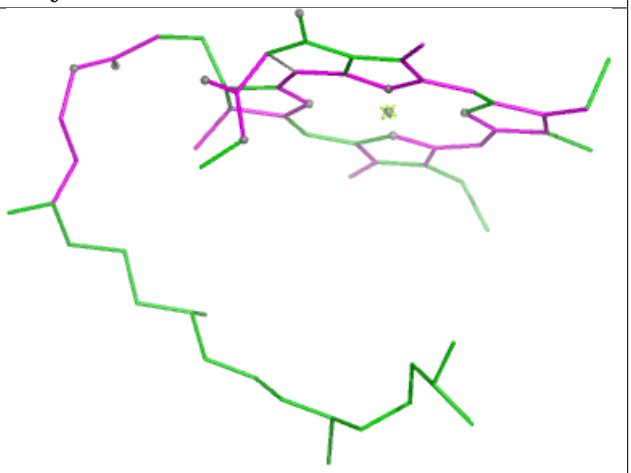


Rings

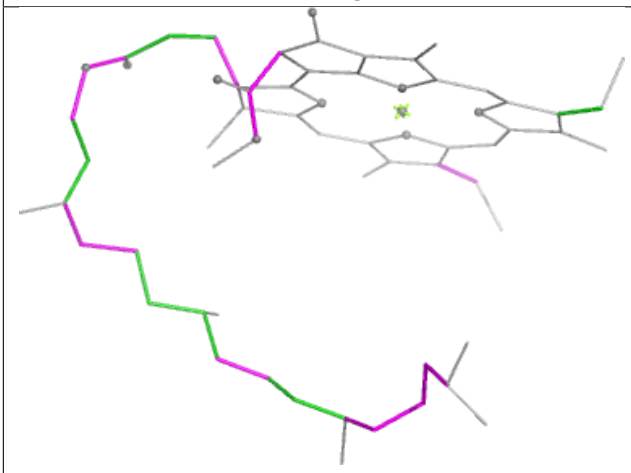
Ligand CLA y 603



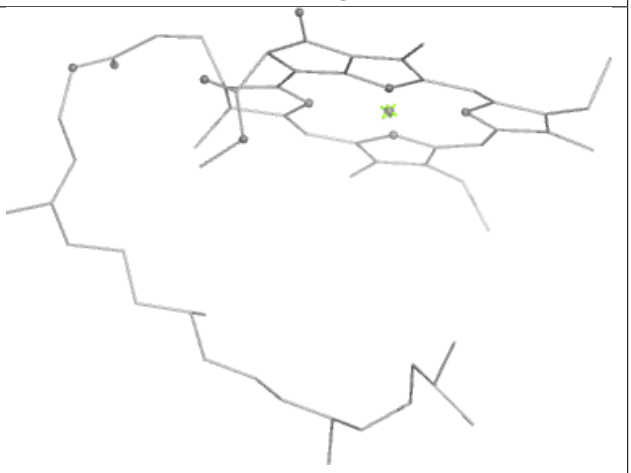
Bond lengths



Bond angles

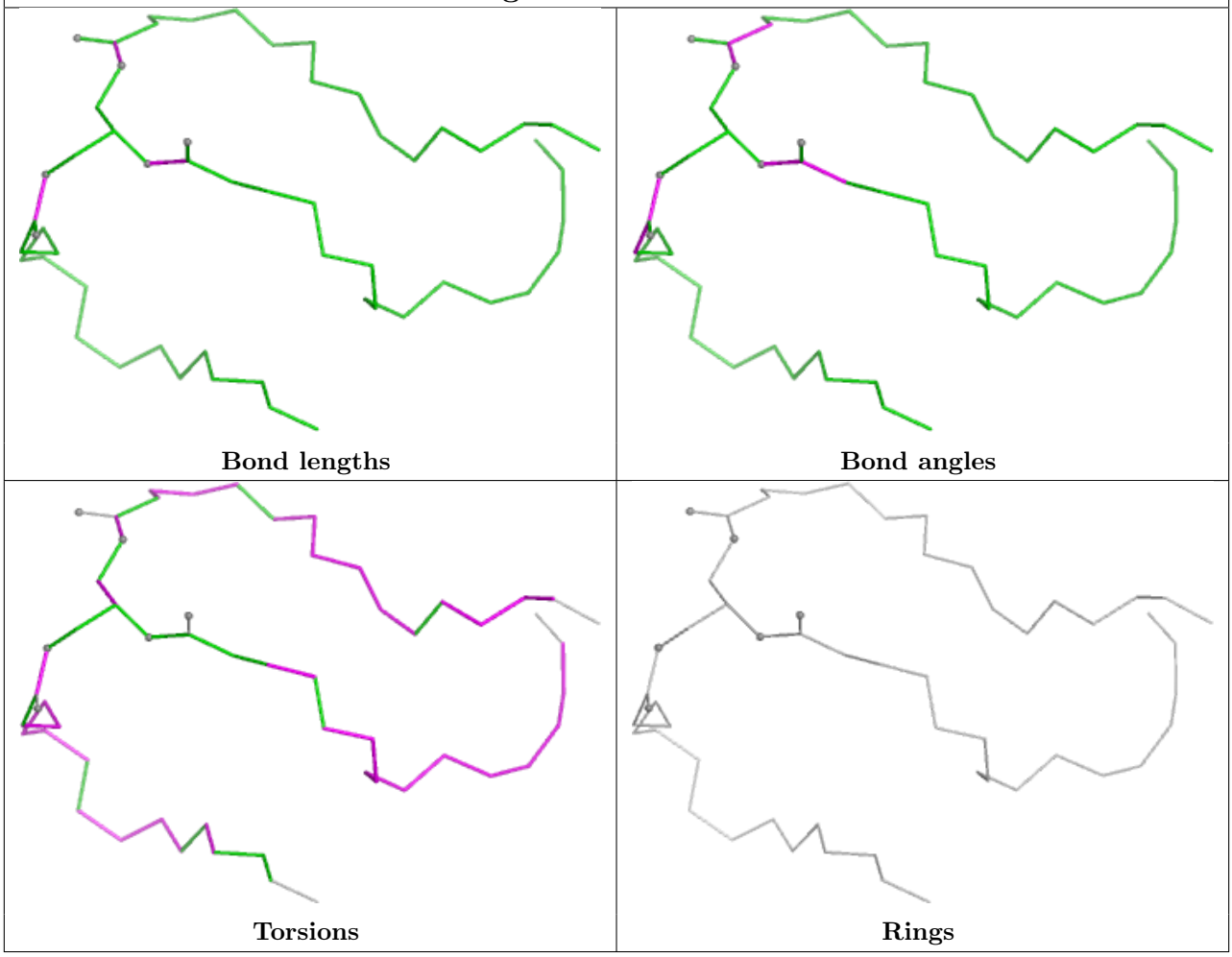


Torsions



Rings

Ligand 4RF k1 101



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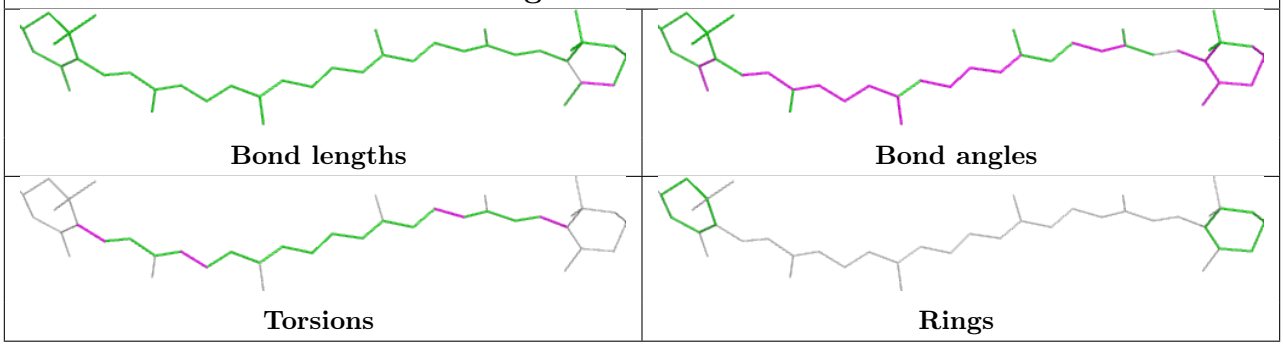

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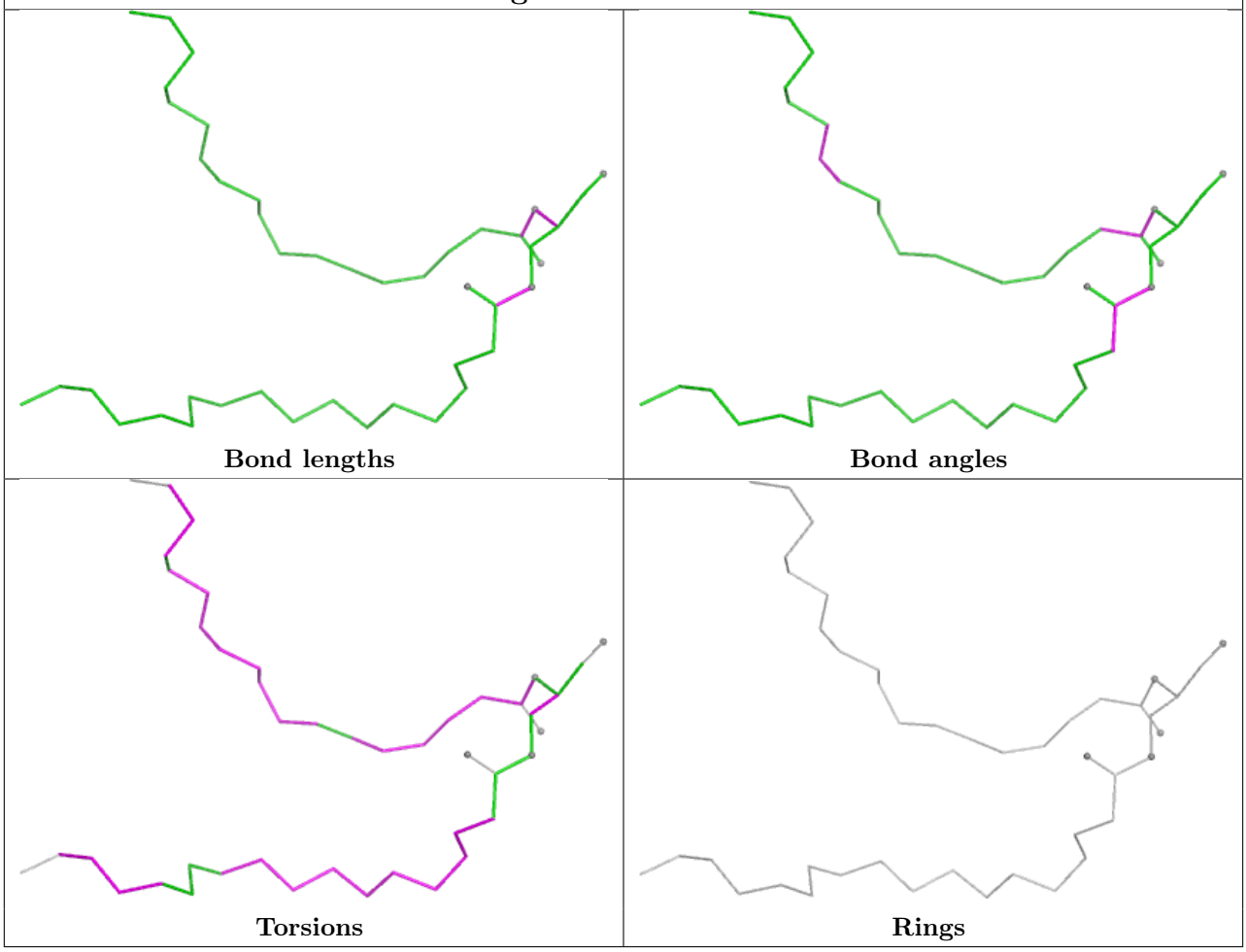

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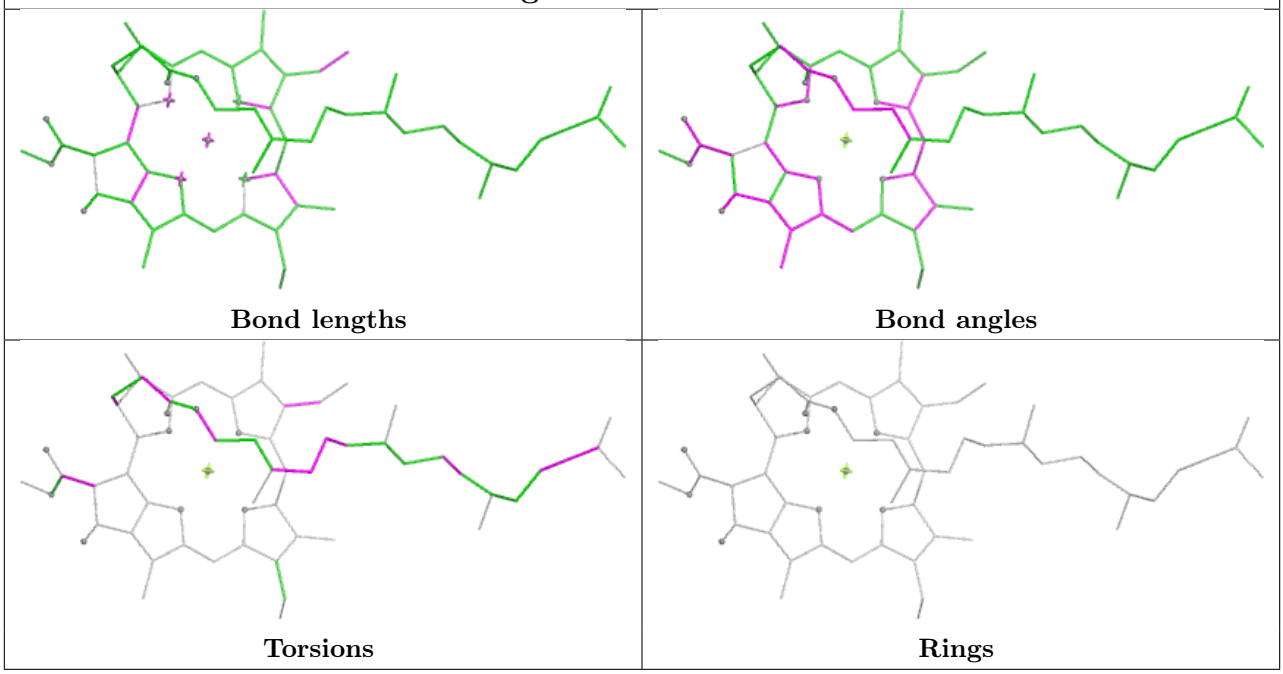
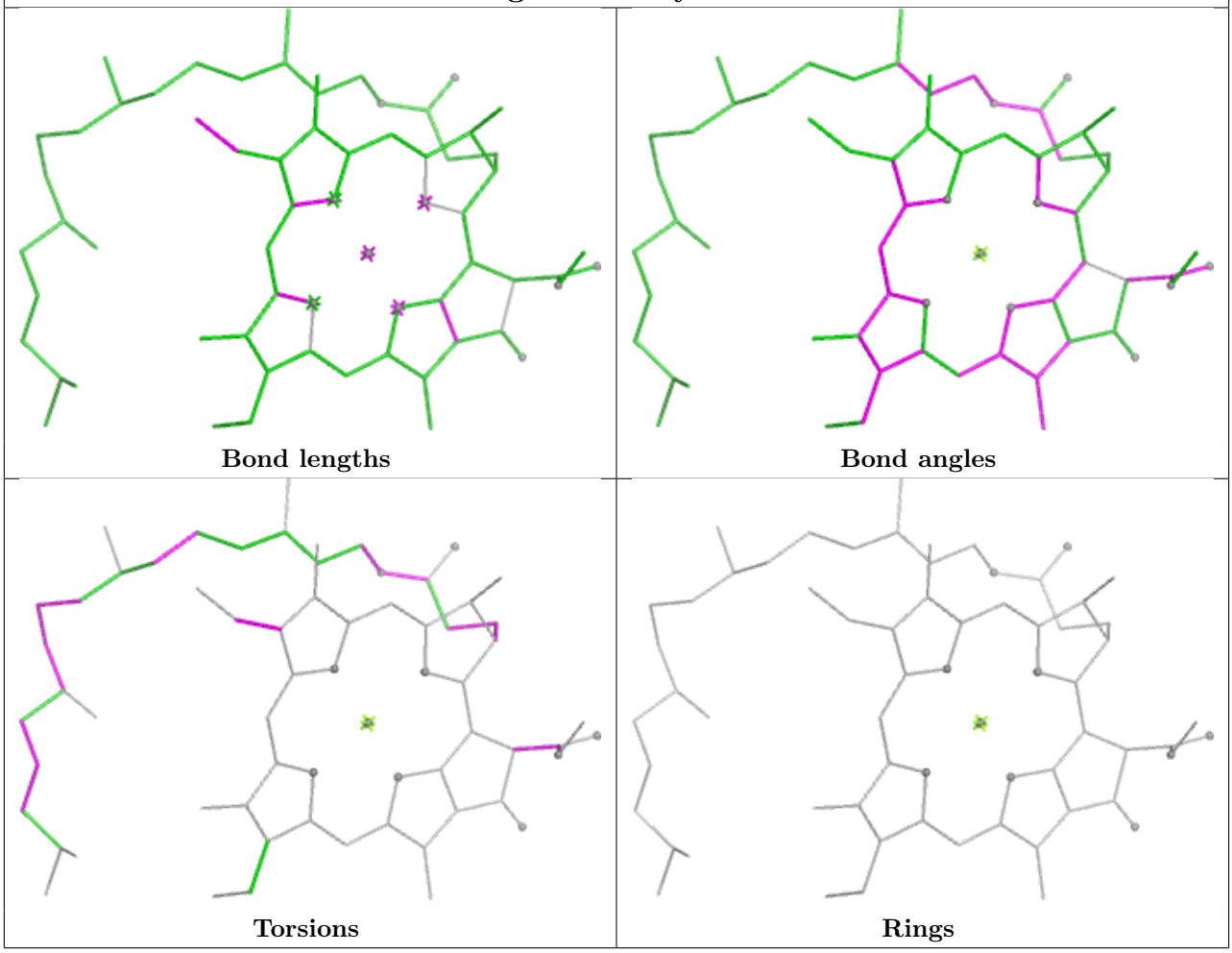


Ligand CLA y 602



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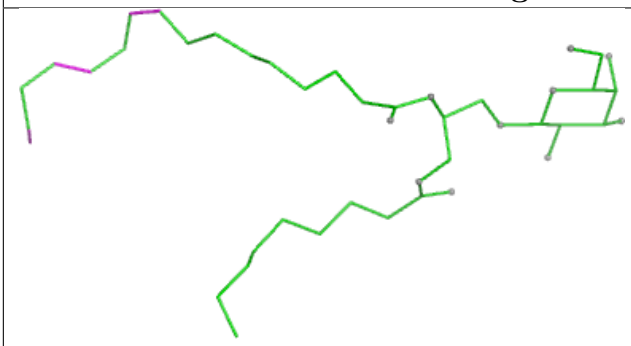
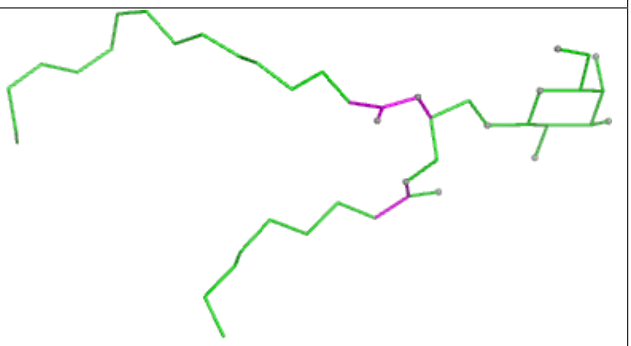
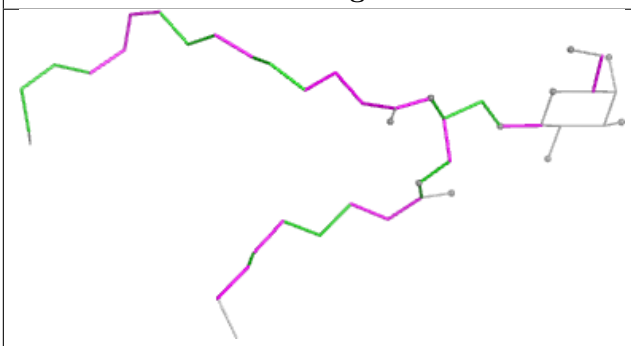
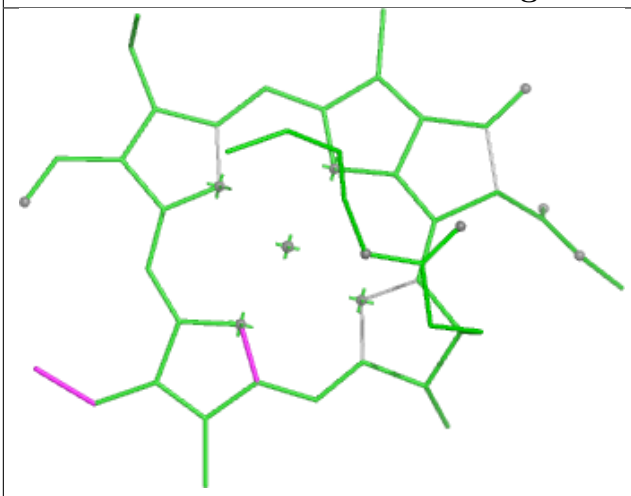
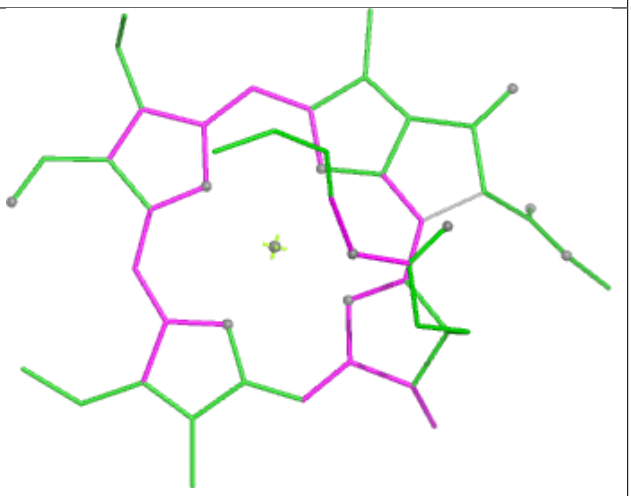
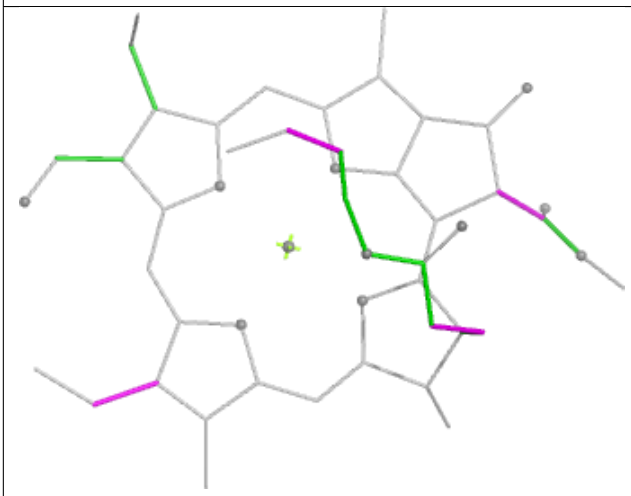
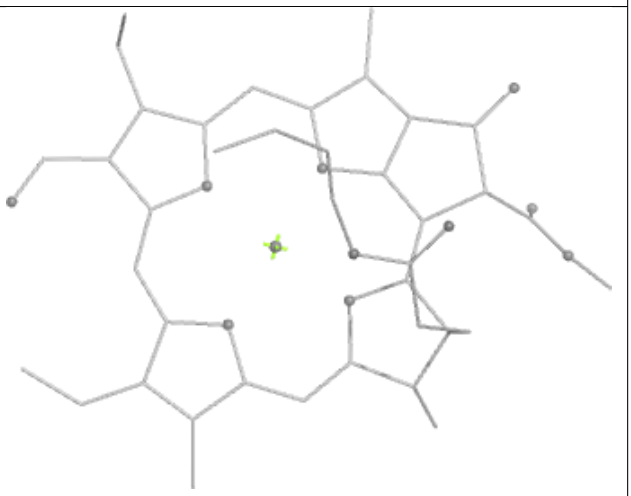
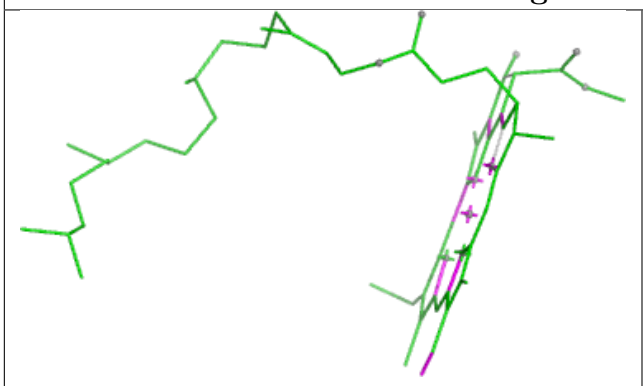
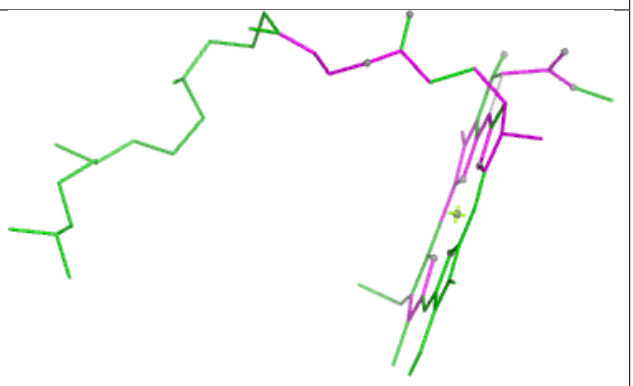
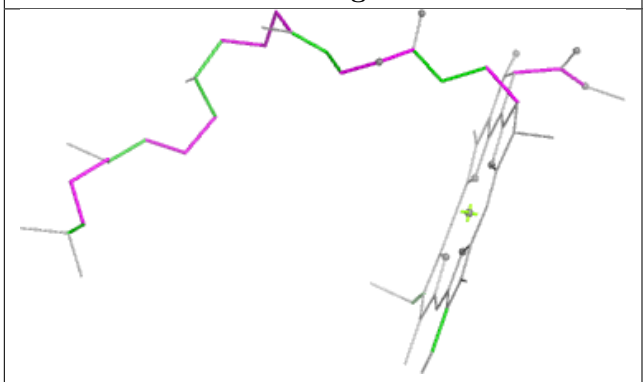
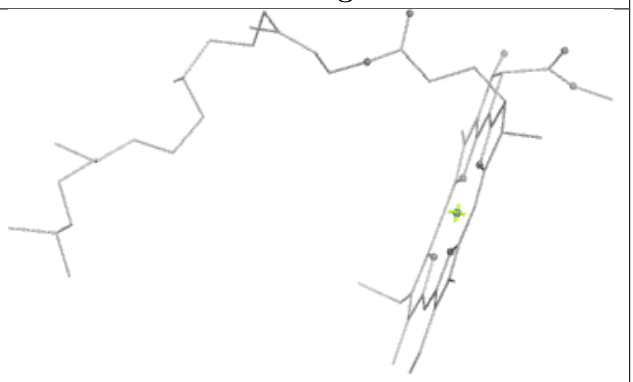
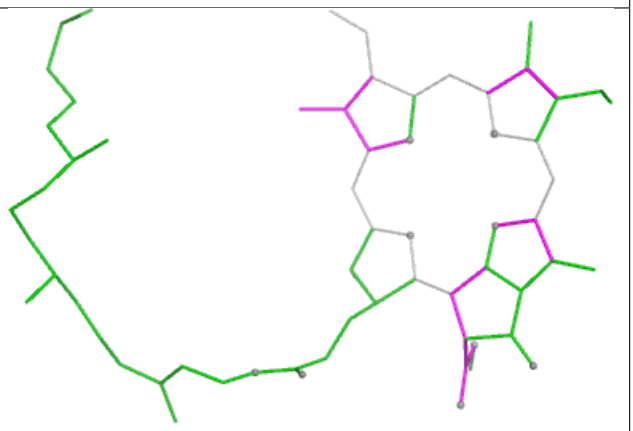
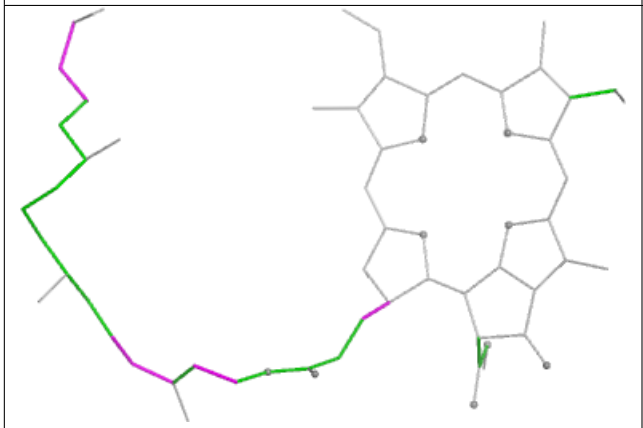
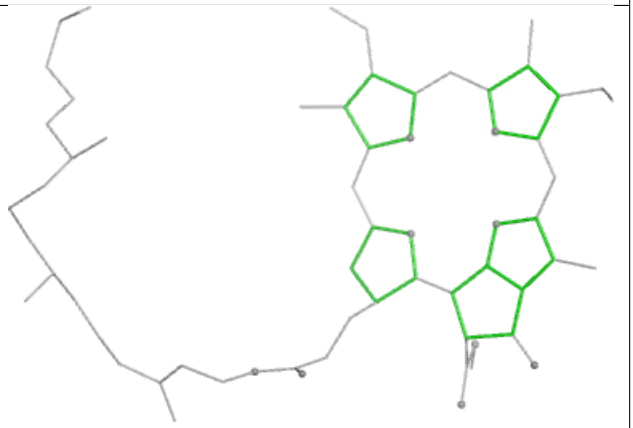
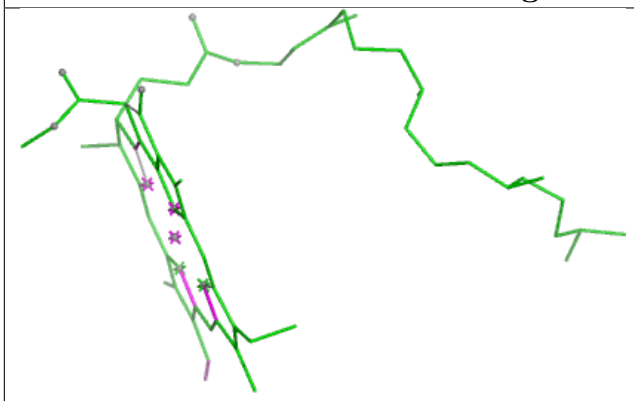
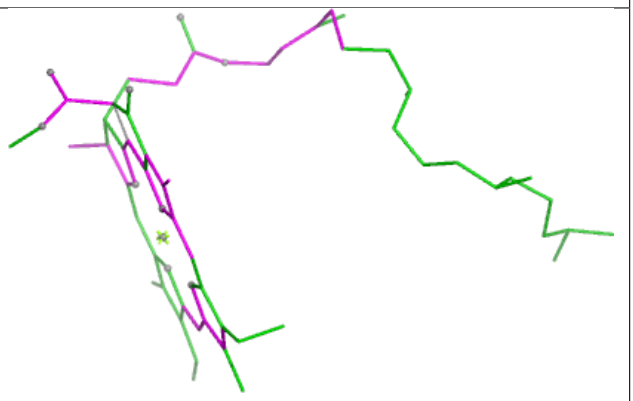
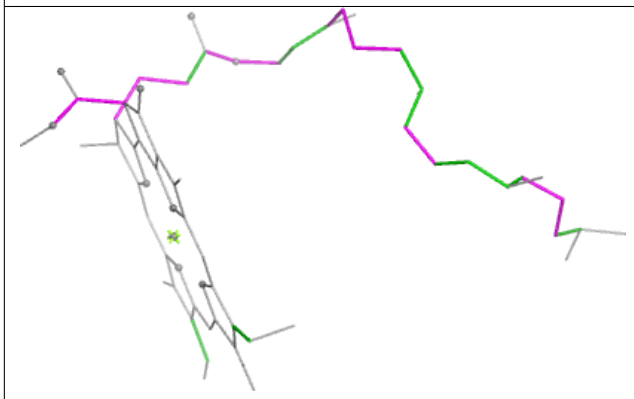
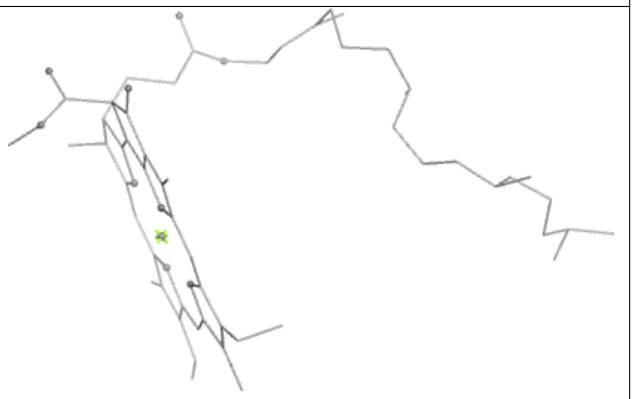
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CHL r1 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO A 408	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c1 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

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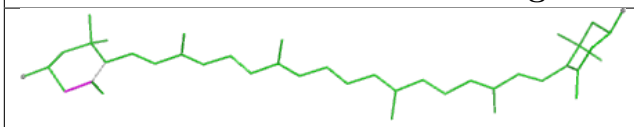
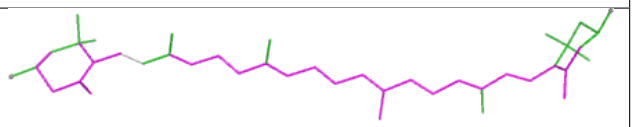
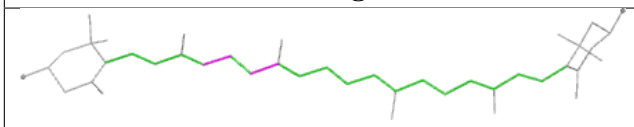
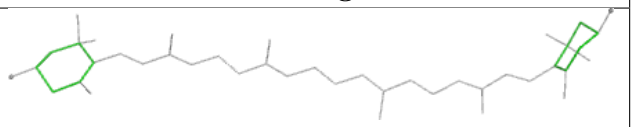
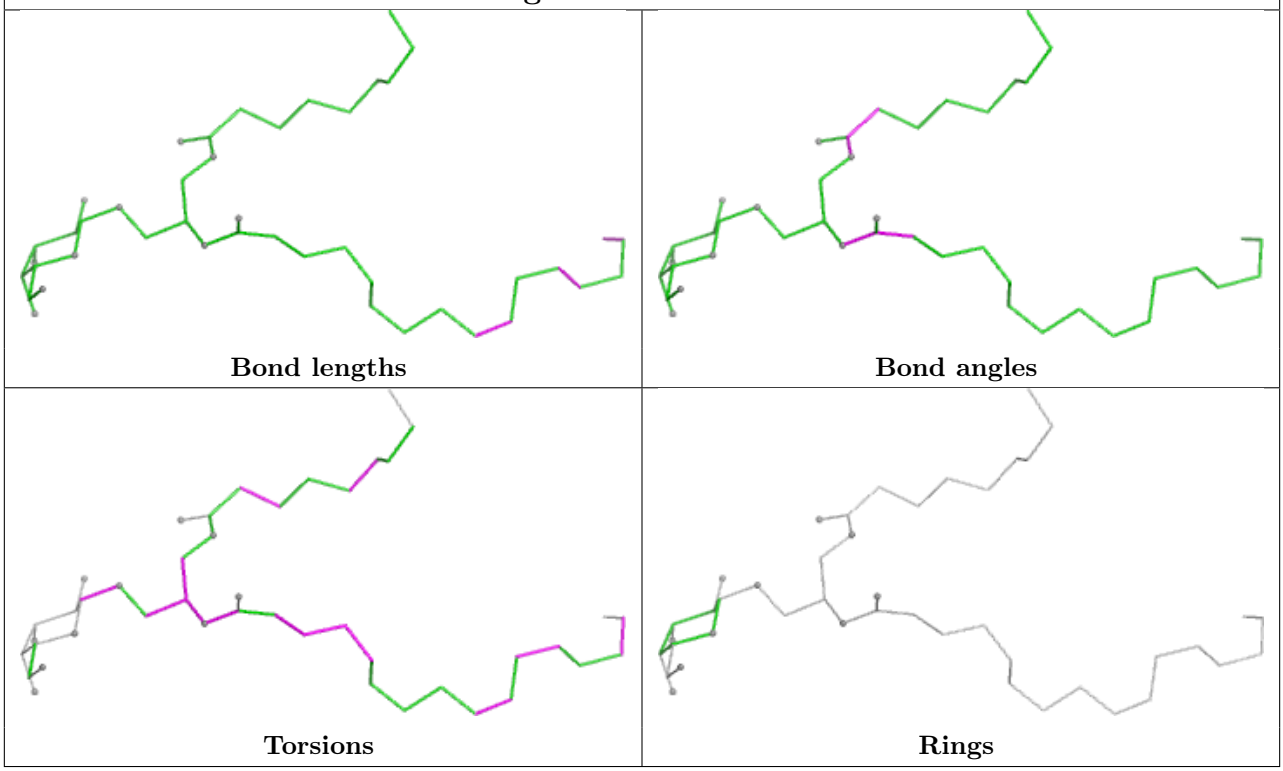
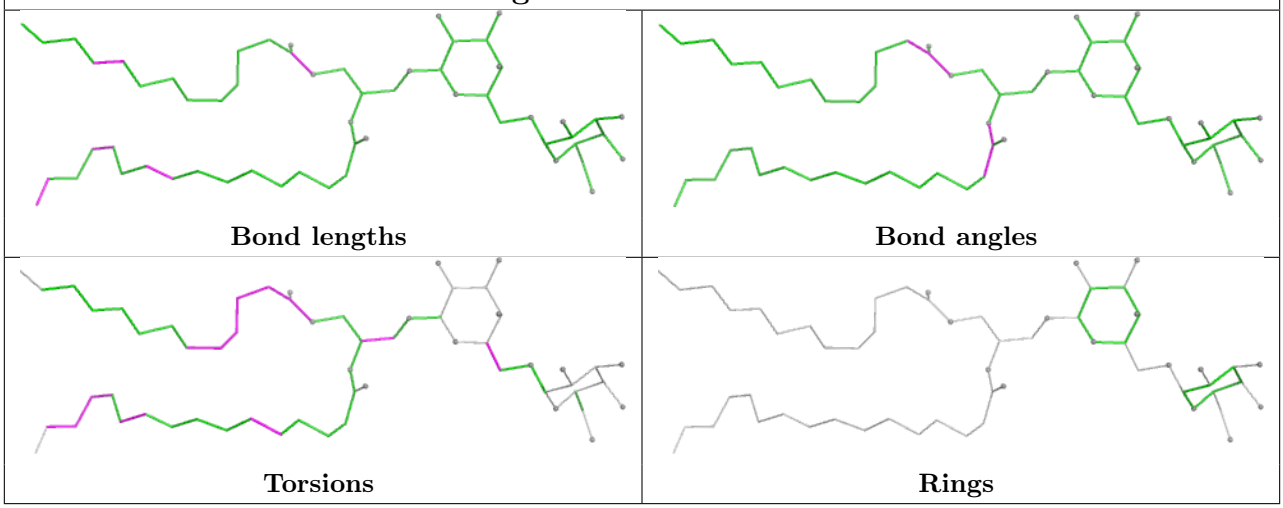
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG b 622



Ligand DGD C1 520



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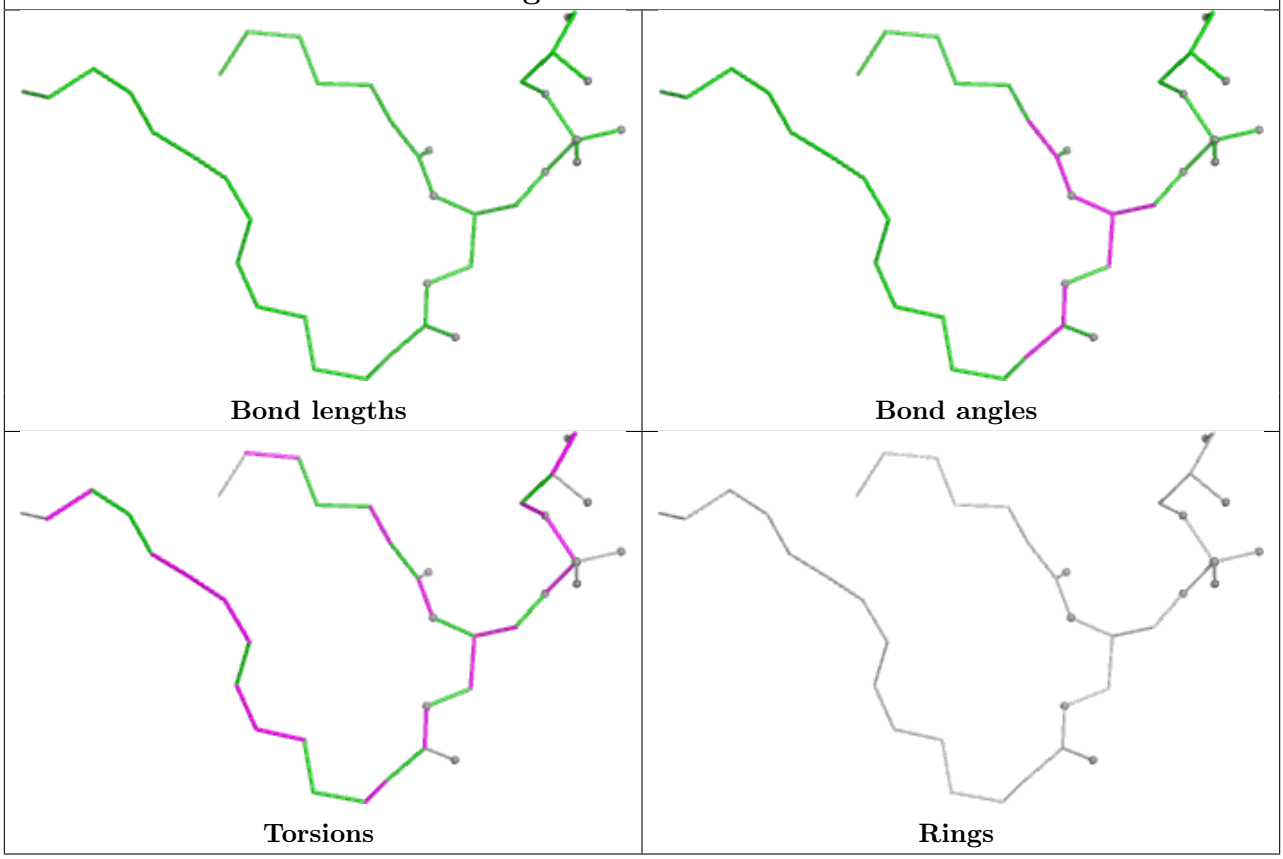
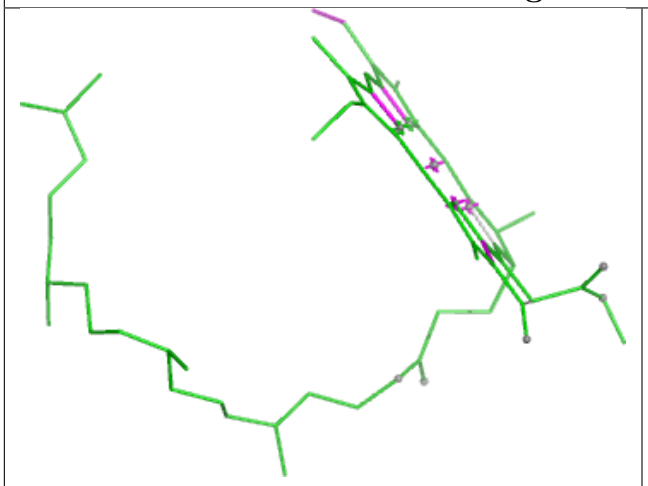
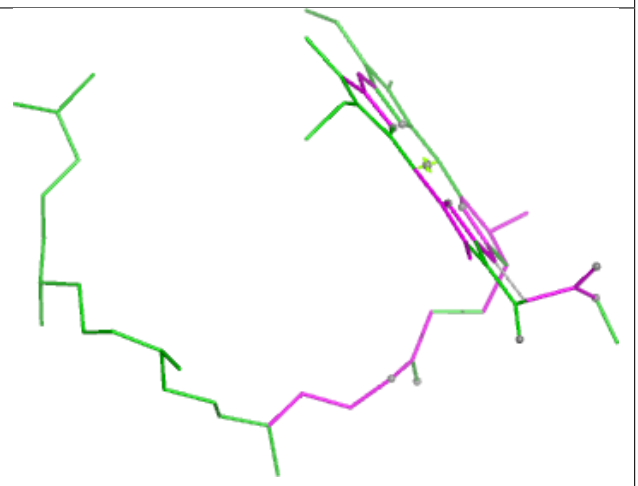


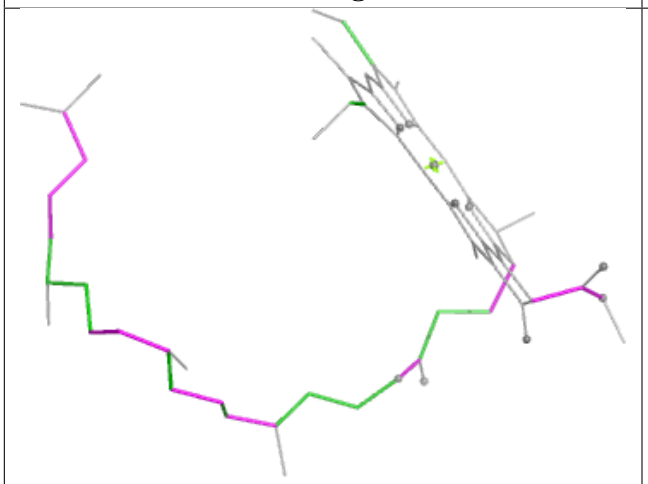
Ligand CLA B 612



Bond lengths



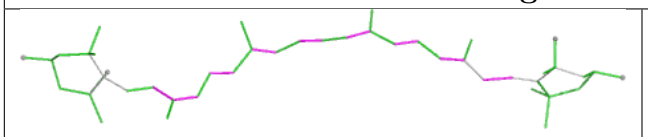
Bond angles



Torsions

Rings

Ligand NEX r1 622



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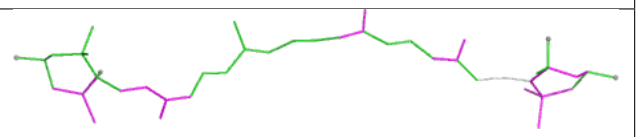
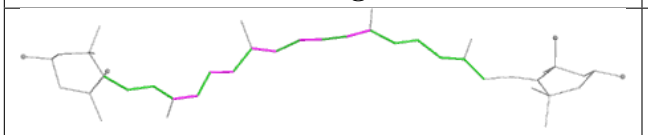


Bond angles



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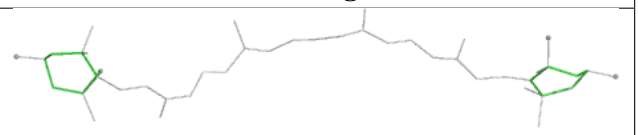
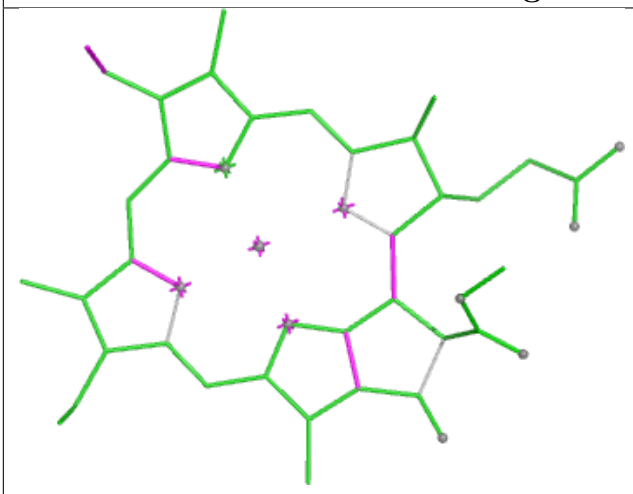


Rings

Ligand CLA N 612



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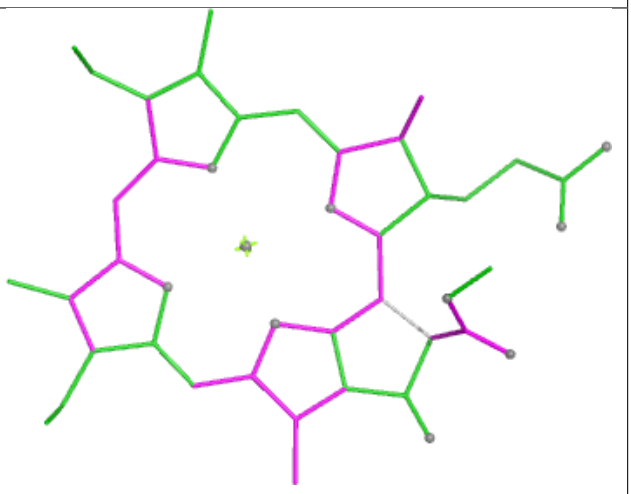

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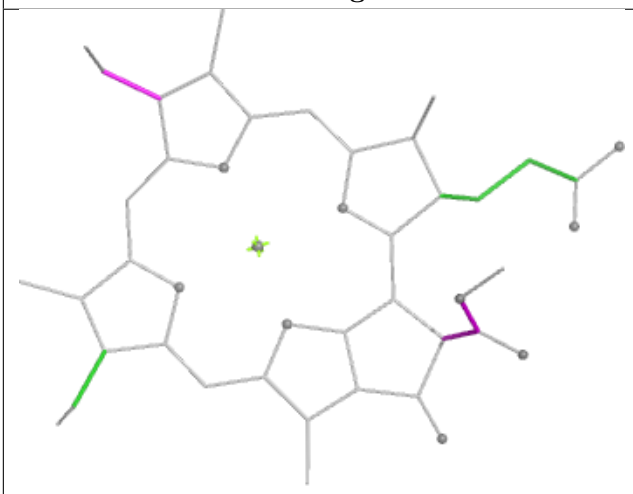

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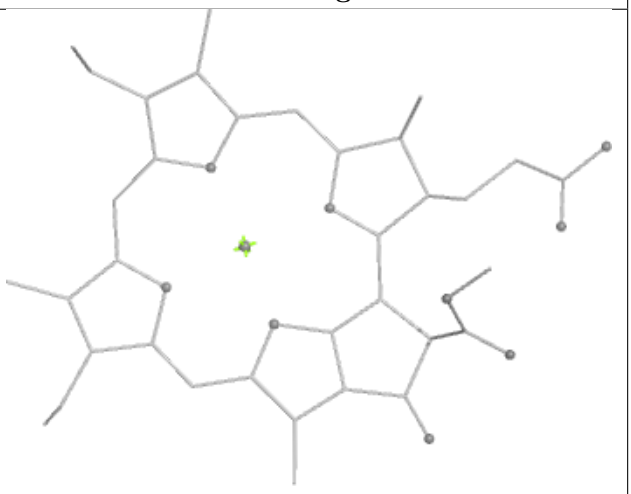

Rings

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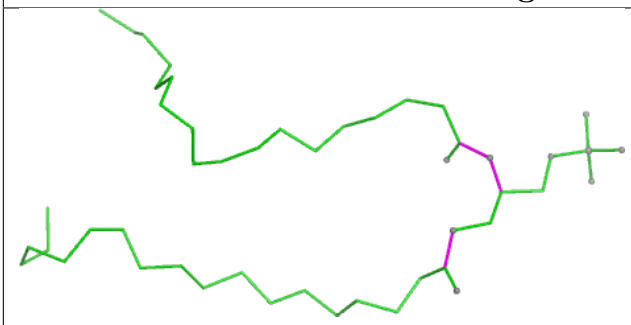
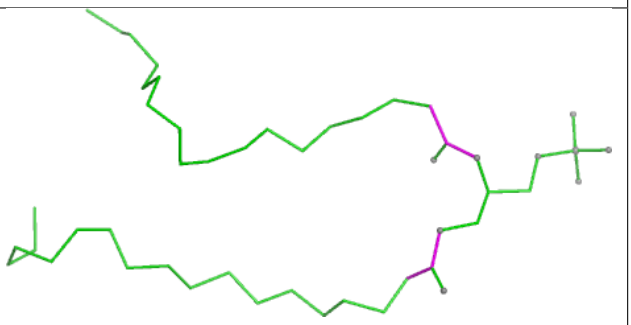
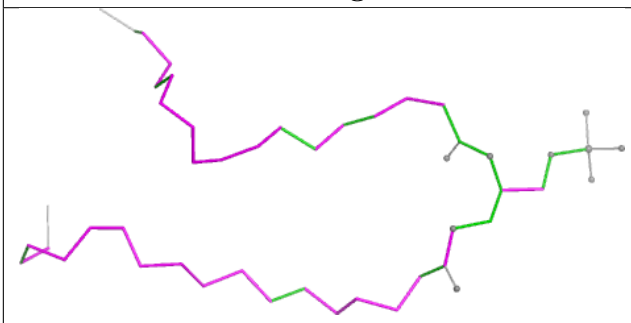
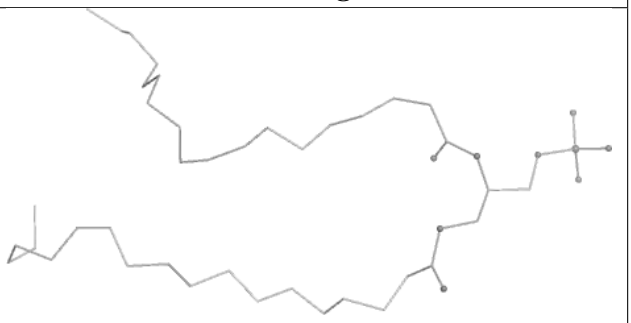
 Bond lengths	 Bond angles
 Torsions	 Rings

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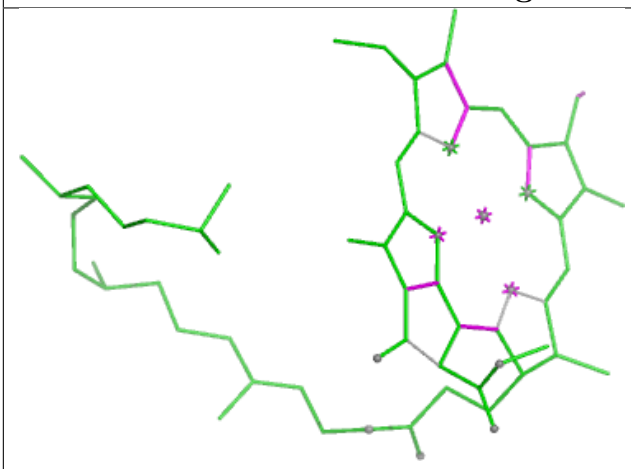
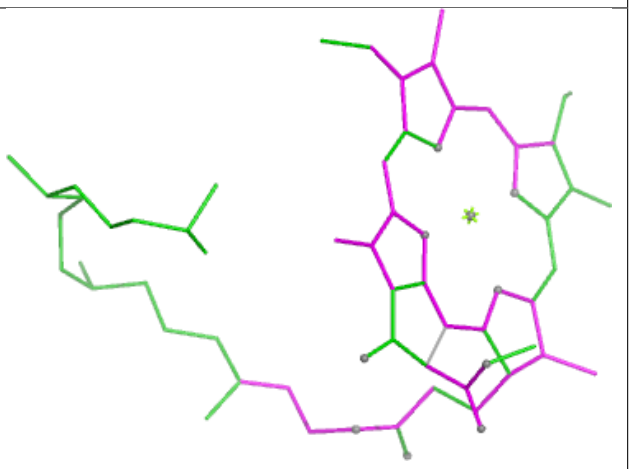
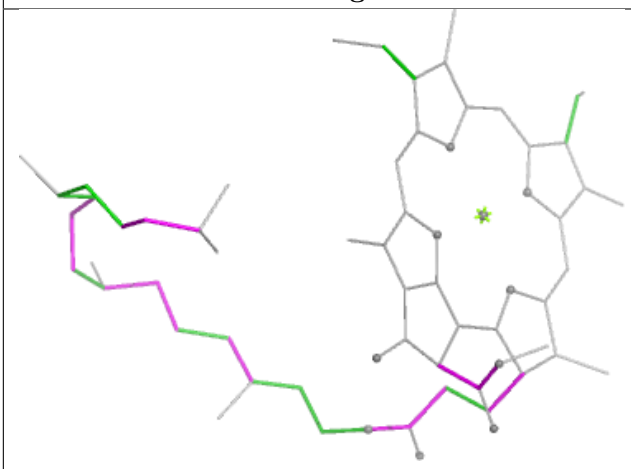
 Bond lengths	 Bond angles
 Torsions	Rings

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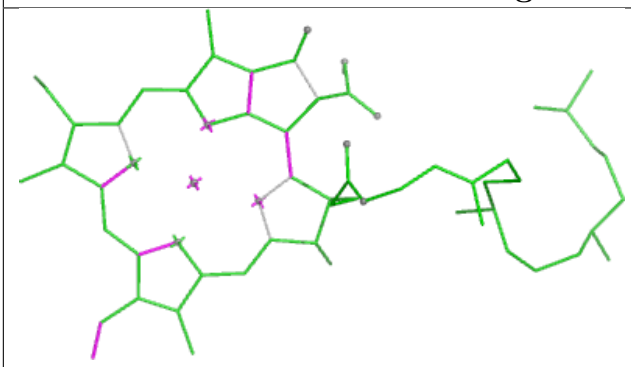
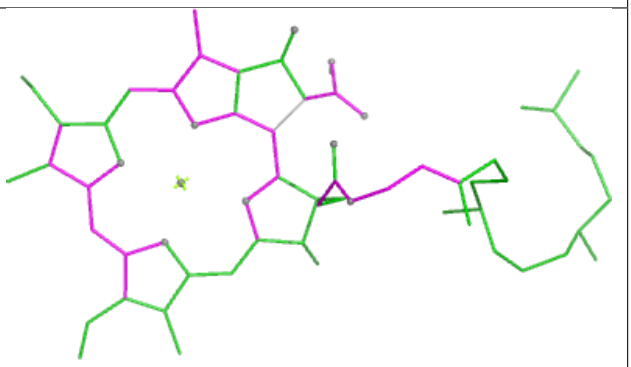
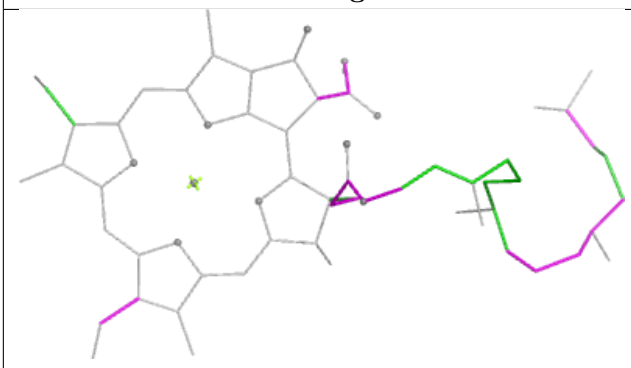
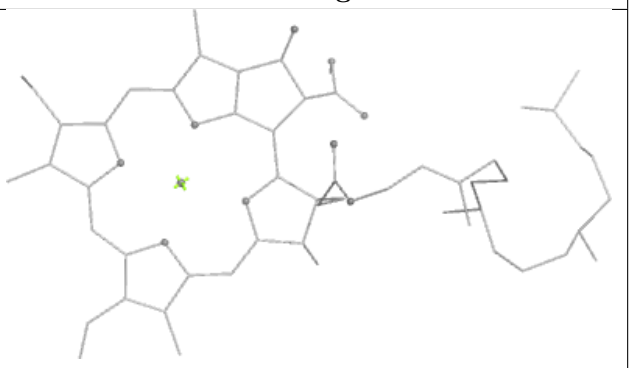
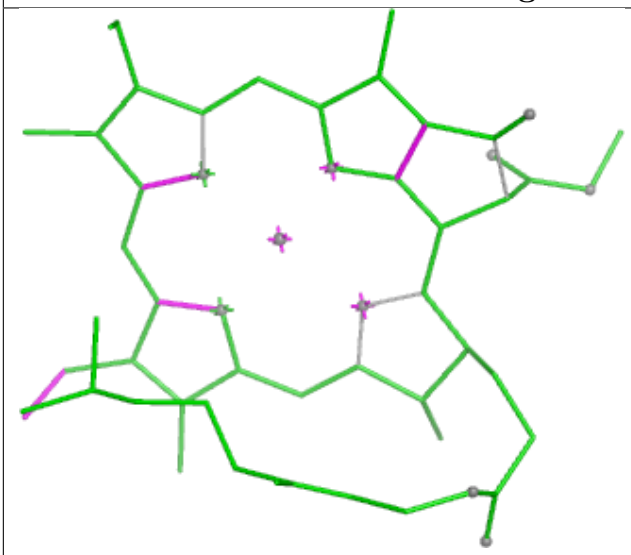
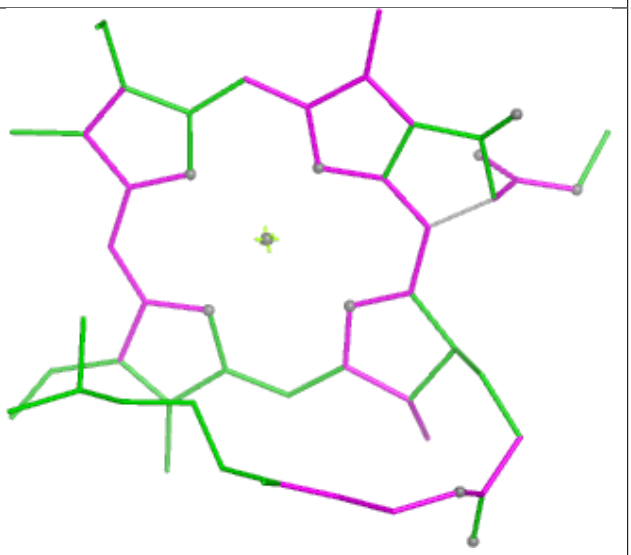
 Bond lengths	 Bond angles
 Torsions	 Rings

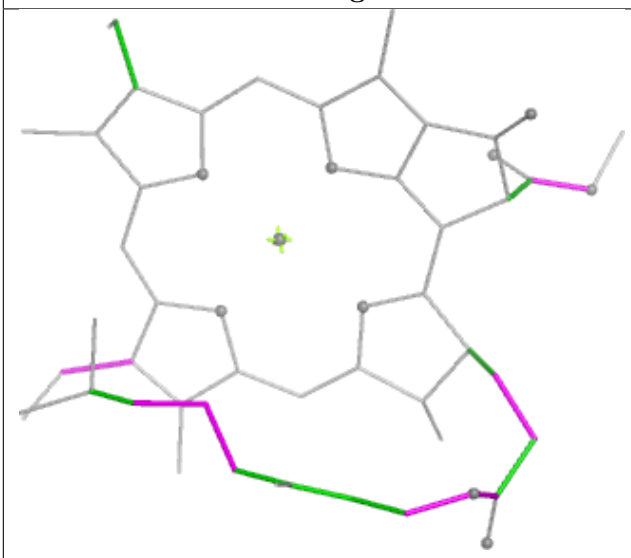
Ligand CLA S1 614



Bond lengths



Bond angles



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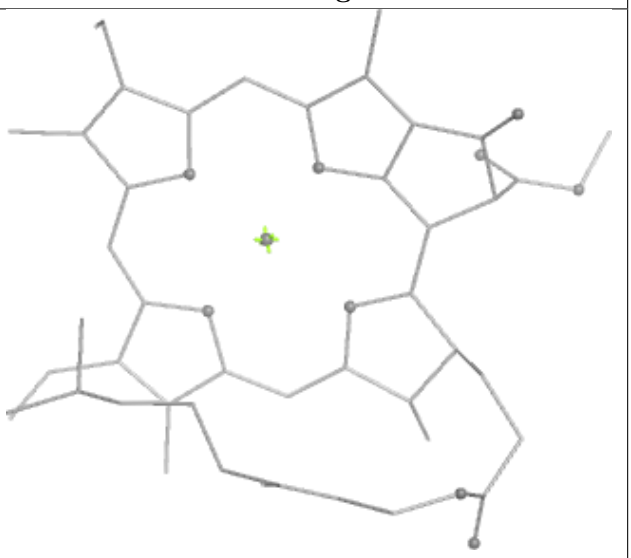
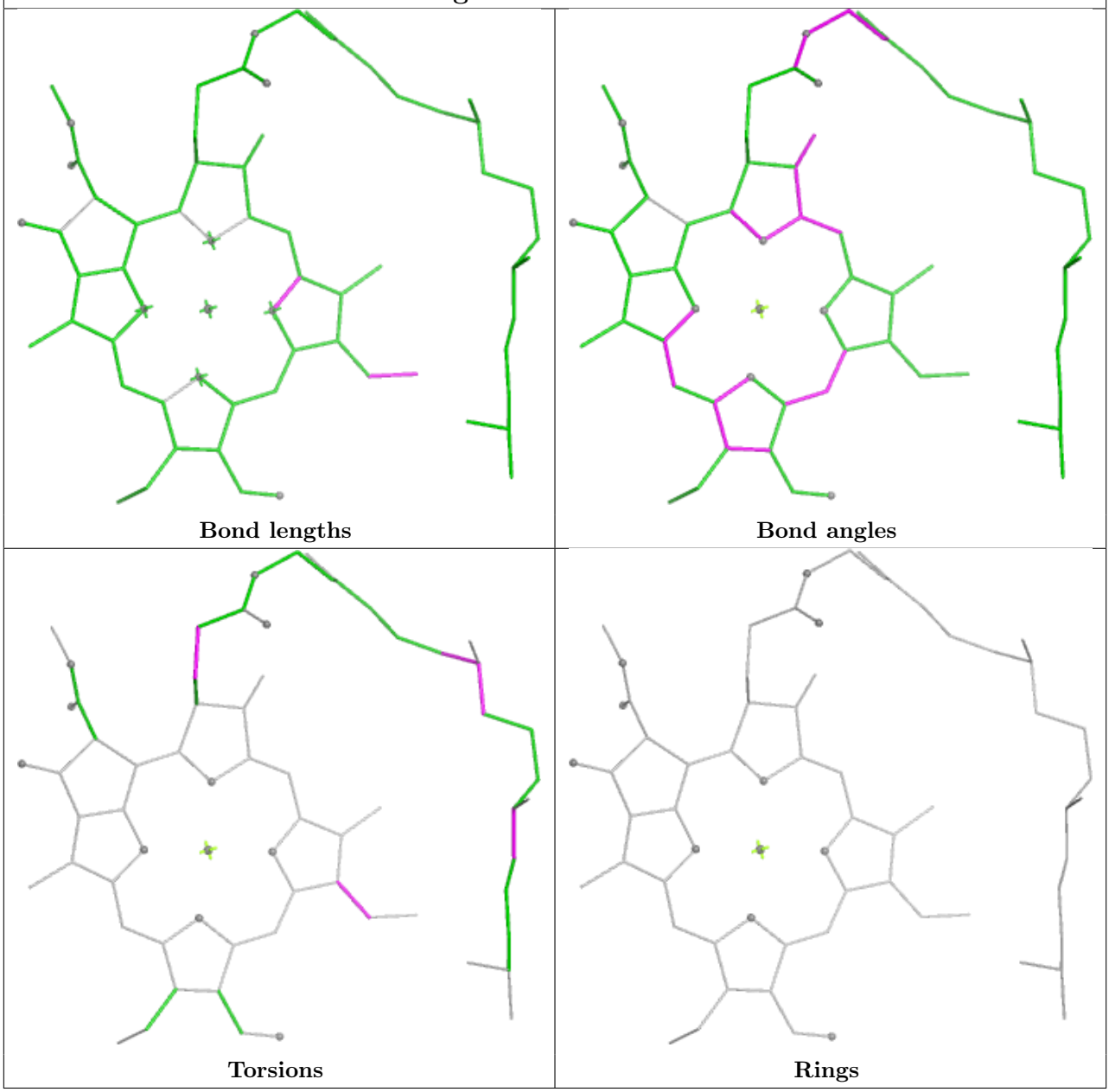
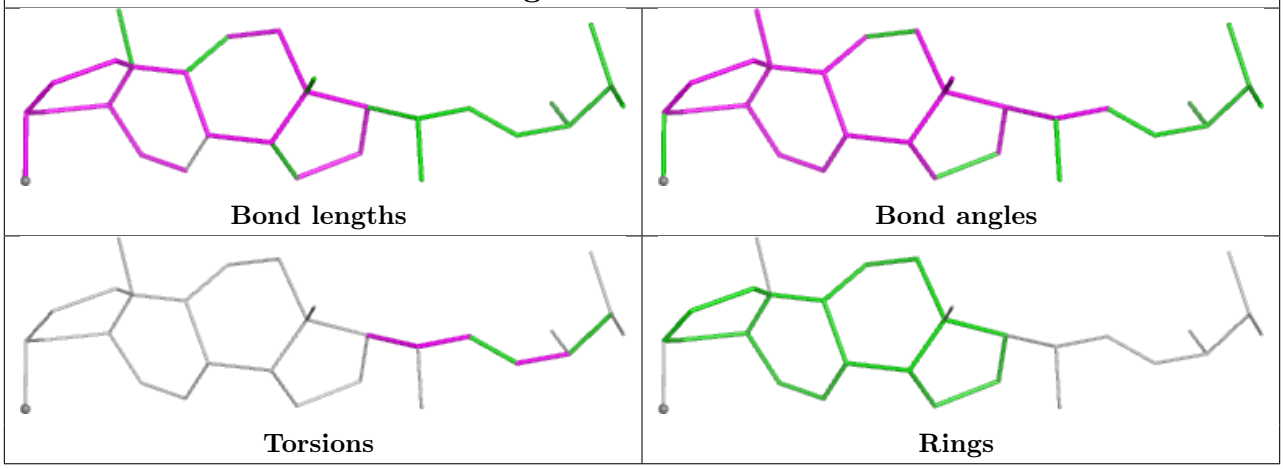


Rings

Ligand CHL Y 607



Ligand ERG R 626



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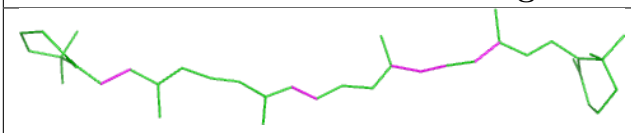
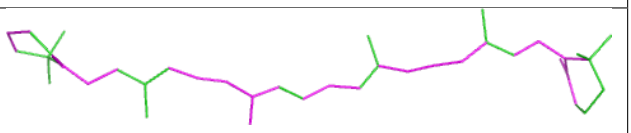
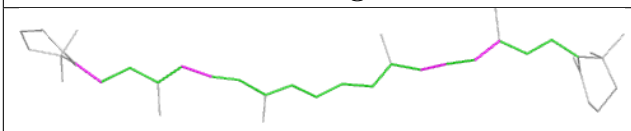
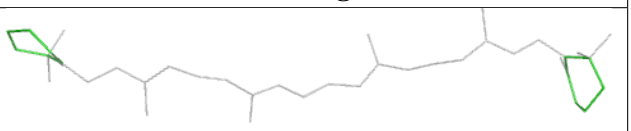
 Bond lengths	 Bond angles
 Torsions	 Rings

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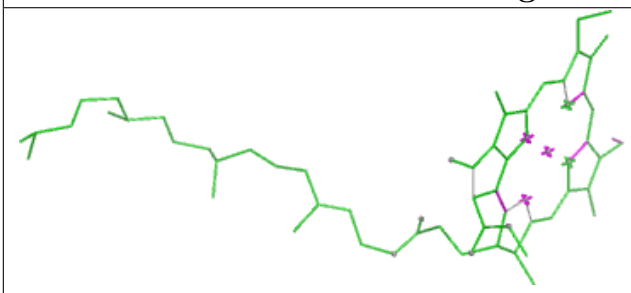
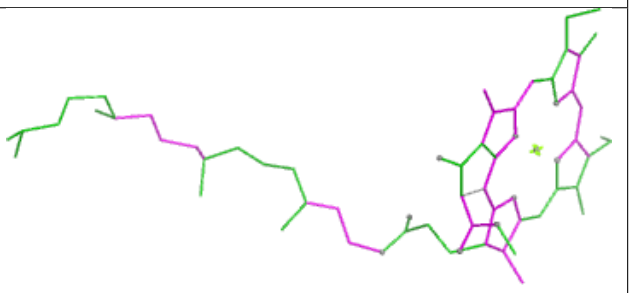
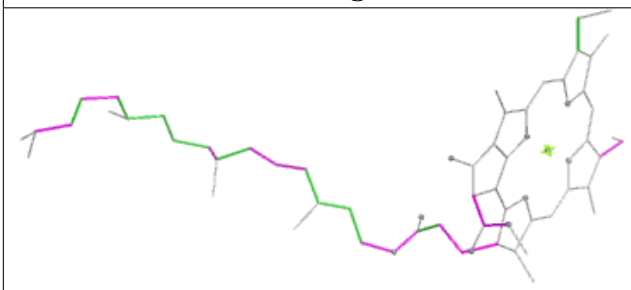
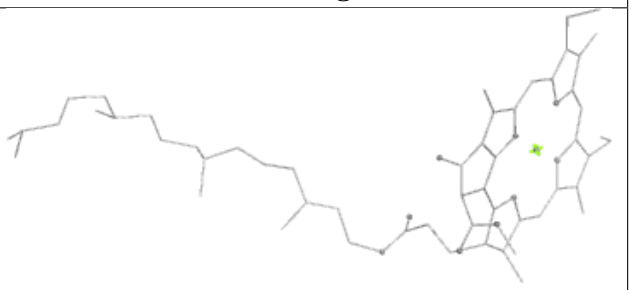
 Bond lengths	 Bond angles
 Torsions	 Rings

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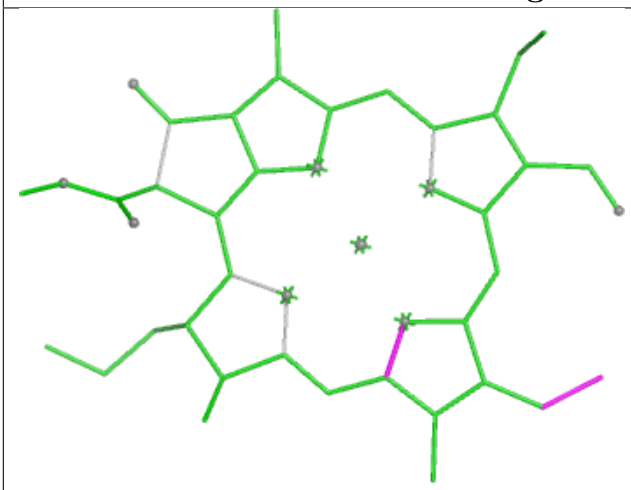
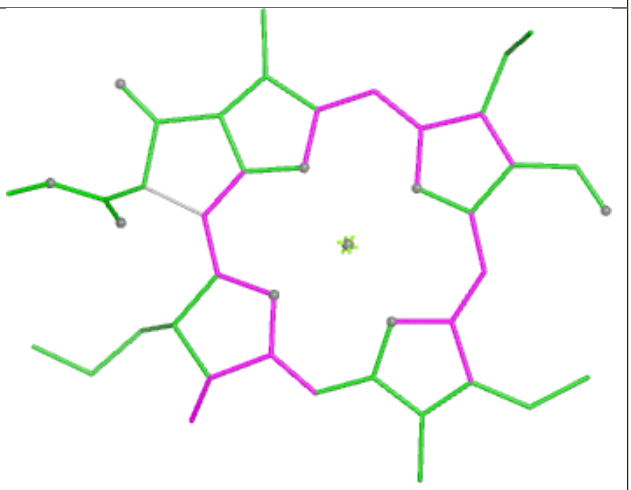
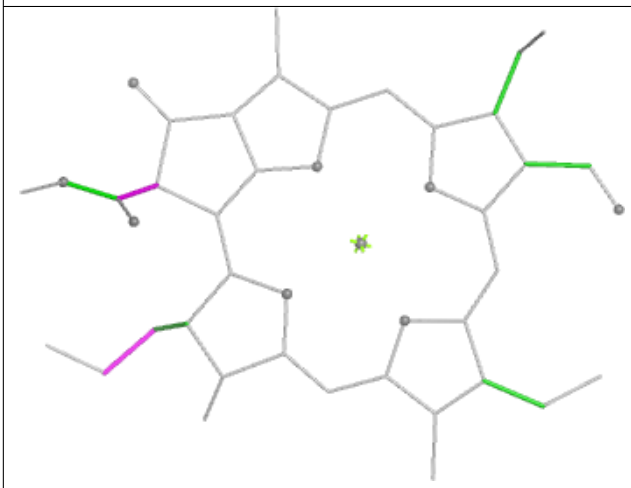
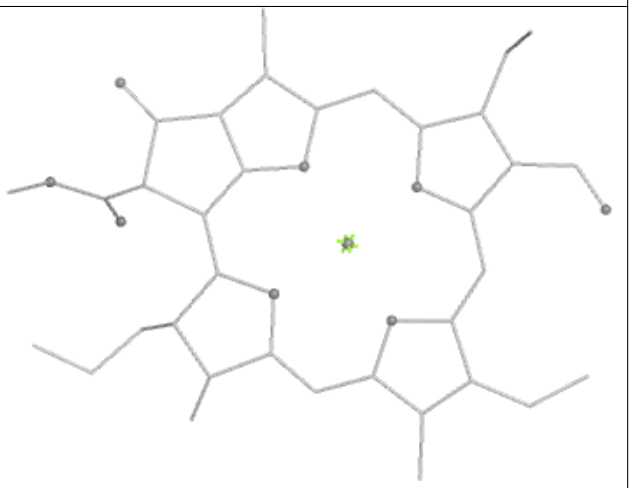
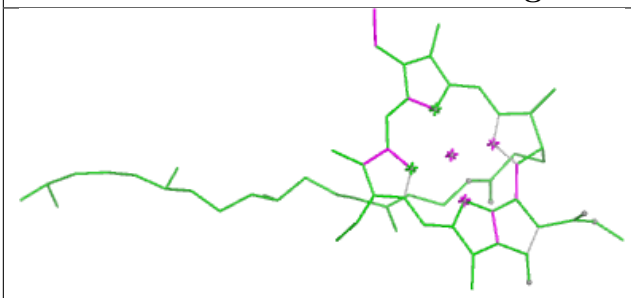
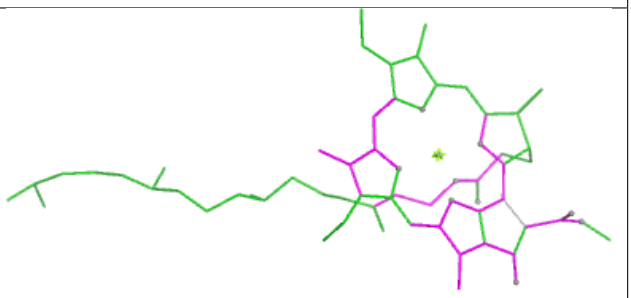
 Bond lengths	 Bond angles
 Torsions	 Rings

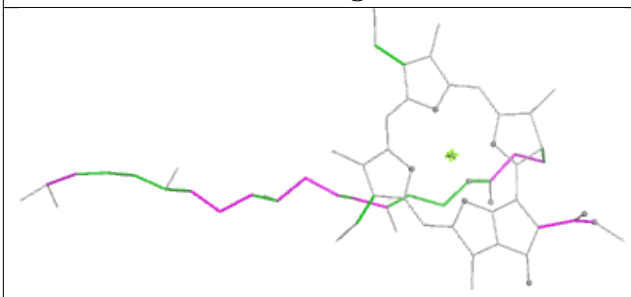
Ligand CLA B 615



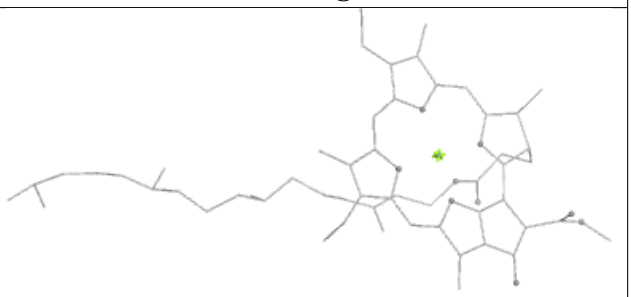
Bond lengths



Bond angles

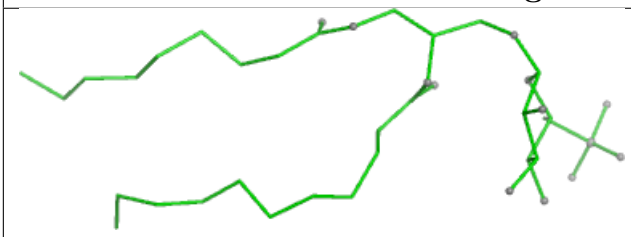


Torsions



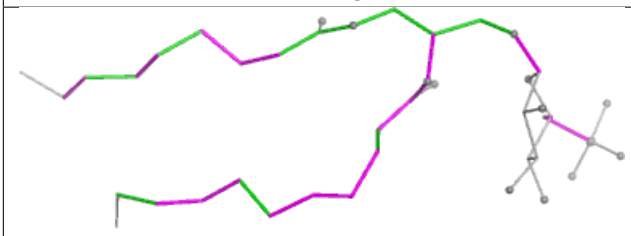
Rings

Ligand SQD B 621



Bond lengths

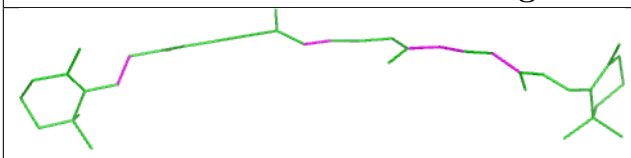
Bond angles



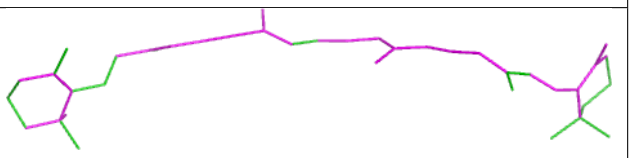
Torsions

Rings

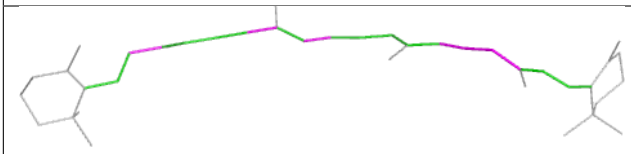
Ligand BCR c1 517



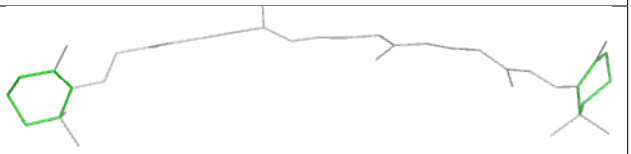
Bond lengths



Bond angles

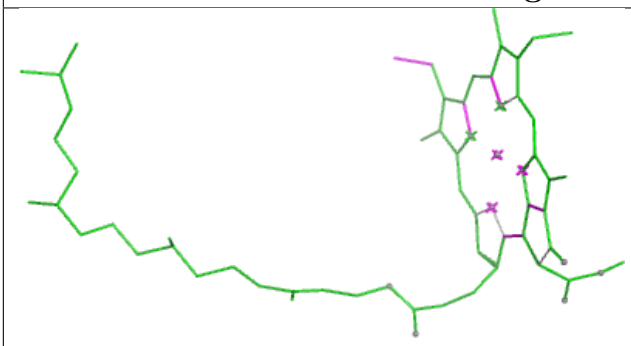


Torsions



Rings

Ligand CLA B 610



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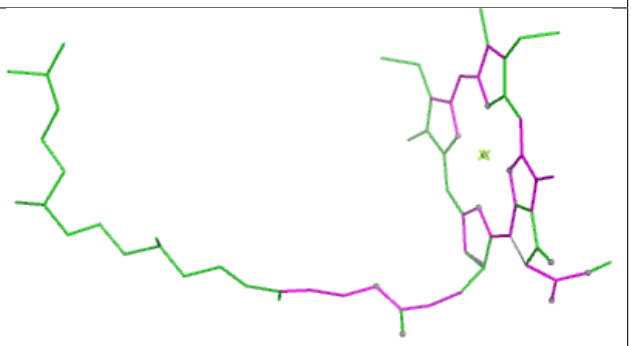
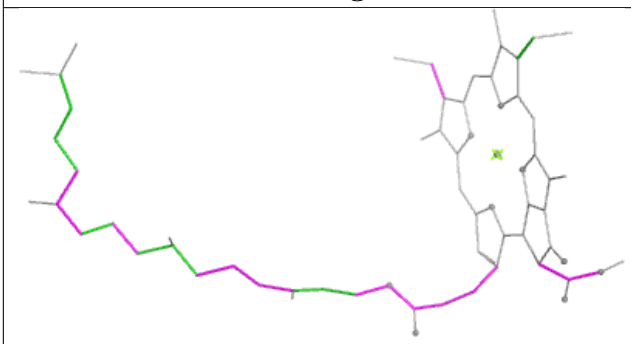


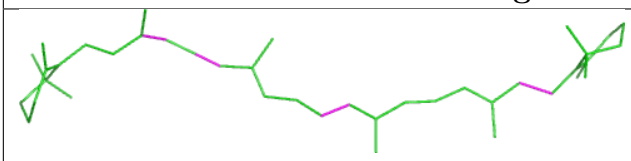
Bond angles



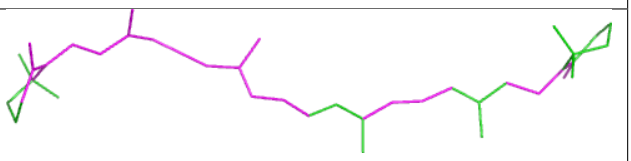
Torsions

Rings

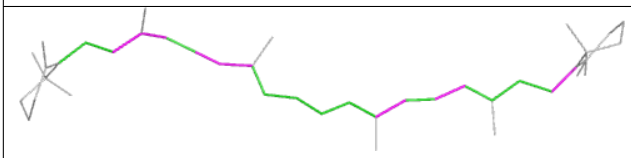
Ligand BCR C1 515



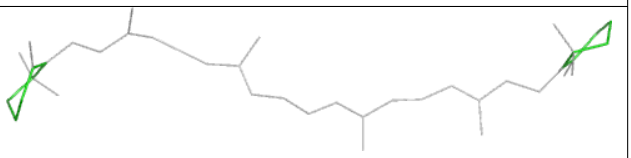
Bond lengths



Bond angles

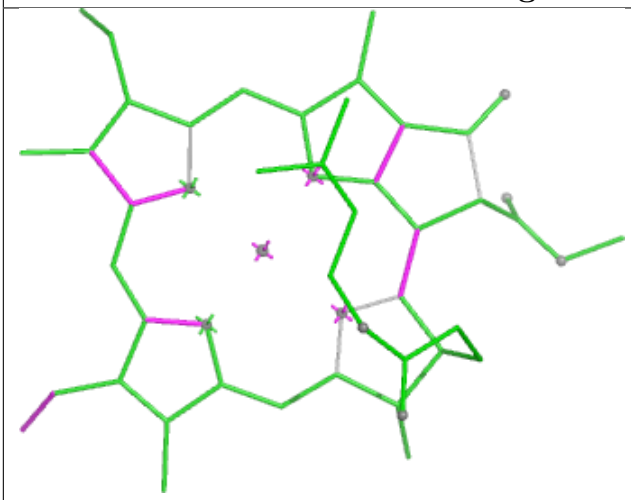


Torsions



Rings

Ligand CLA S1 605



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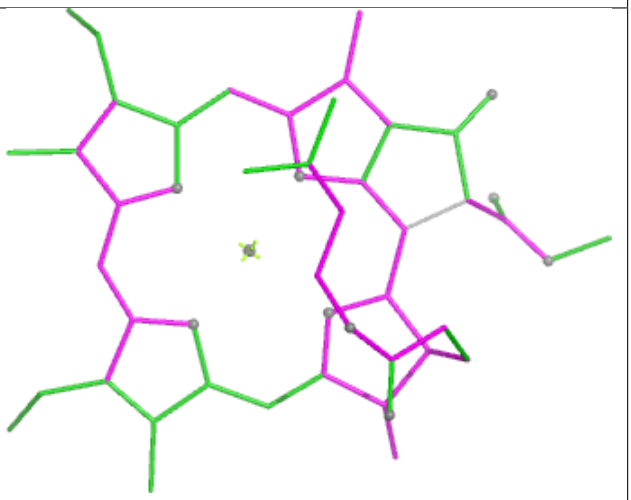
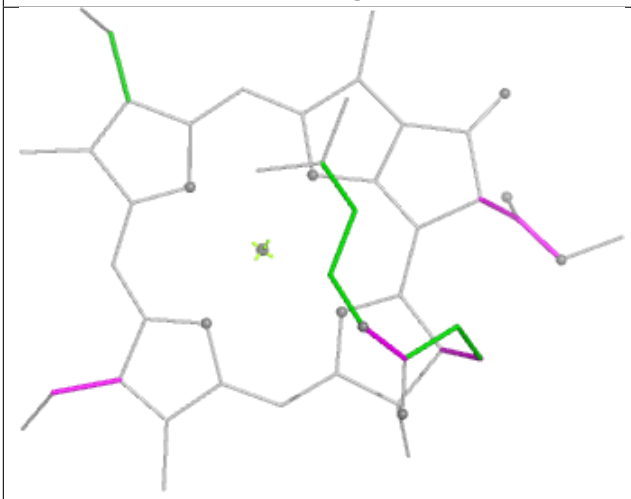


Bond angles



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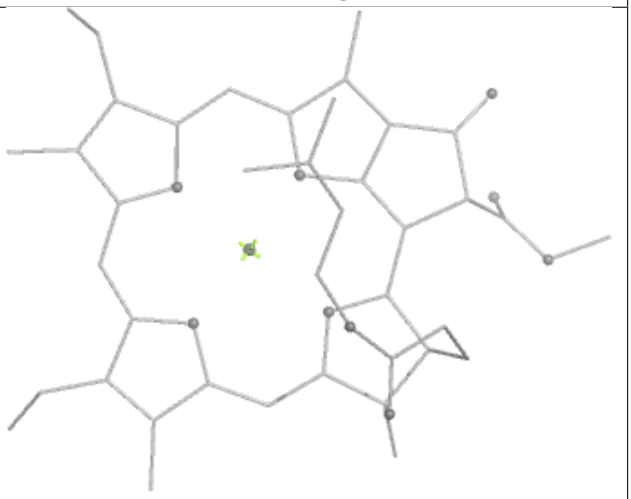
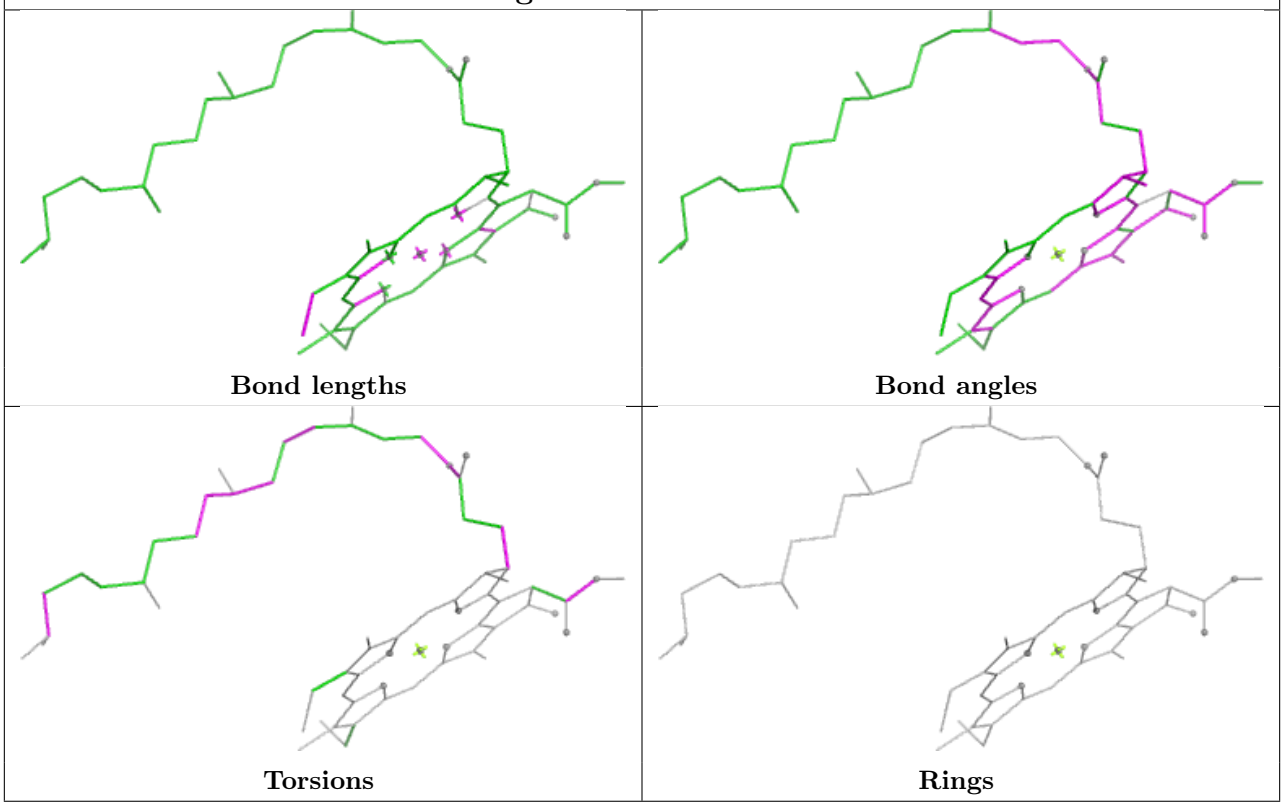
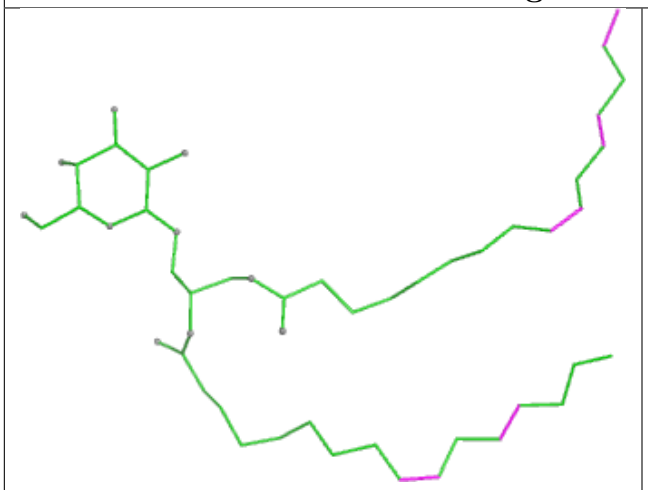


Rings

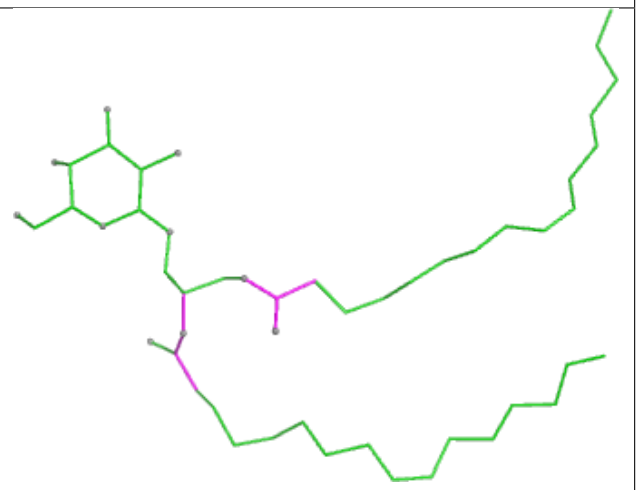
Ligand CLA Y1 614



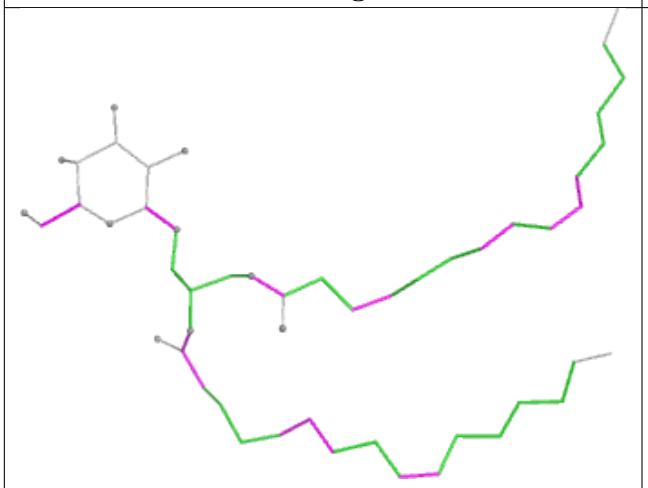
Ligand LMG c 521



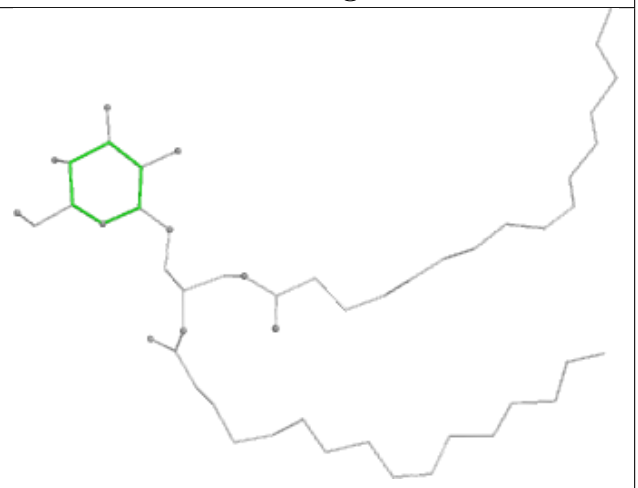
Bond lengths



Bond angles

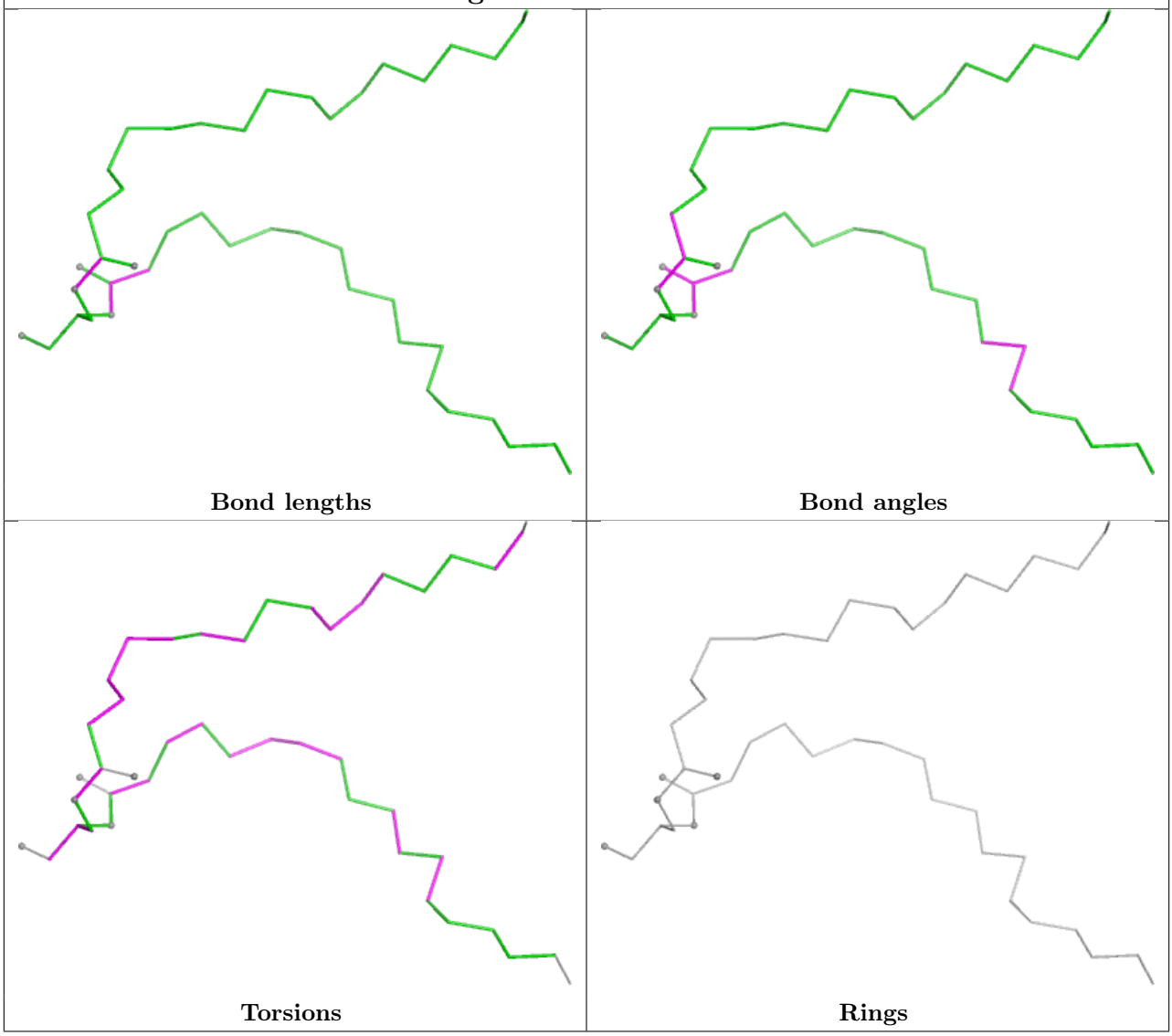


Torsions

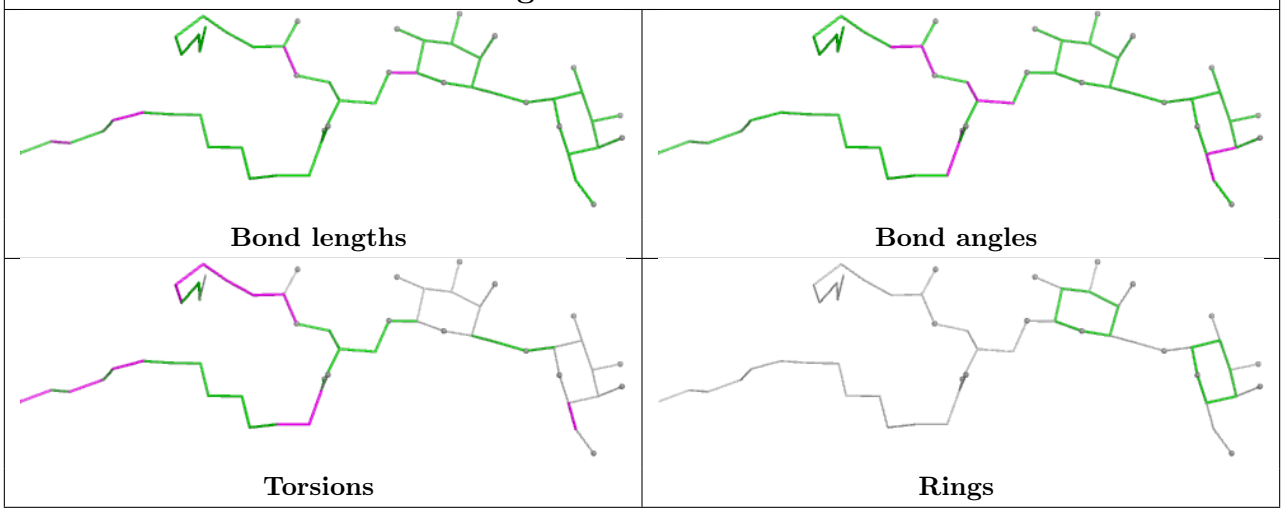


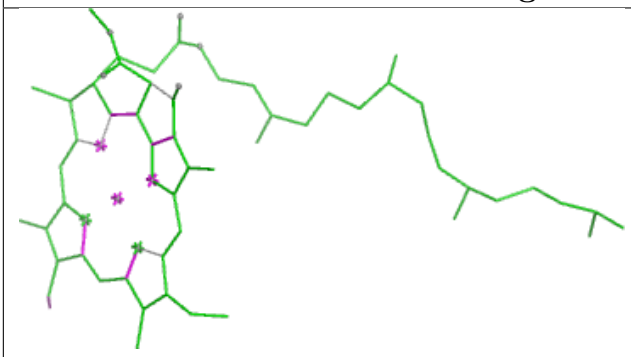
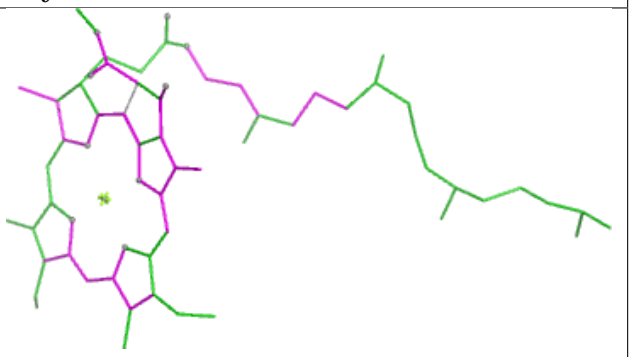
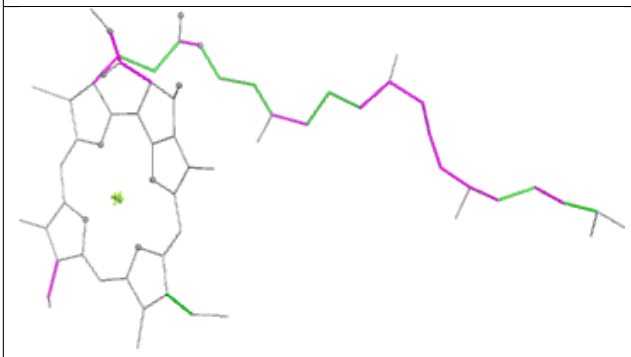
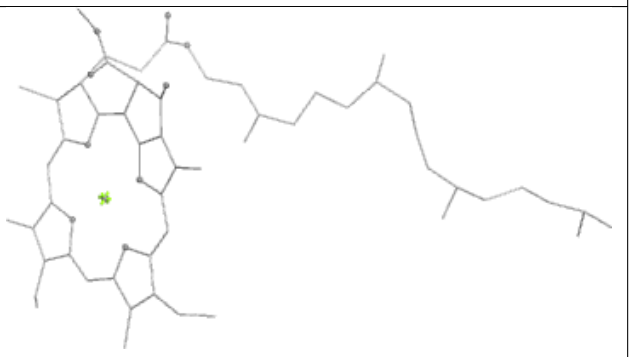
Rings

Ligand DGA C1 524



Ligand DGD c1 518



Ligand CLA y1 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

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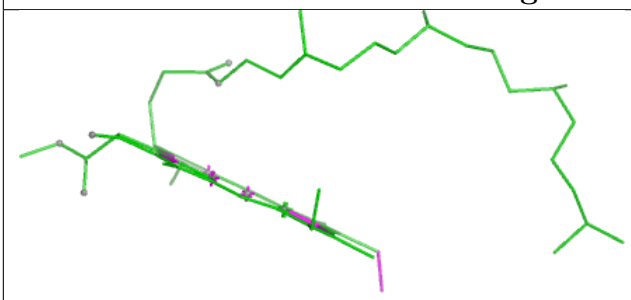
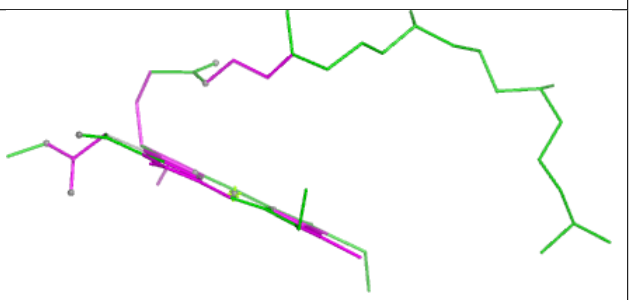
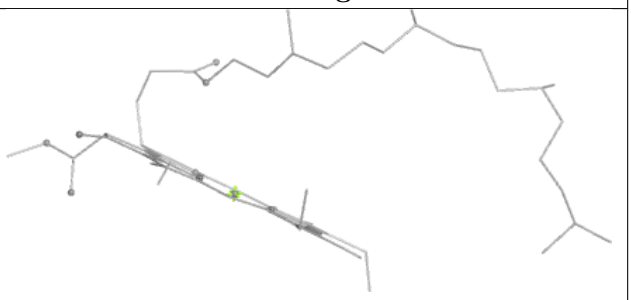
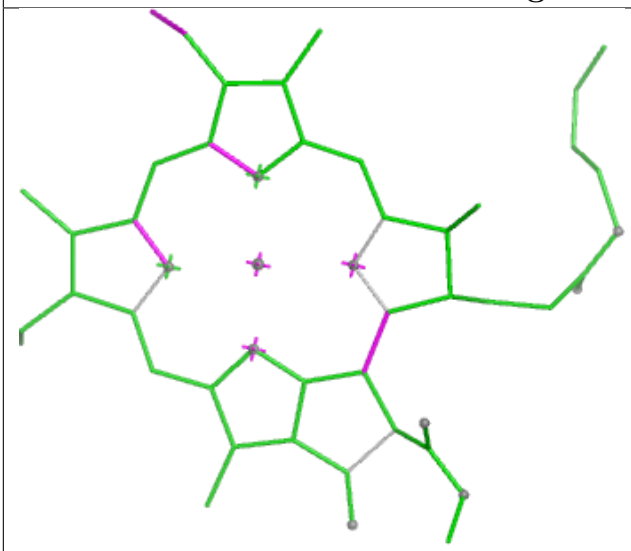
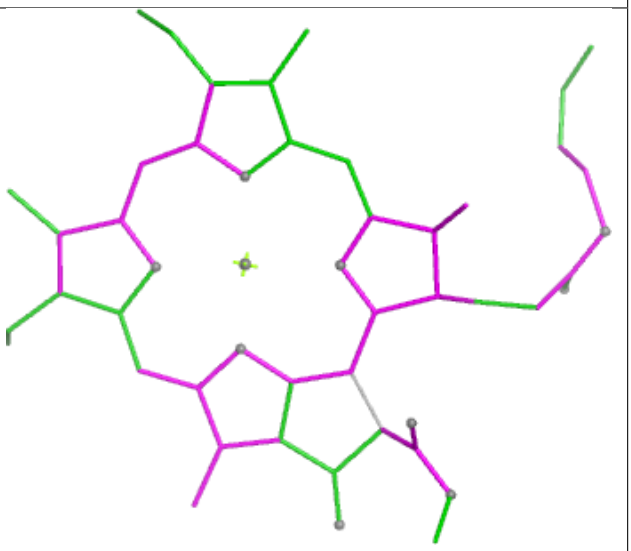
 Bond lengths	 Bond angles
Torsions	 Rings

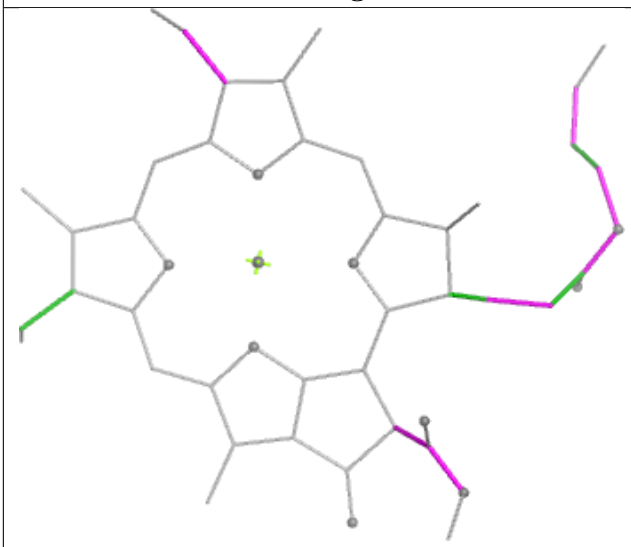
Ligand CLA n 611



Bond lengths



Bond angles



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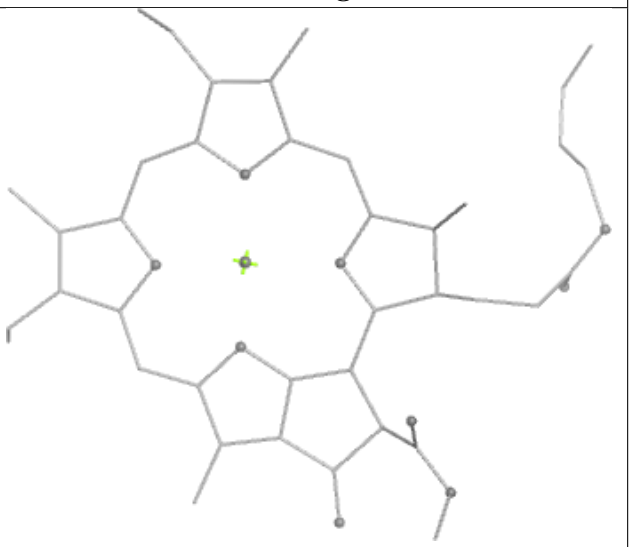
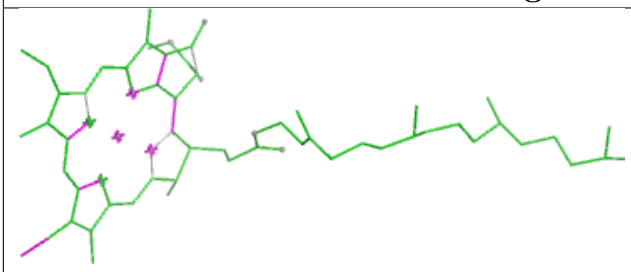
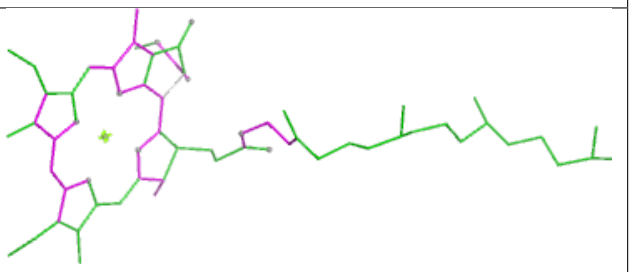
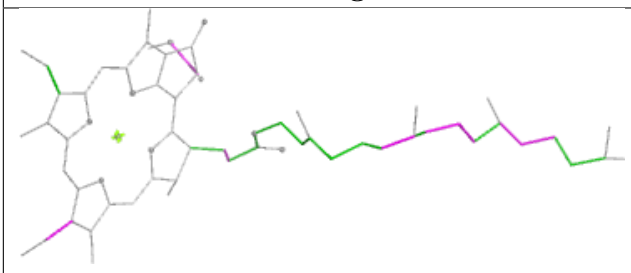
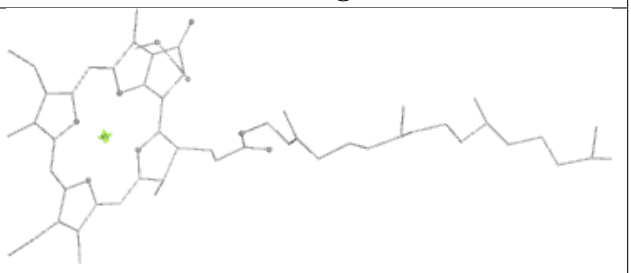
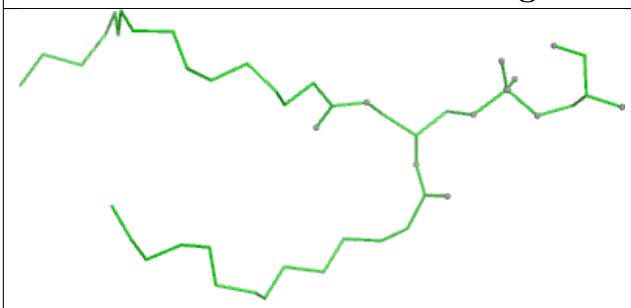
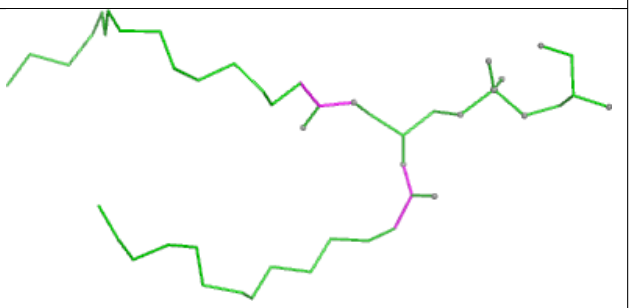
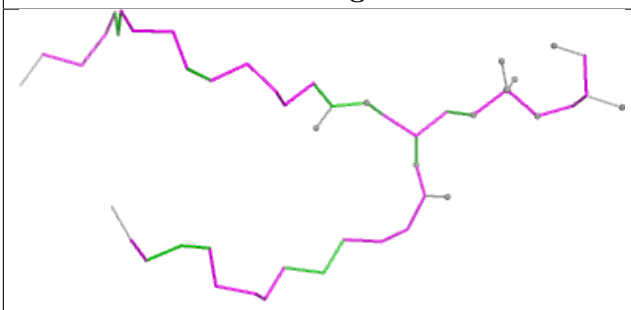
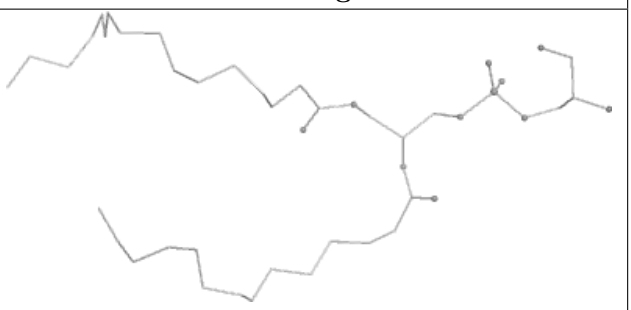
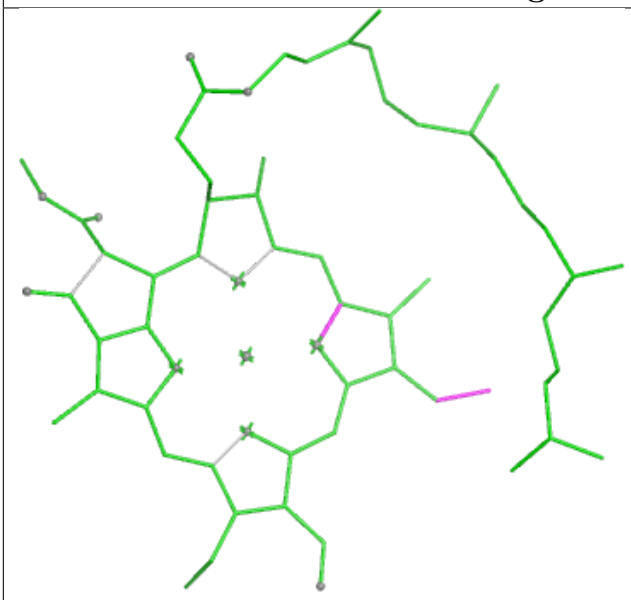


Rings

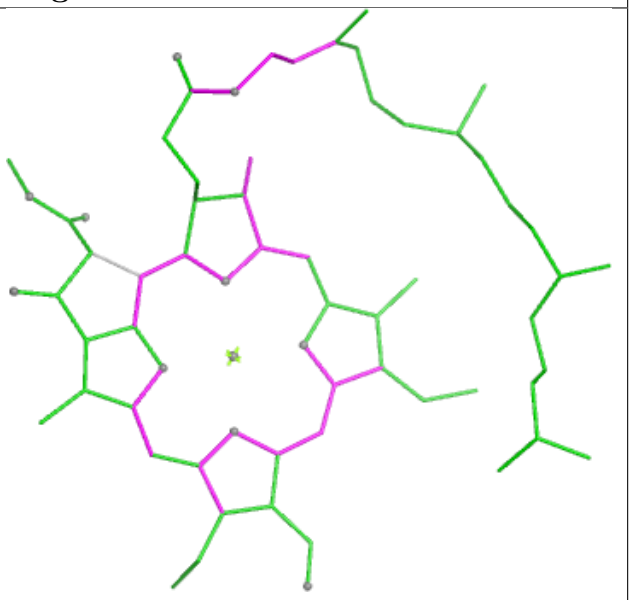
Ligand CLA C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG c1 525	
 Bond lengths	 Bond angles
 Torsions	 Rings

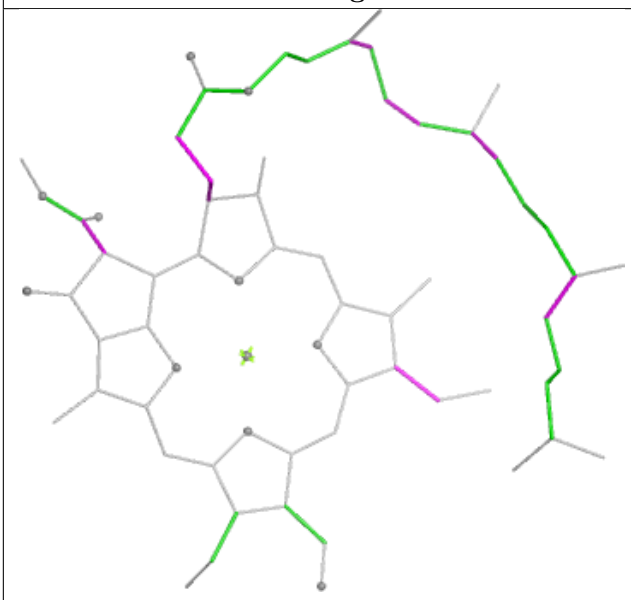
Ligand CHL g 607



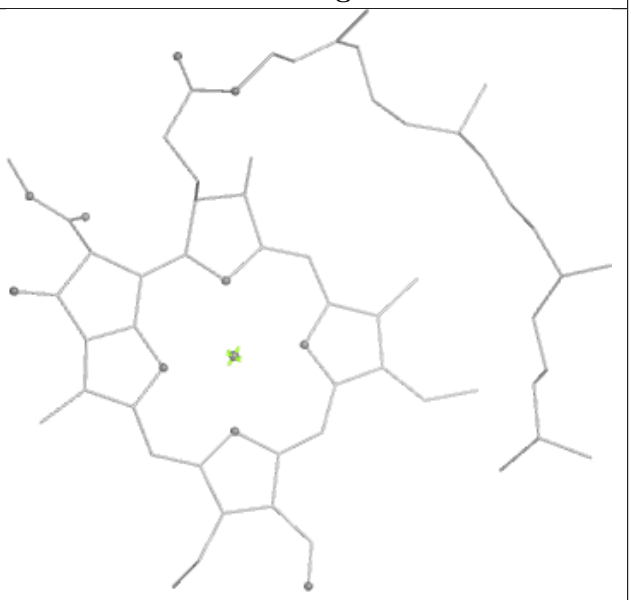
Bond lengths



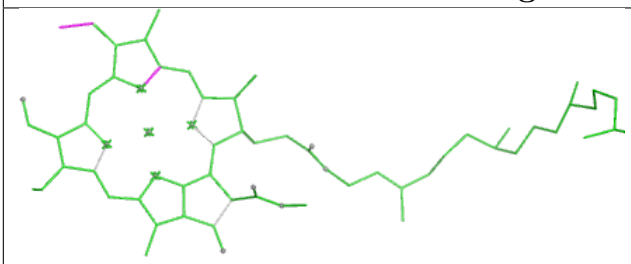
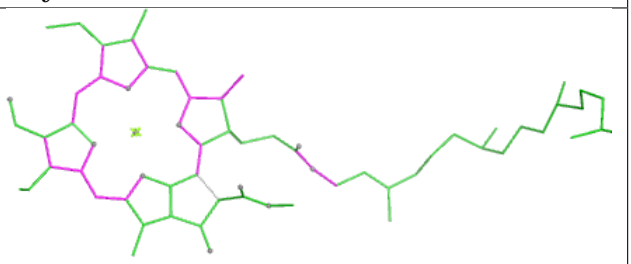
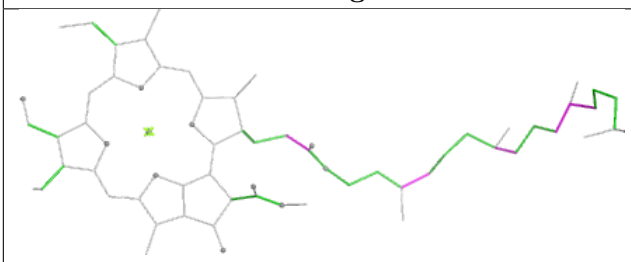
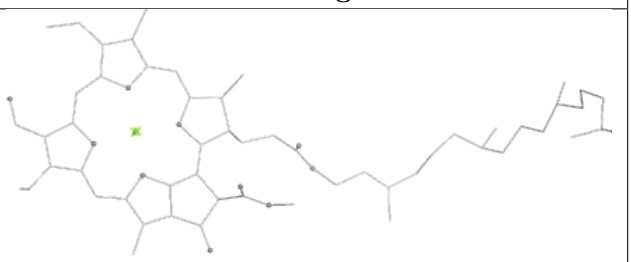
Bond angles

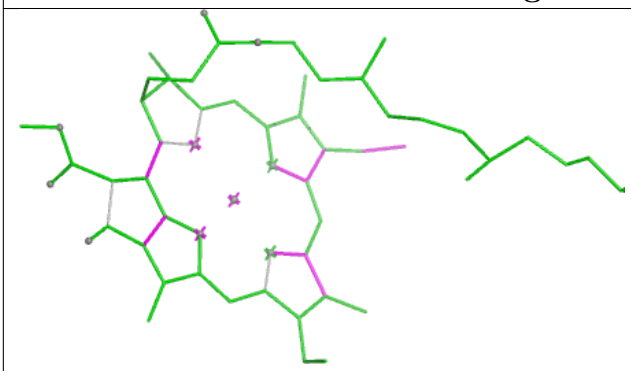
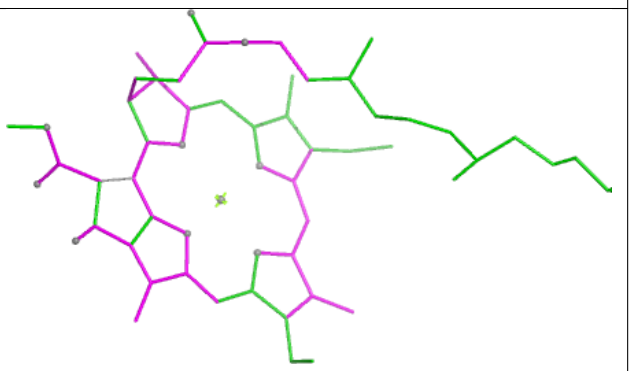
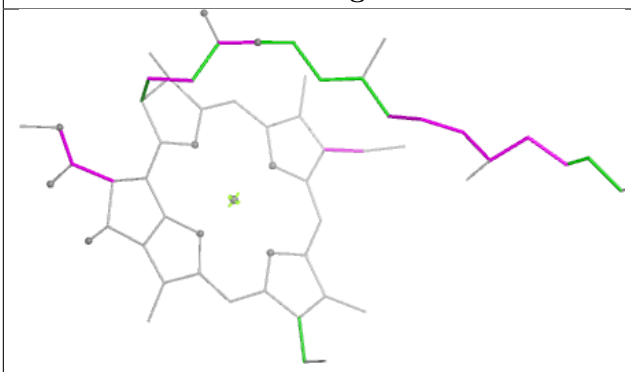
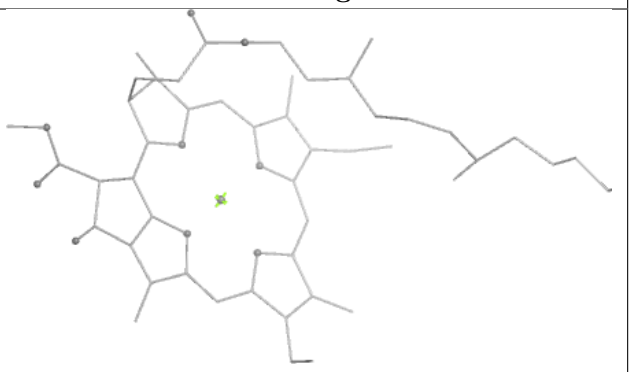


Torsions

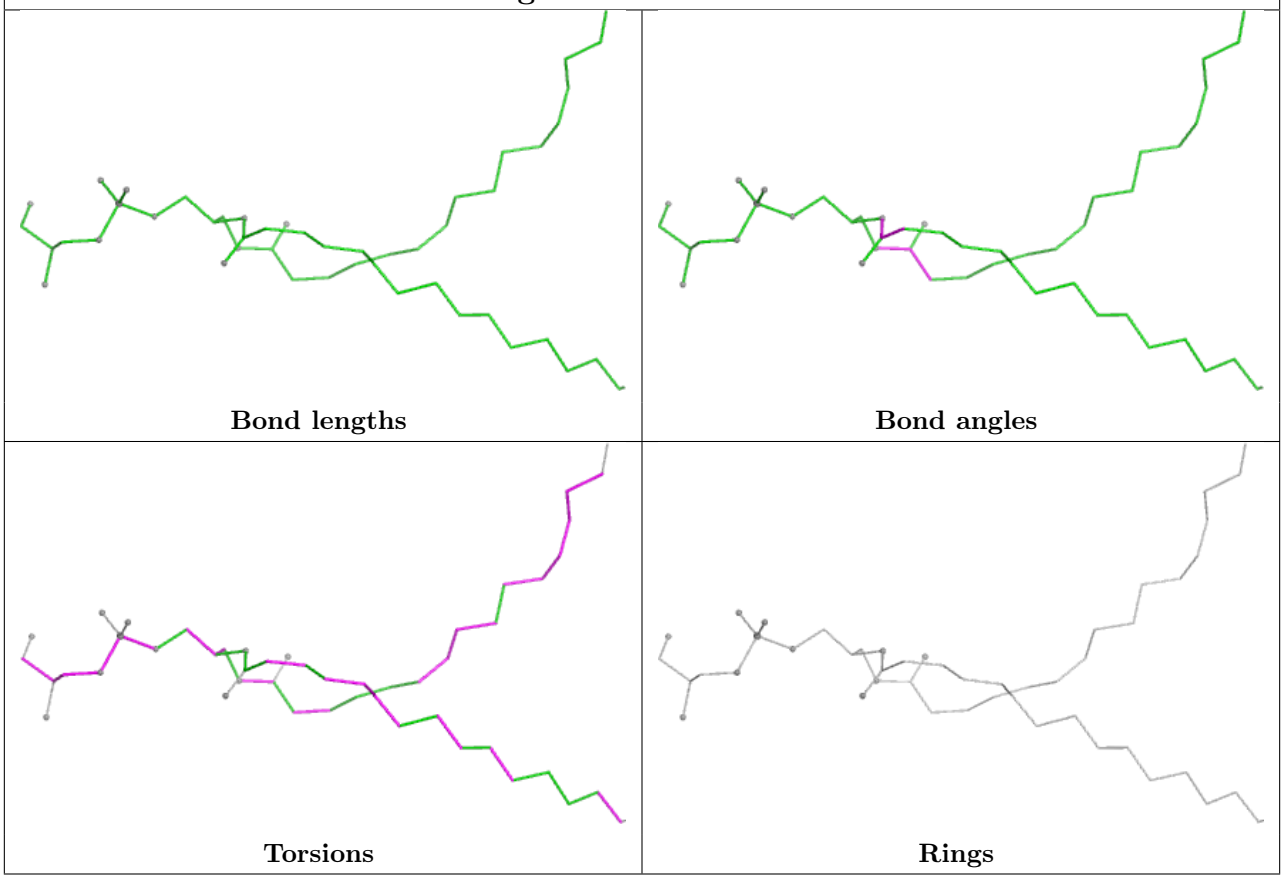


Rings

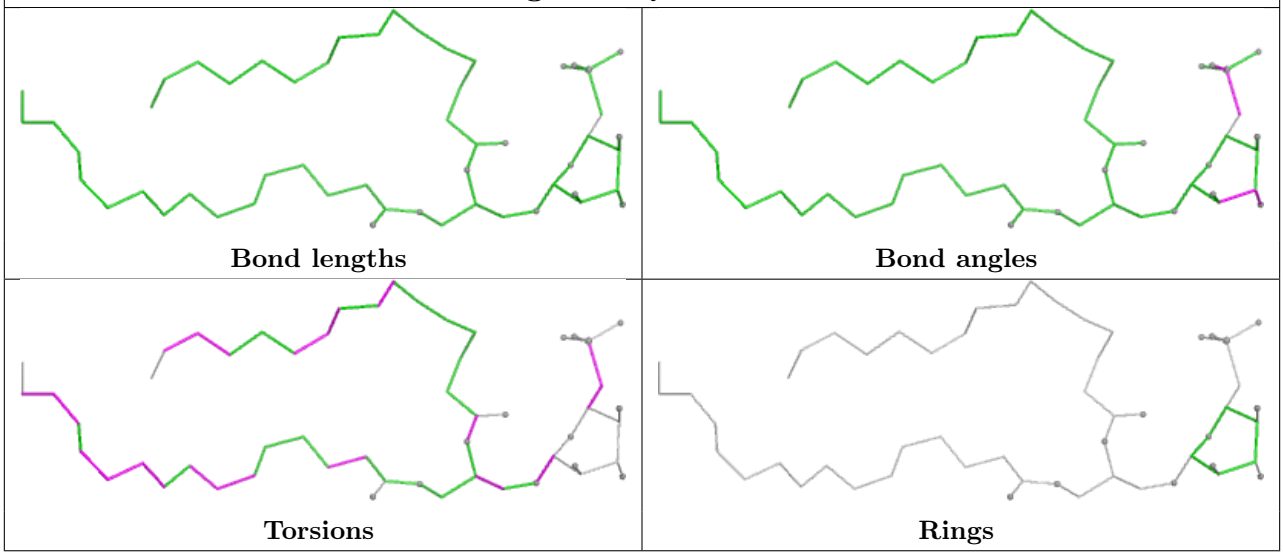
Ligand CHL y1 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

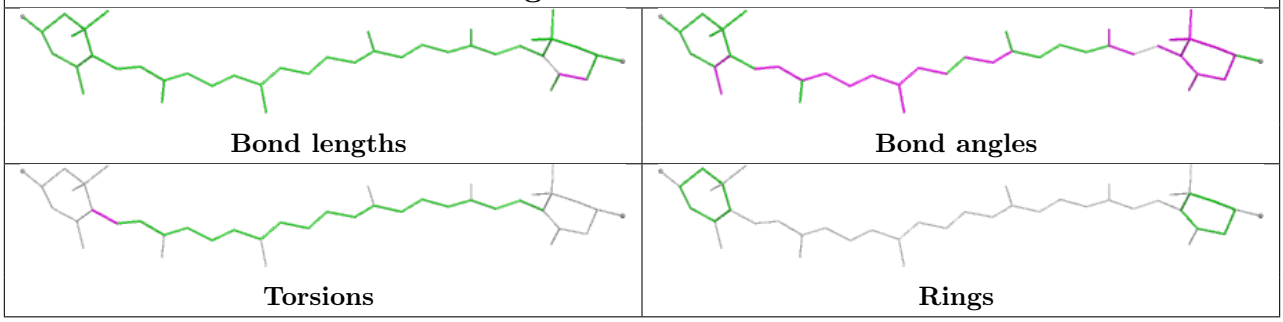
Ligand LHG d1 409



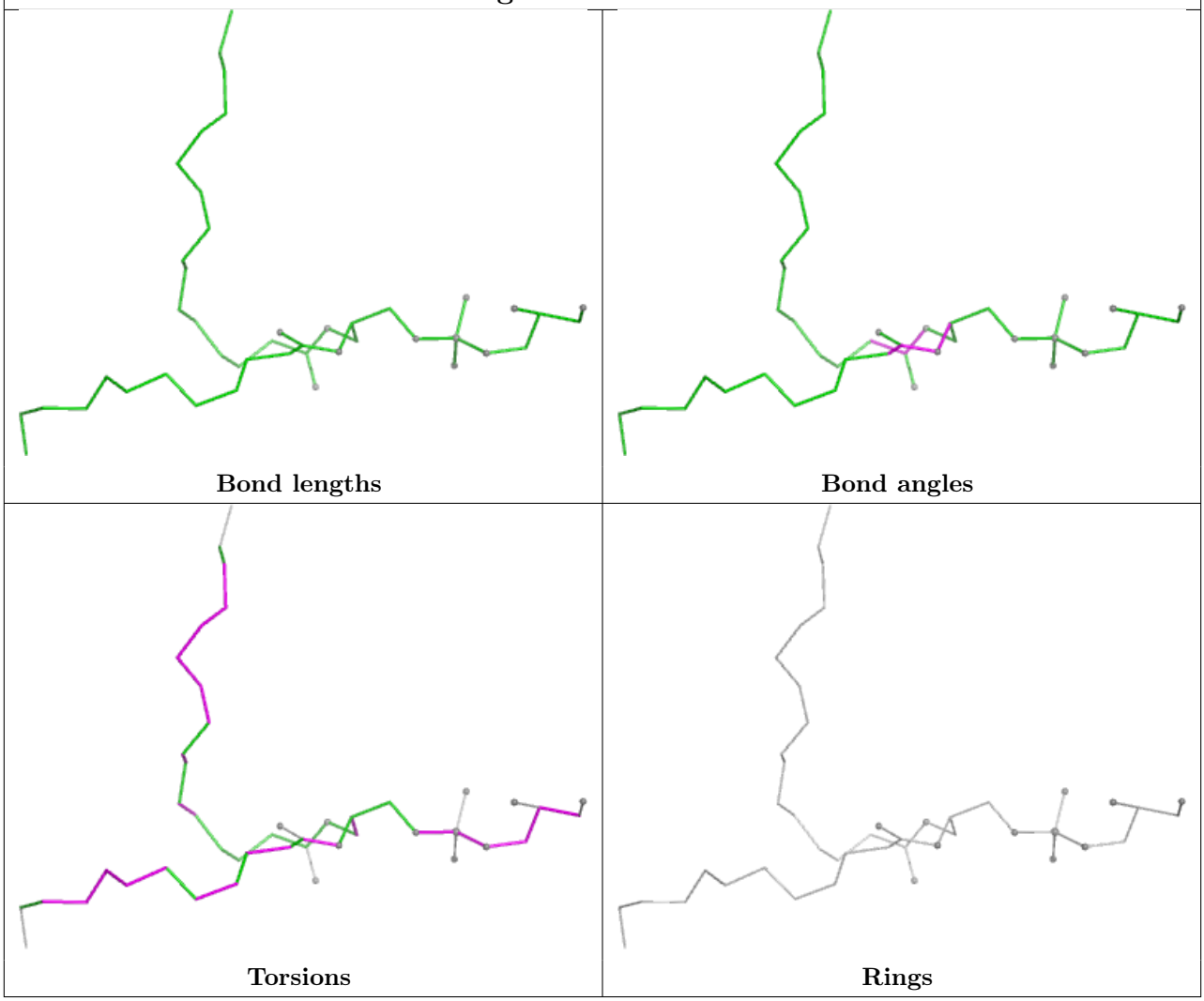
Ligand SQD B 626



Ligand LUT N 620



Ligand LHG s 624



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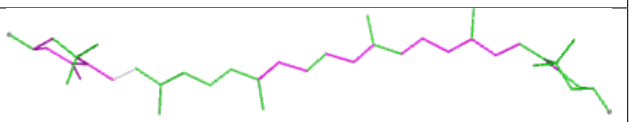
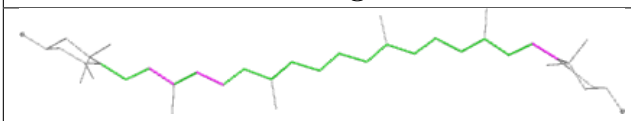
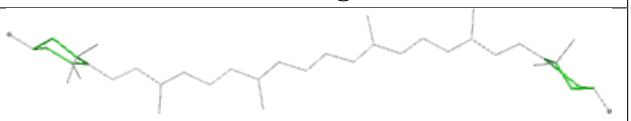
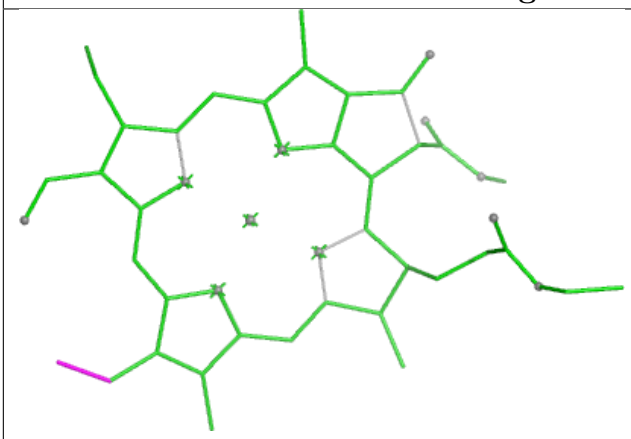
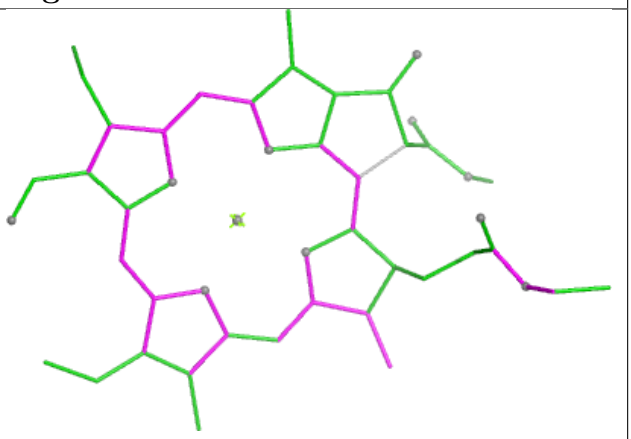
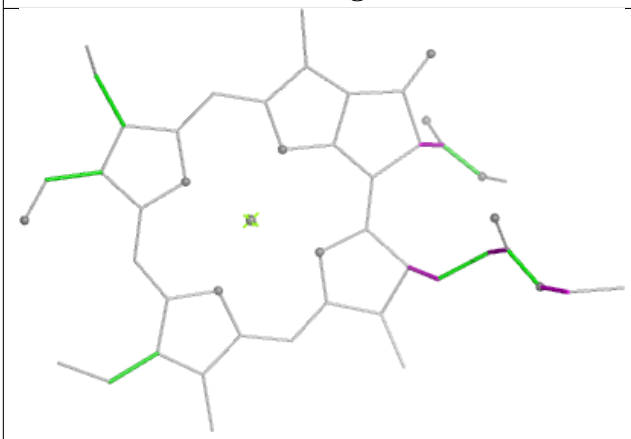
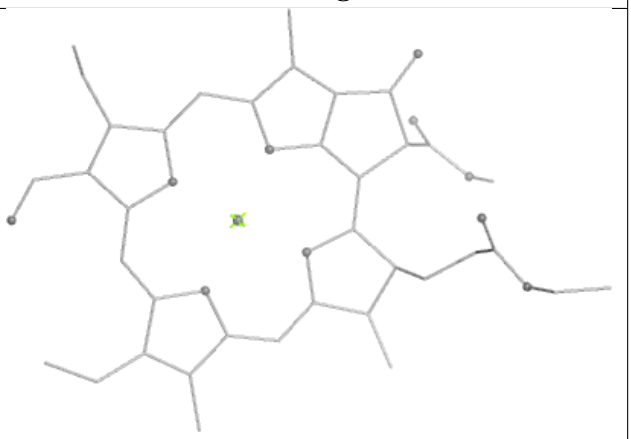
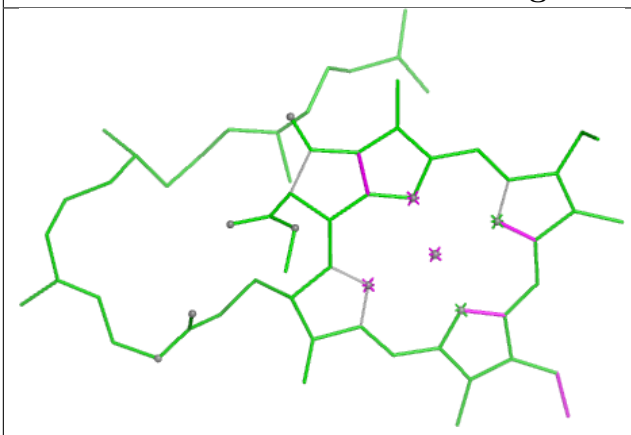
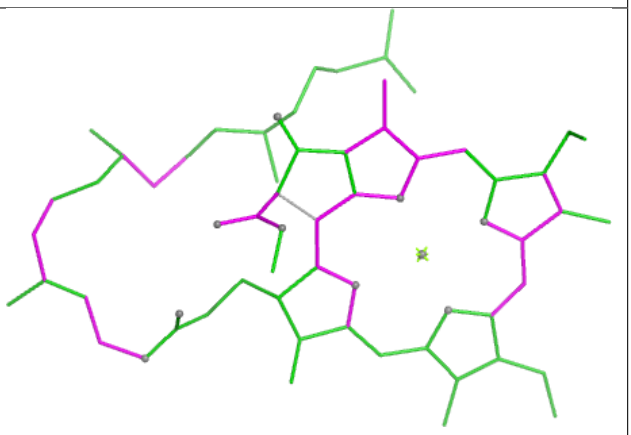
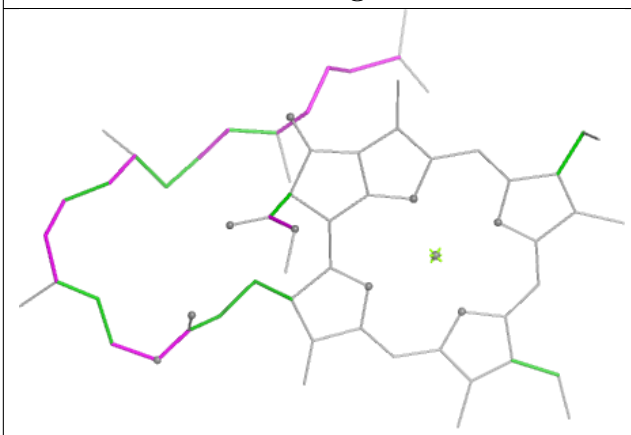
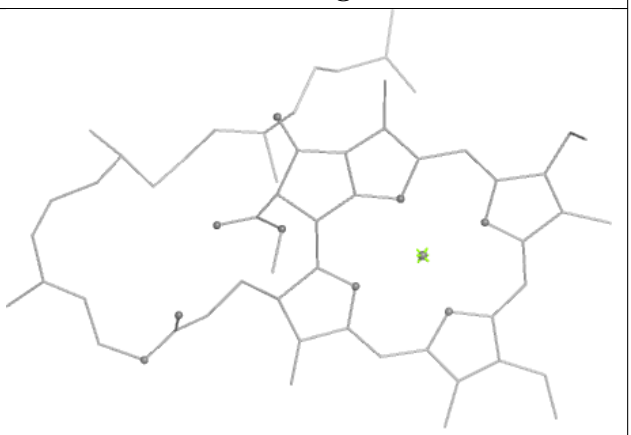
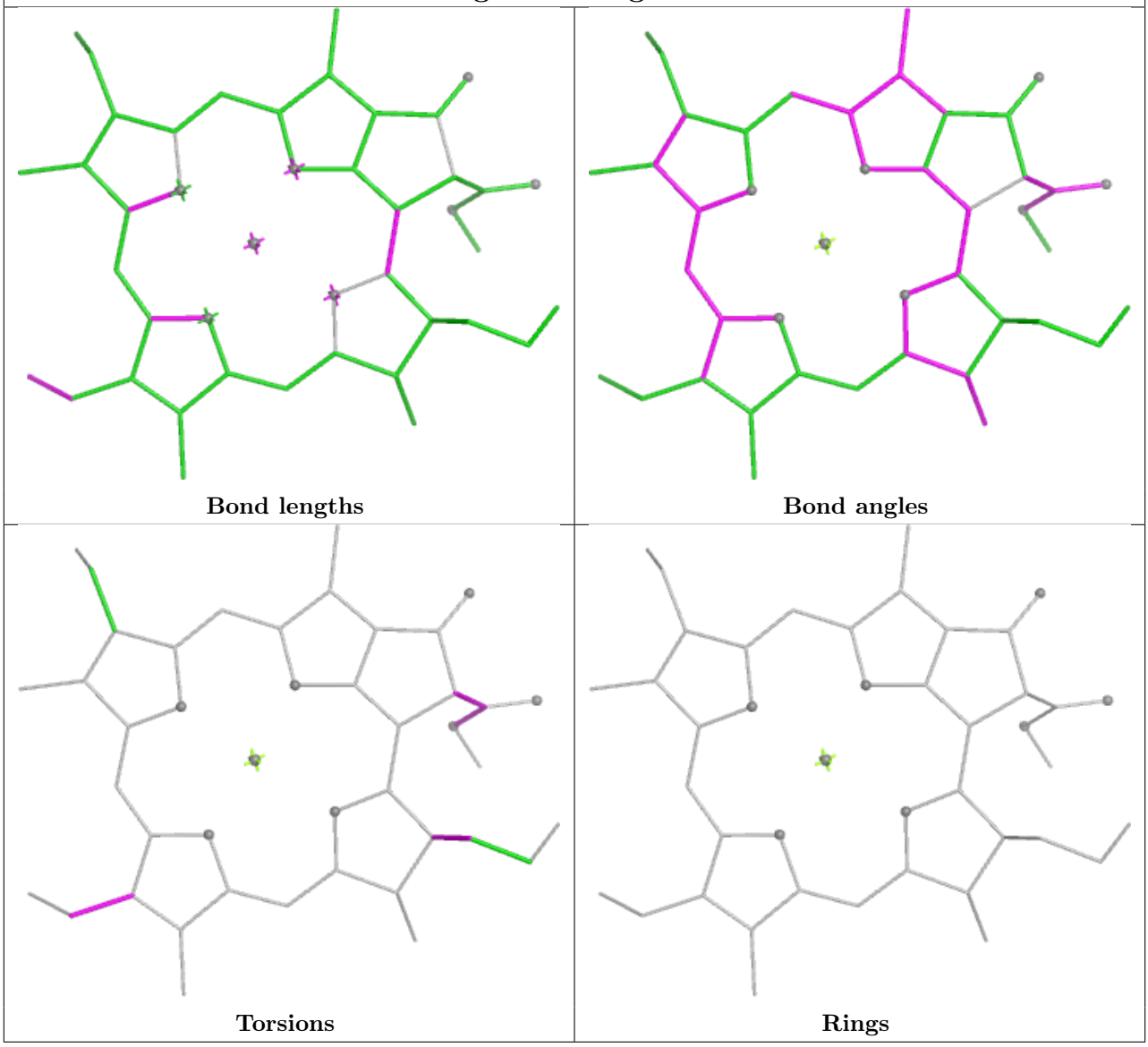
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL g1 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 612



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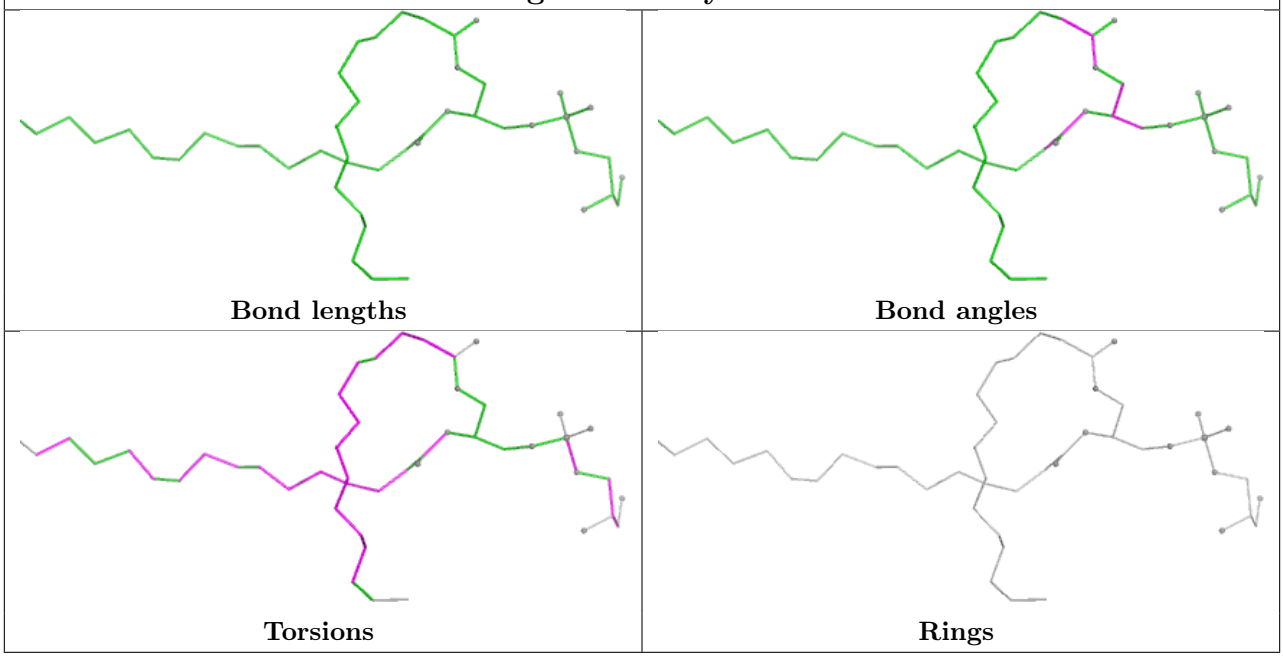

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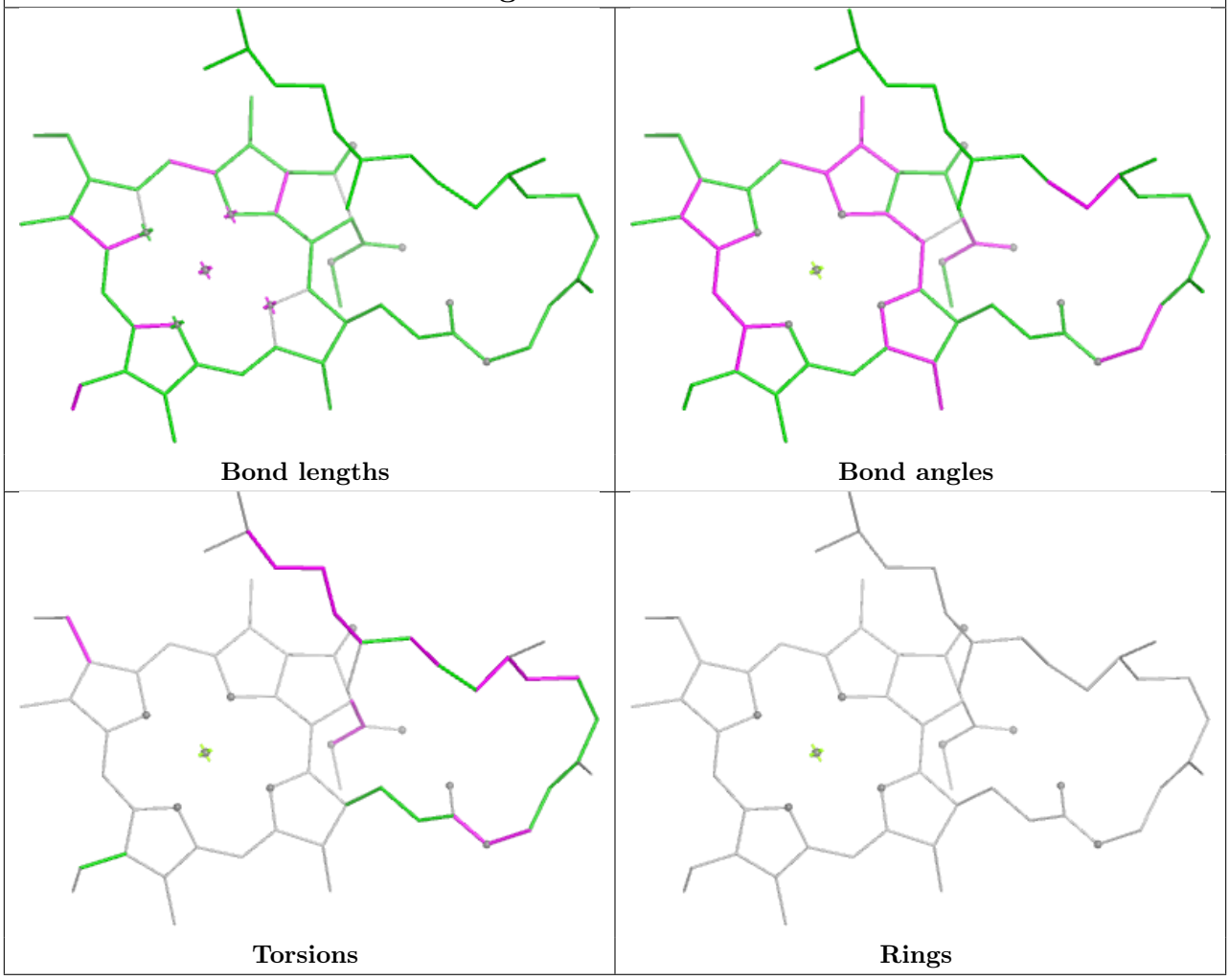

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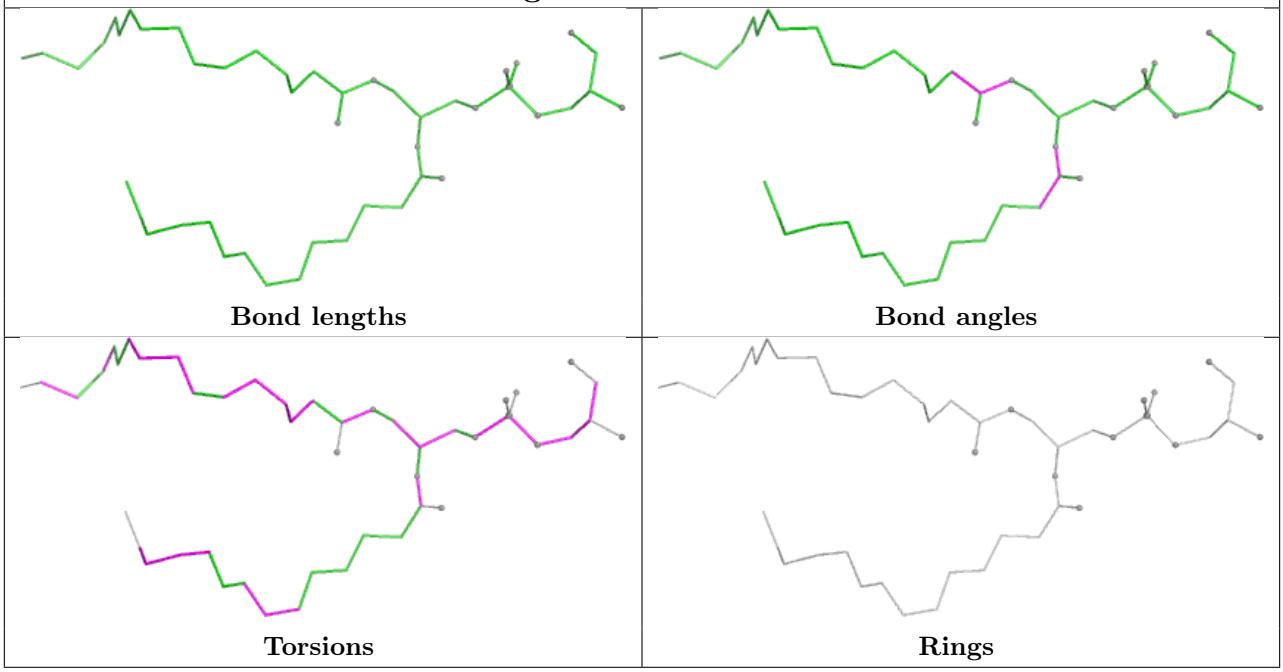

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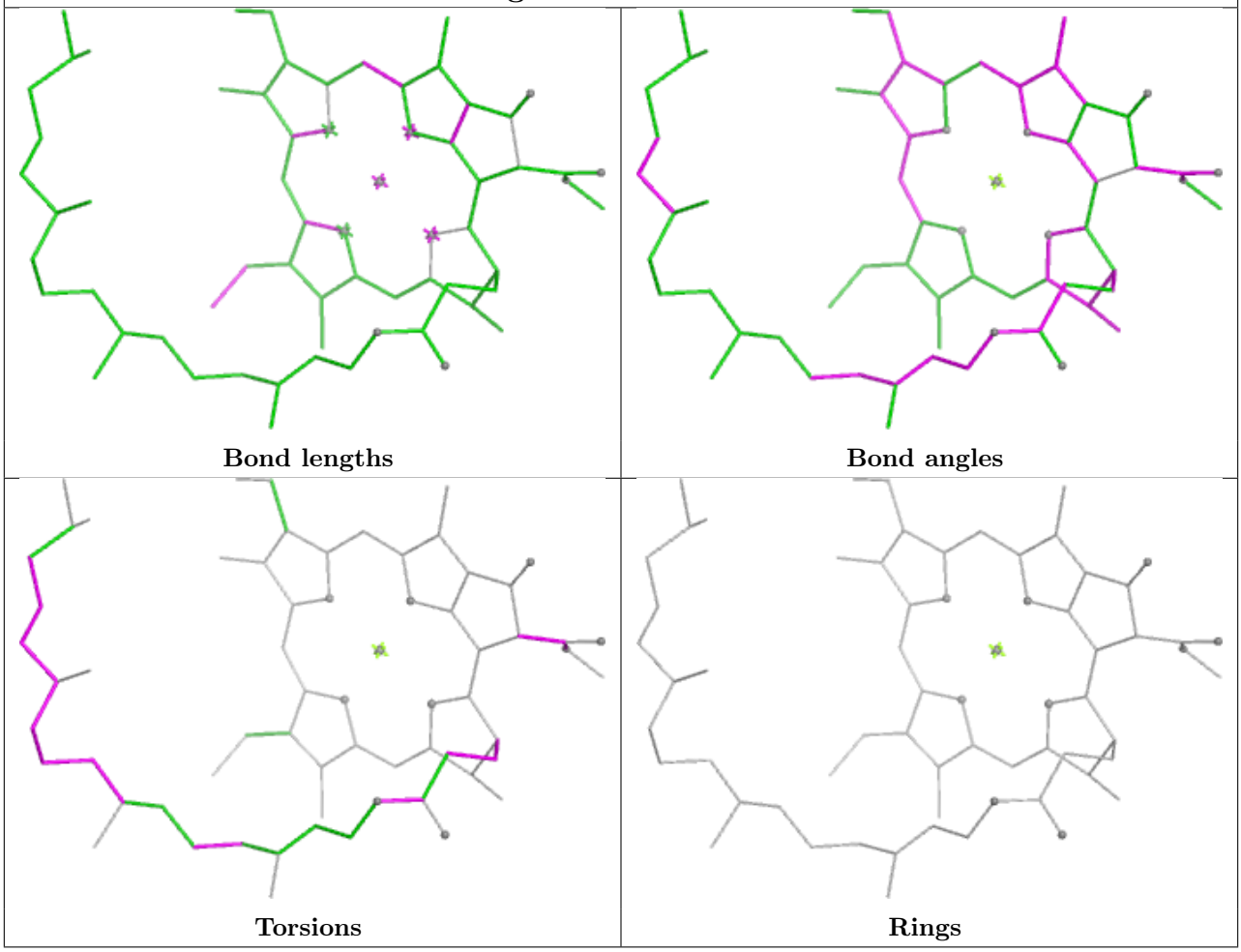

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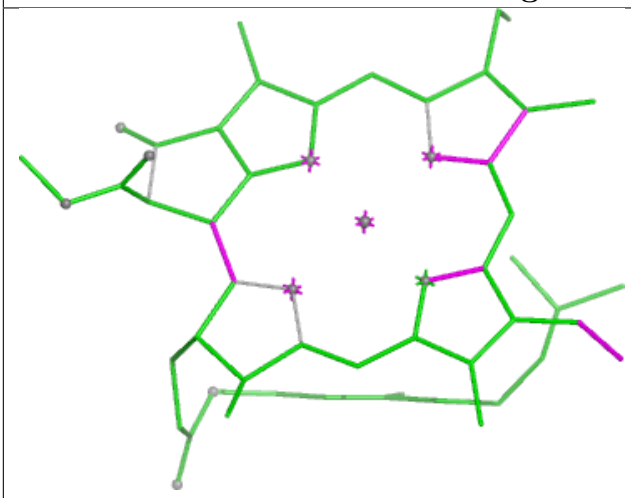
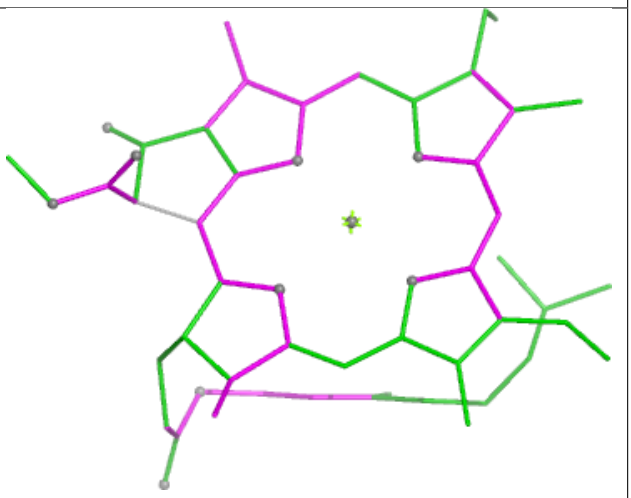
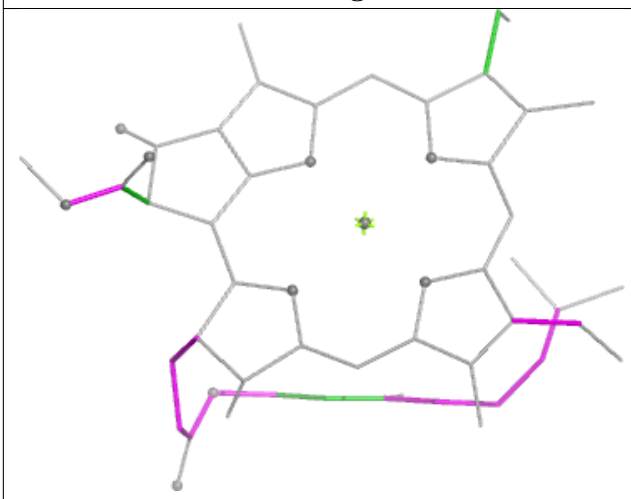
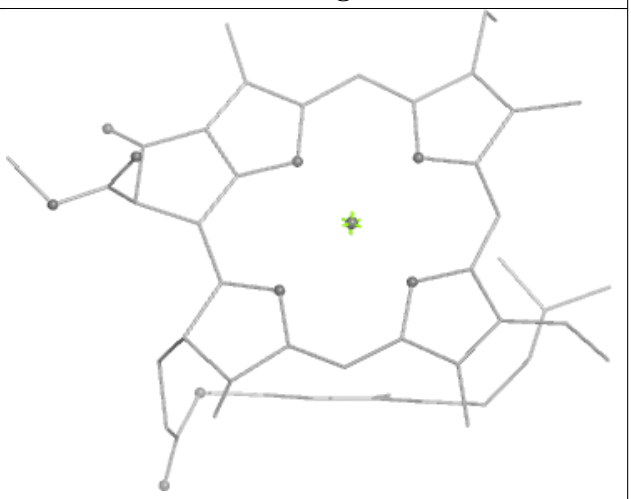
 Bond lengths	 Bond angles
 Torsions	 Rings

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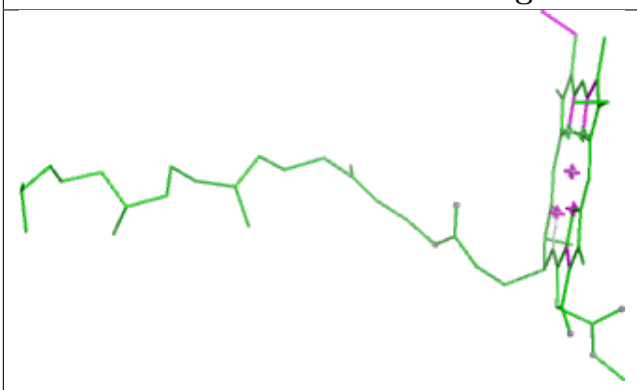
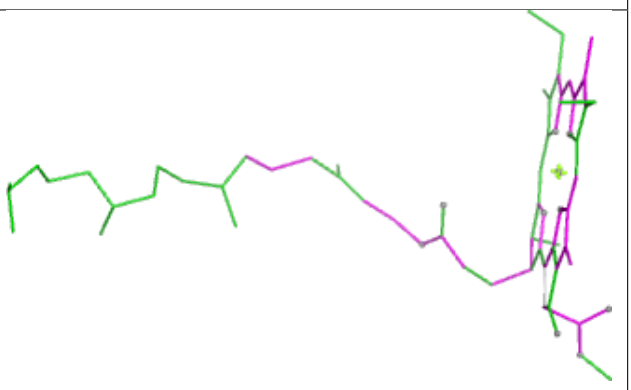
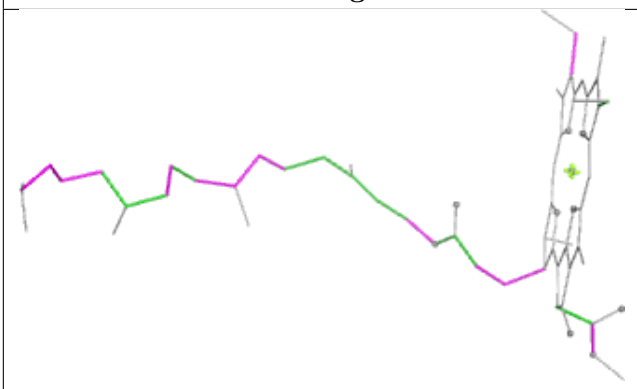
 Bond lengths	 Bond angles
 Torsions	Rings

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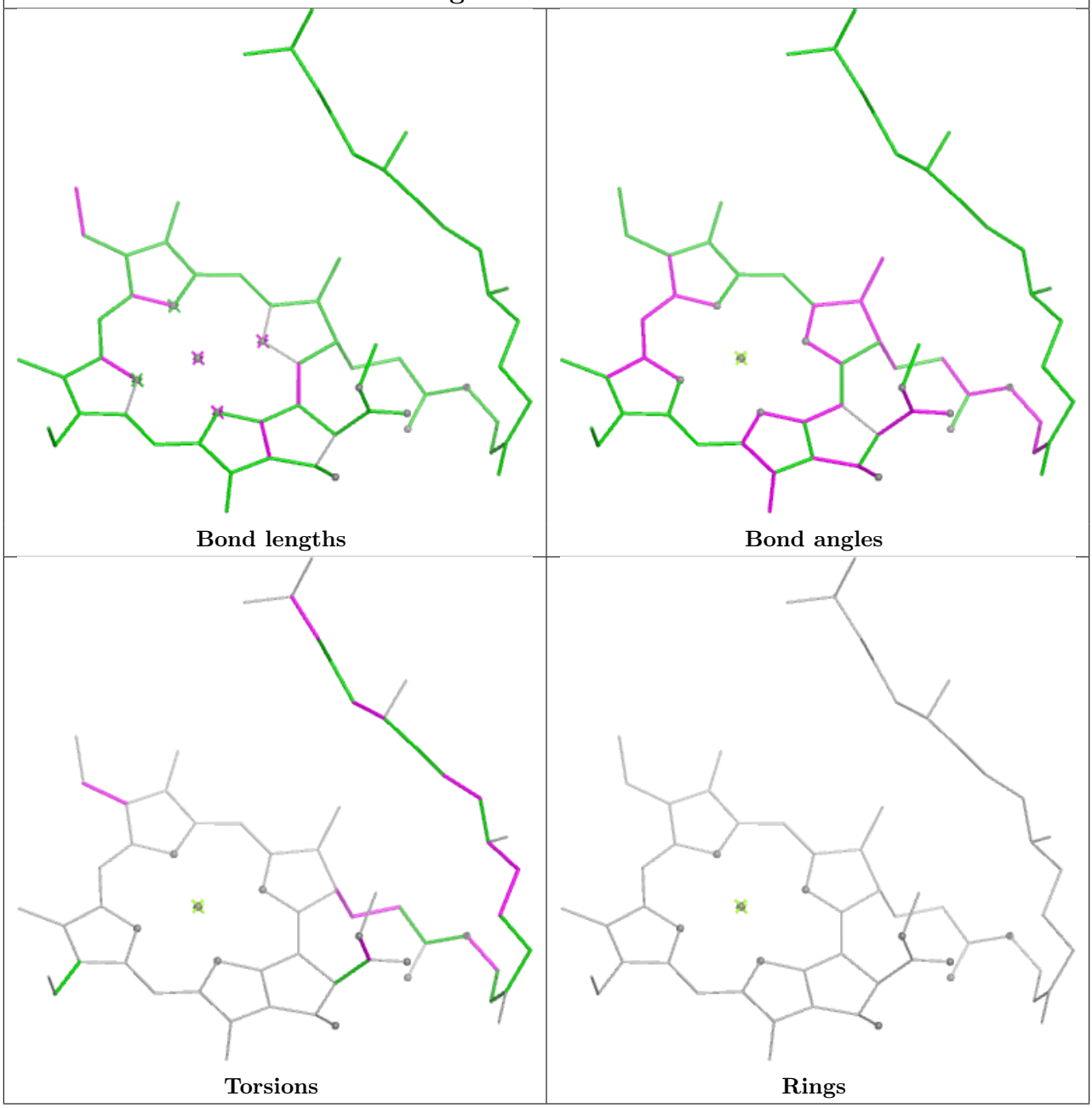
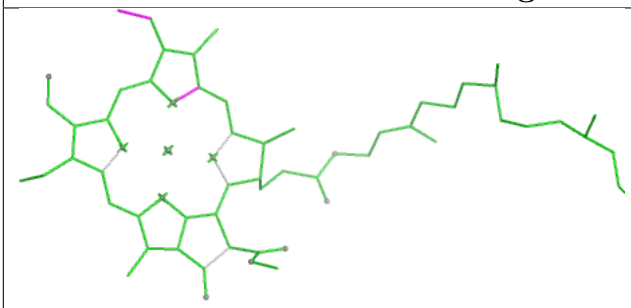
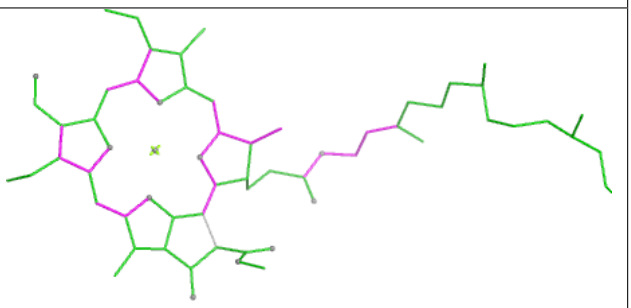


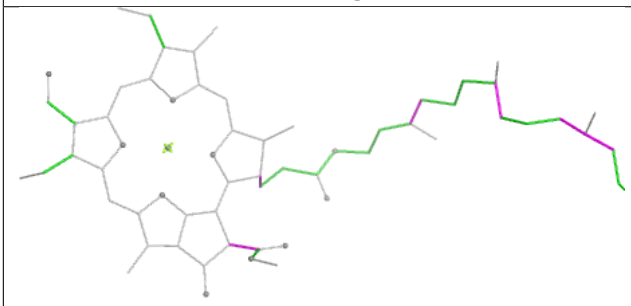
Ligand CHL n1 601



Bond lengths



Bond angles



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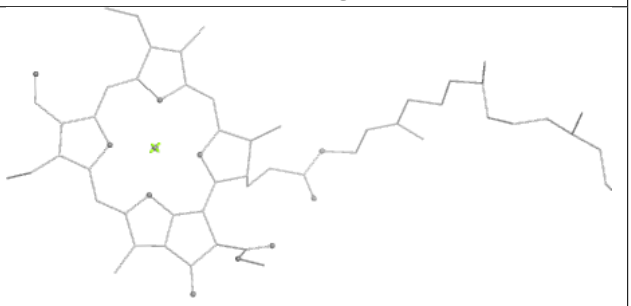
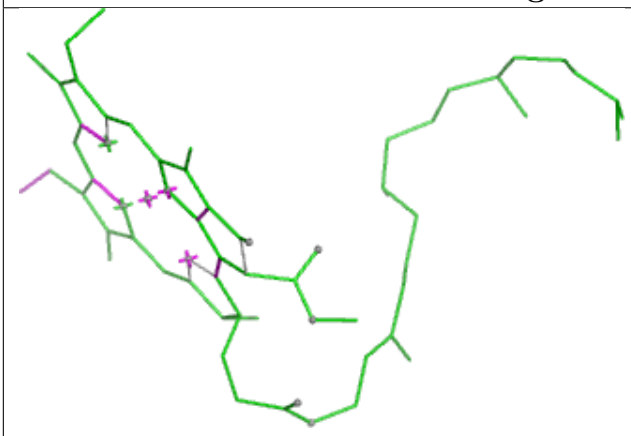


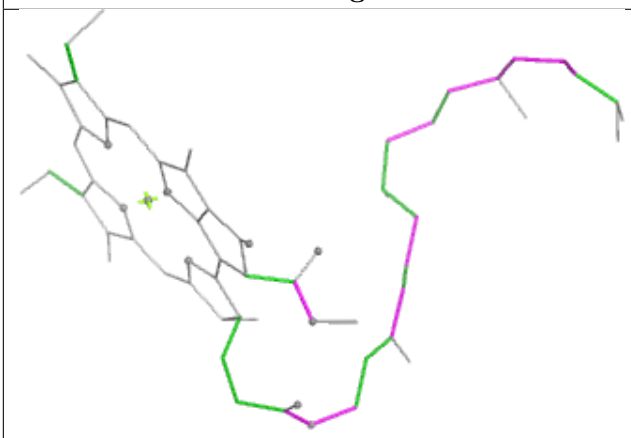
Rings

Ligand CLA b 614



Bond lengths

Bond angles



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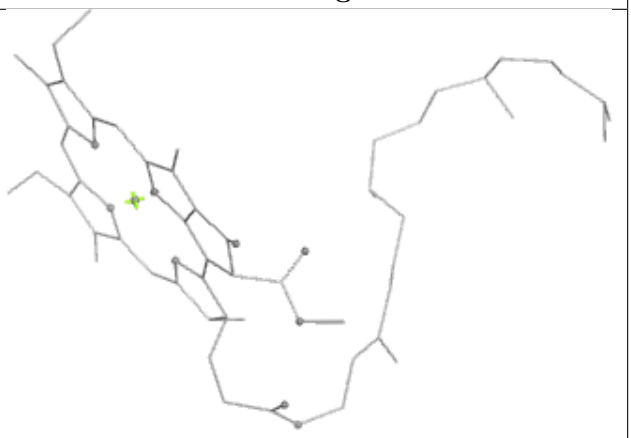
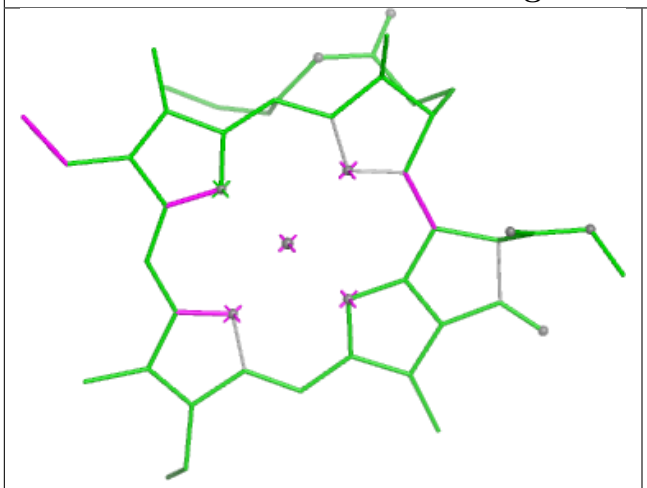
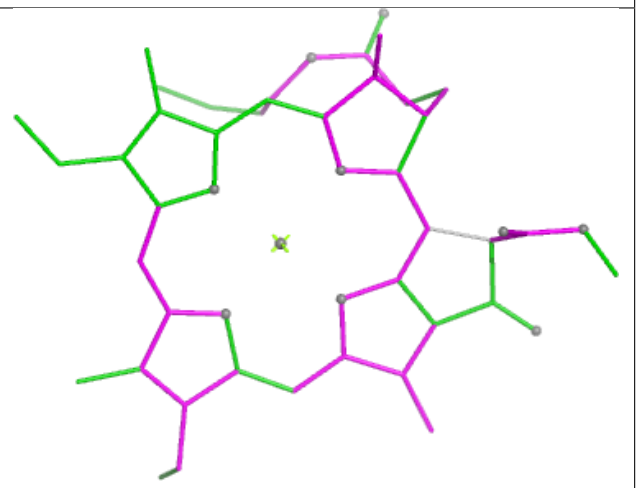


Rings

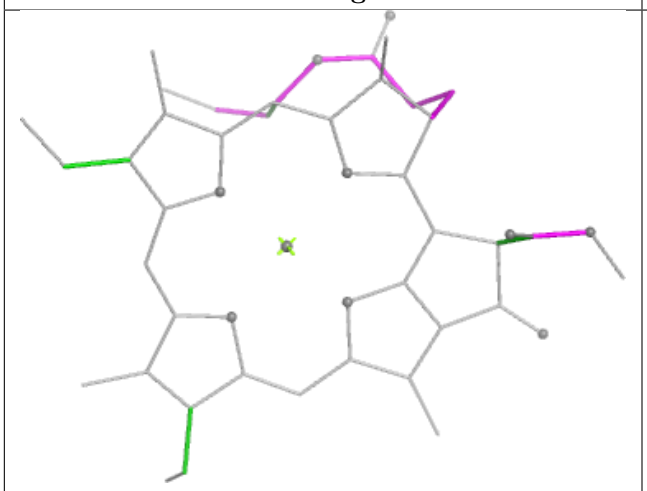
Ligand CLA G 614



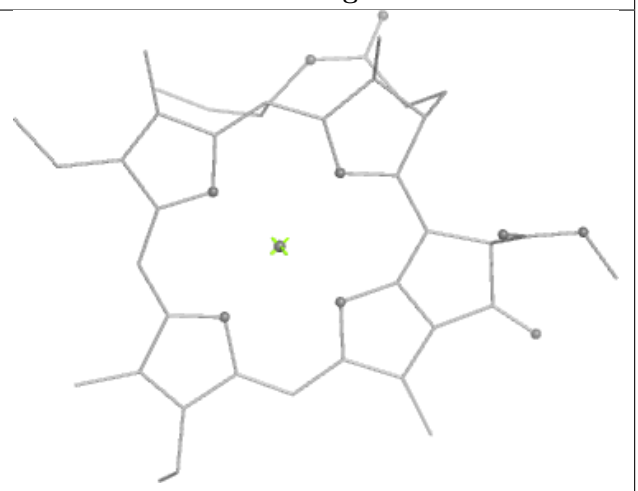
Bond lengths



Bond angles



Torsions

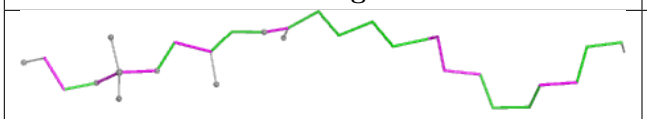


Rings

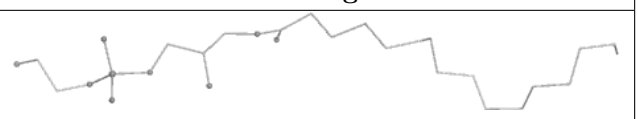
Ligand LPX S 625

Bond lengths

Bond angles

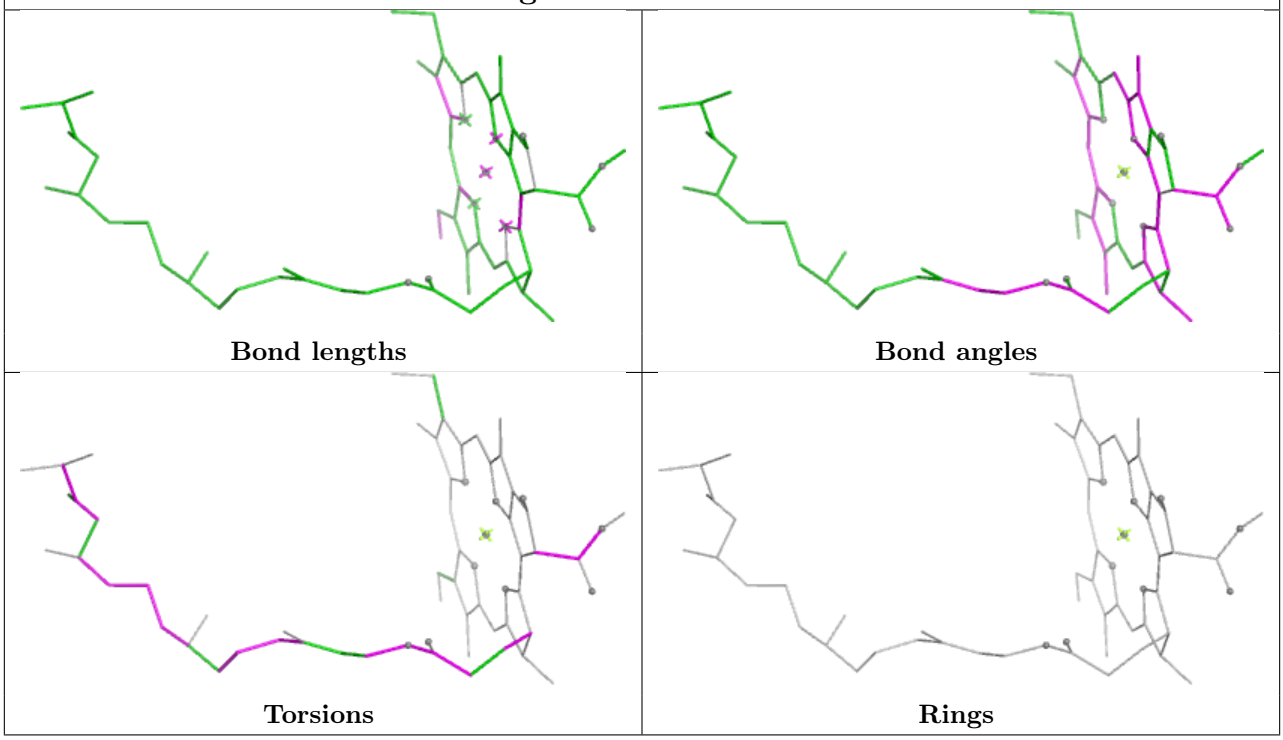


Torsions

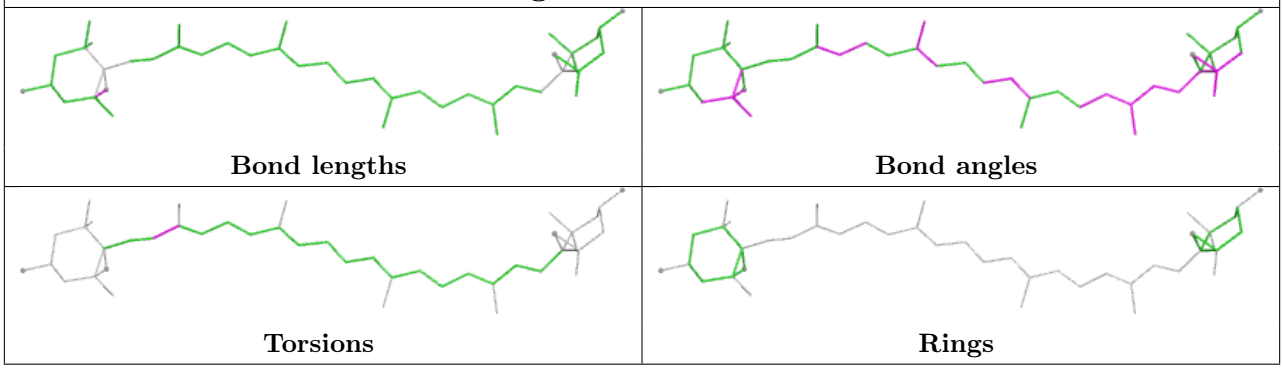


Rings

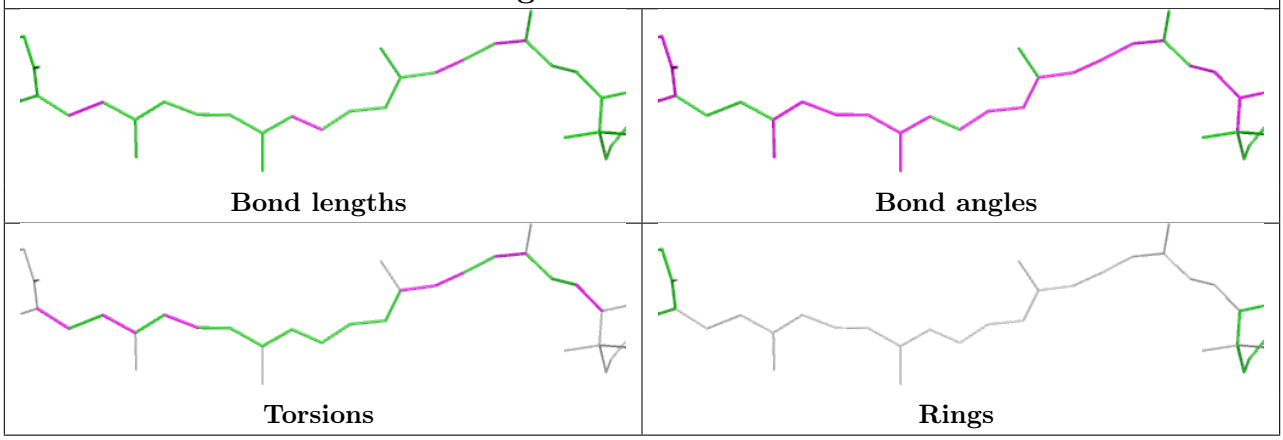
Ligand CLA b1 608



Ligand XAT r 621



Ligand BCR b1 618



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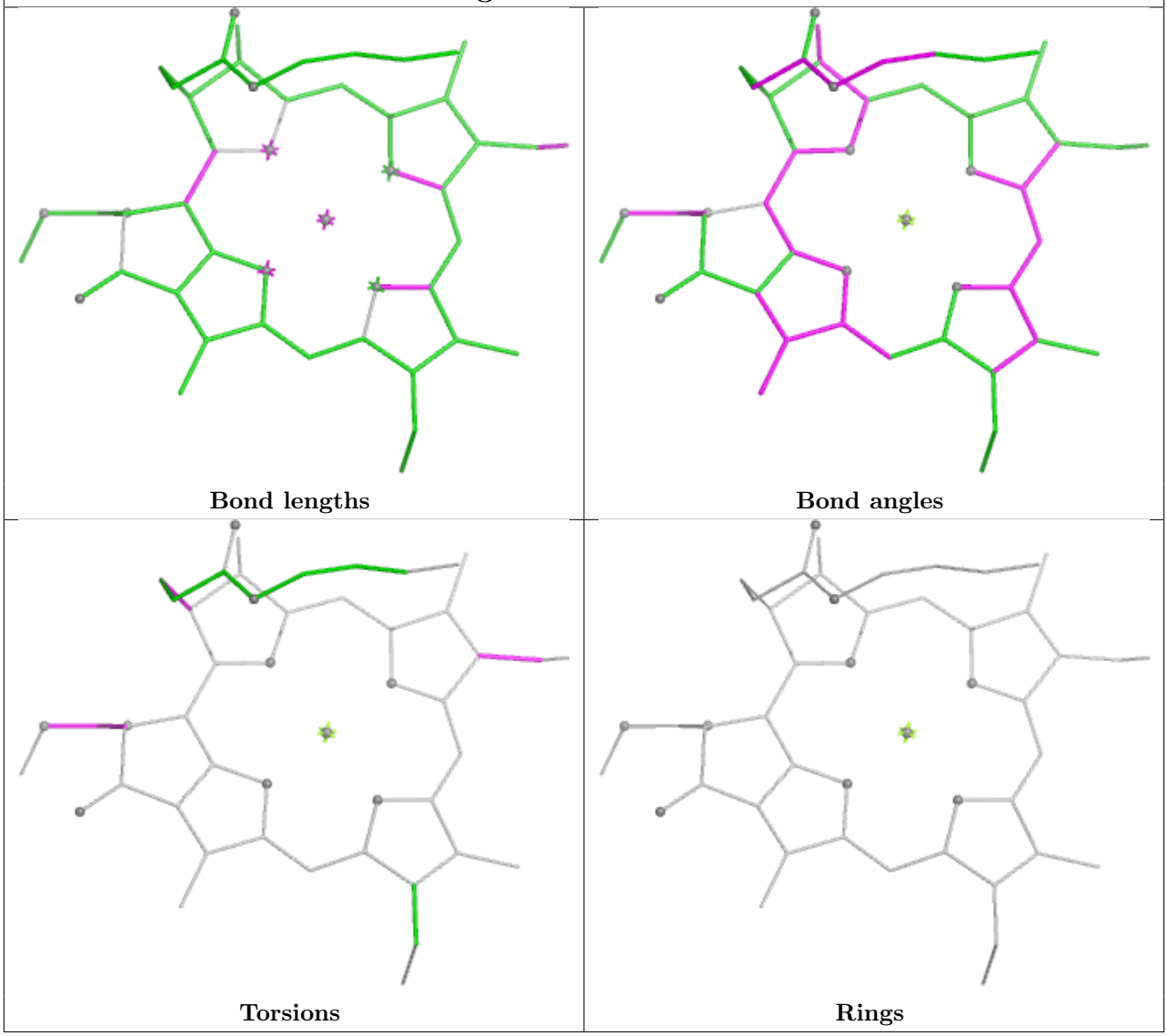
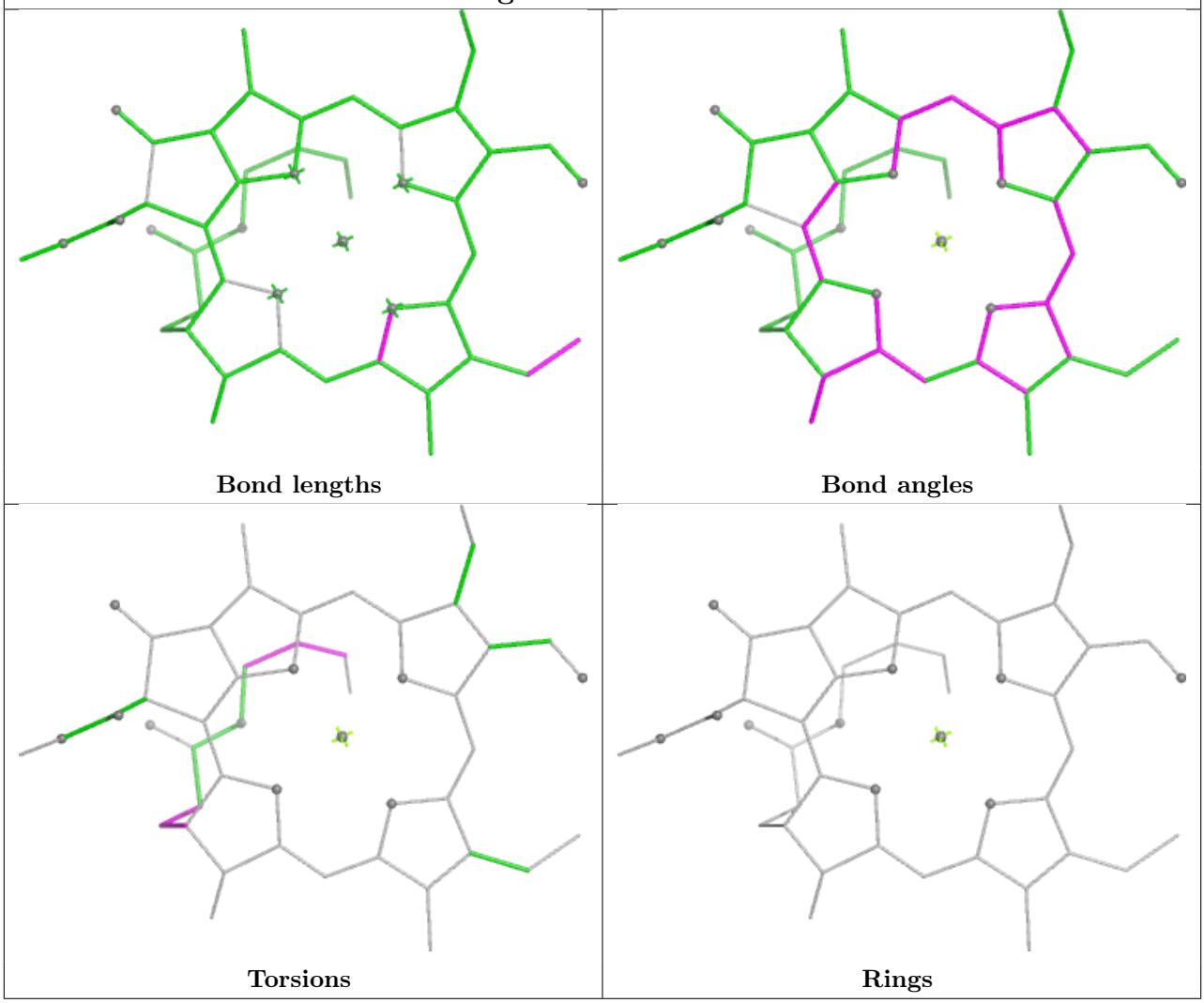
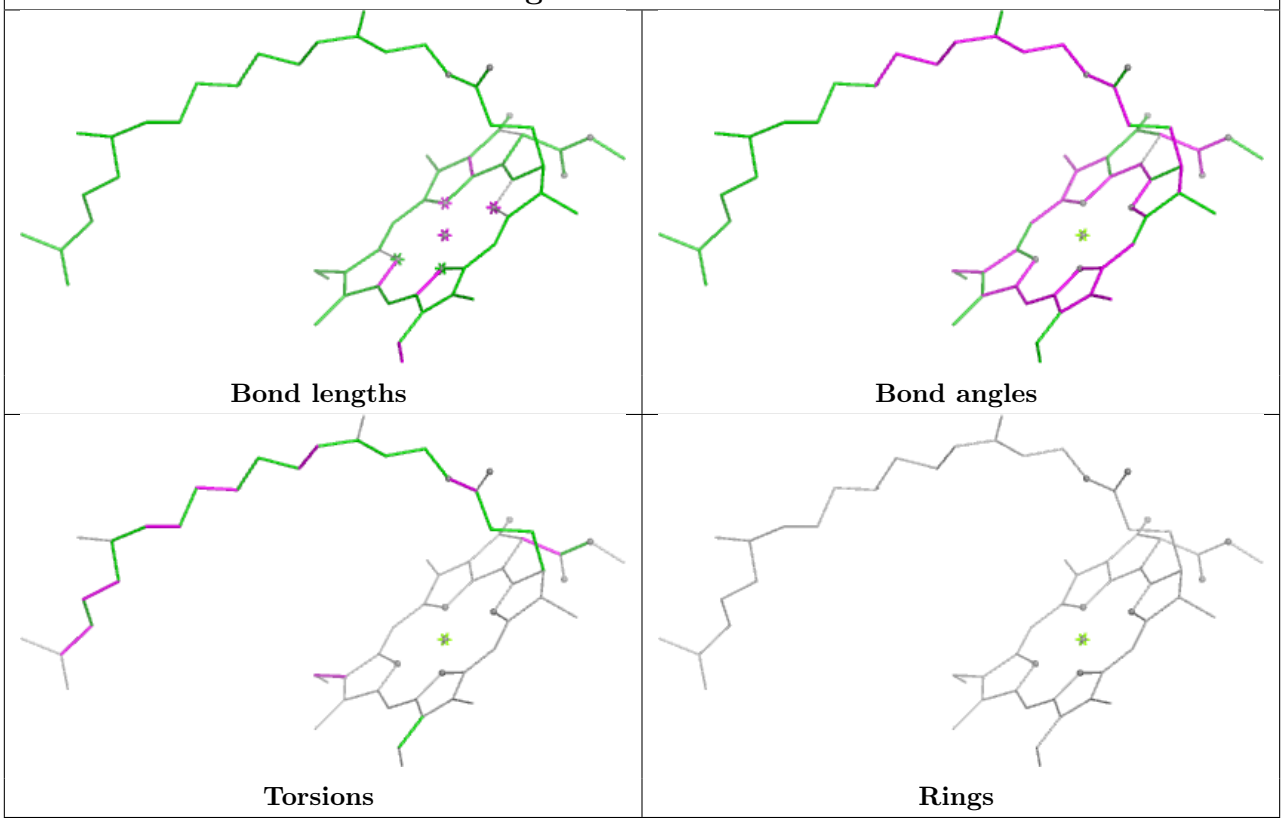


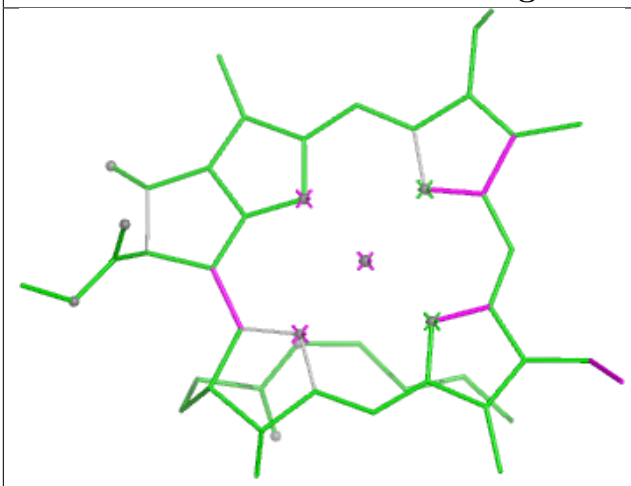
Ligand CHL r 607



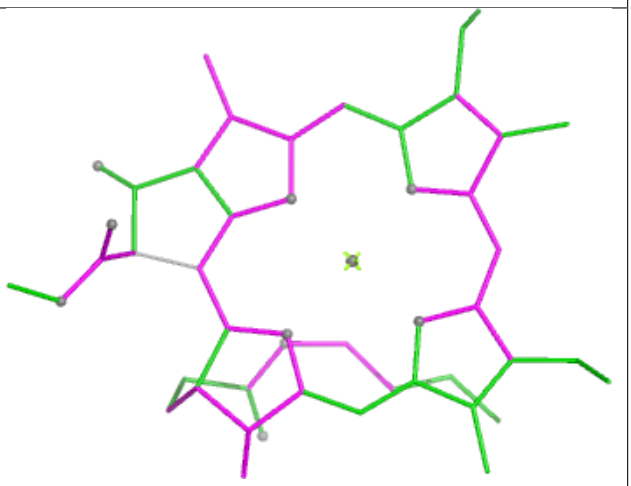
Ligand CLA C 508



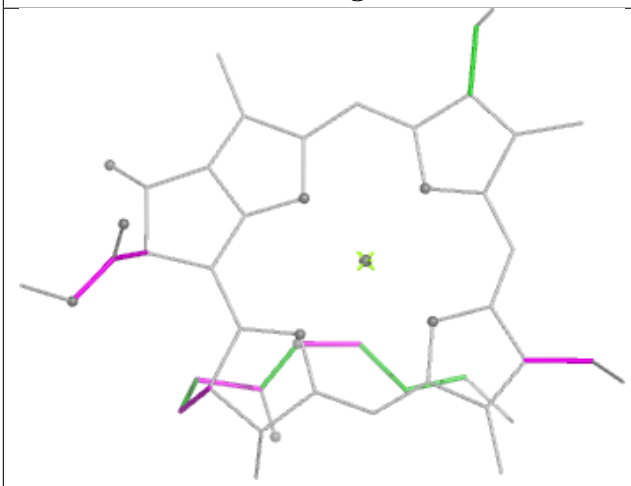
Ligand CLA n1 614



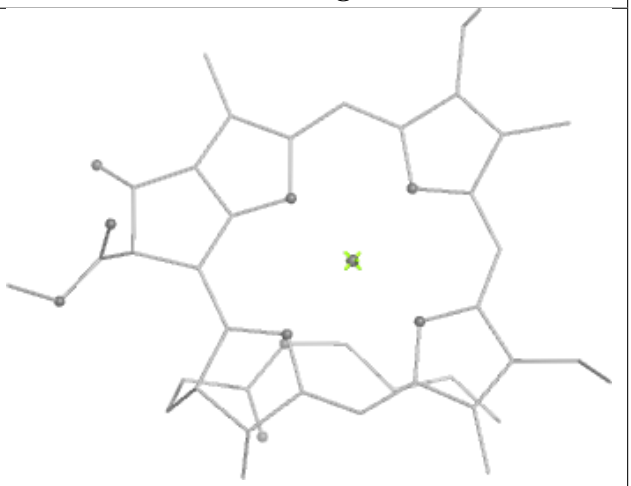
Bond lengths



Bond angles

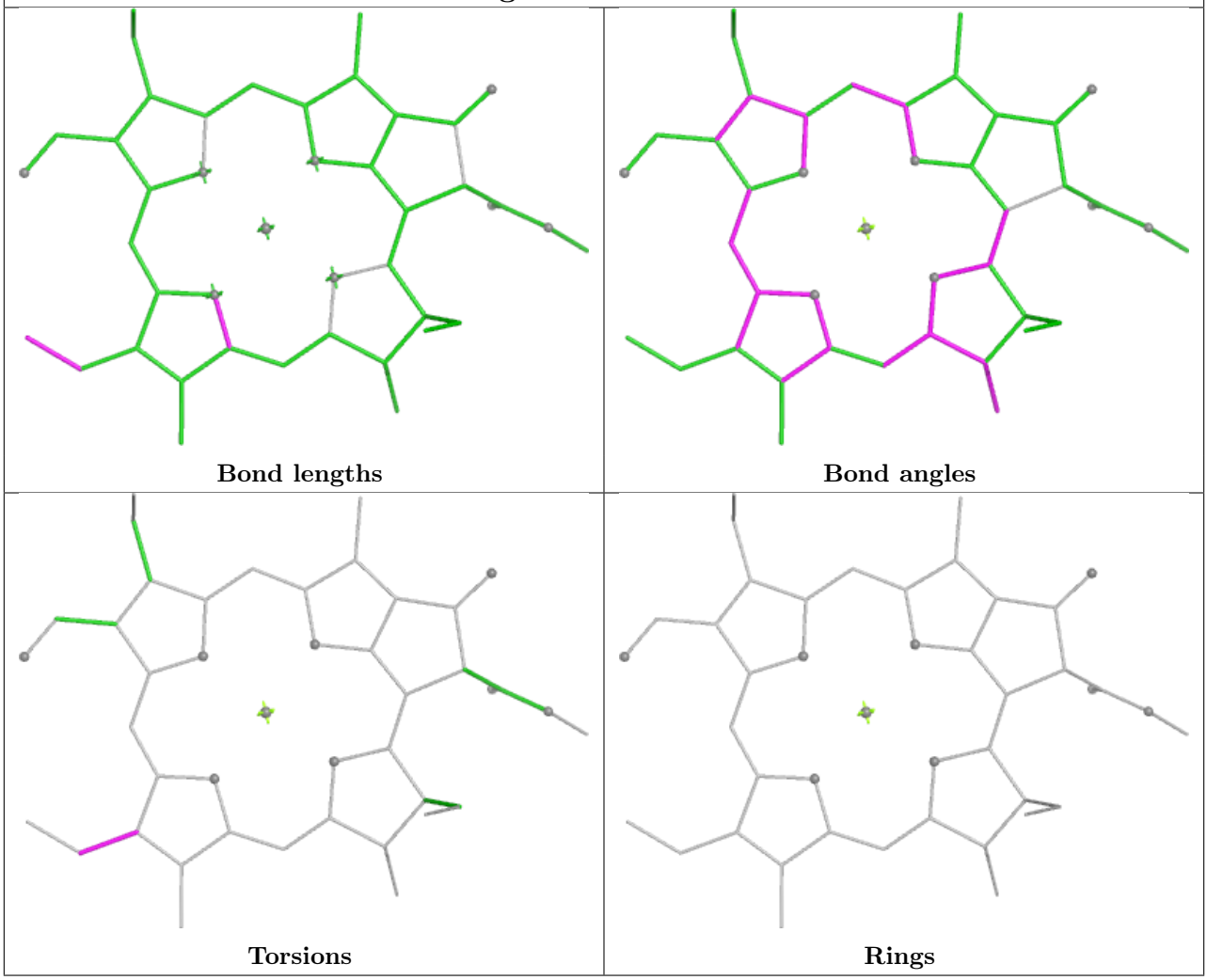


Torsions

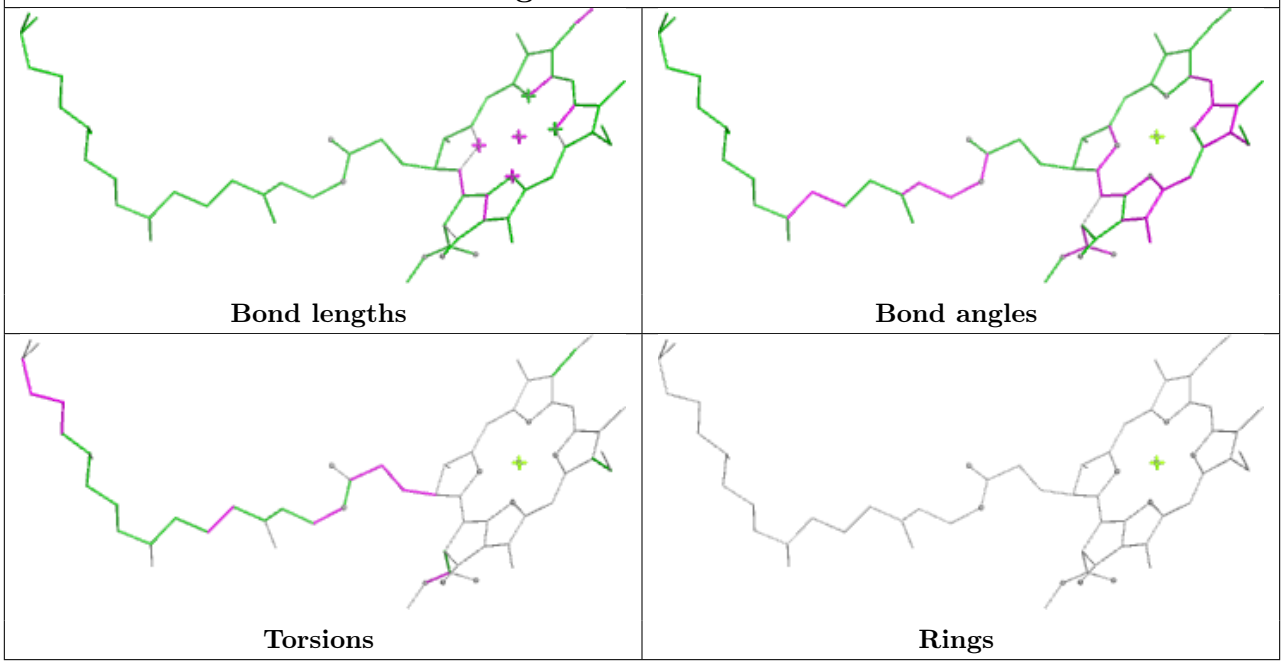


Rings

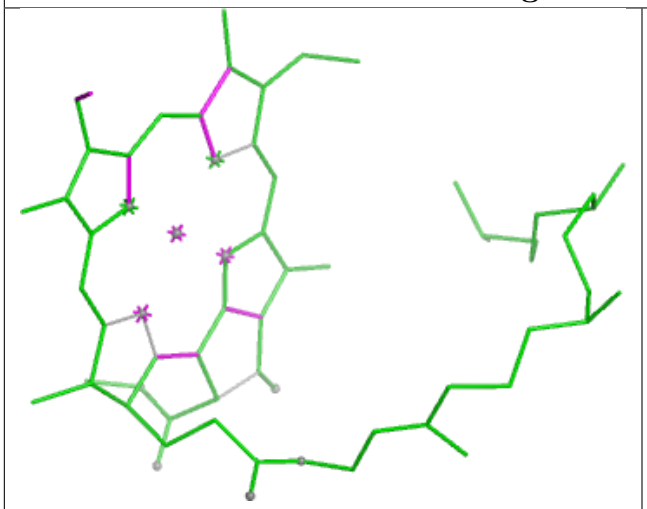
Ligand CHL s 607



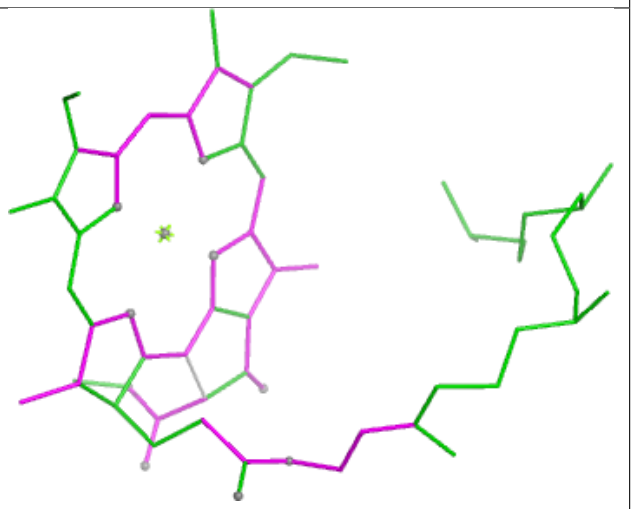
Ligand CLA A1 405



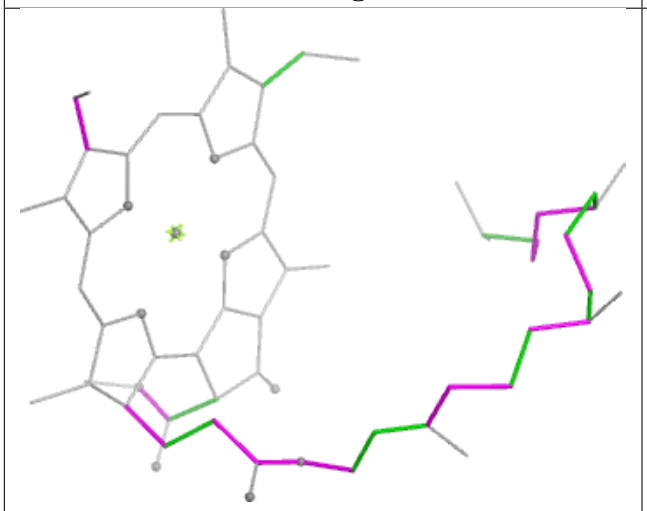
Ligand CLA c1 503



Bond lengths



Bond angles



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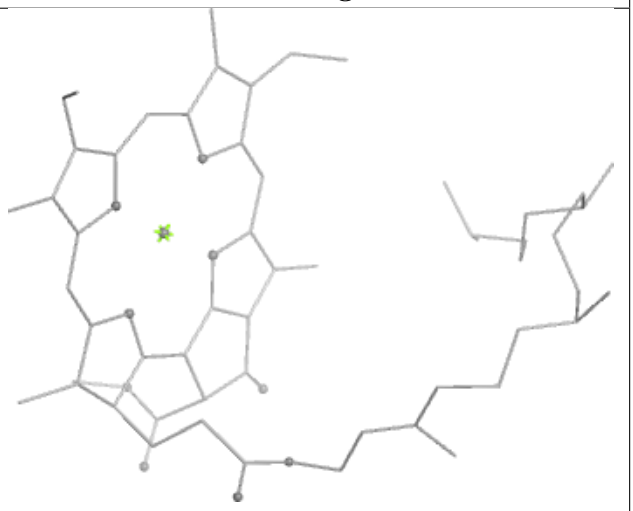
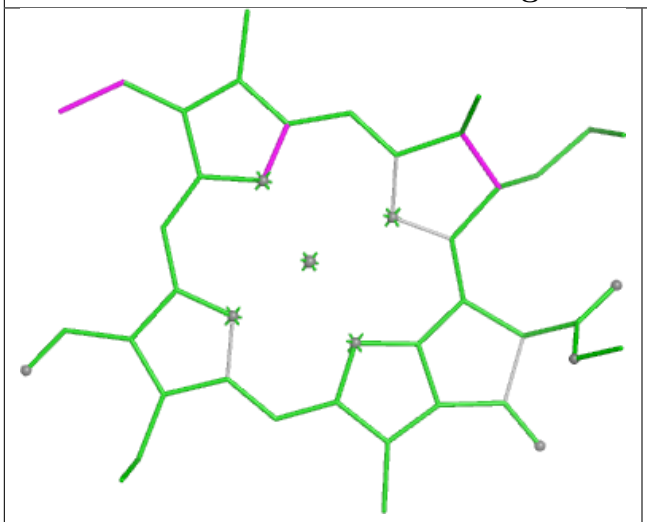
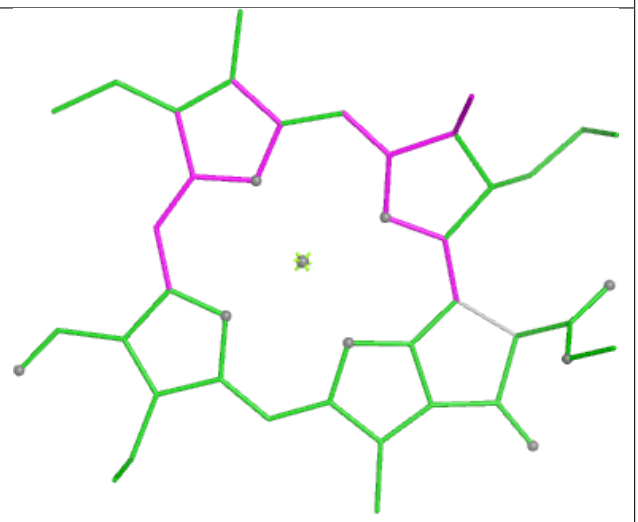


Rings

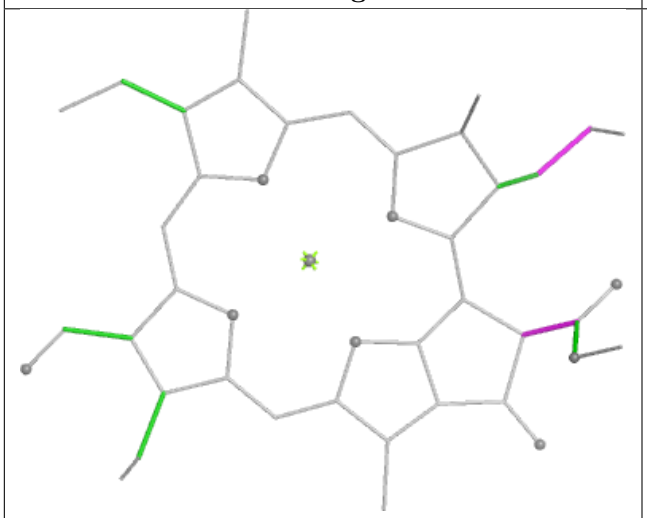
Ligand CHL r1 606



Bond lengths



Bond angles



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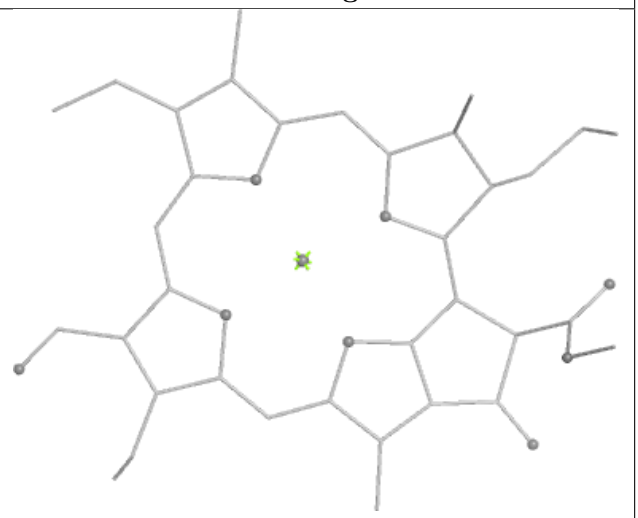
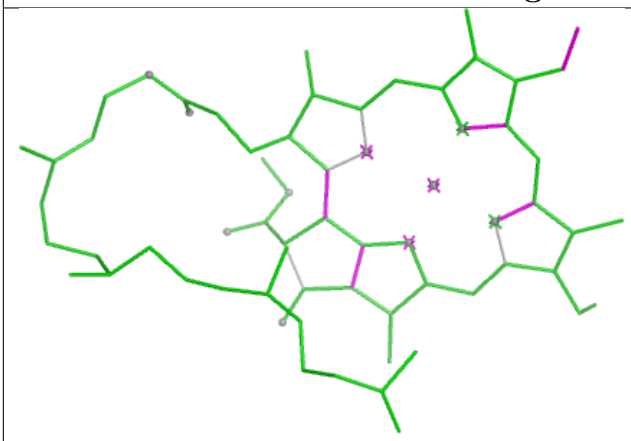
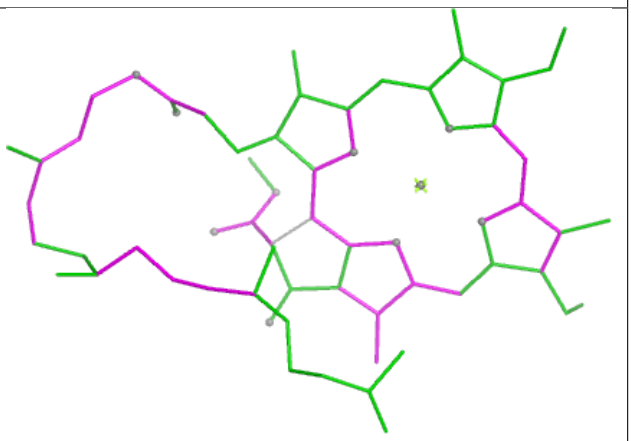


Rings

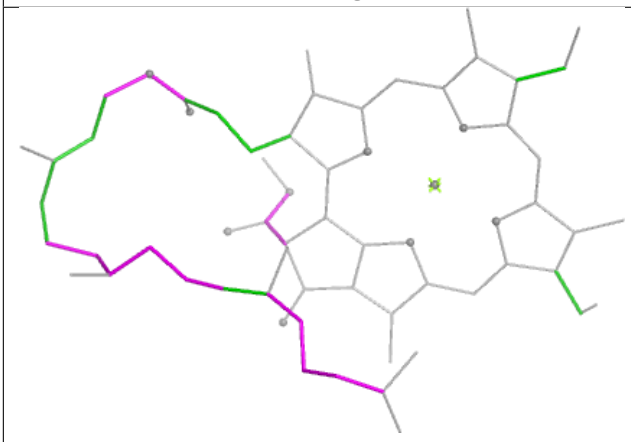
Ligand CLA C 509



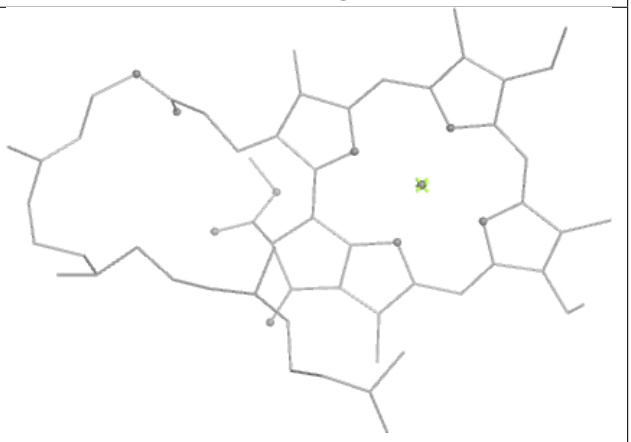
Bond lengths



Bond angles

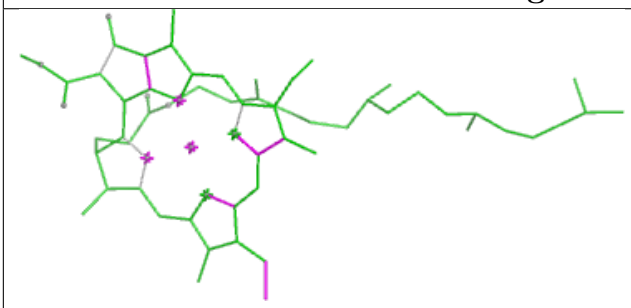


Torsions



Rings

Ligand CLA b 615



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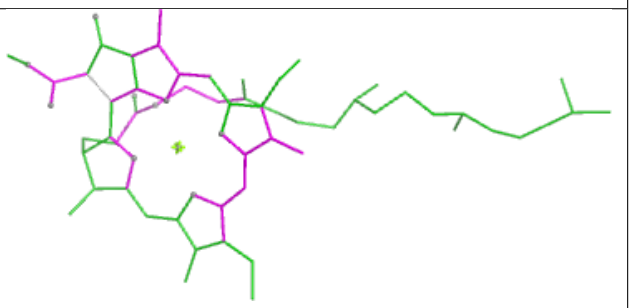

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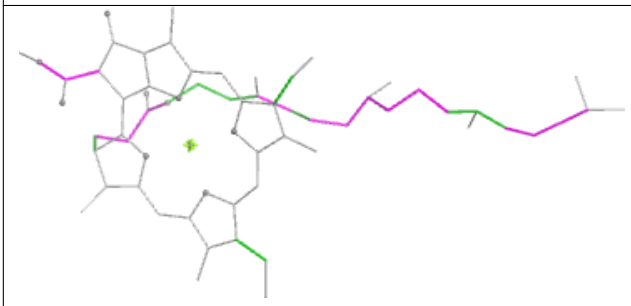

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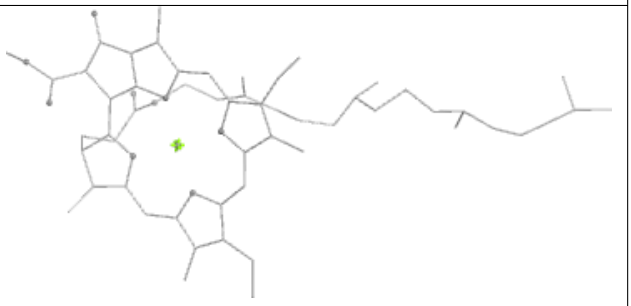
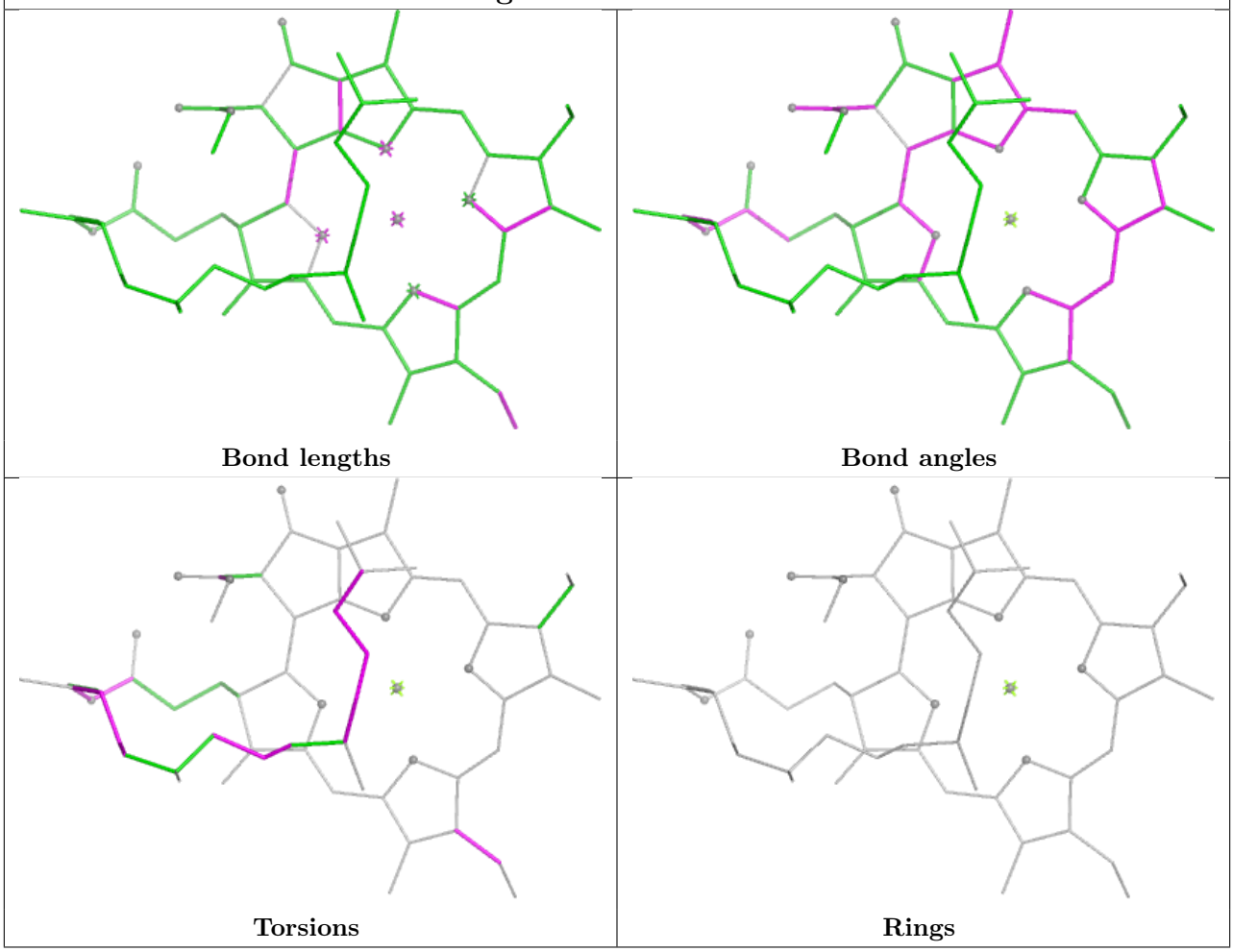
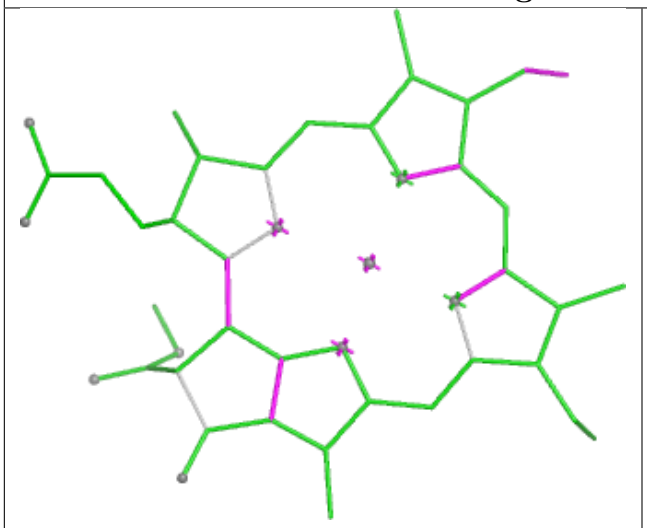


Rings

Ligand CLA C1 510



Ligand CLA N1 612



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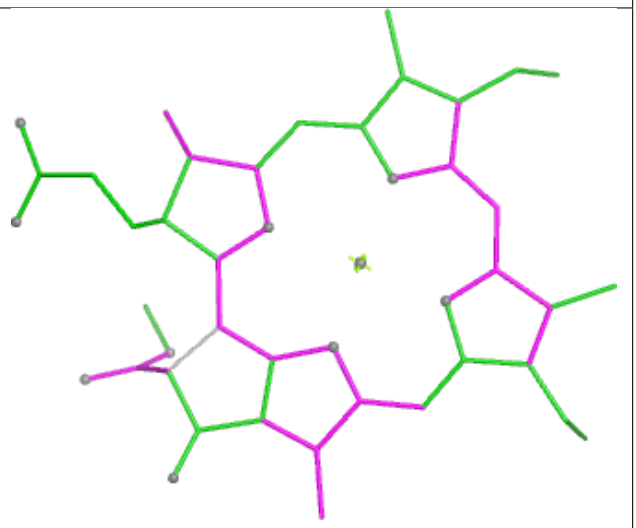
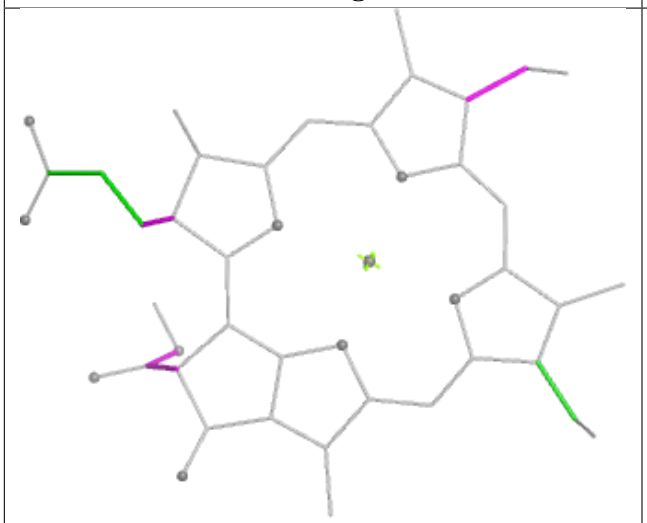


Bond angles



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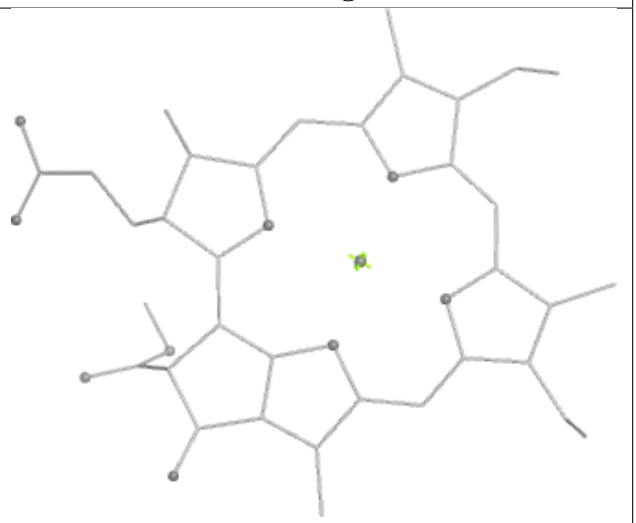
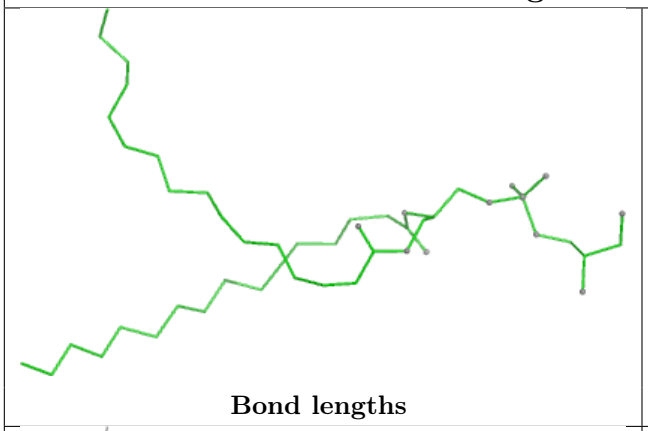


Rings

Ligand LHG d 409



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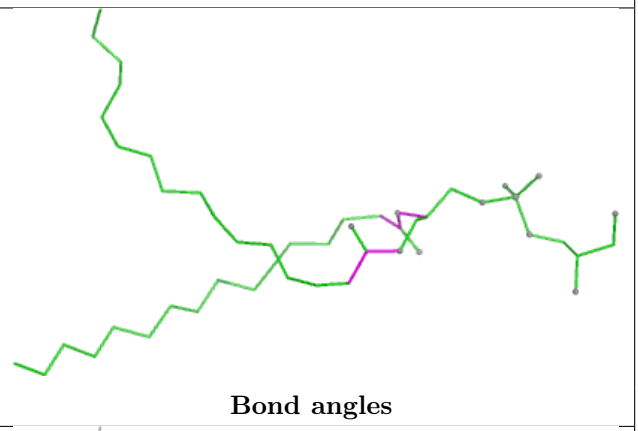

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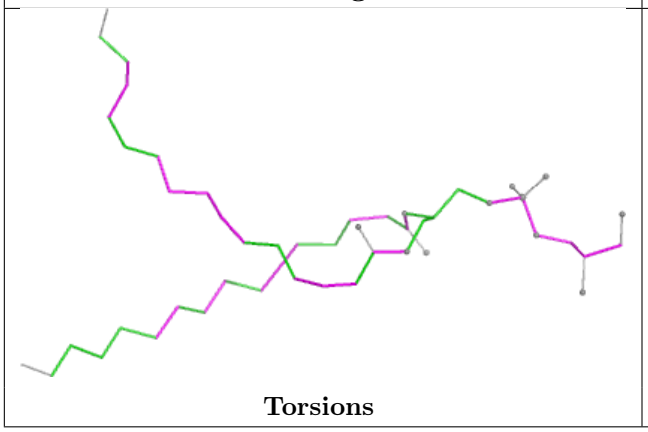

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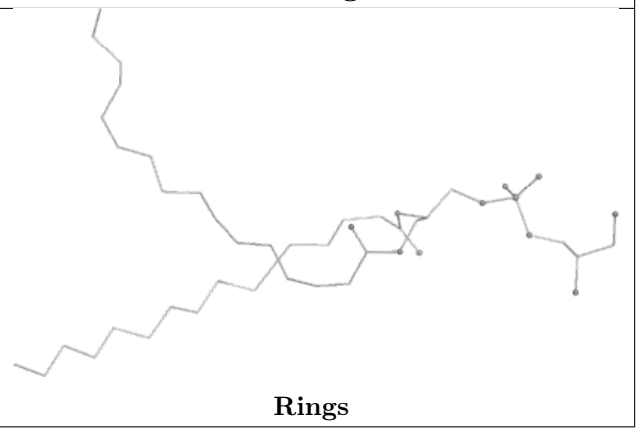
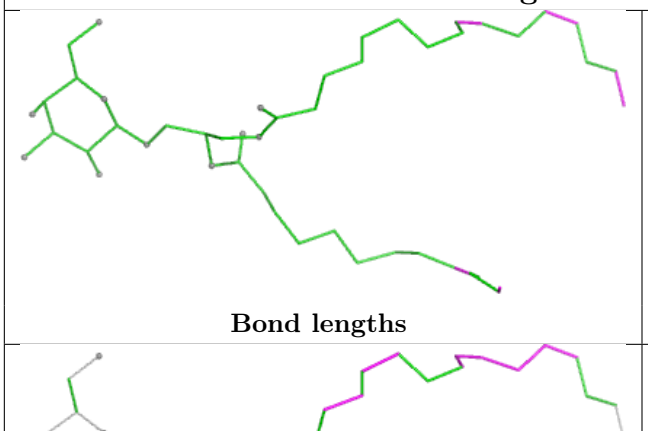


Rings

Ligand LMG A 413



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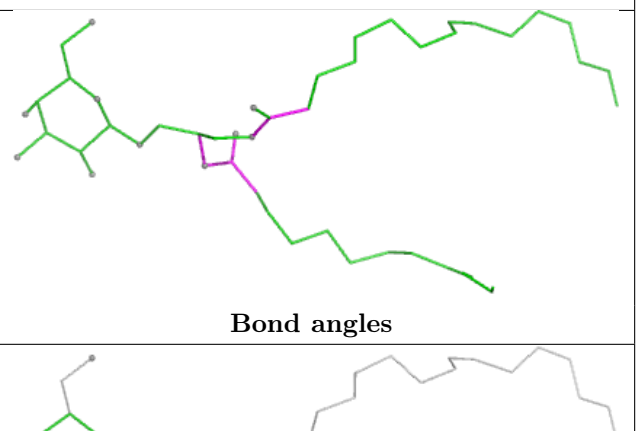
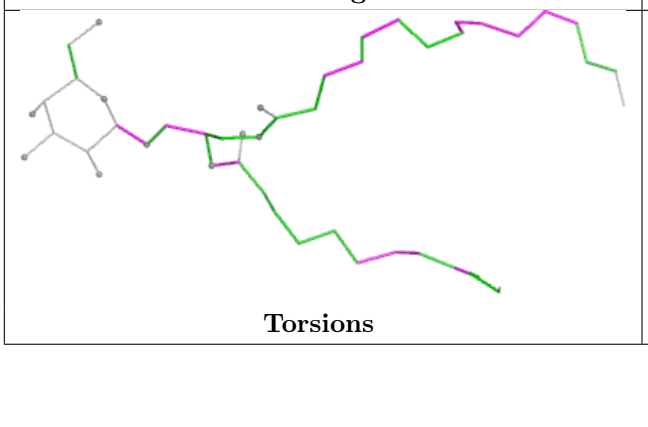


Bond angles



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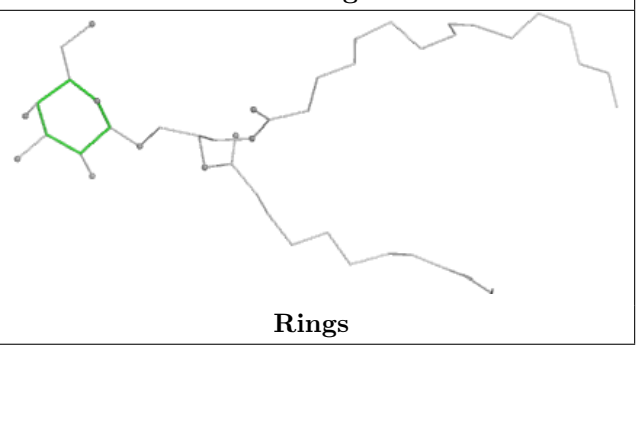
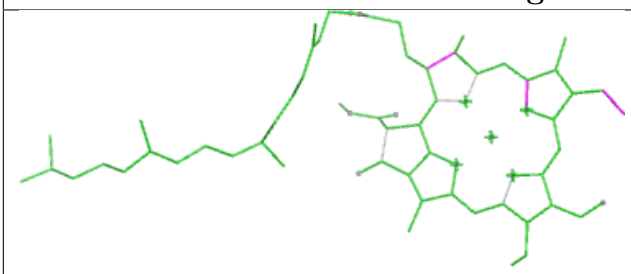
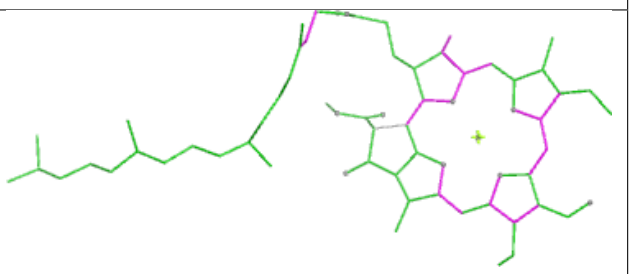
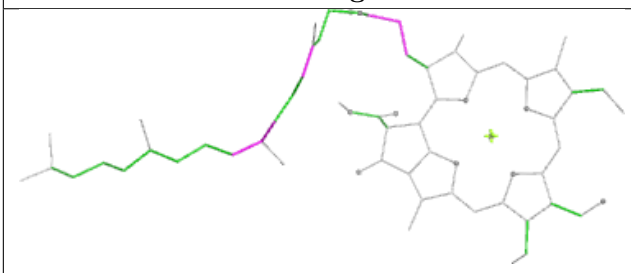
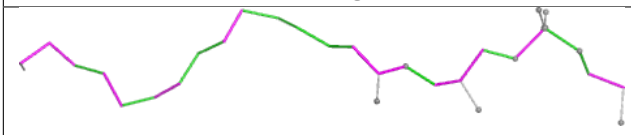
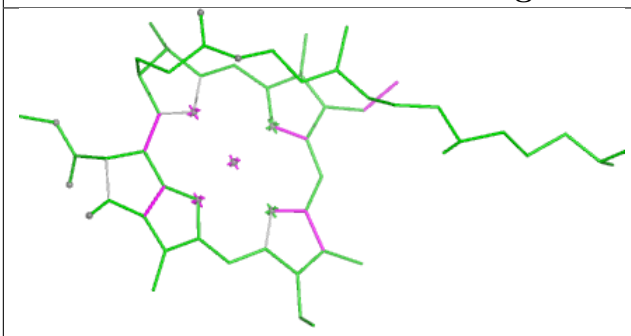


Rings

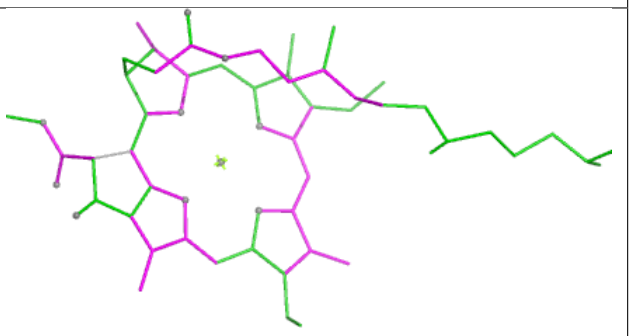
Ligand CHL n 605	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand LPX S1 625	
Bond lengths	Bond angles
 Torsions	Rings

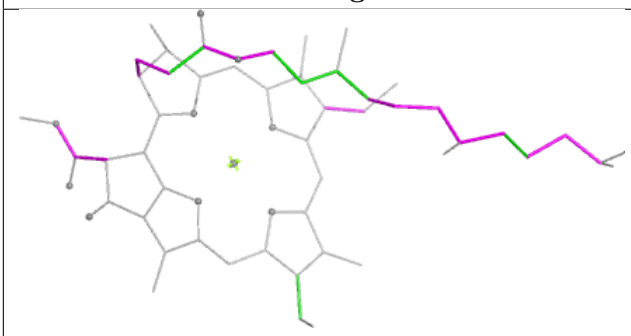
Ligand CLA R1 610



Bond lengths



Bond angles



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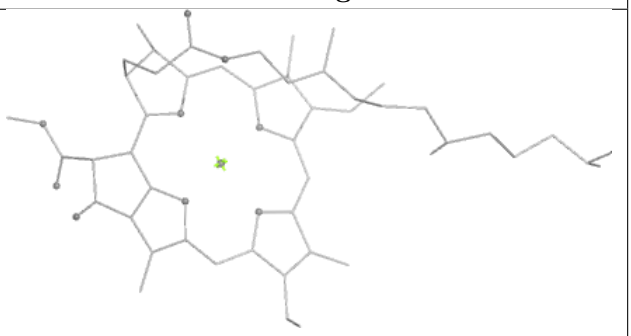
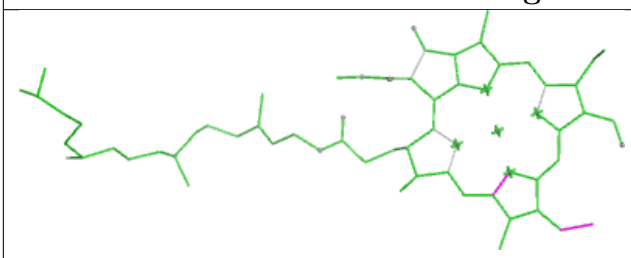


Rings

Ligand CHL Y 606



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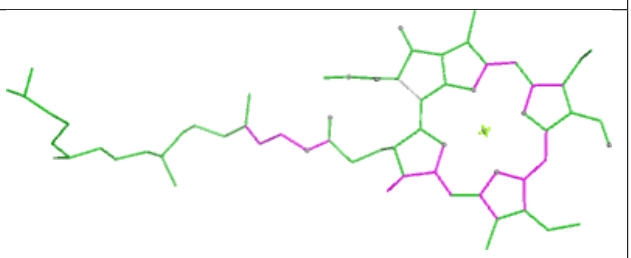
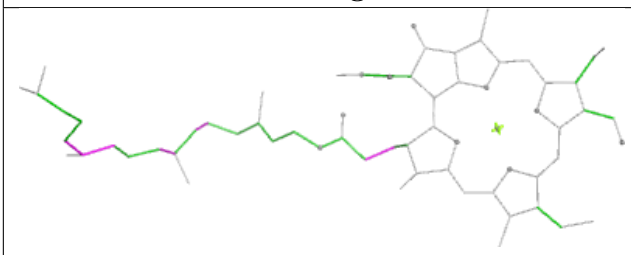


Bond angles



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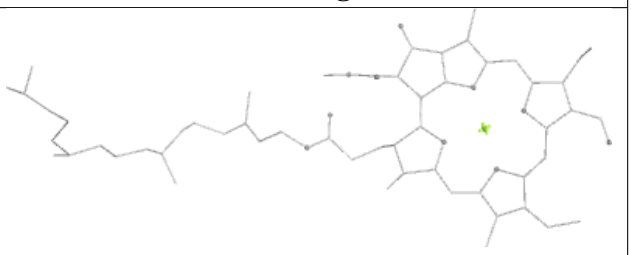
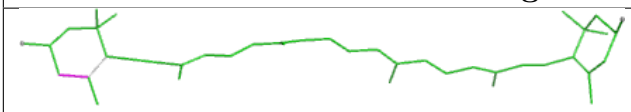


Rings

Ligand LUT s1 620



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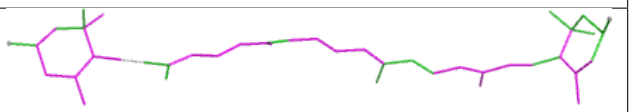
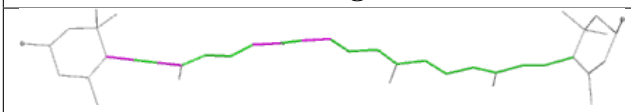


Bond angles



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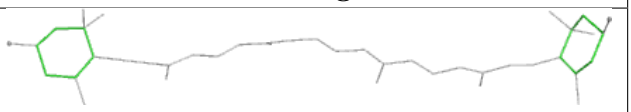

Rings

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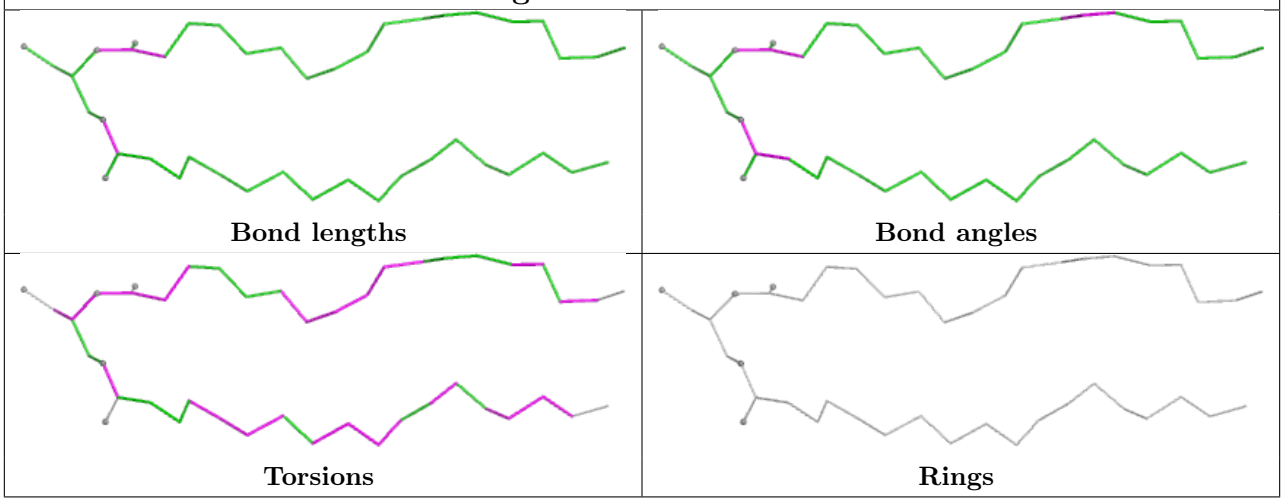
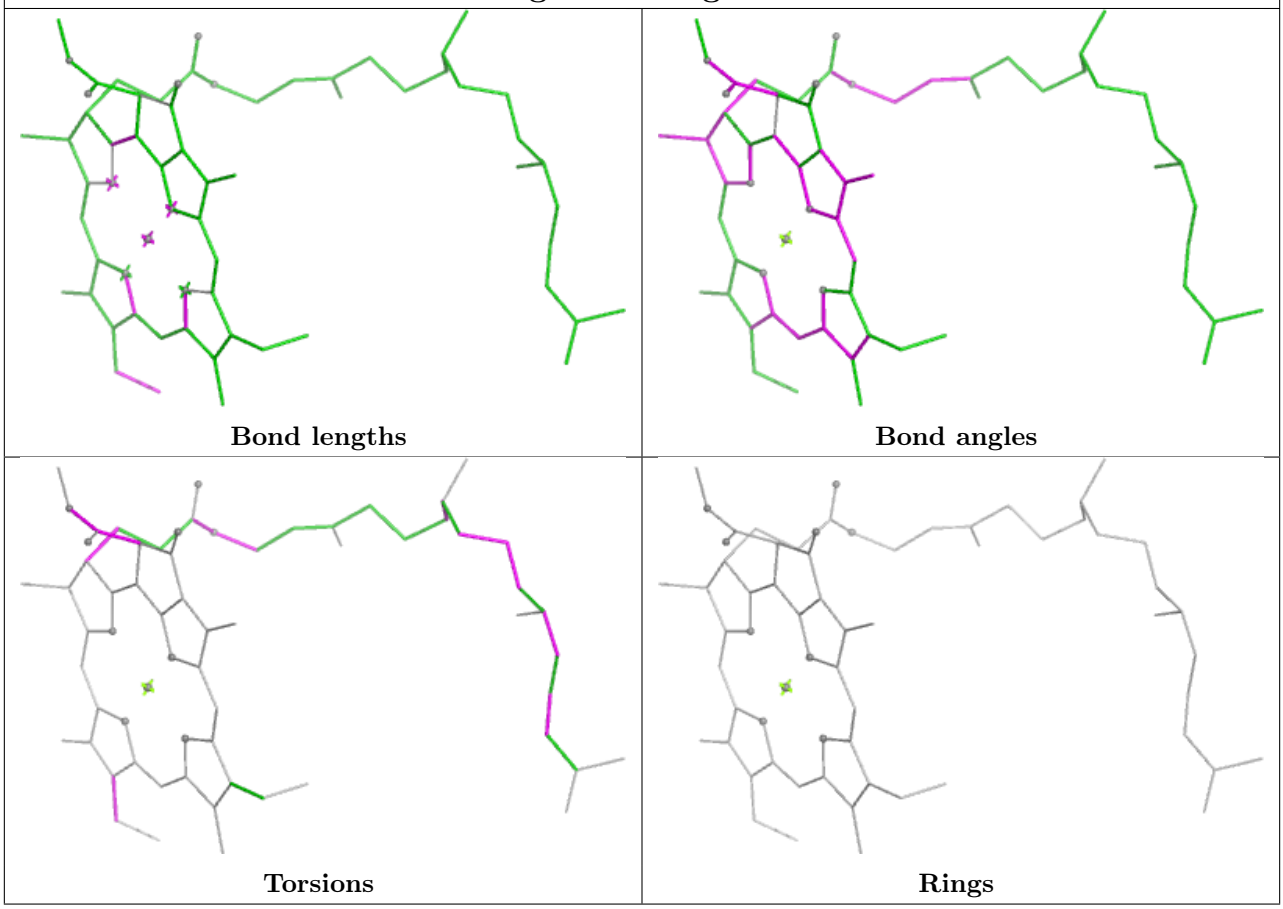
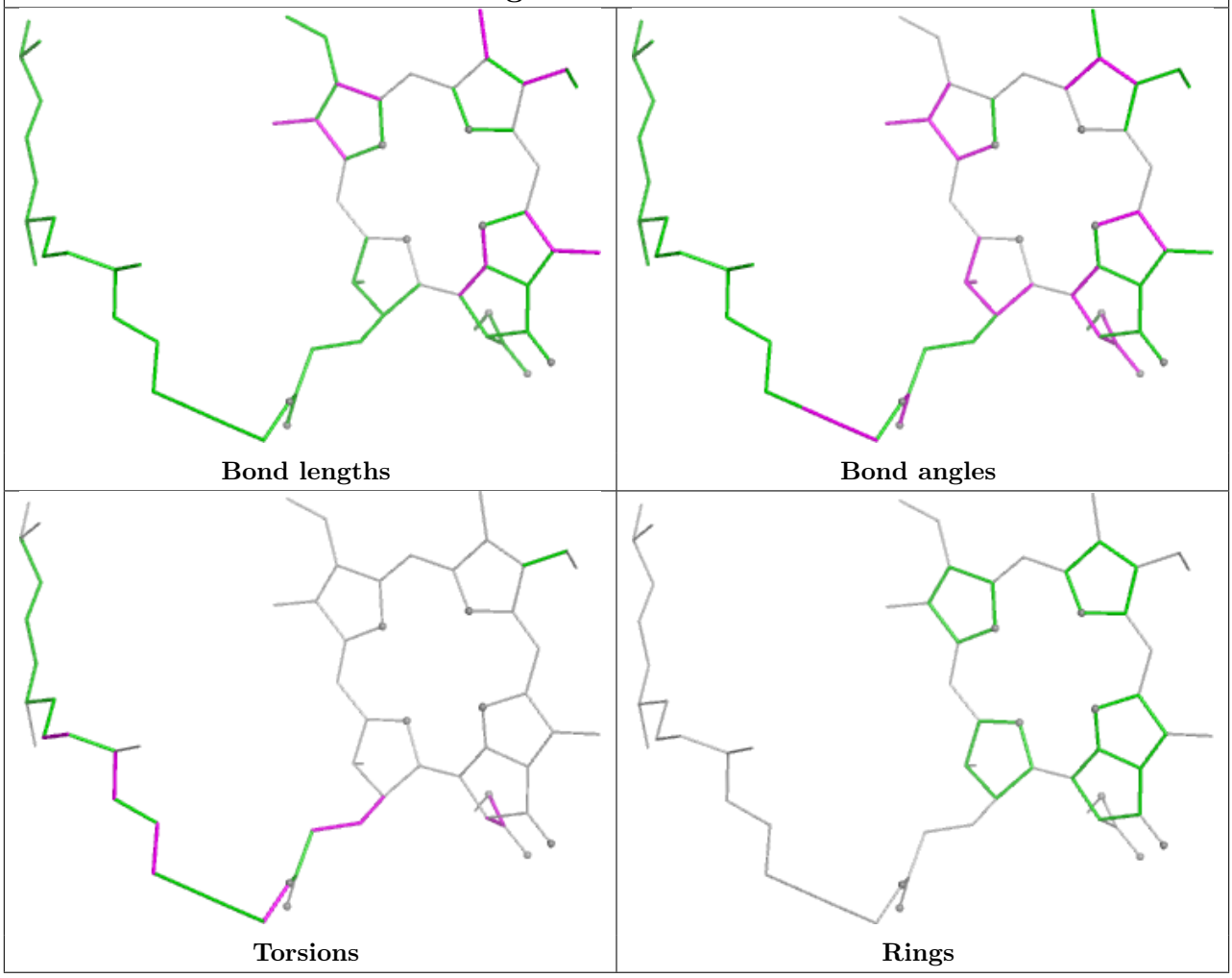


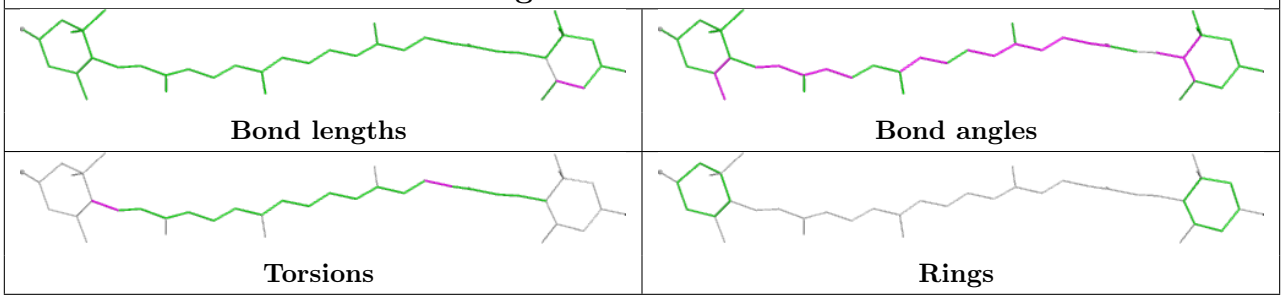
Ligand CLA g 611

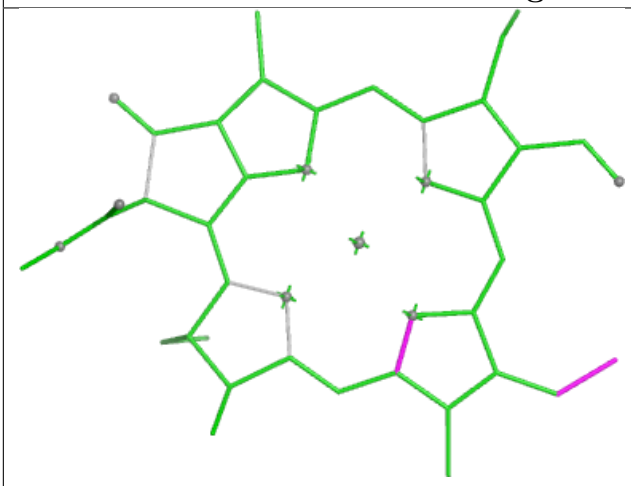
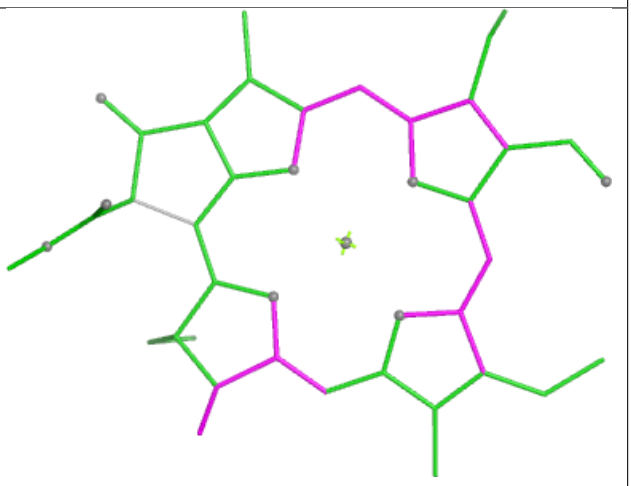
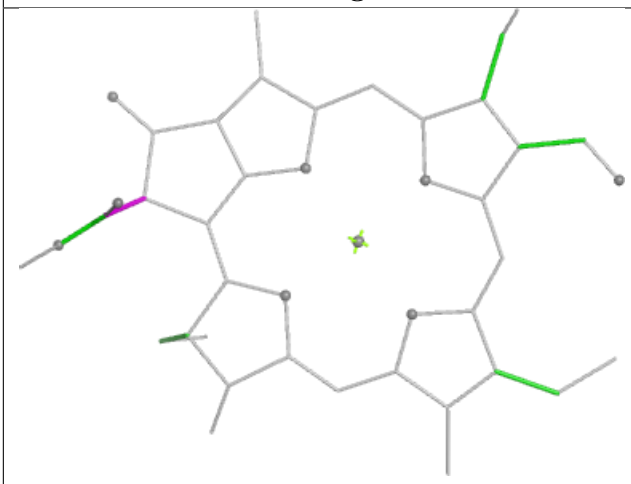
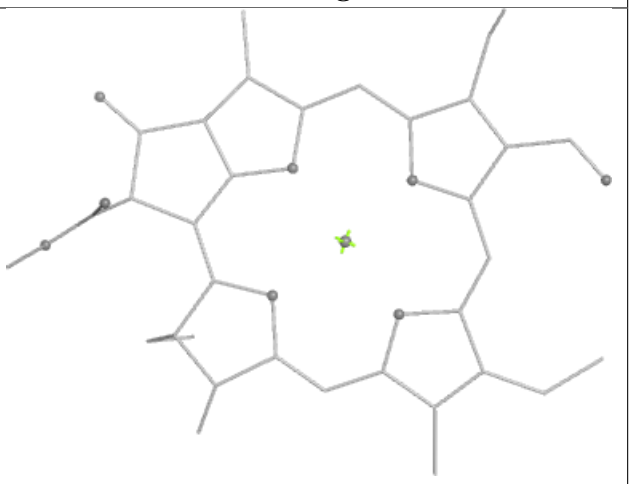


Ligand PHO a 409

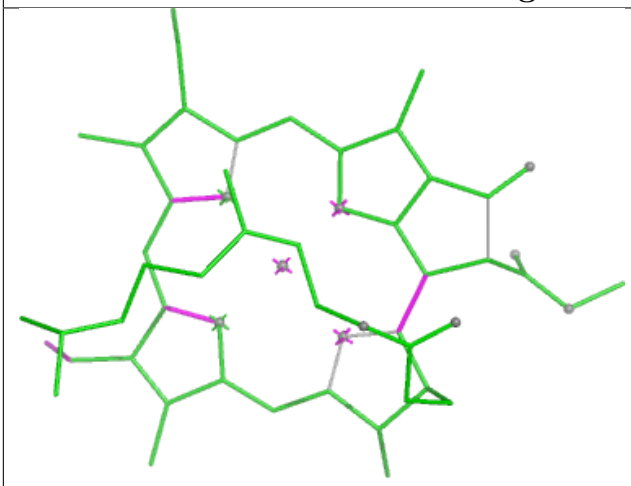


Ligand LUT G1 621



Ligand CHL S 607	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA S1 613



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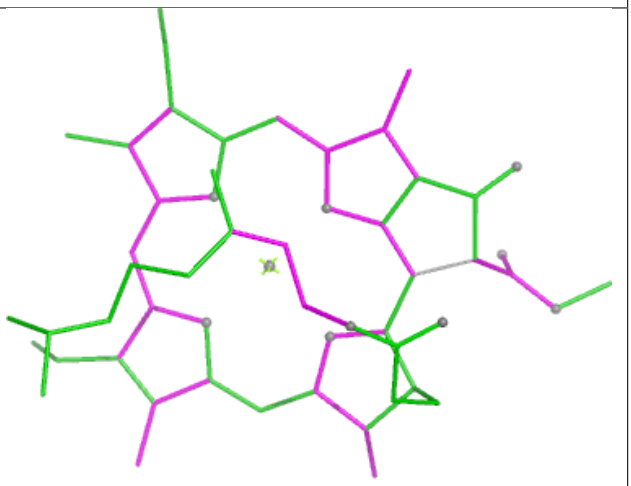
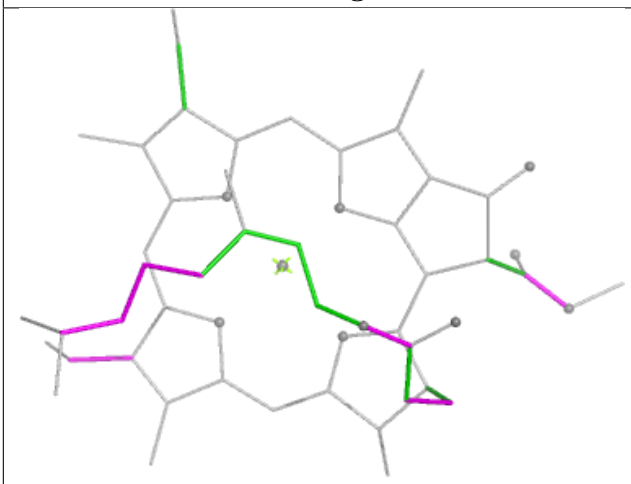
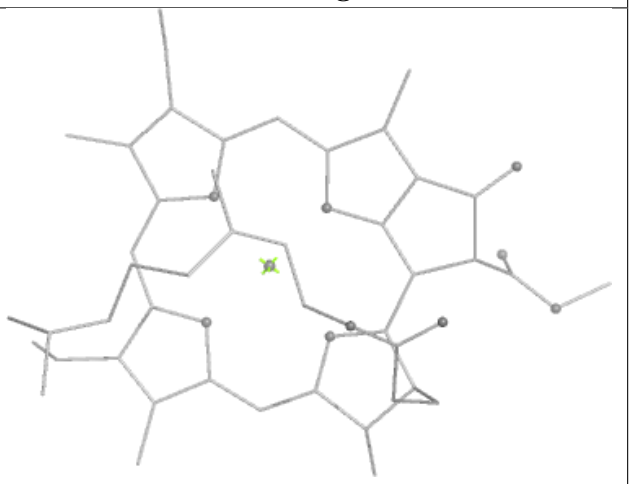


Bond angles

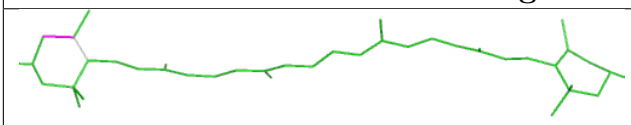


Torsions



Rings

Ligand LUT y1 621



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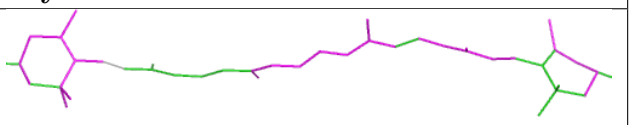
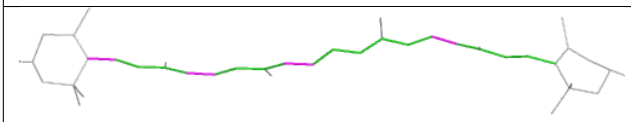


Bond angles



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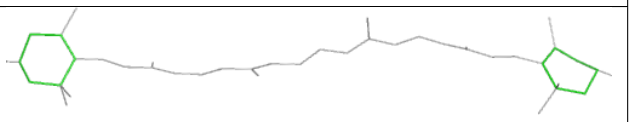
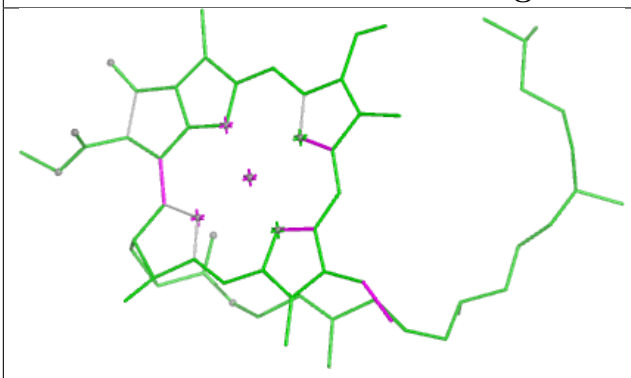
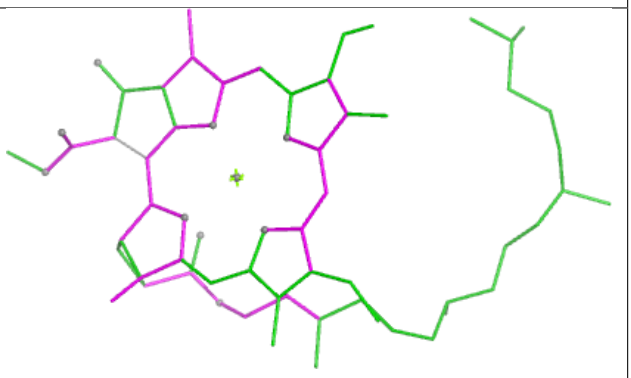
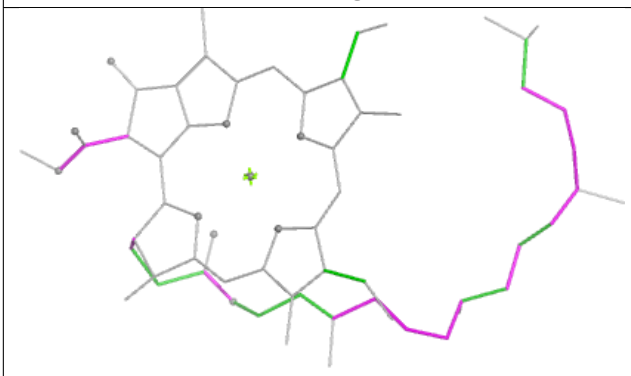
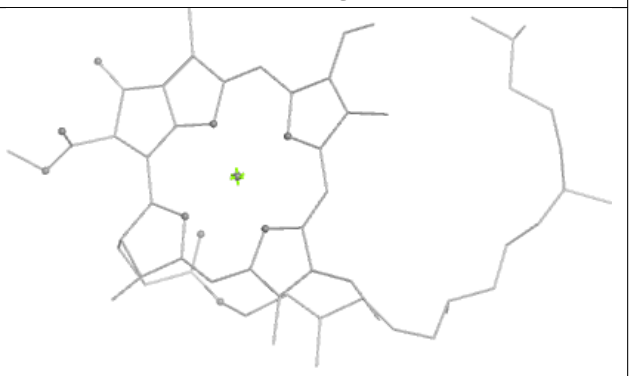
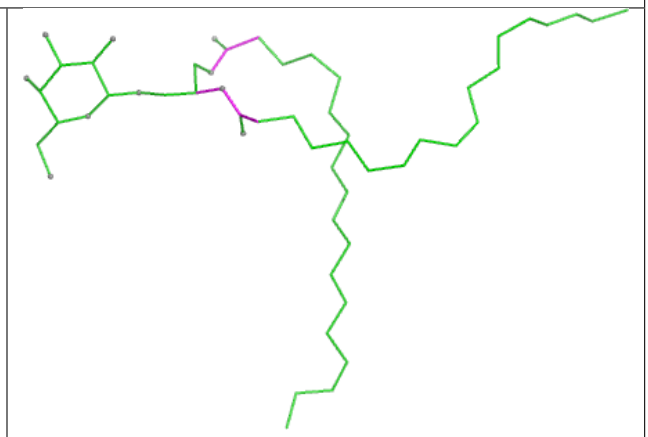


Rings

Ligand CLA N1 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG c1 523

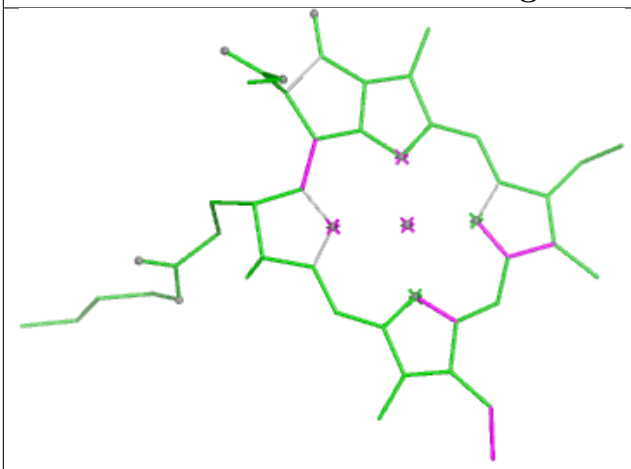
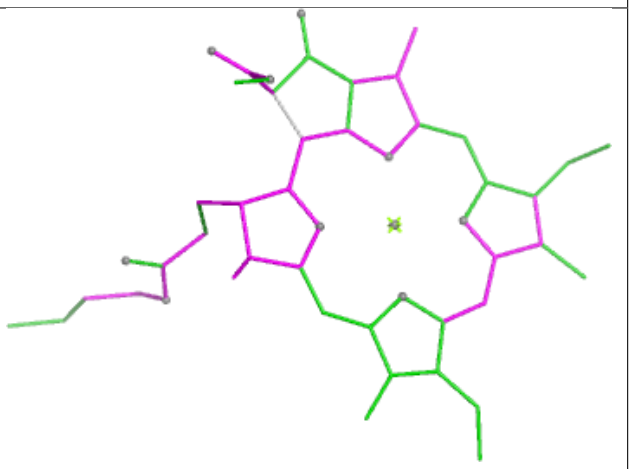
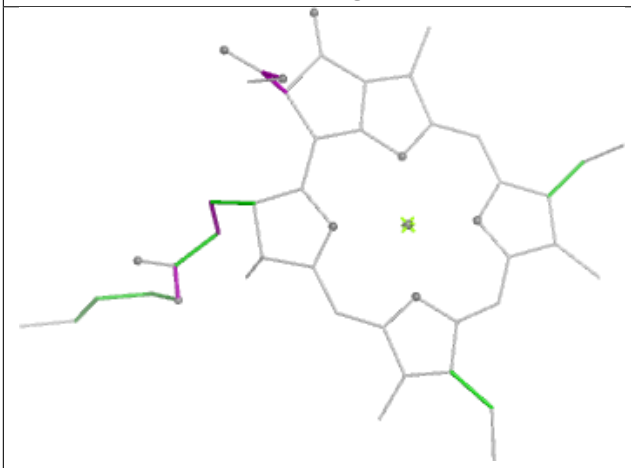
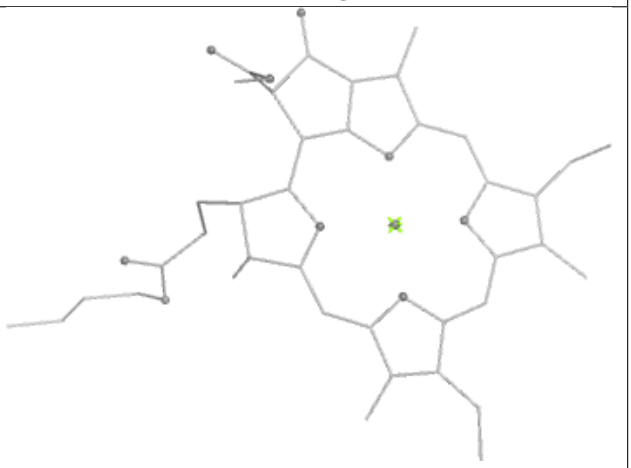
Bond lengths



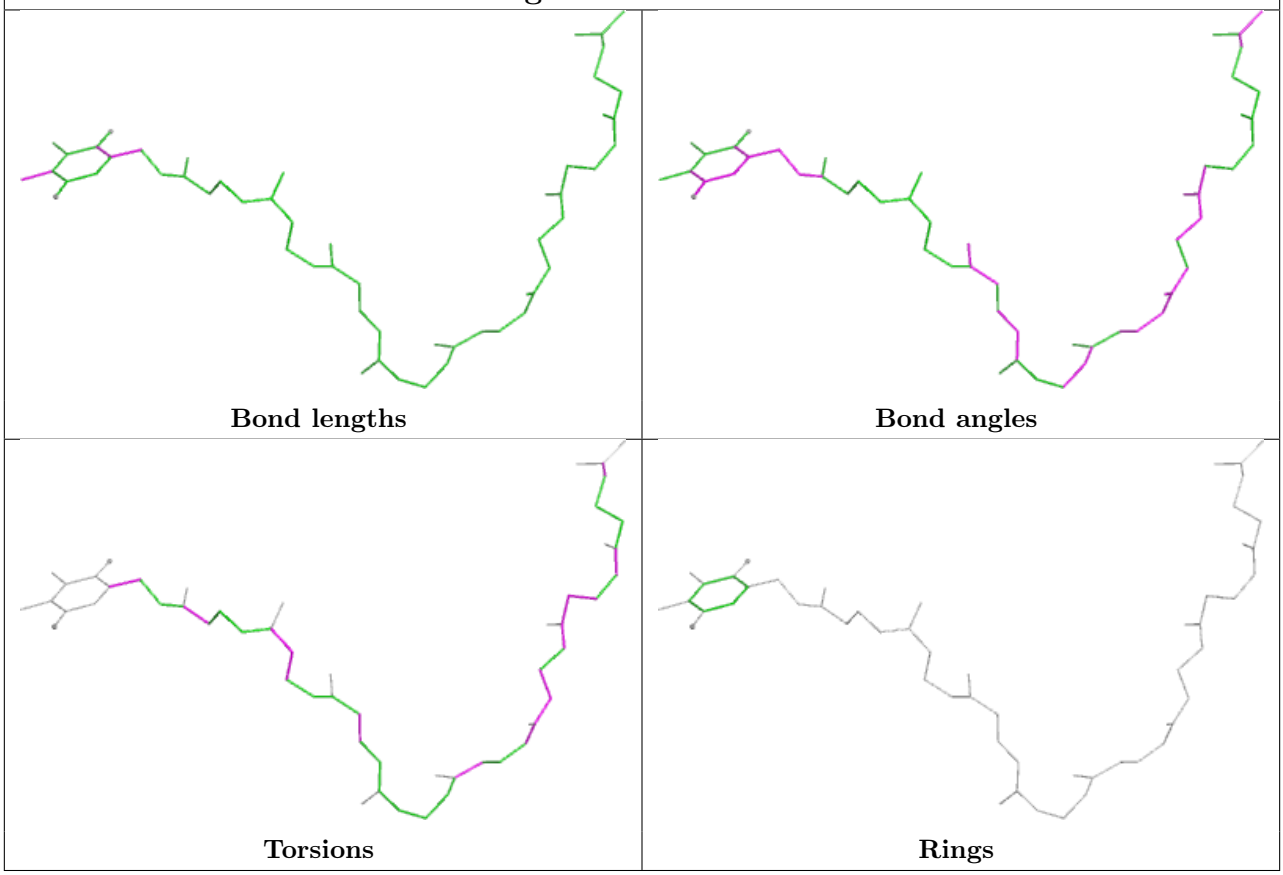
Bond angles

Torsions

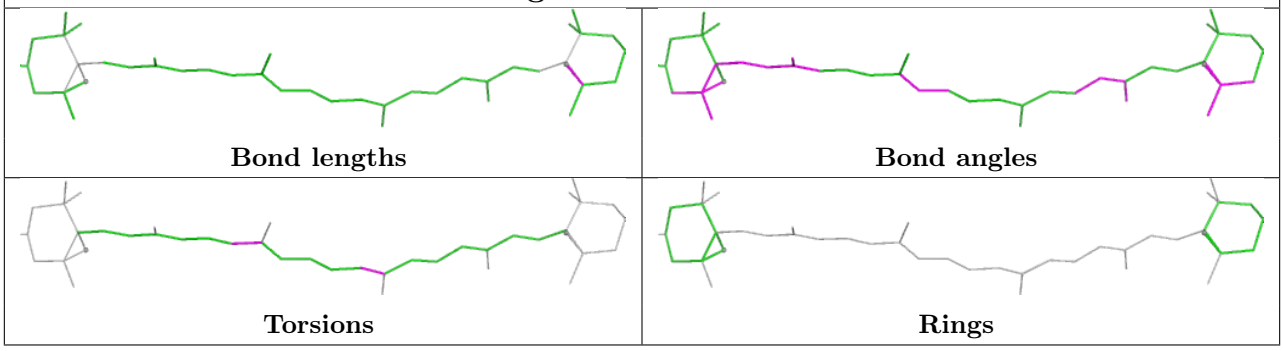
Rings

Ligand CLA a1 407	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

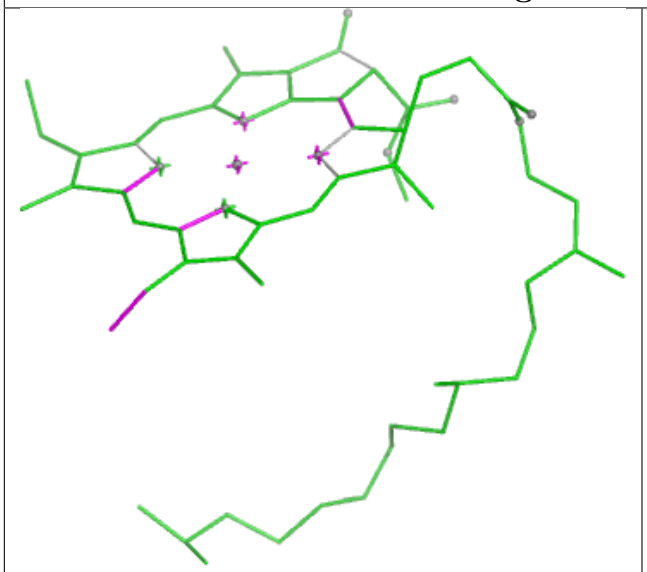
Ligand PL9 d1 405



Ligand XAT n 622



Ligand CLA G1 603



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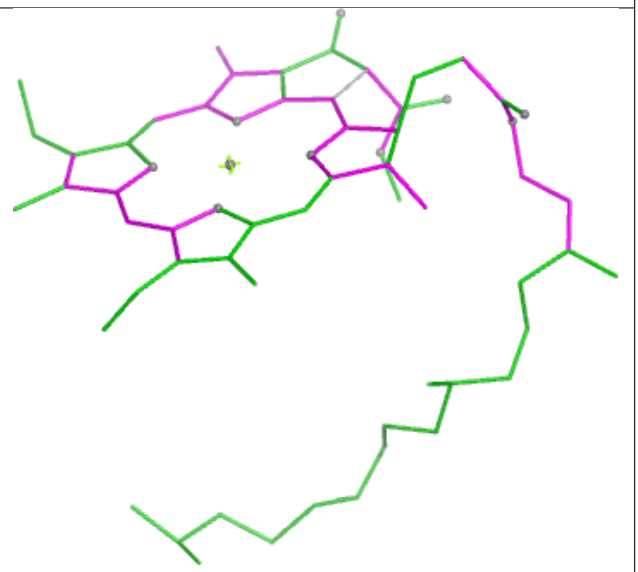
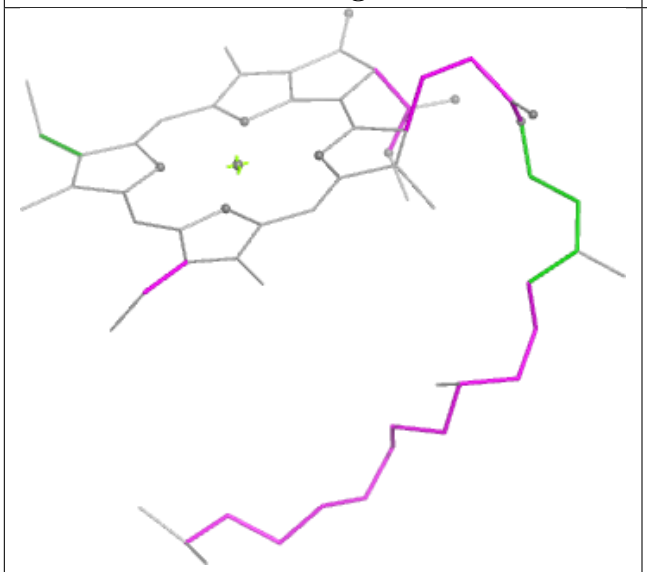


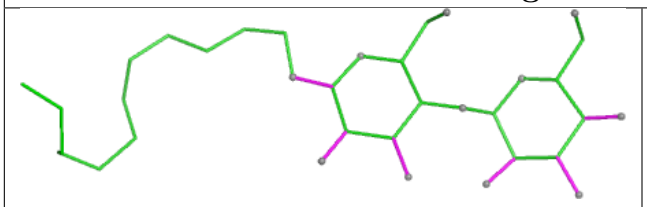
Bond angles



Torsions

Rings

Ligand LMT R 625



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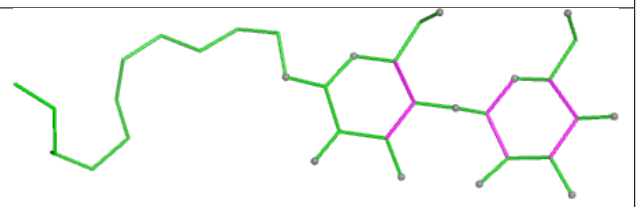

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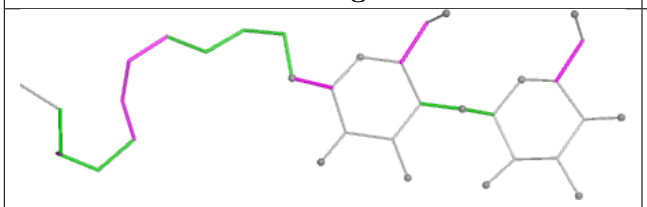

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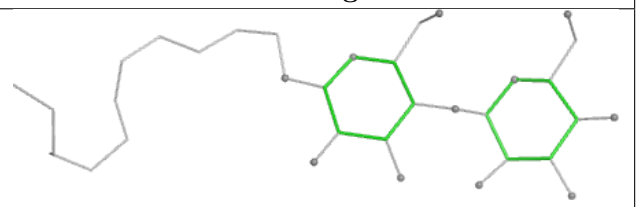

Rings

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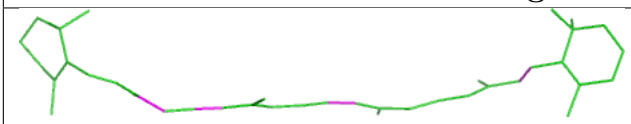

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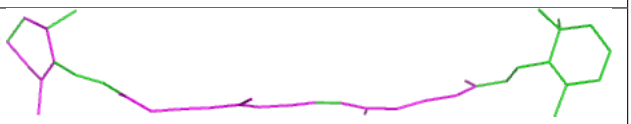

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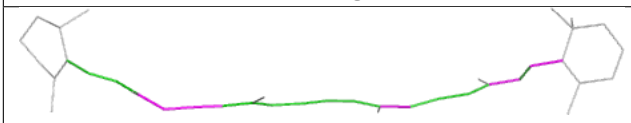

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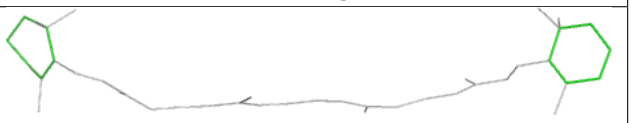
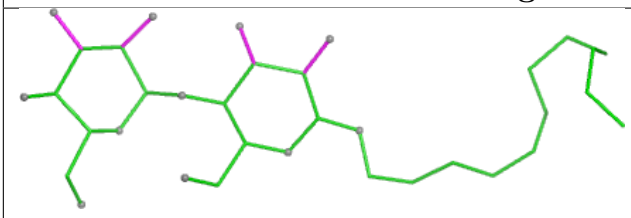


Rings

Ligand LMT r1 625



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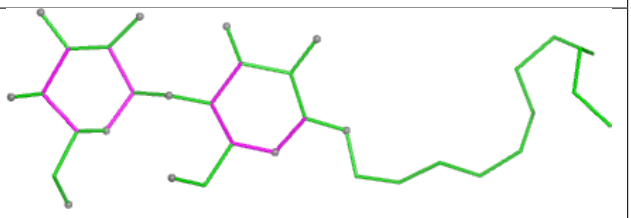

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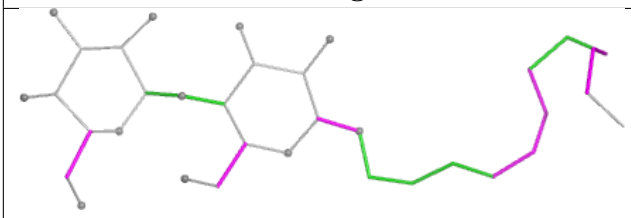

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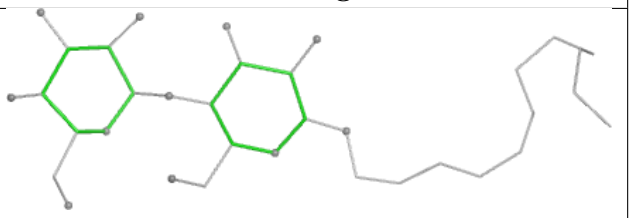
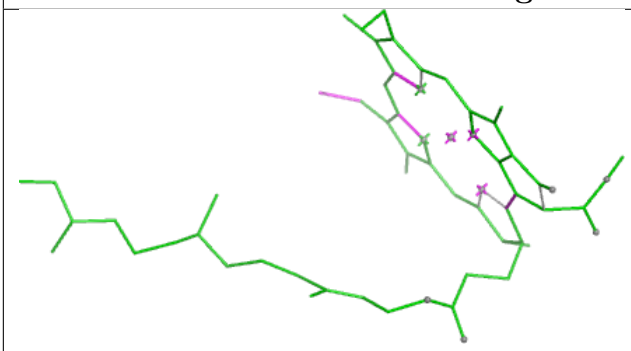


Rings

Ligand CLA C1 504



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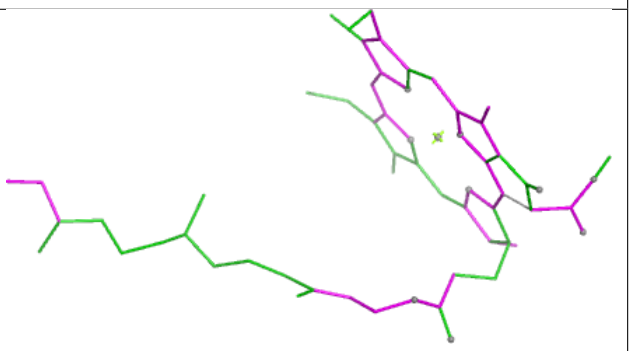

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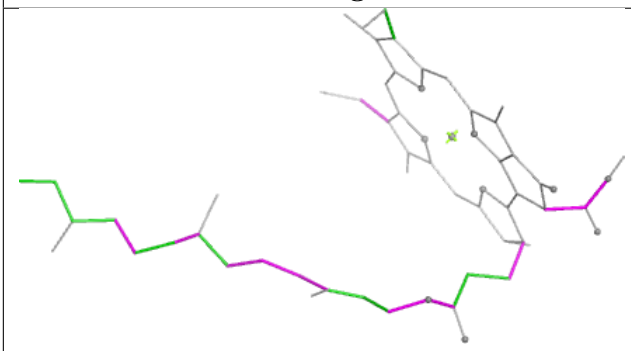
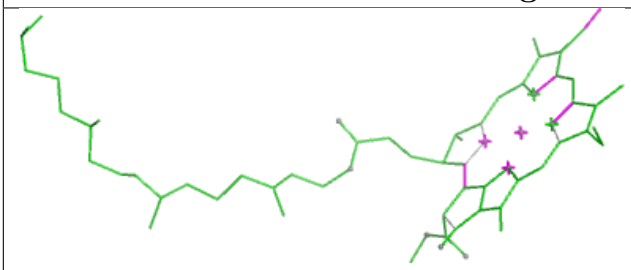


Torsions

Rings

Ligand CLA a1 405



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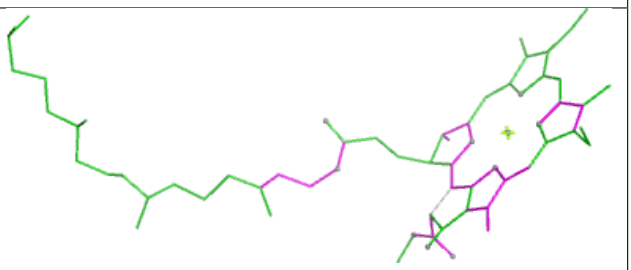

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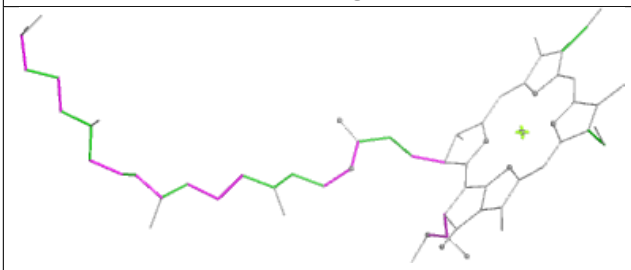

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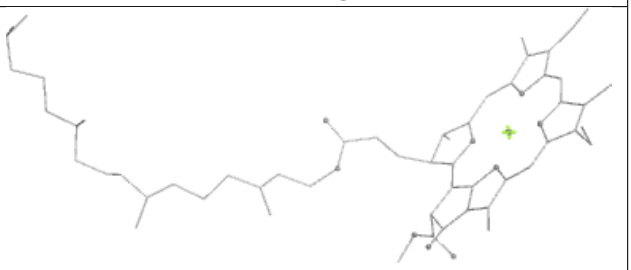
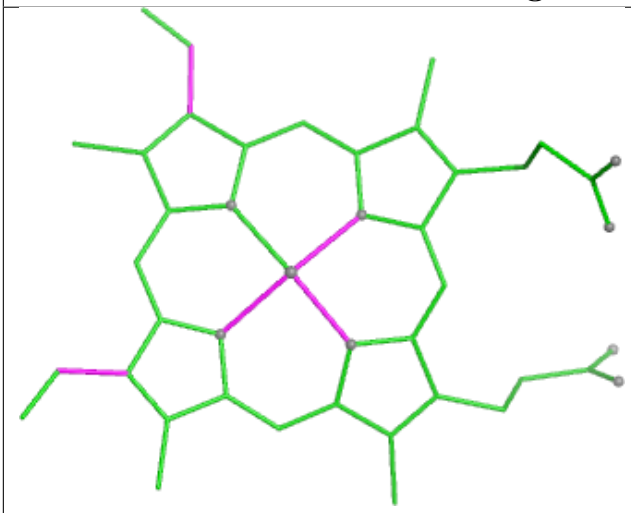


Rings

Ligand HEM f 101



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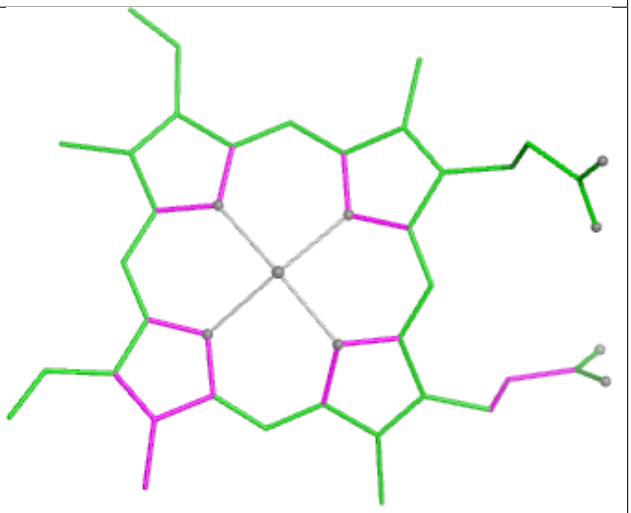

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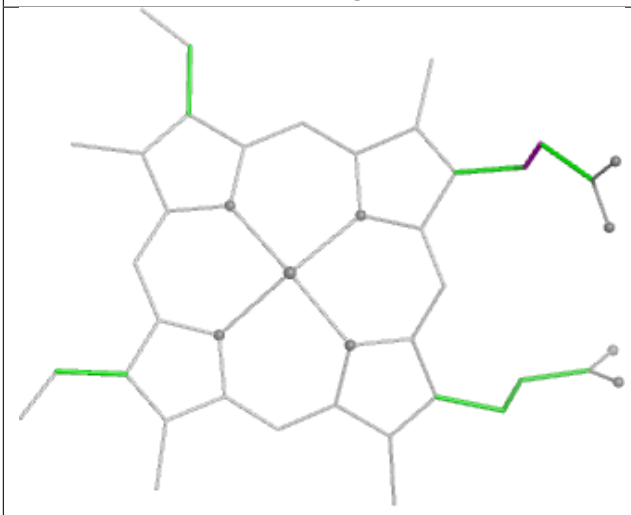

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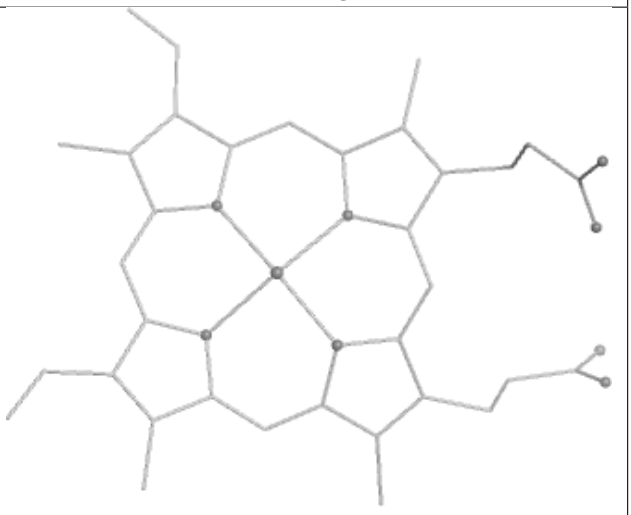
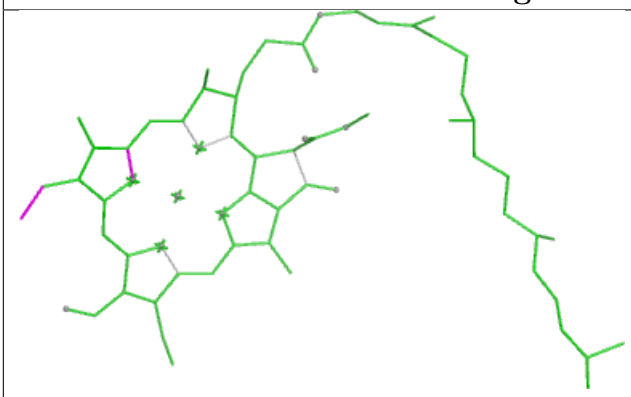
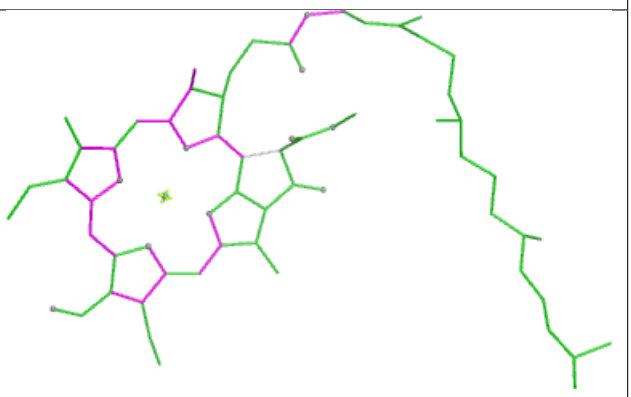
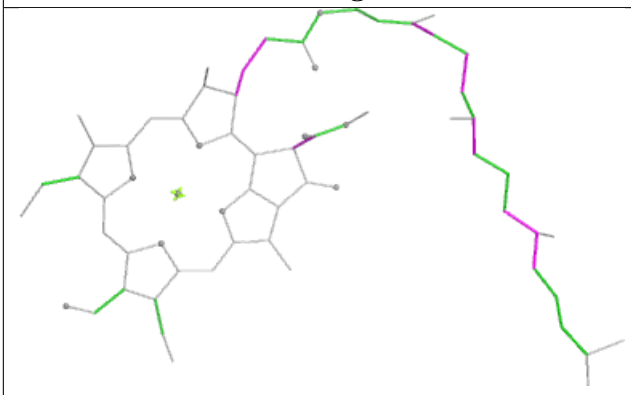
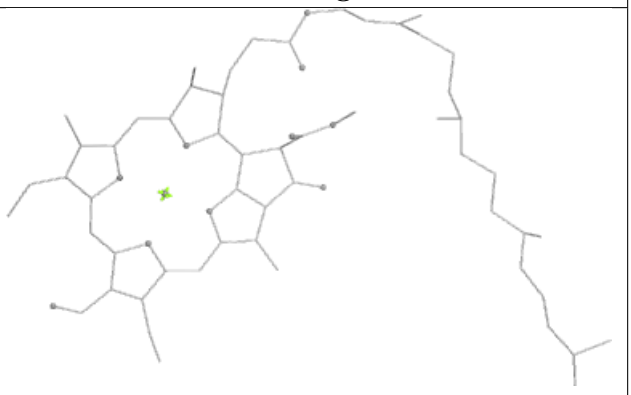
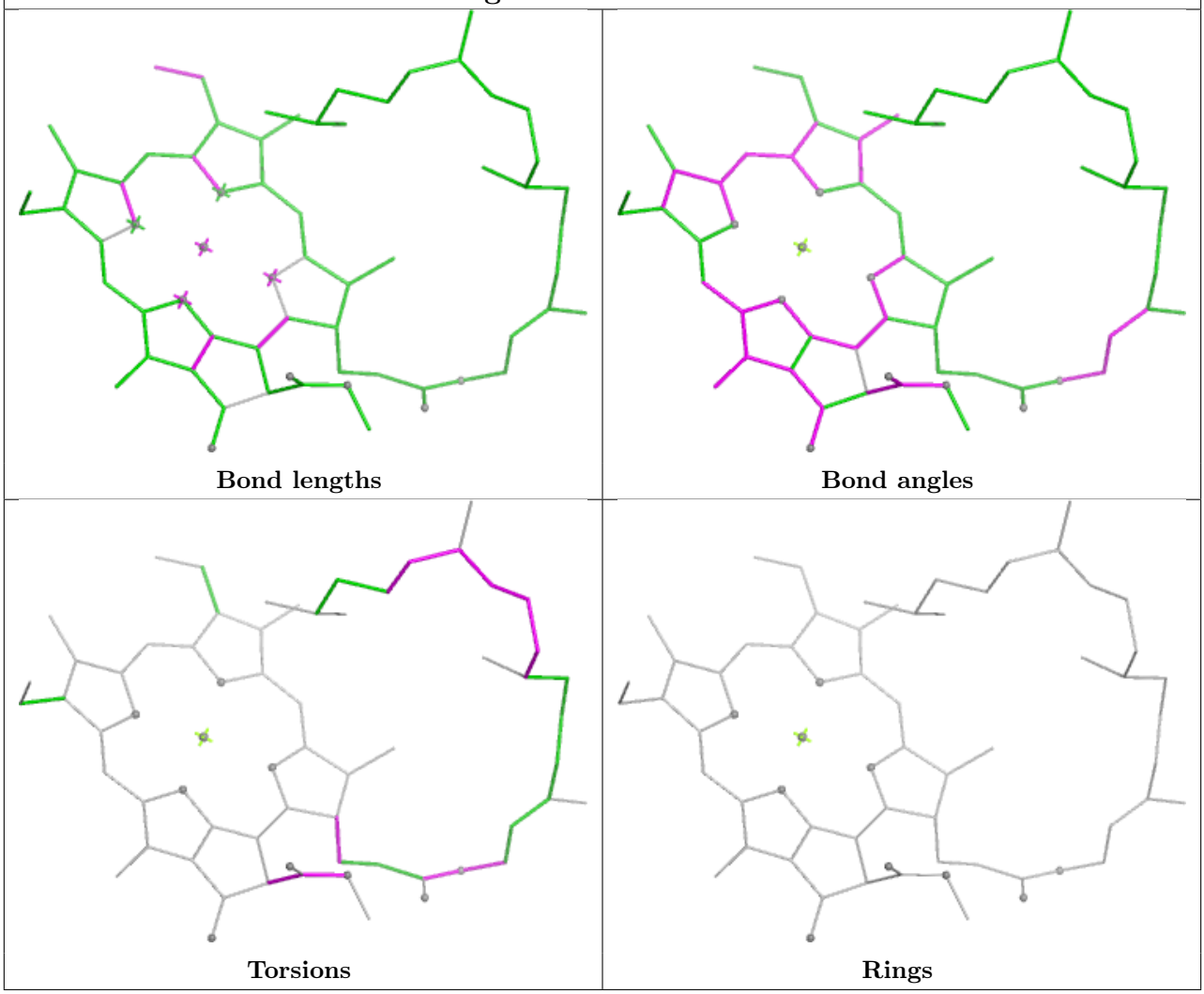


Rings

Ligand CHL N1 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 616



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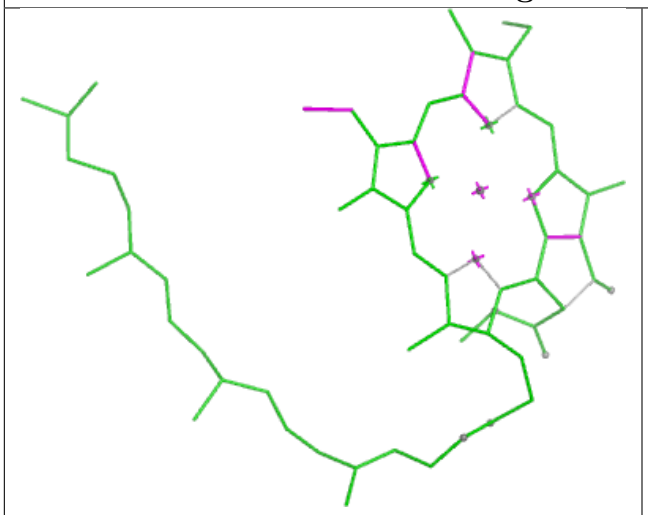

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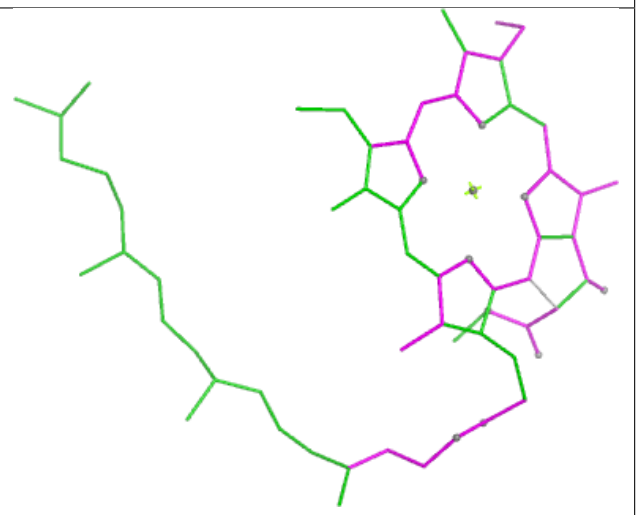
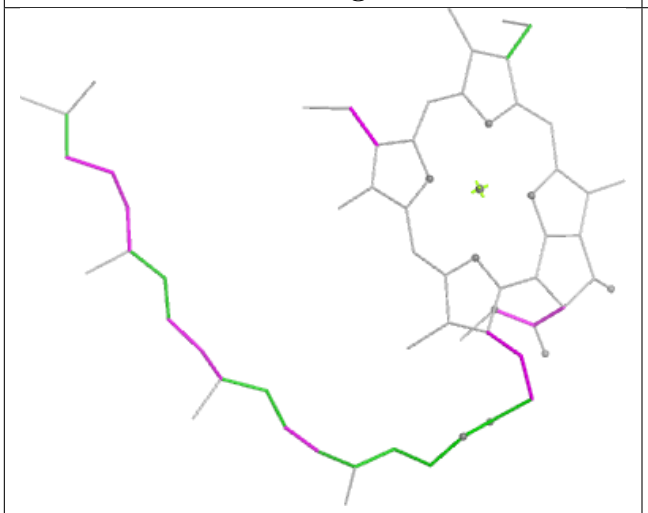


Bond angles



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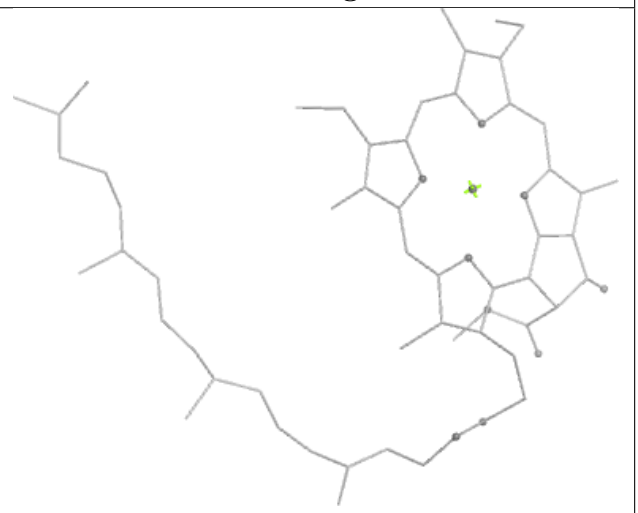
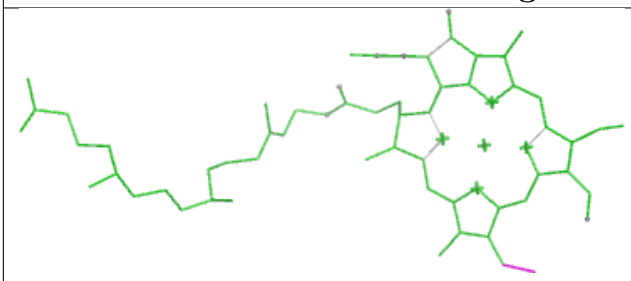
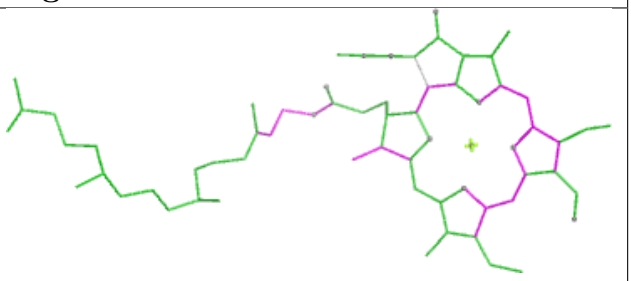
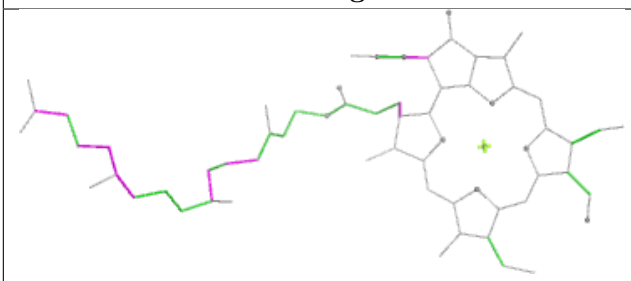
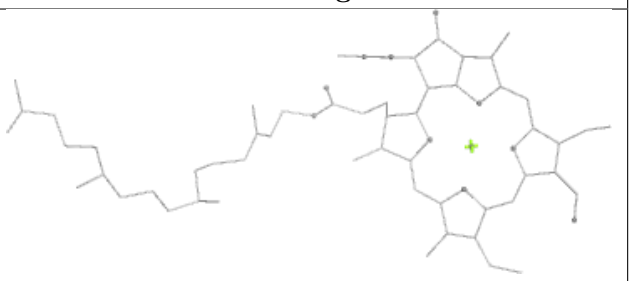


Rings

Ligand CHL g1 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

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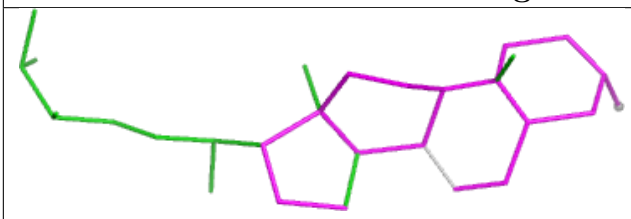
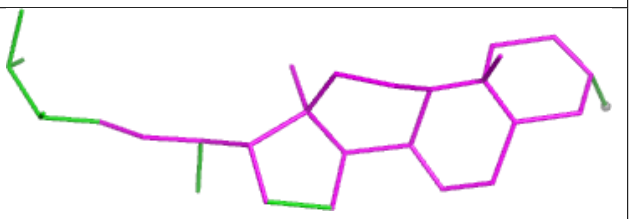
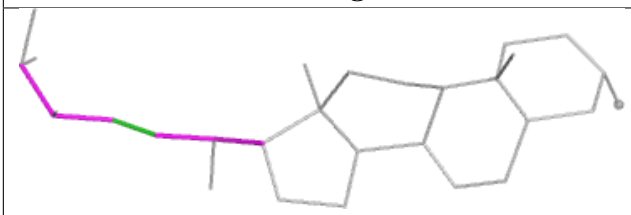
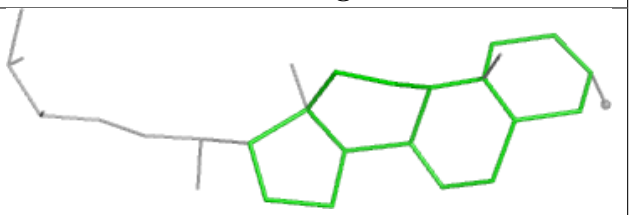
 Bond lengths	 Bond angles
 Torsions	 Rings

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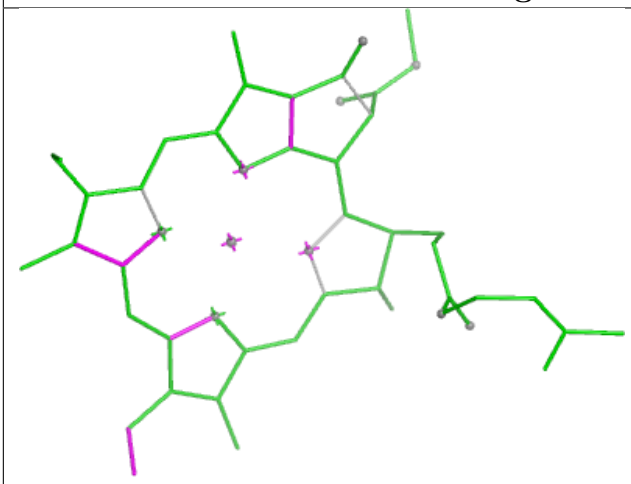
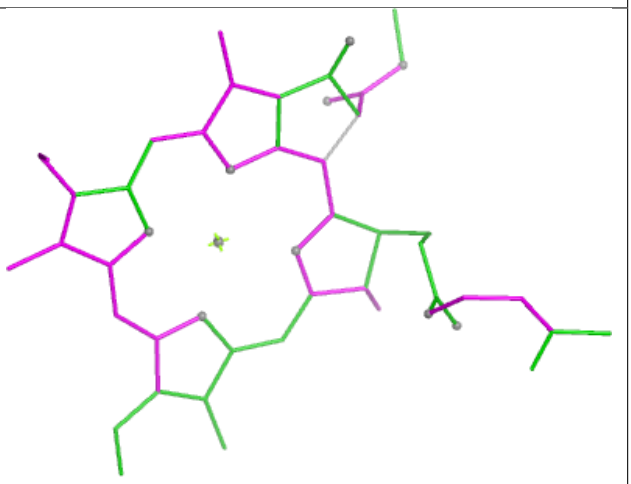
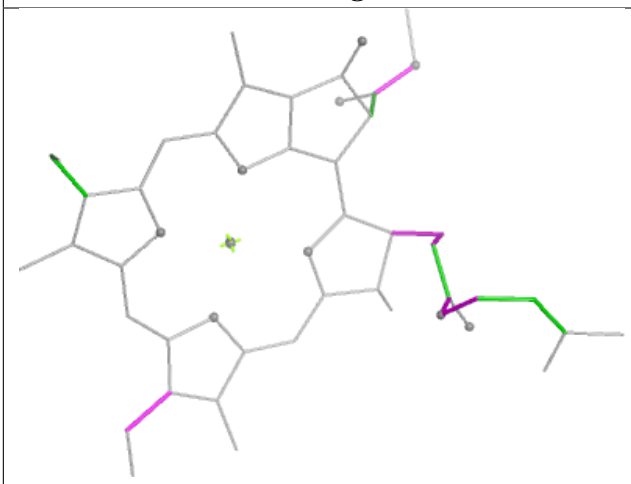
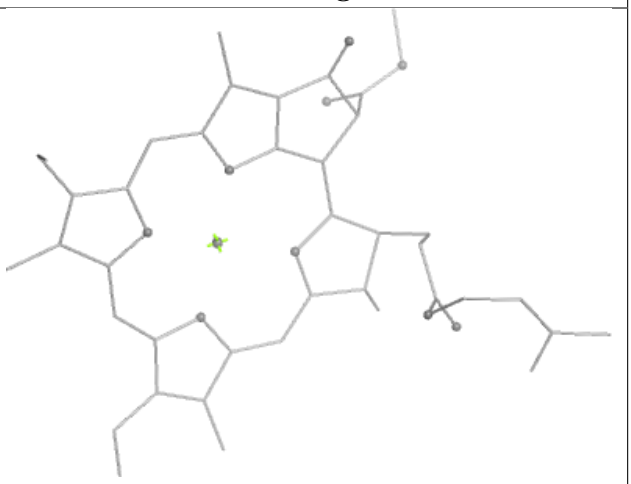
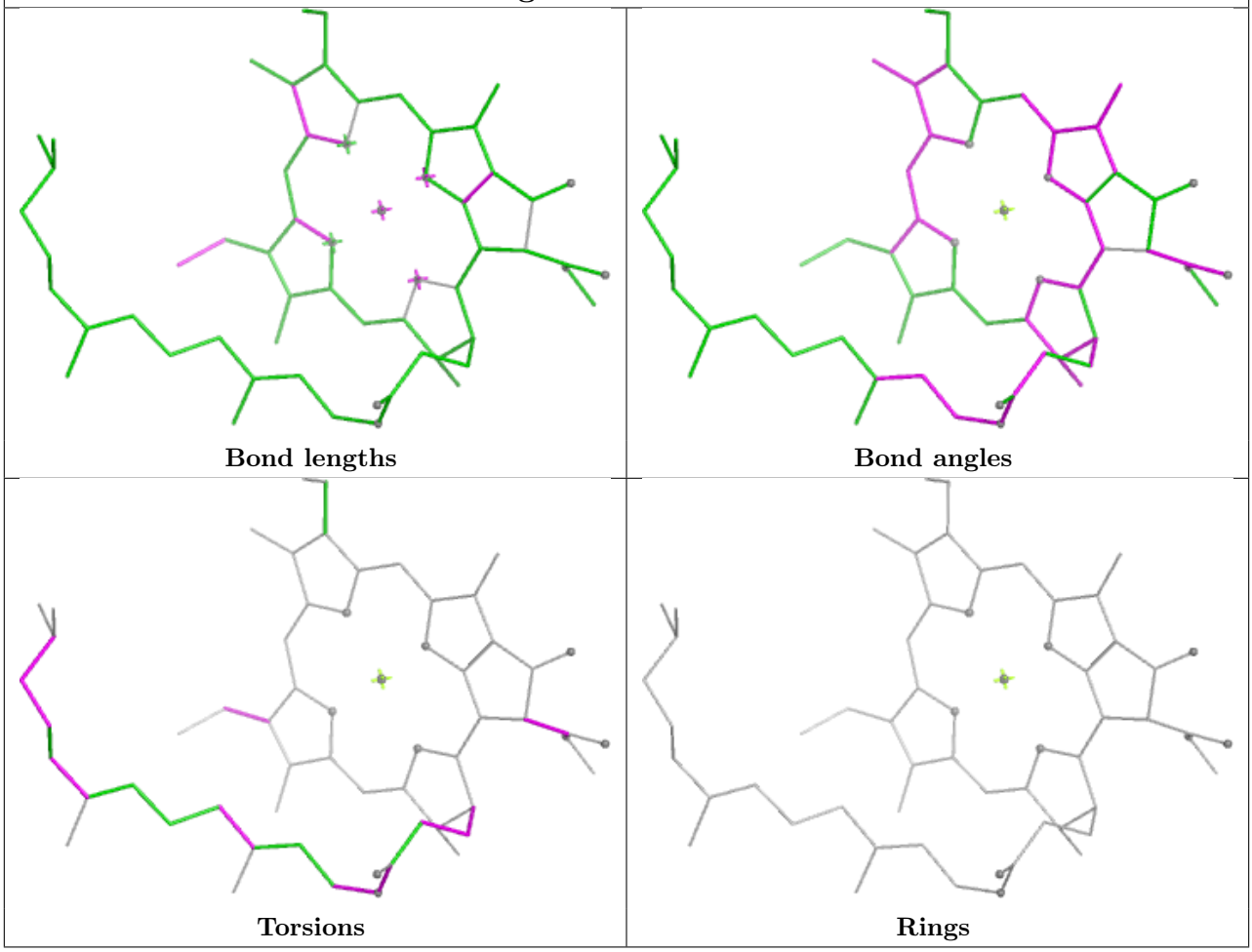
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 602



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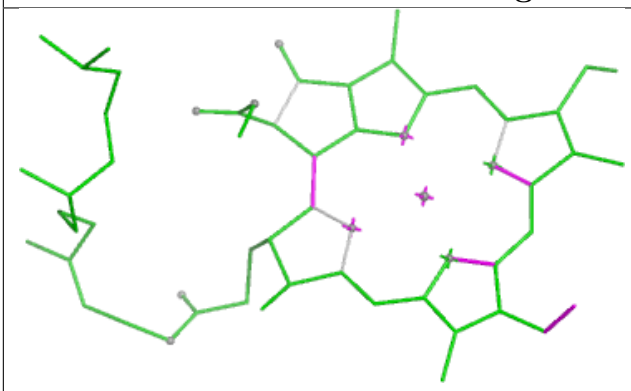
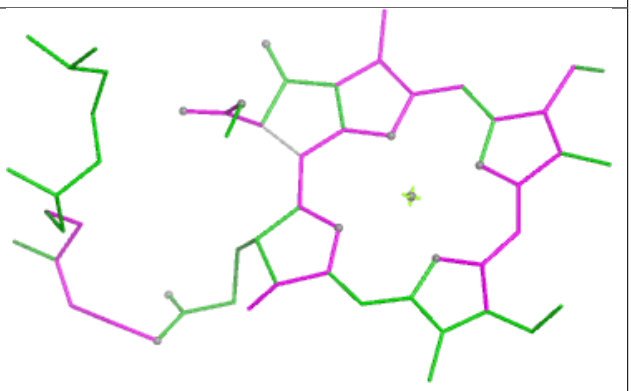
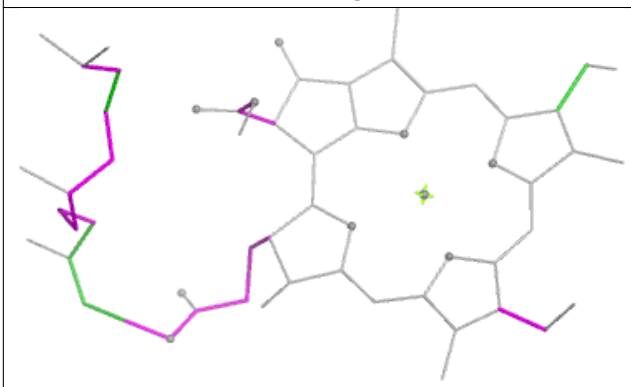
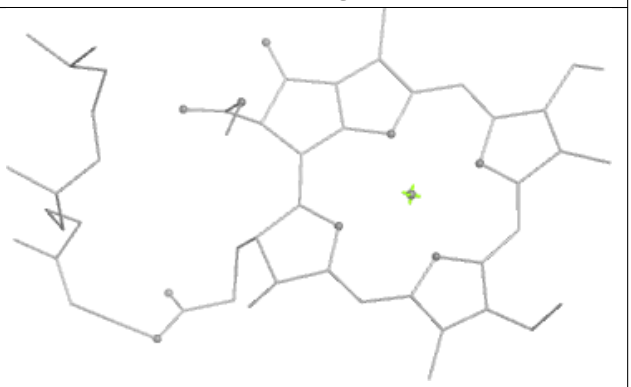
 Bond lengths	 Bond angles
 Torsions	 Rings

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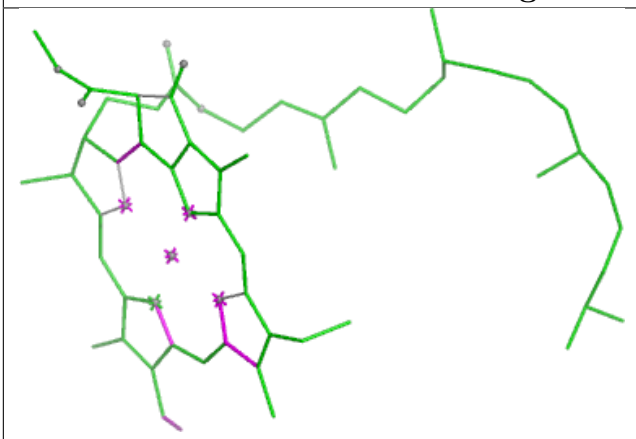
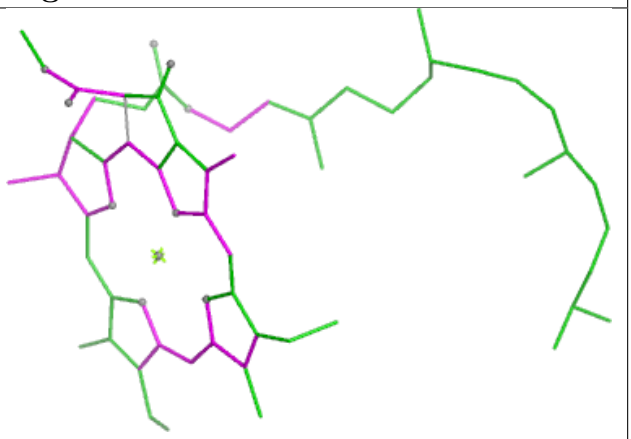
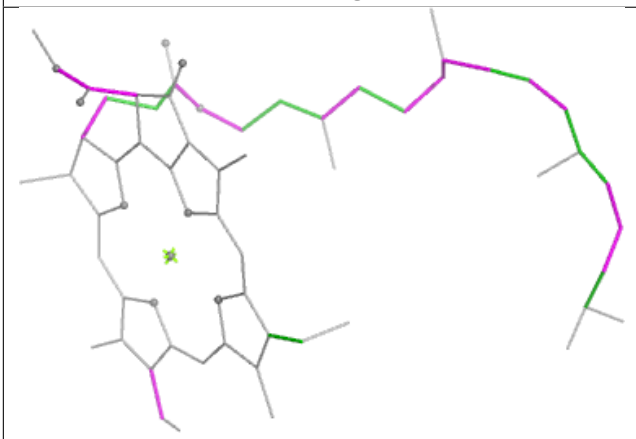
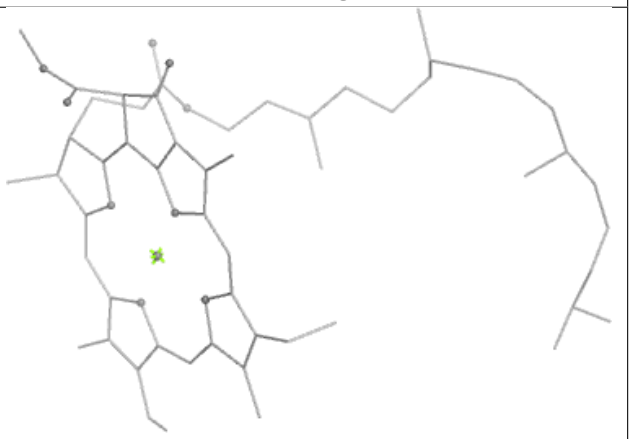
 Bond lengths	 Bond angles
 Torsions	 Rings

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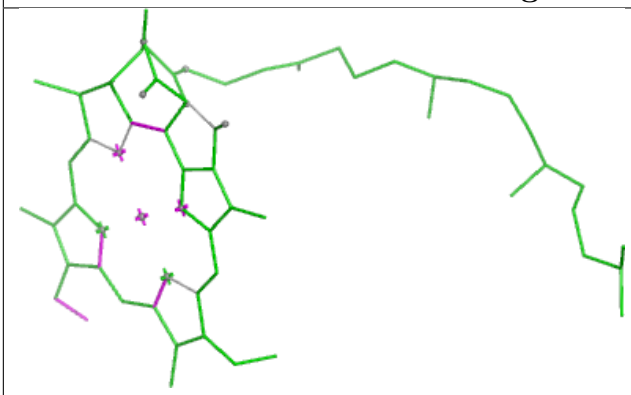

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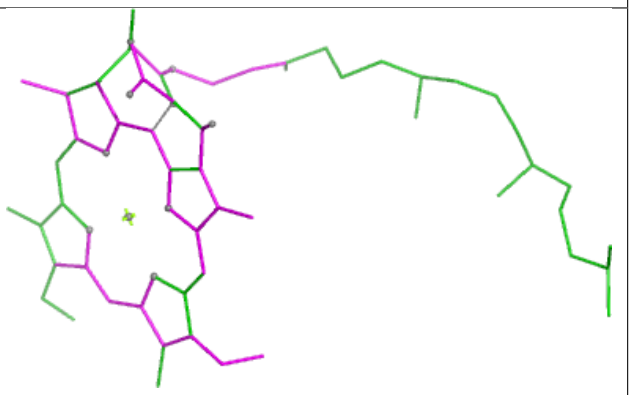

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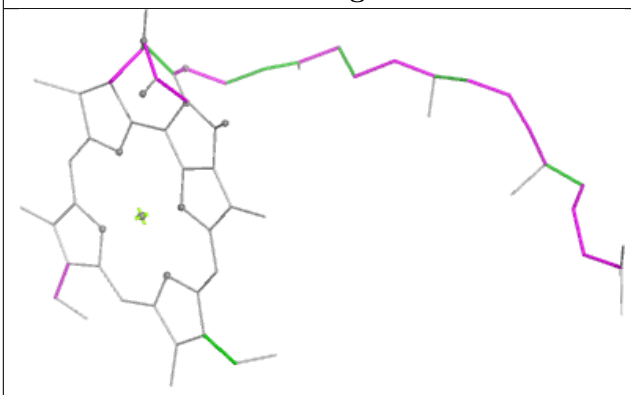

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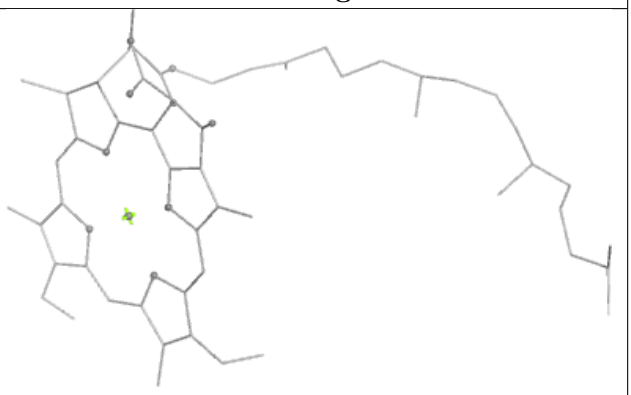
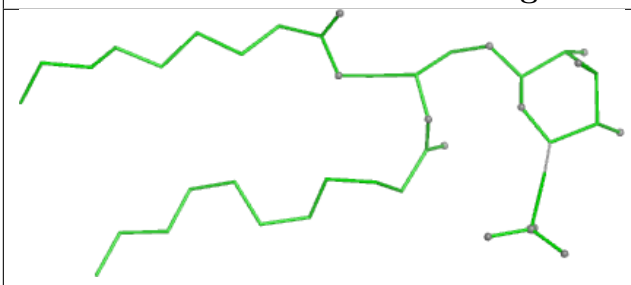


Rings

Ligand SQD M 101



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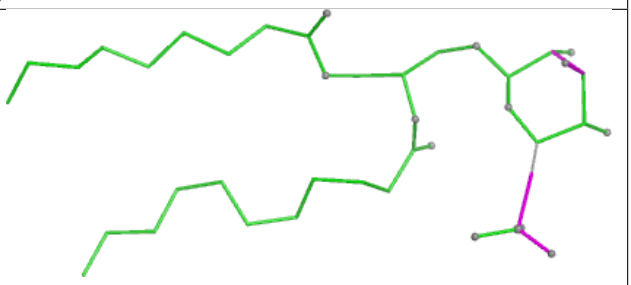

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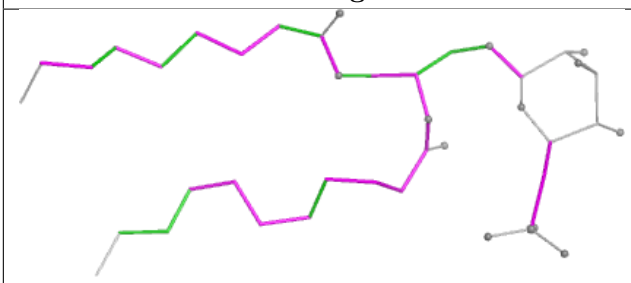

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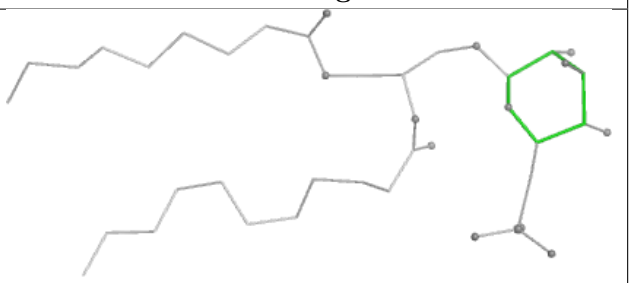
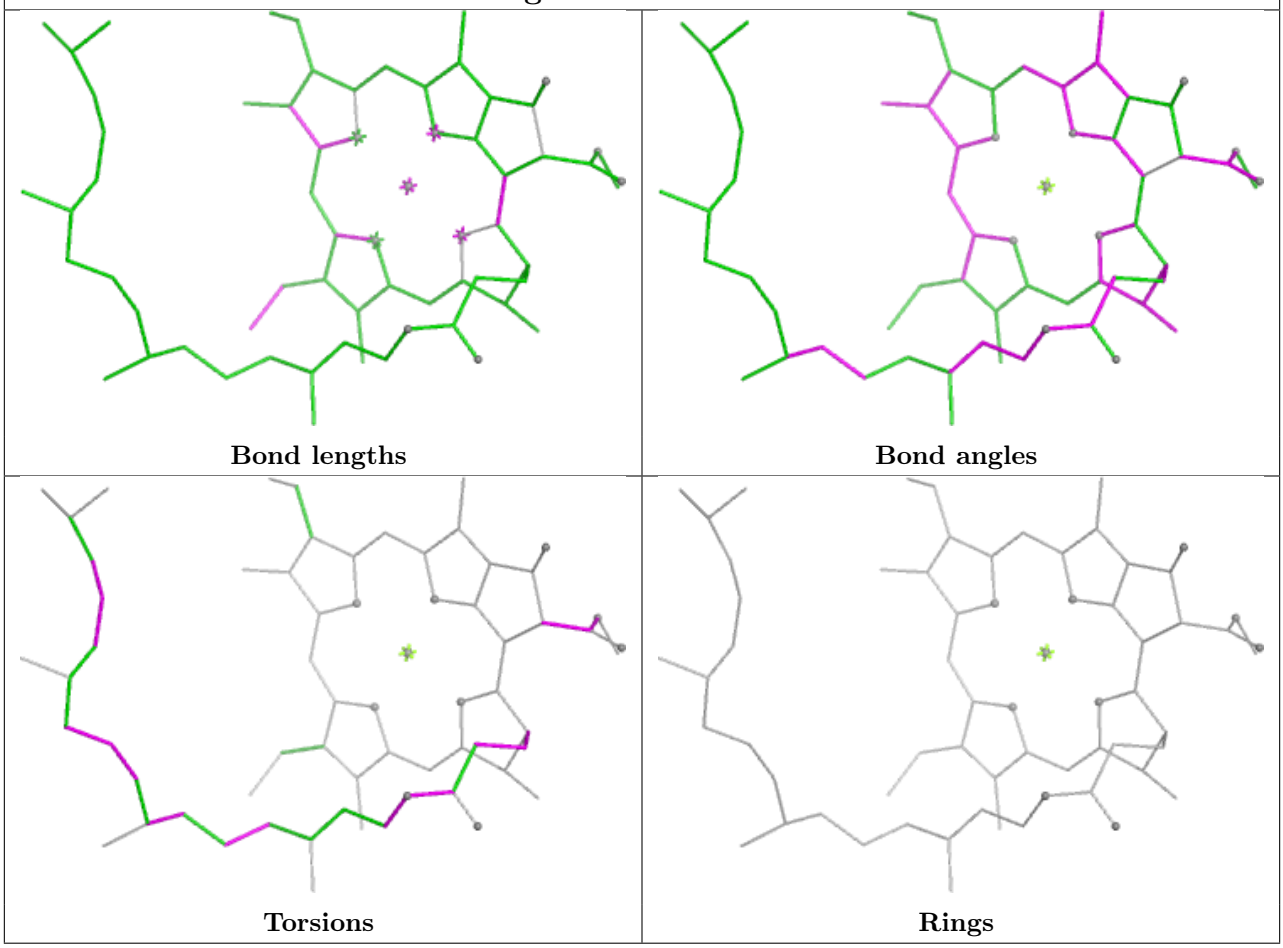
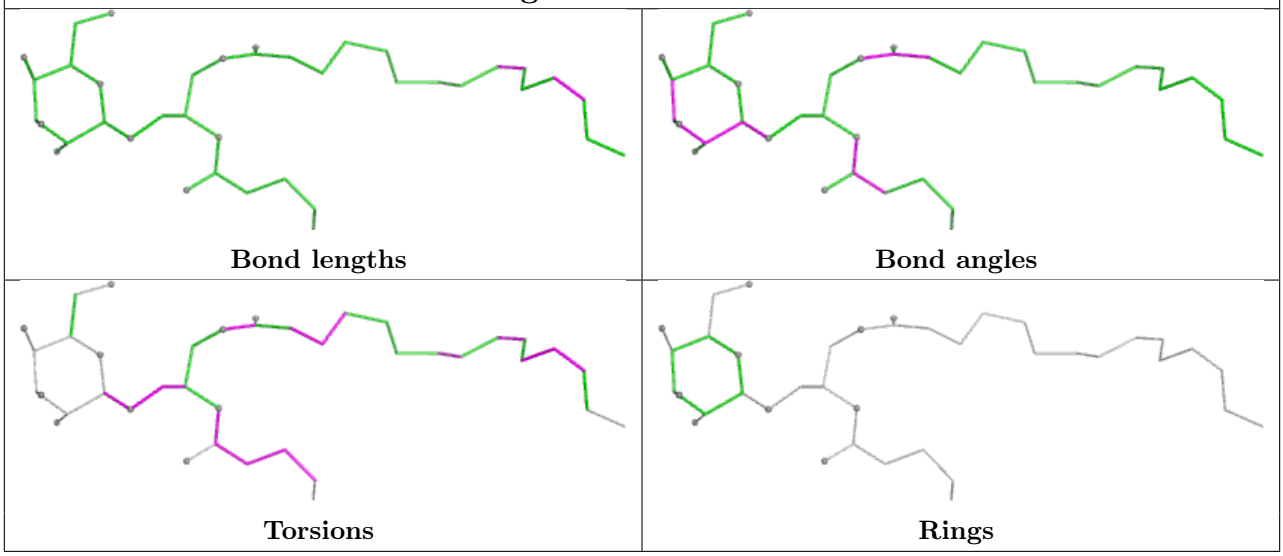


Rings

Ligand CLA N 602



Ligand LMG w 201



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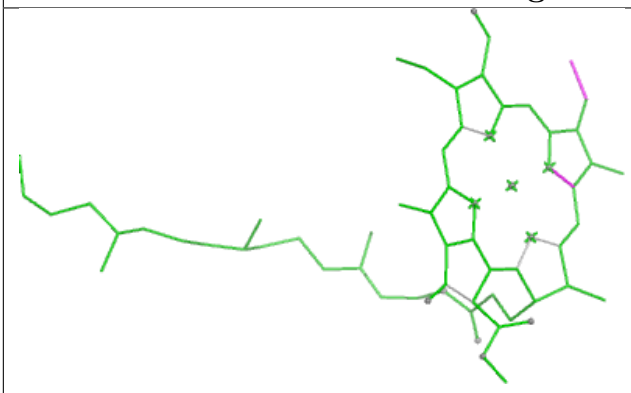
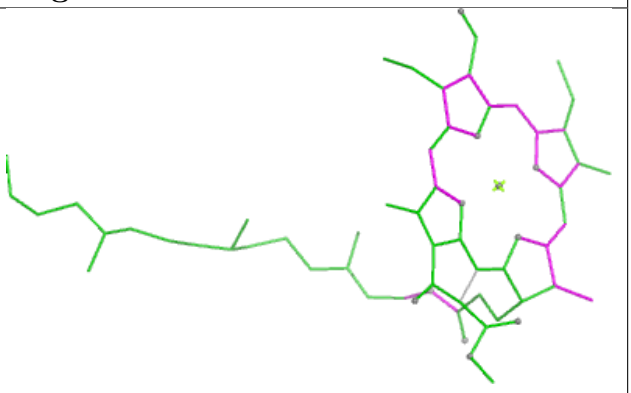
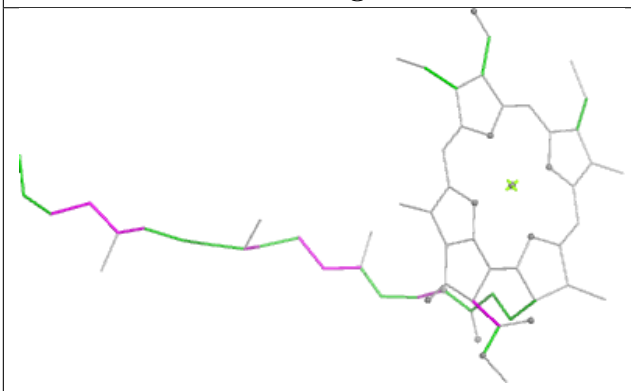
 Bond lengths	 Bond angles
 Torsions	Rings

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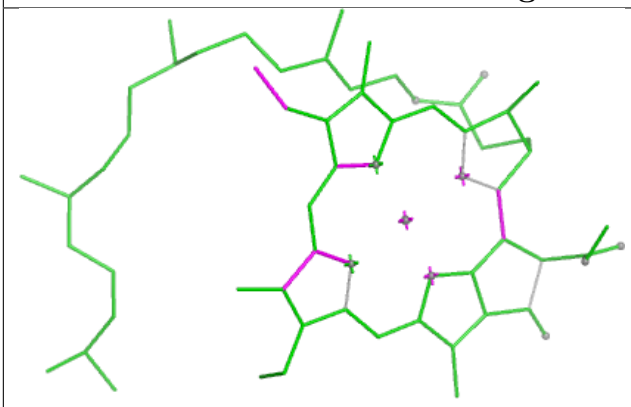
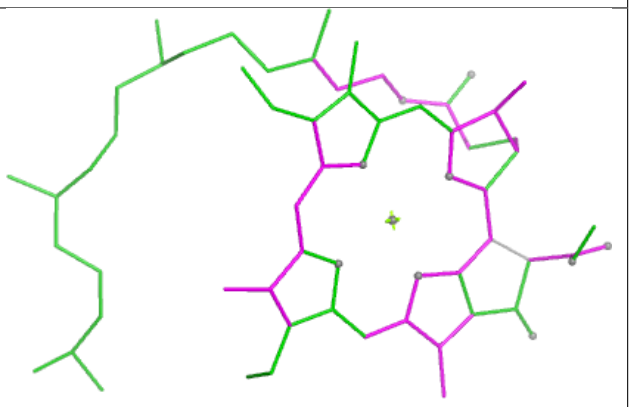
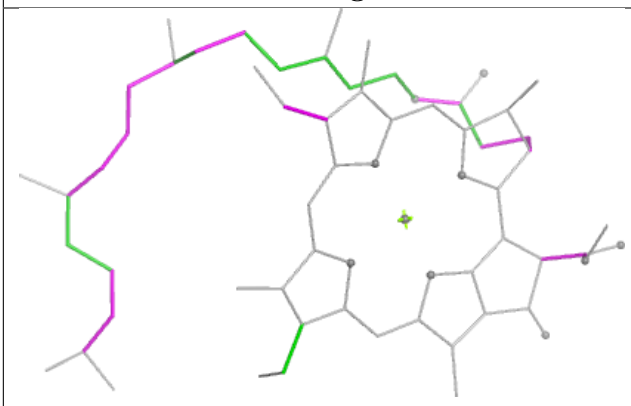
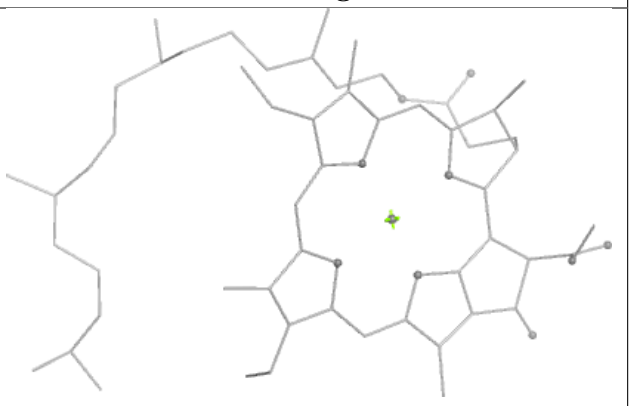
 Bond lengths	 Bond angles
 Torsions	 Rings

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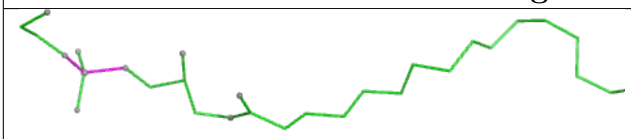
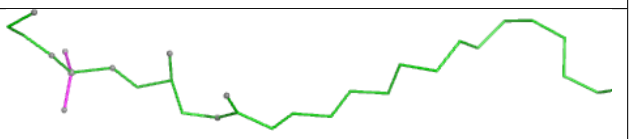
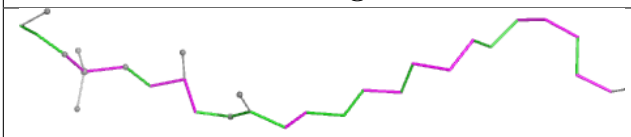
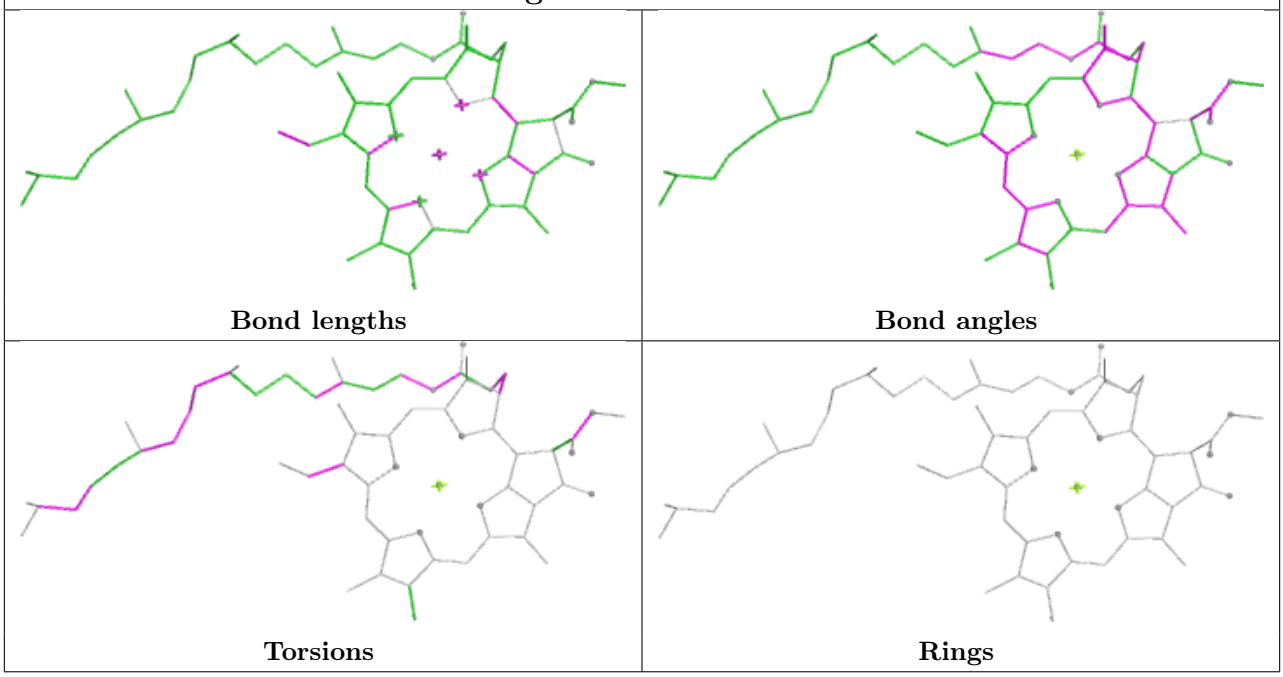
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA C 501



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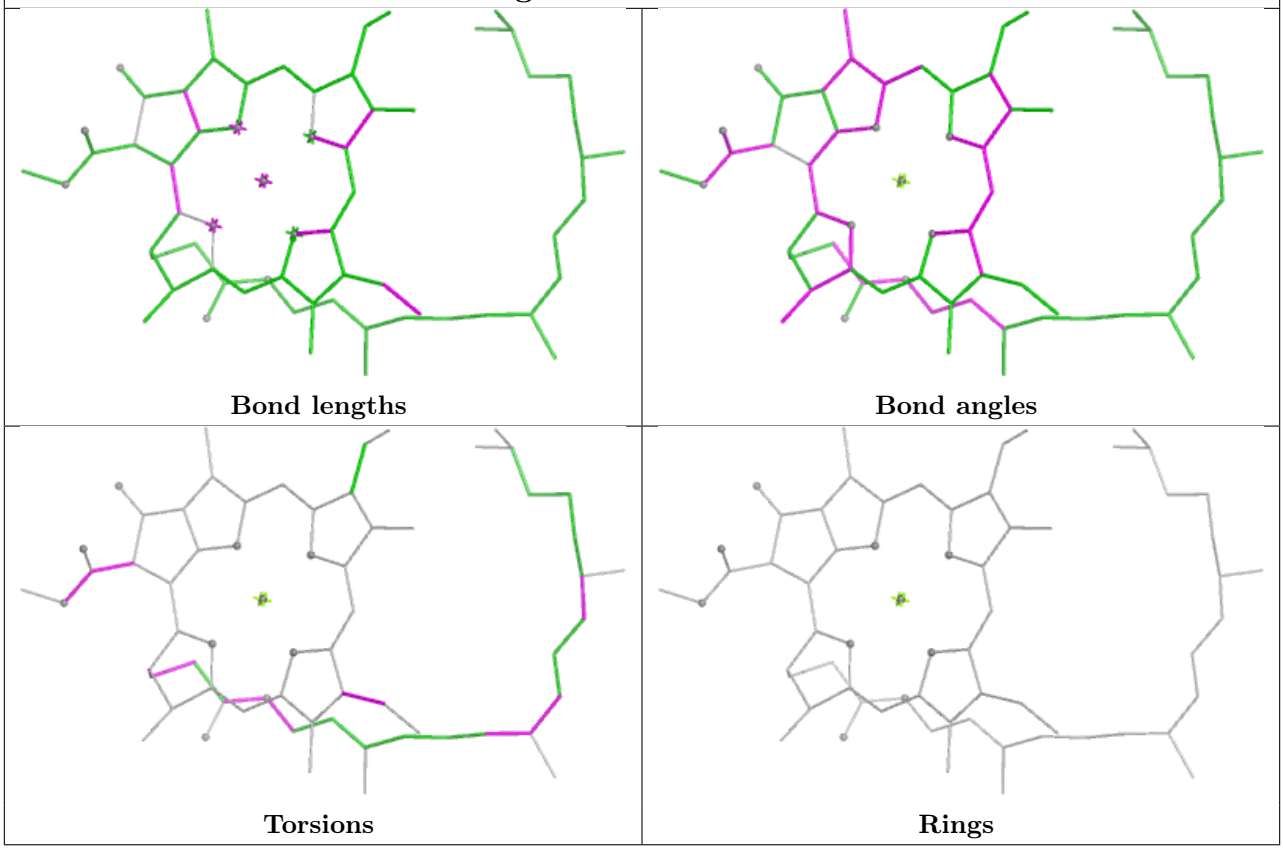

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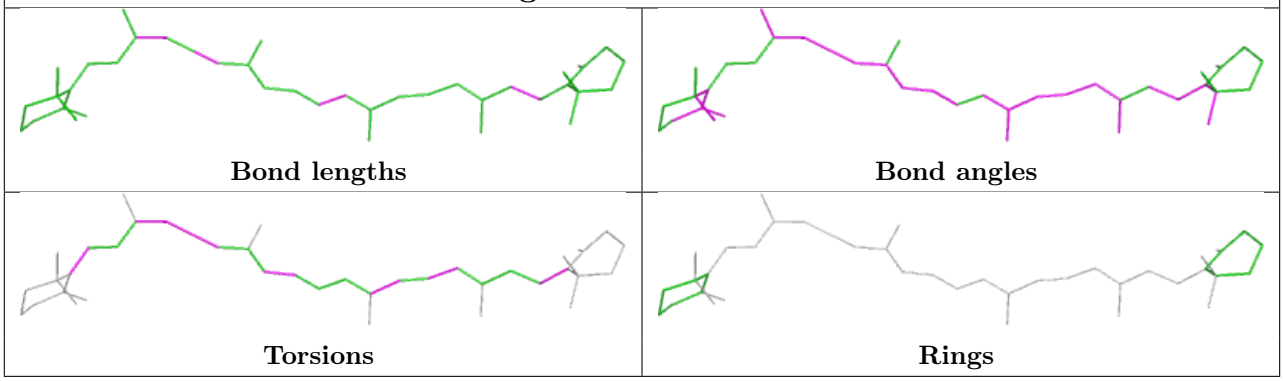

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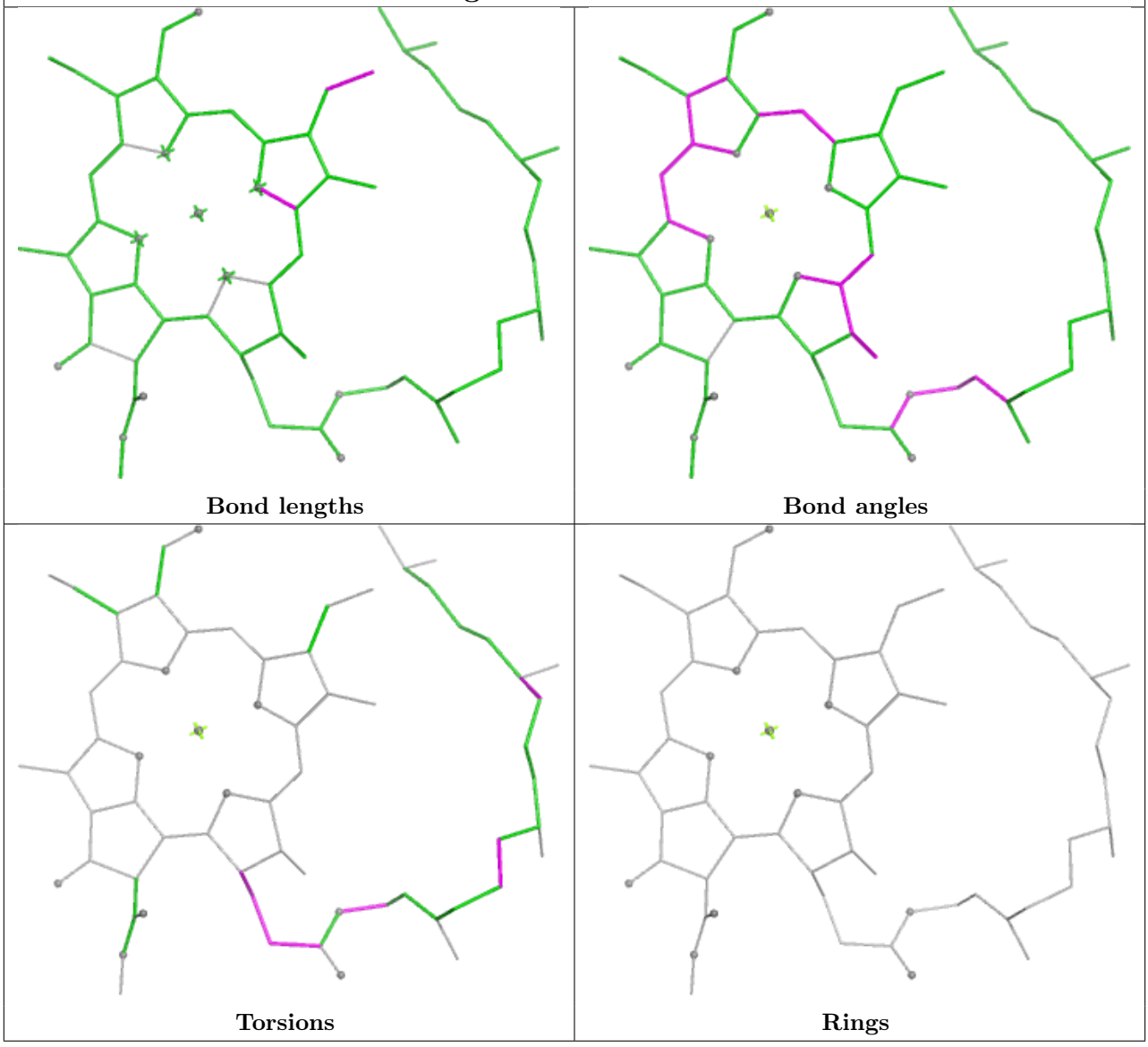

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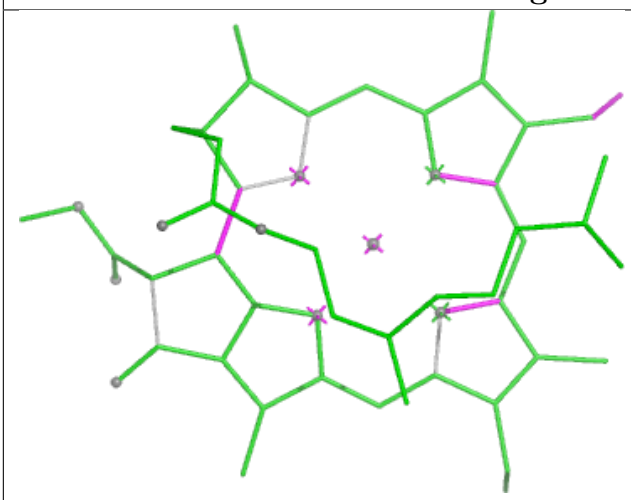
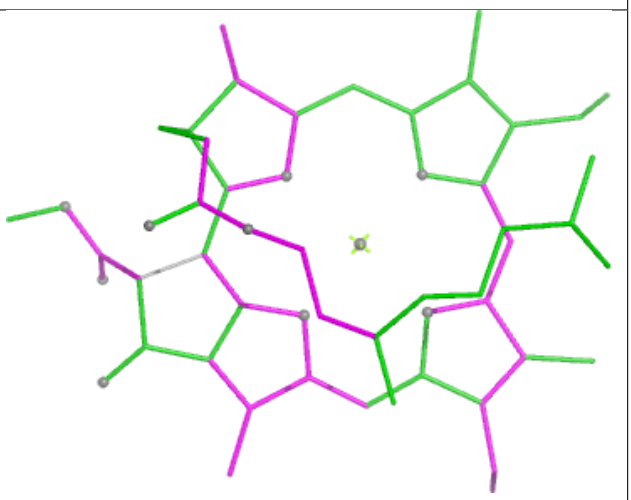
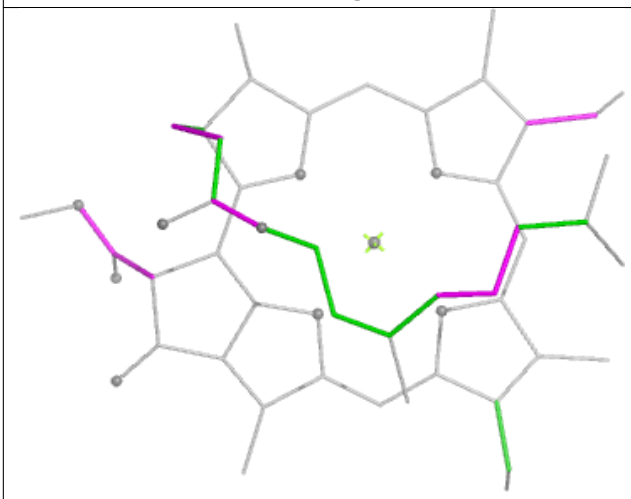


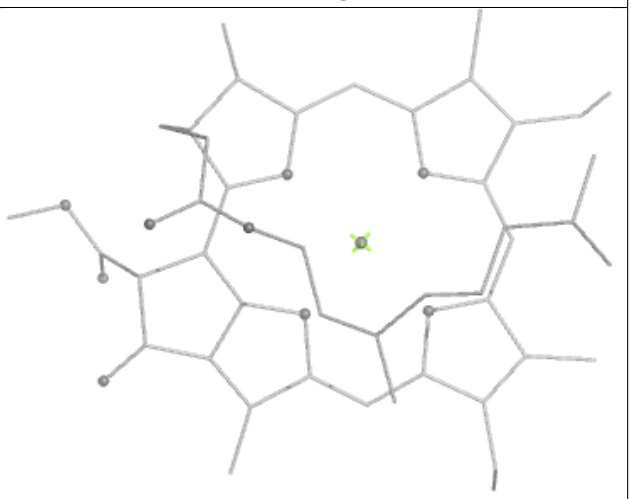
Bond lengths



Bond angles

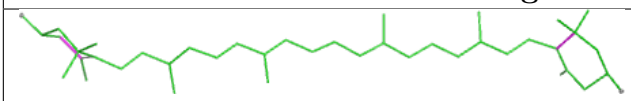


Torsions



Rings

Ligand LUT r1 620



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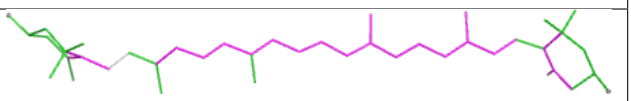
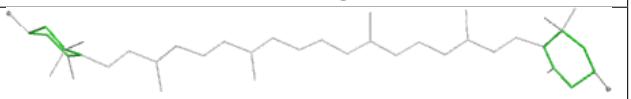


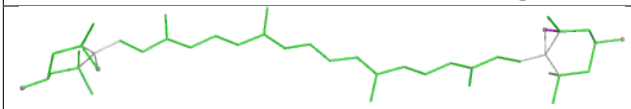
Bond angles

Torsions



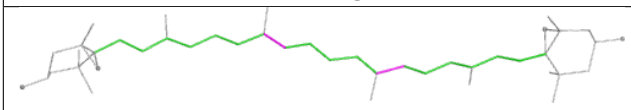
Rings

Ligand XAT R1 621



Bond lengths

Bond angles



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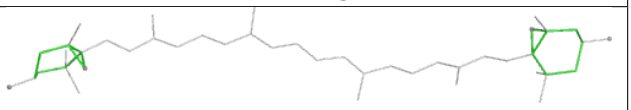
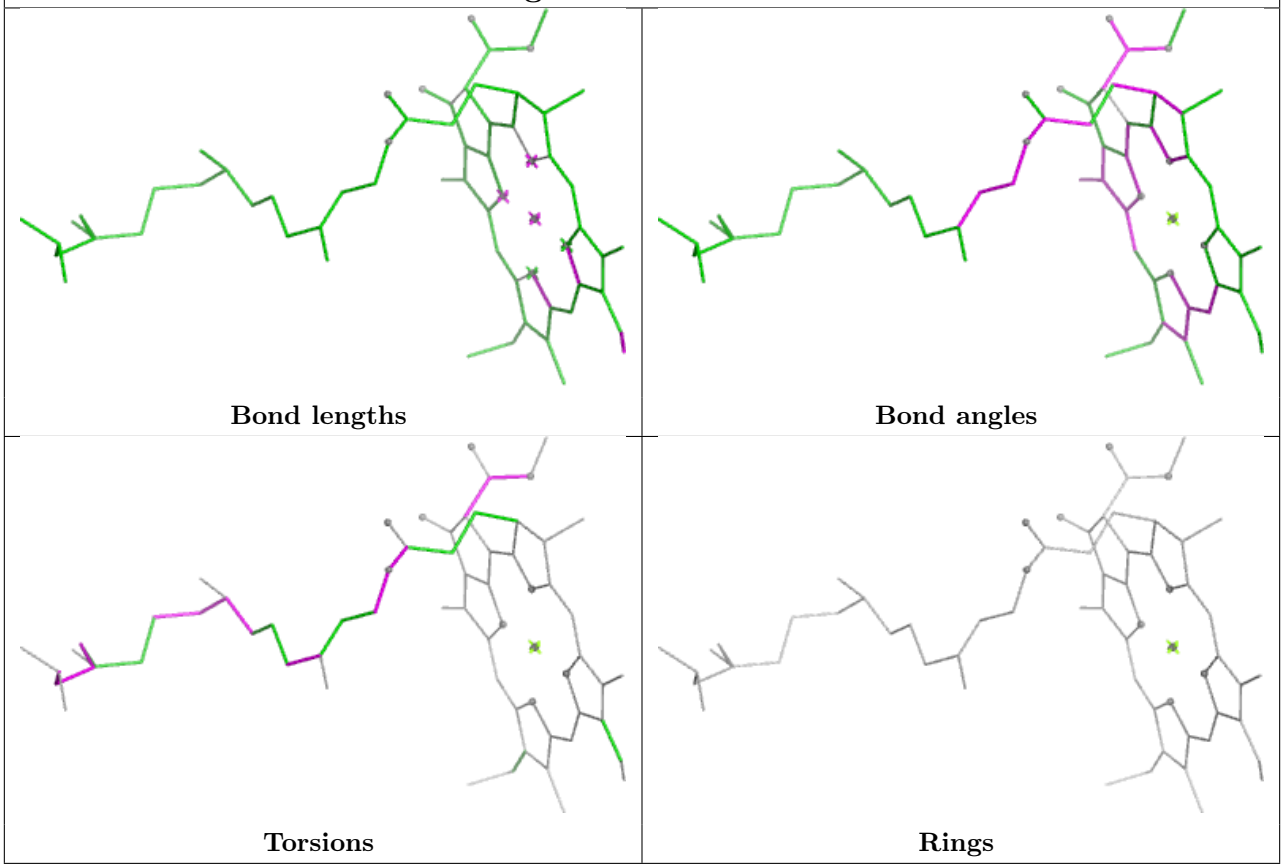
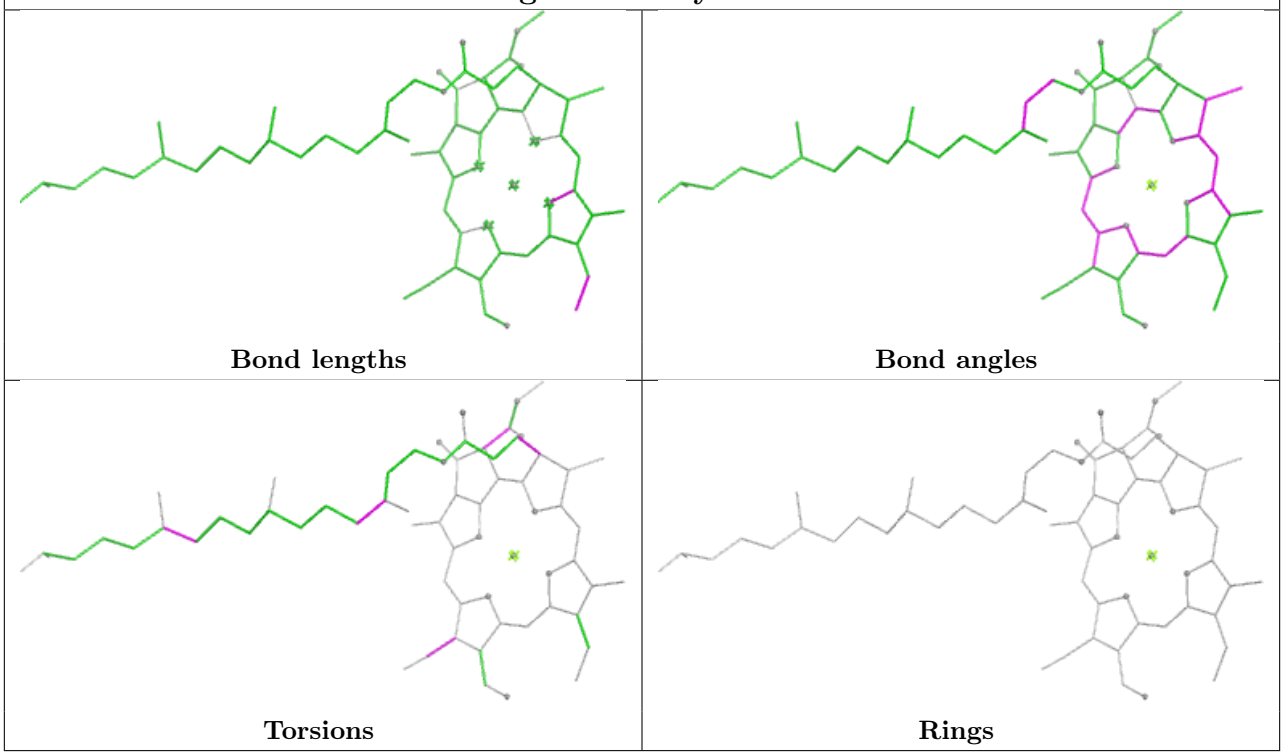


Rings

Ligand CLA Y 604



Ligand CHL y1 609



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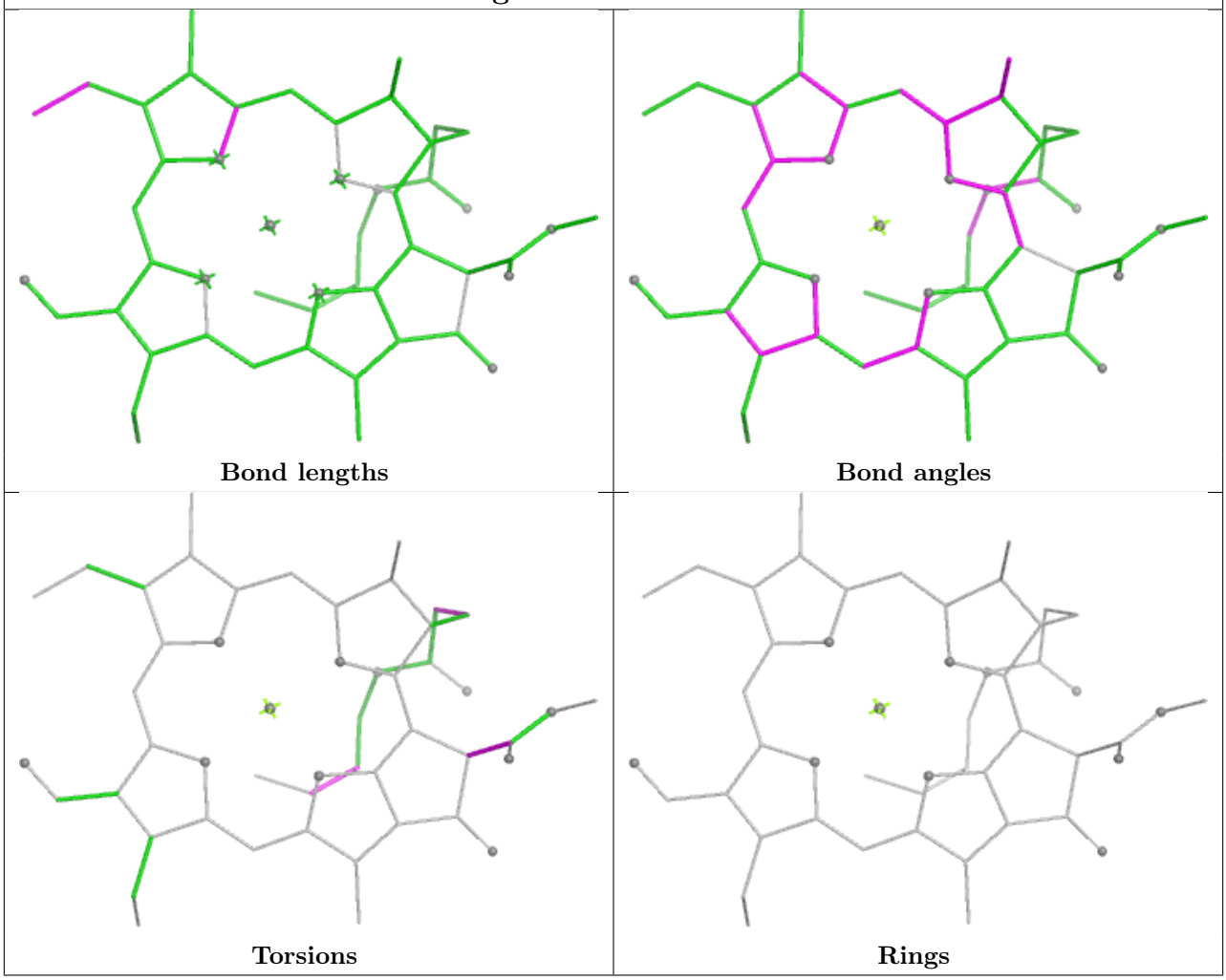

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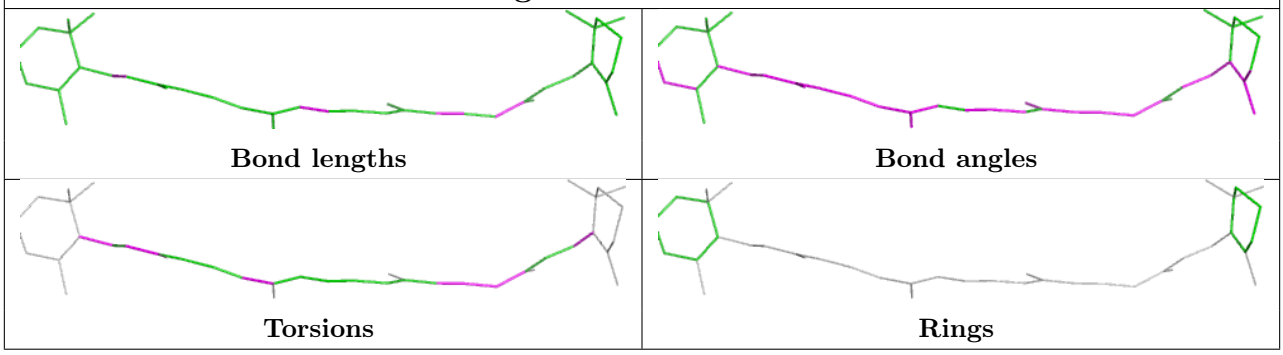

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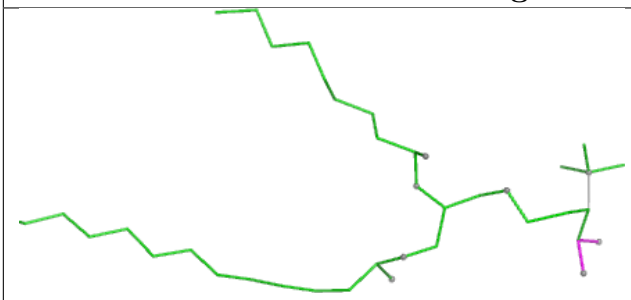
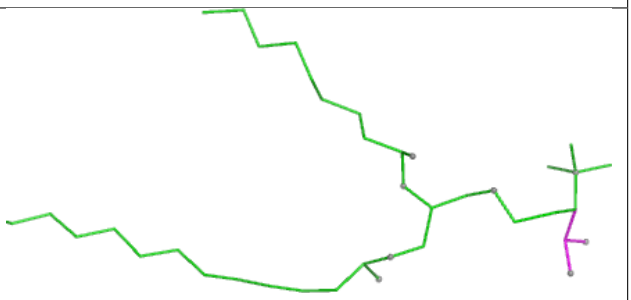
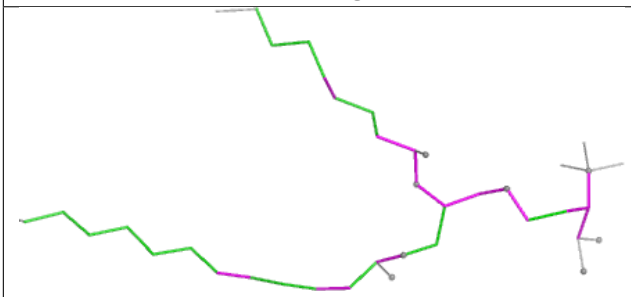
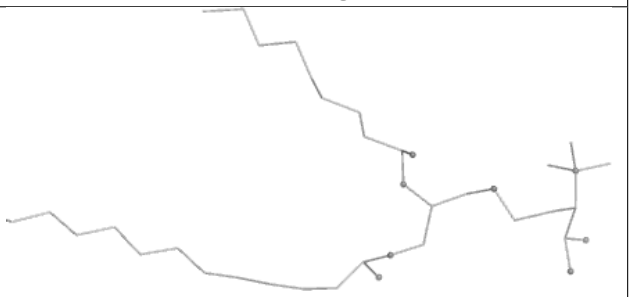
 Bond lengths	 Bond angles
 Torsions	 Rings

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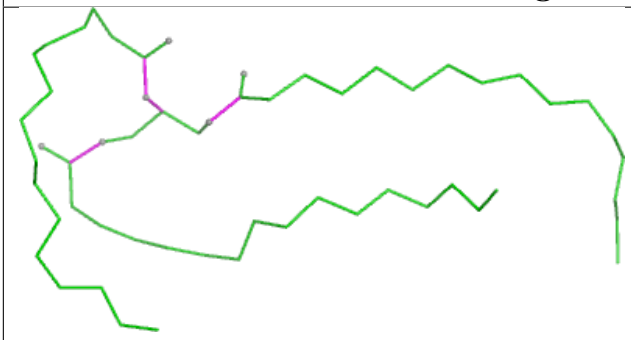
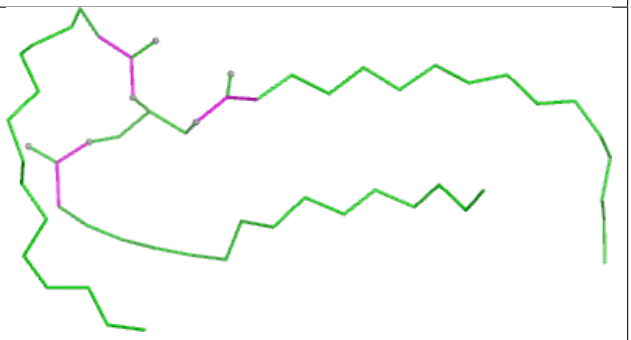
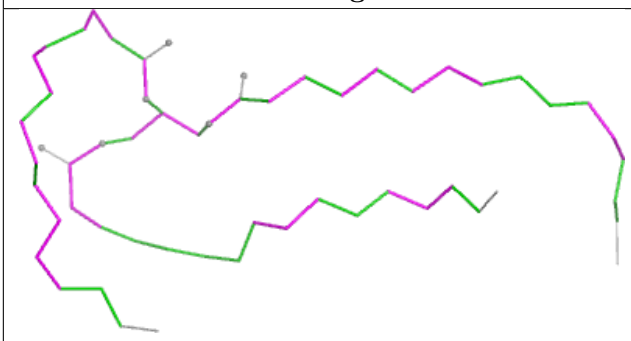
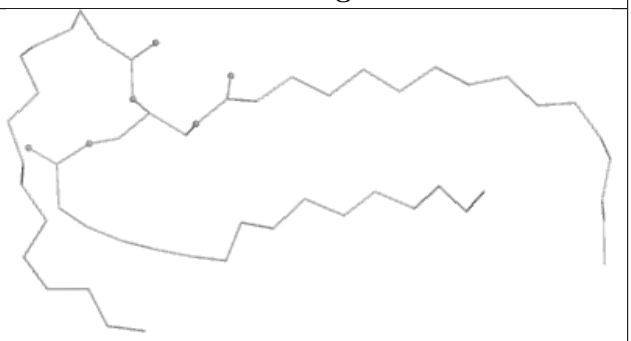
 Bond lengths	 Bond angles
 Torsions	 Rings

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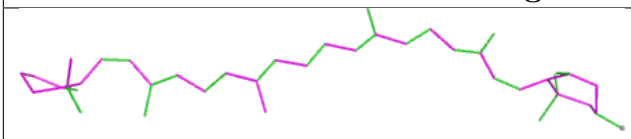
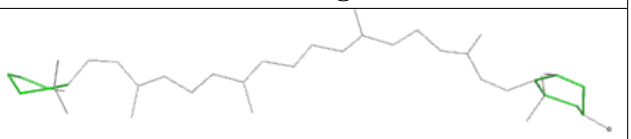
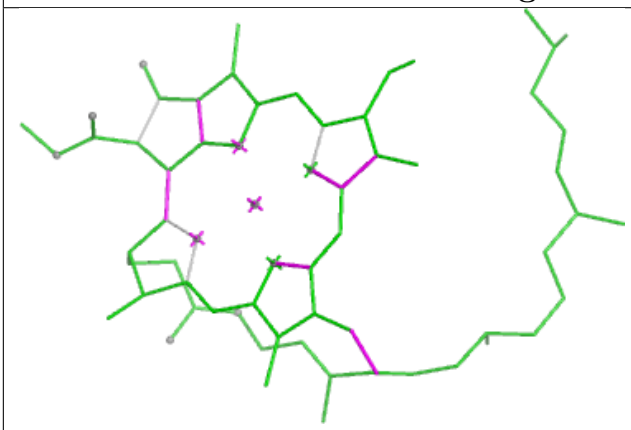
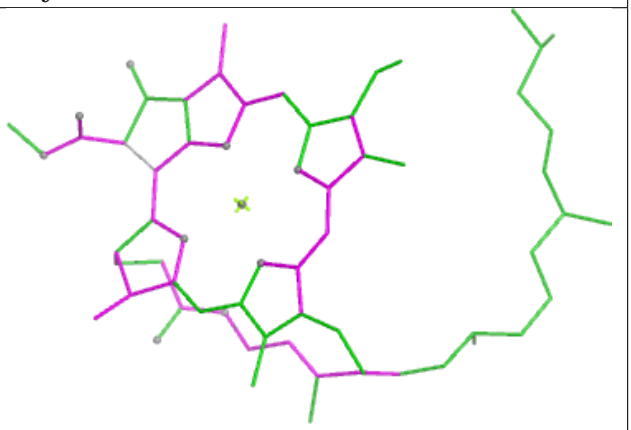
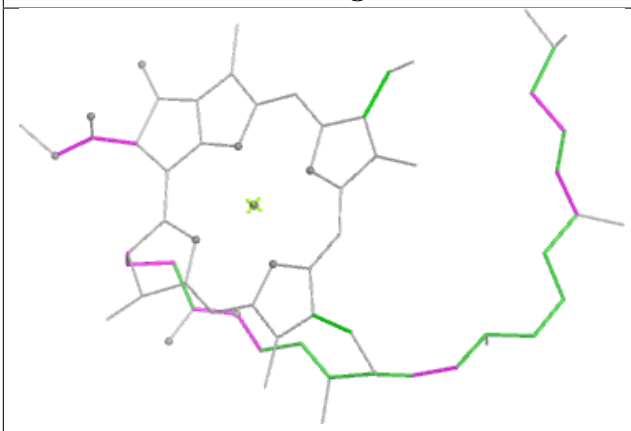
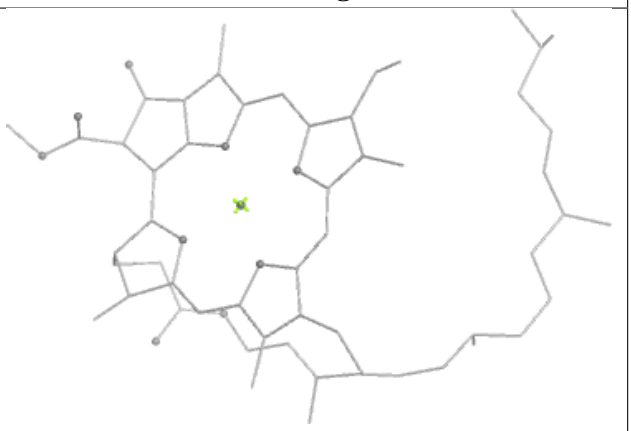
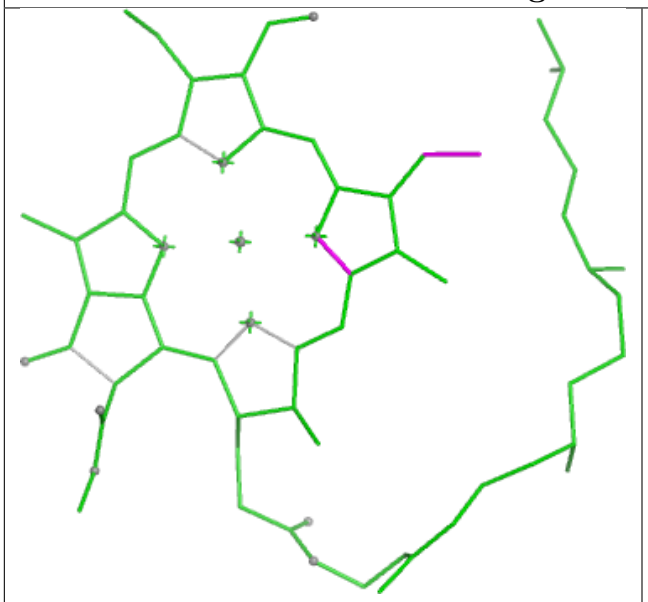
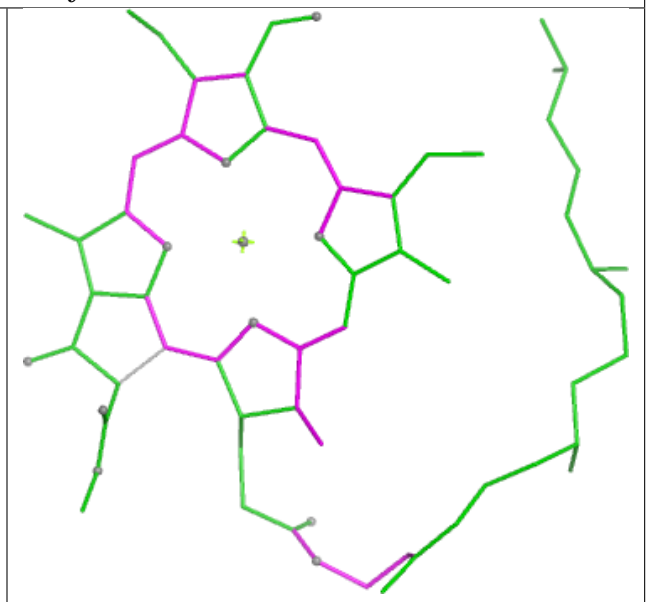
 Bond lengths	Bond angles
Torsions	 Rings

Ligand CLA y1 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

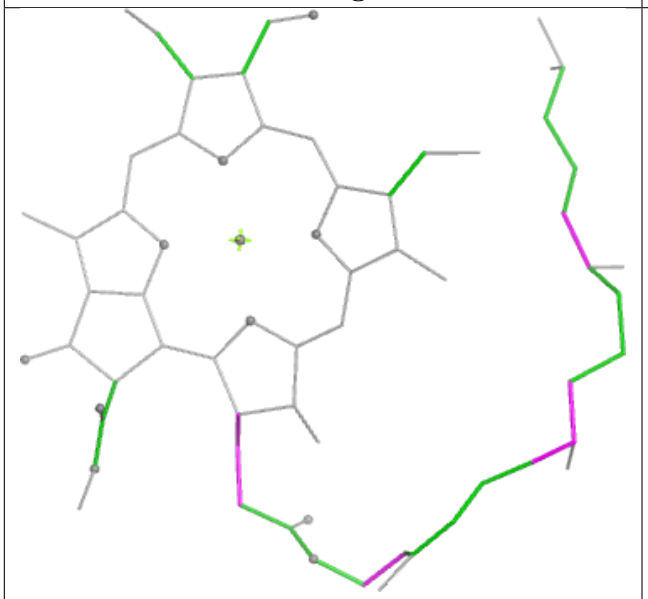
Ligand CHL y 607



Bond lengths



Bond angles



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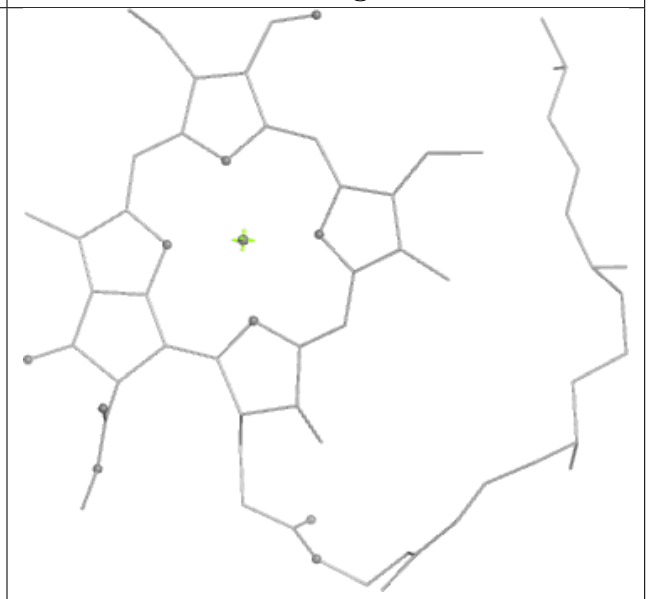
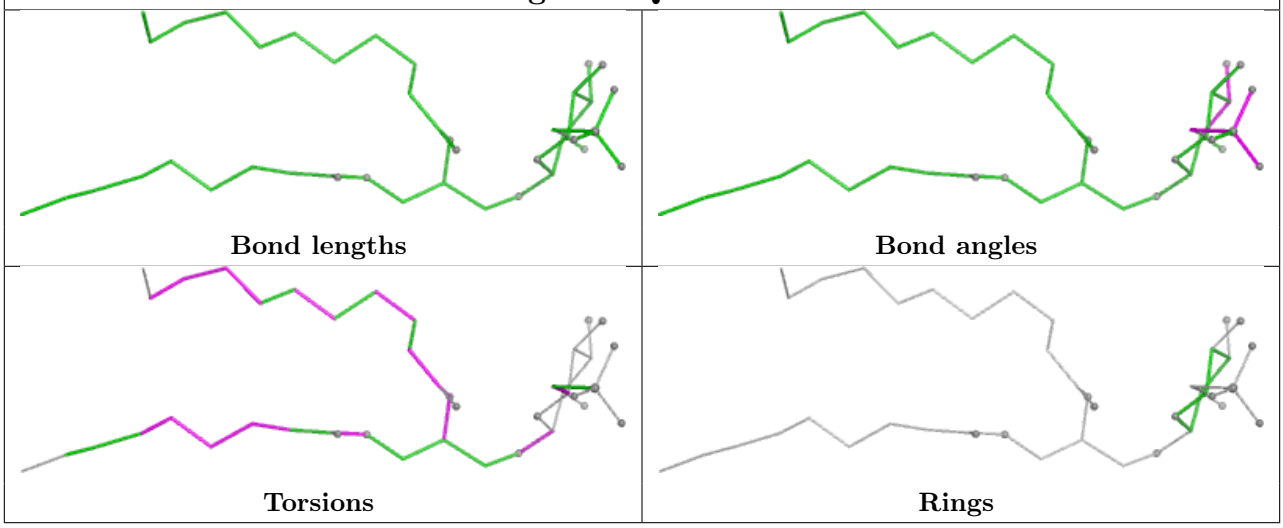
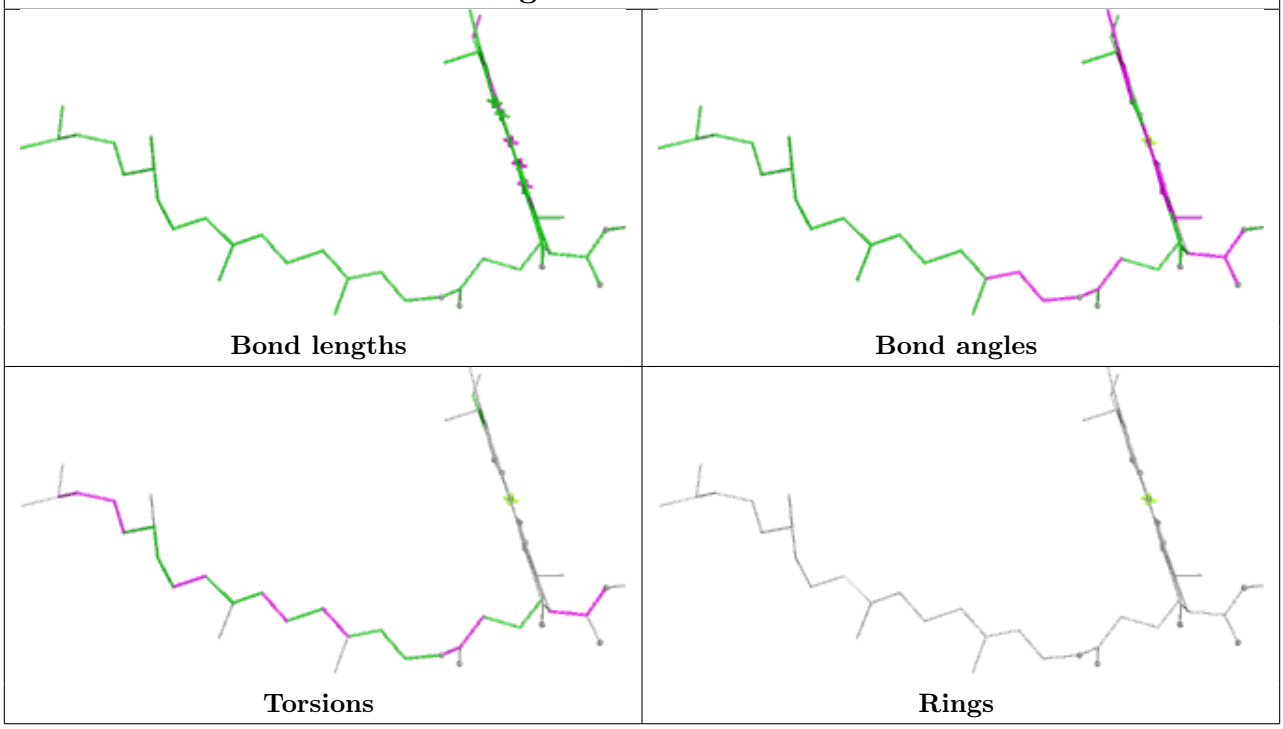


Rings

Ligand SQD b 621



Ligand CLA b1 606



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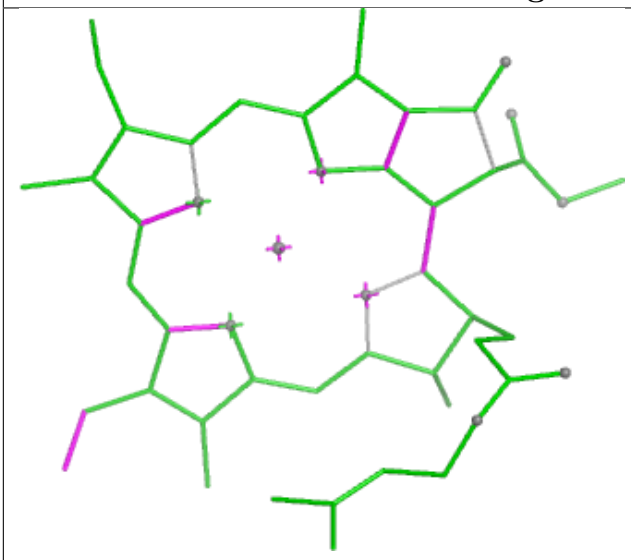

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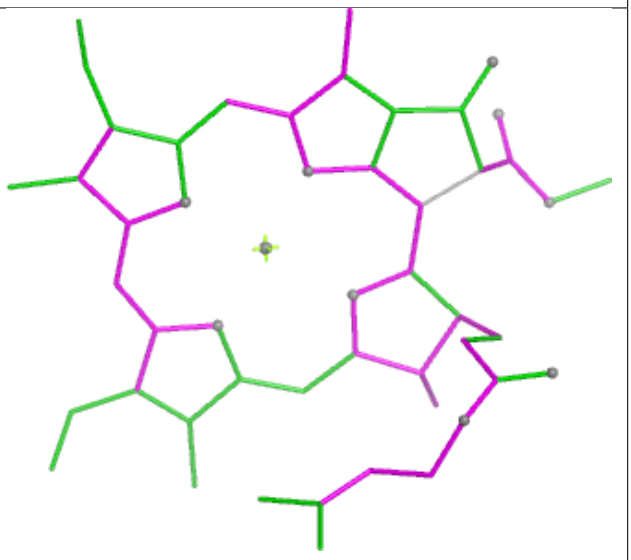
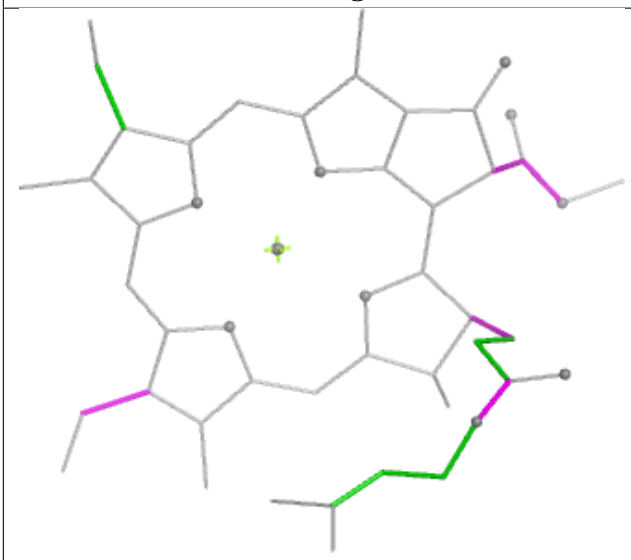


Bond angles



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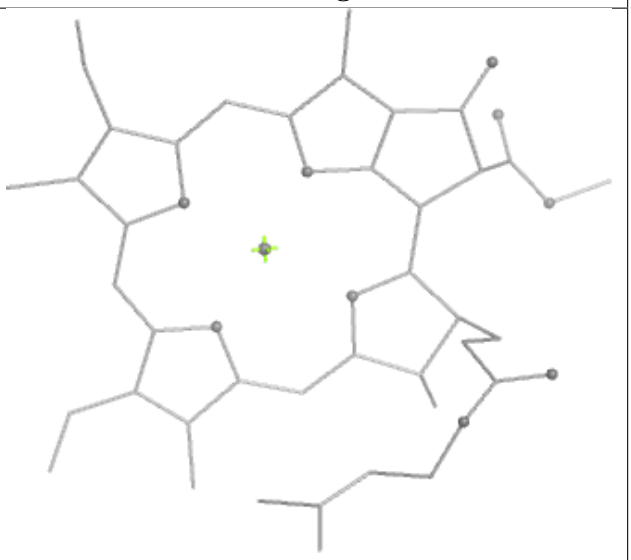
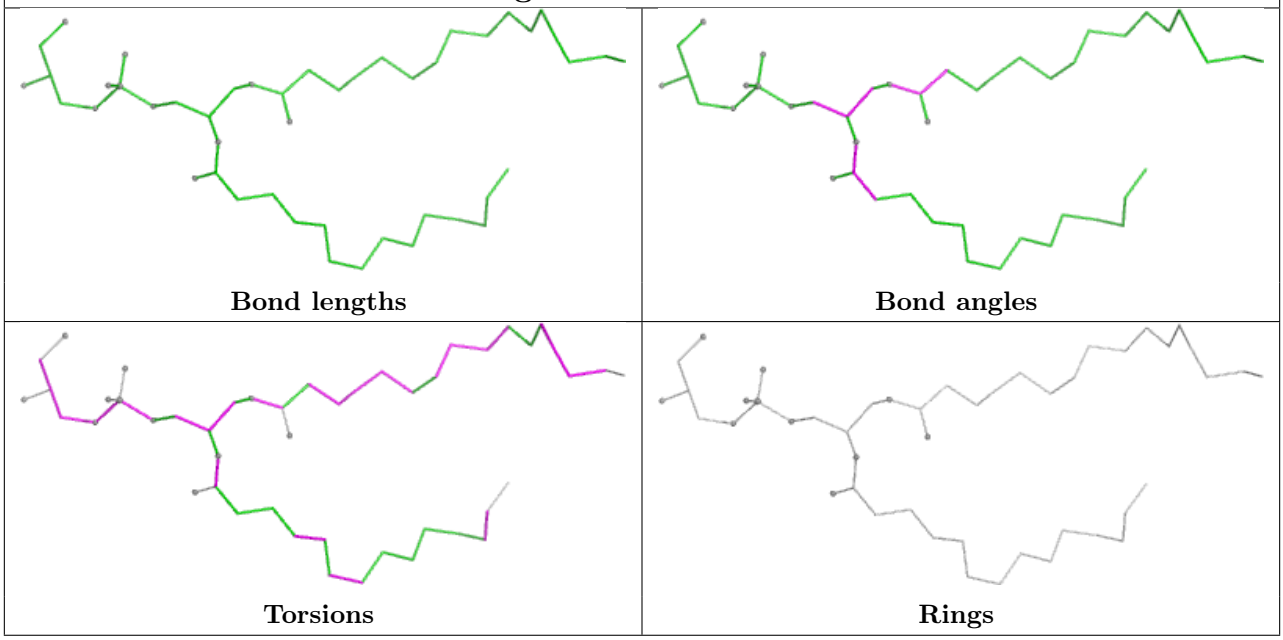


Rings

Ligand LHG C1 525



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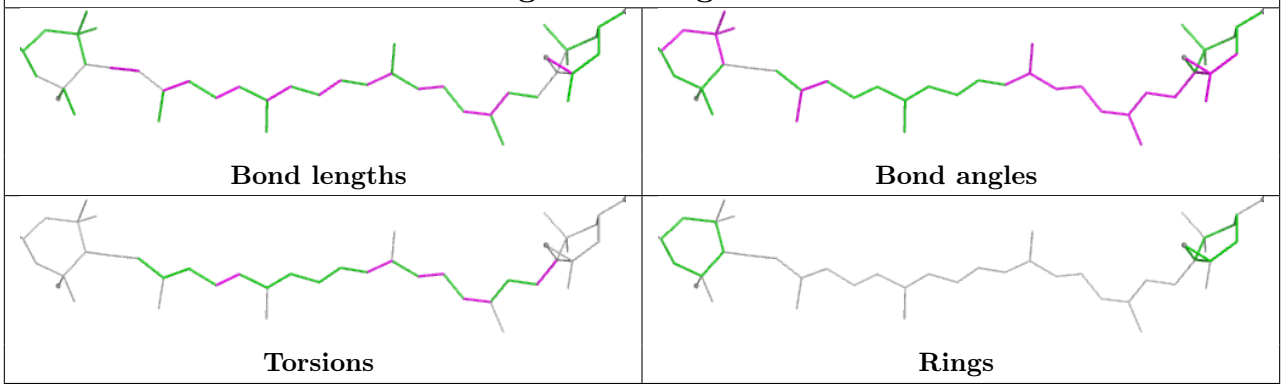
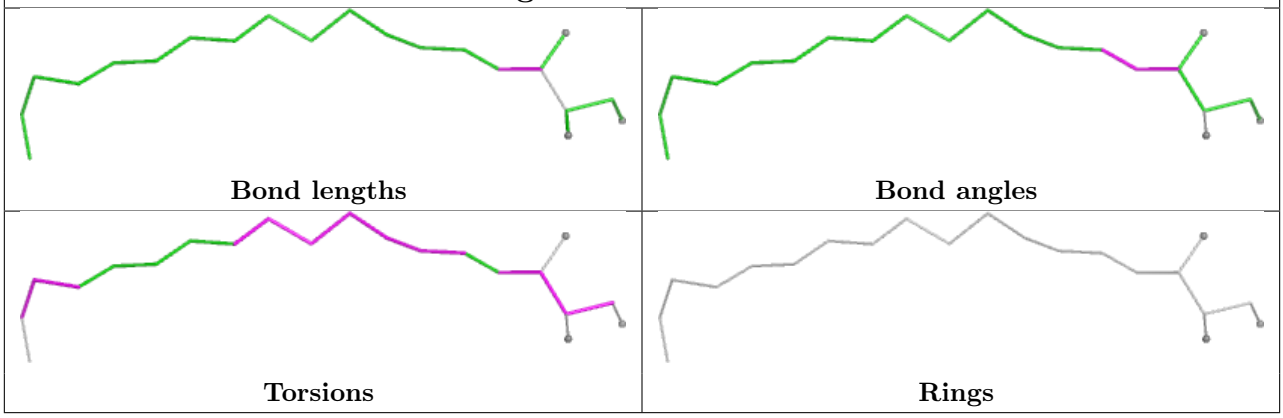
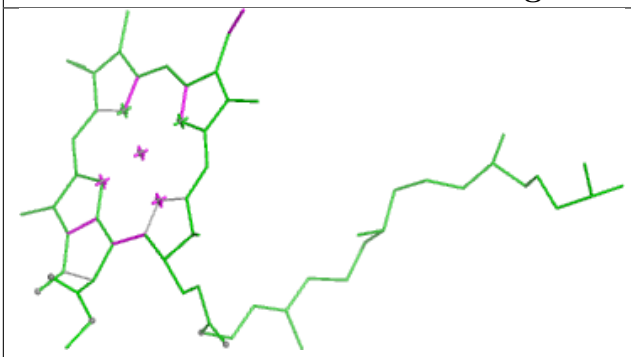


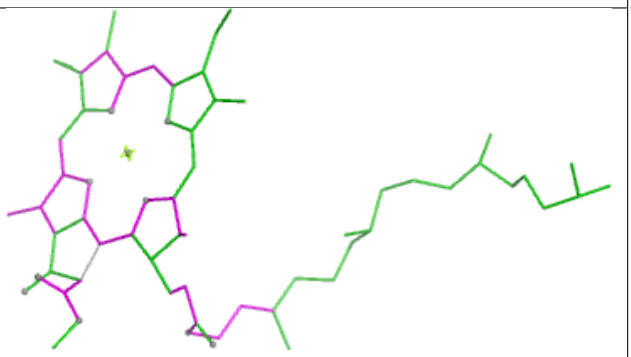
Ligand SPH A1 414



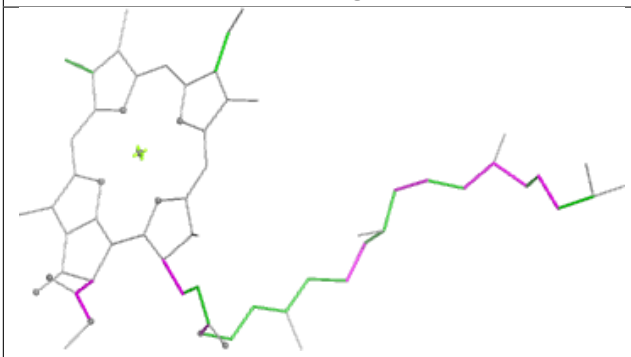
Ligand CLA C 511



Bond lengths



Bond angles



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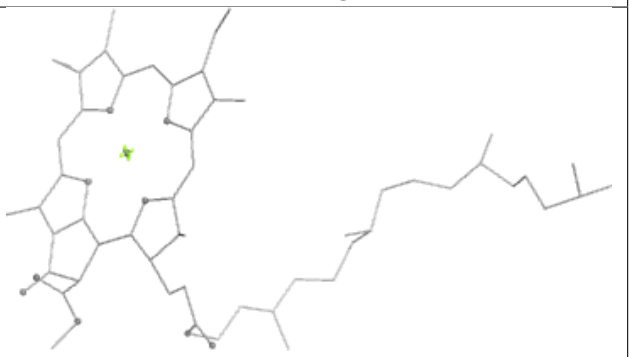
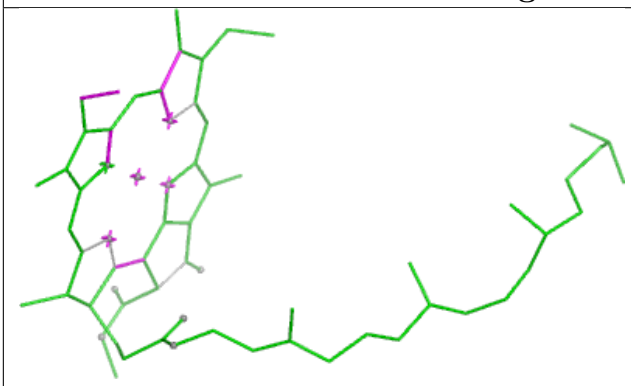


Rings

Ligand CLA S1 611



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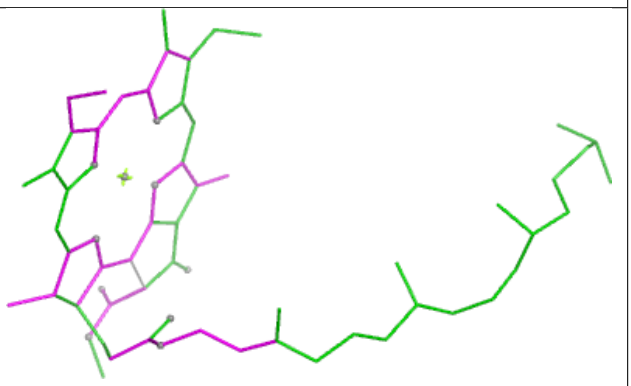

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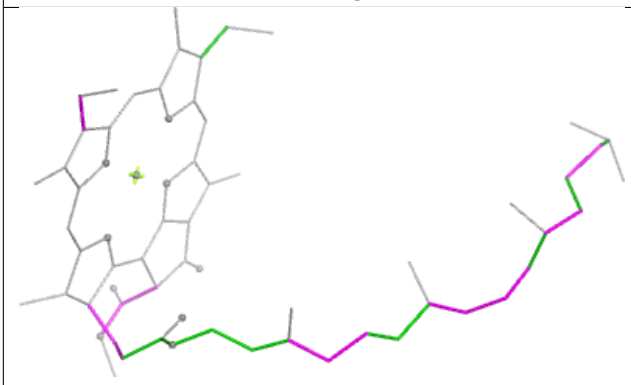

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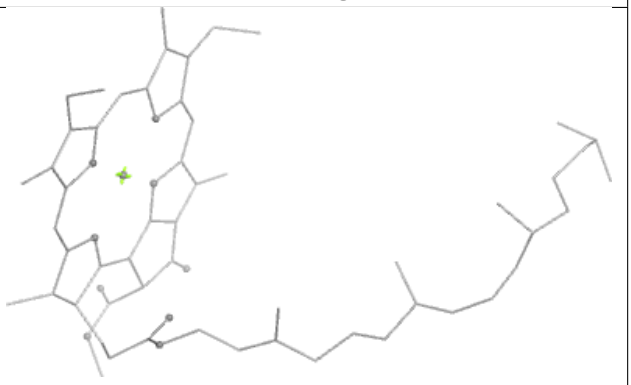
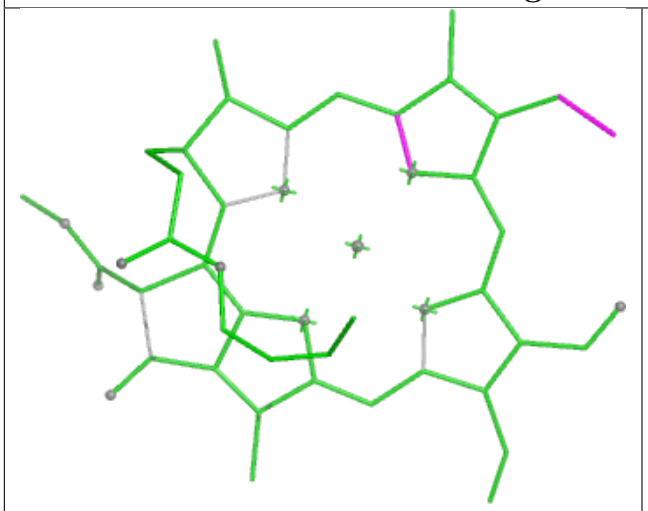


Rings

Ligand CHL R 607



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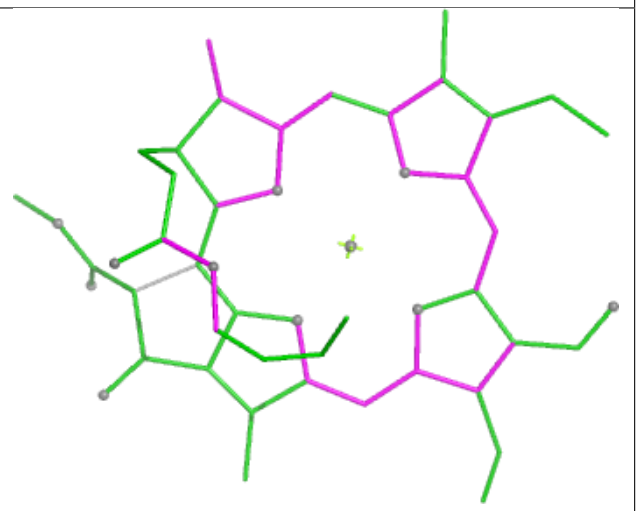

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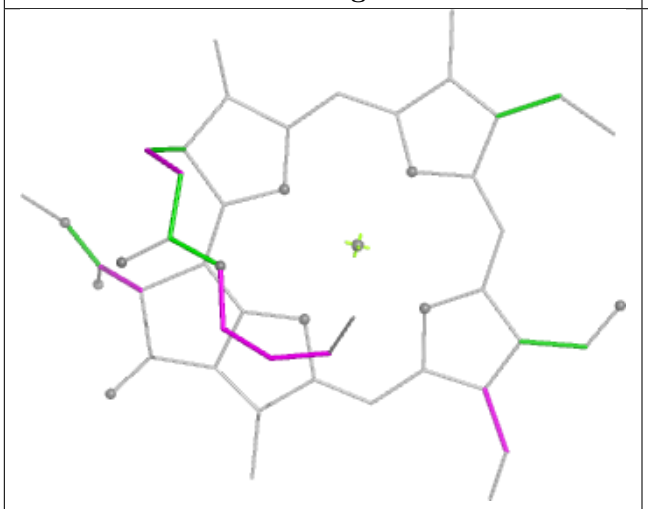

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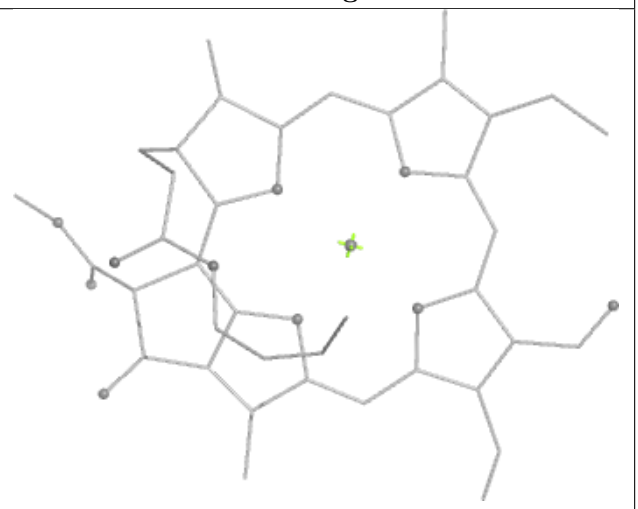
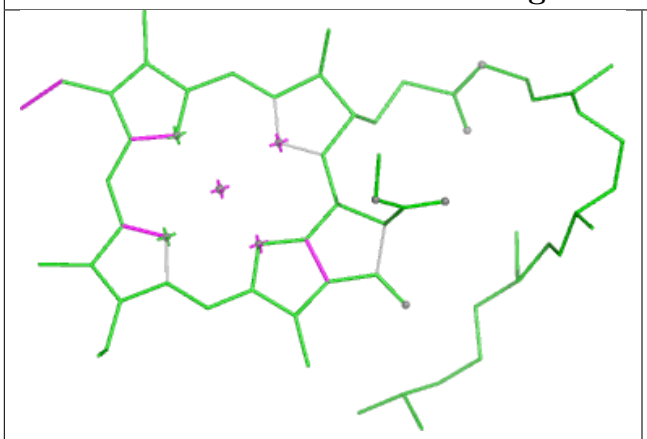


Rings

Ligand CLA b 611



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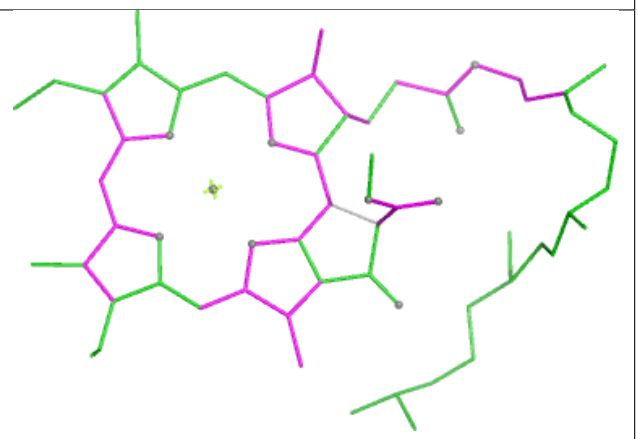

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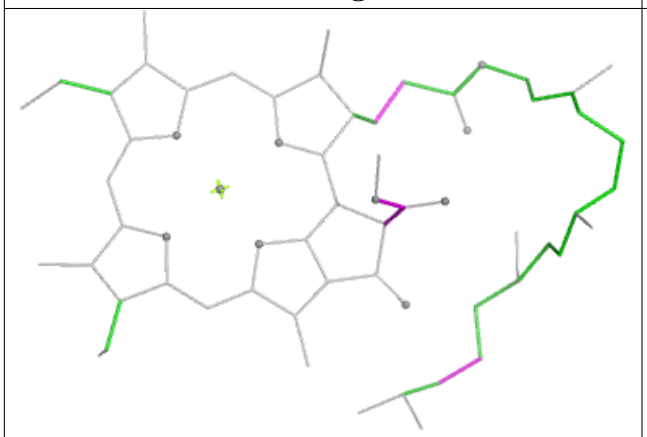

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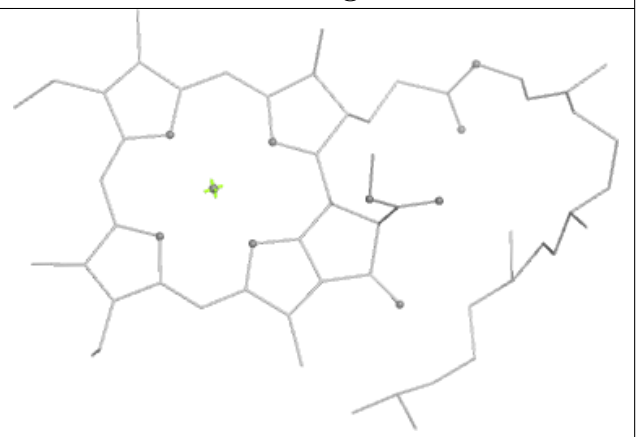
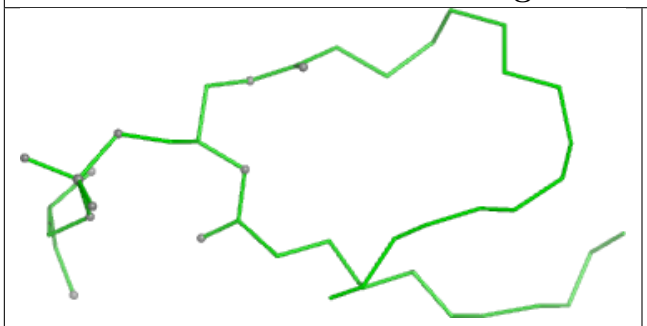


Rings

Ligand LHG D1 408



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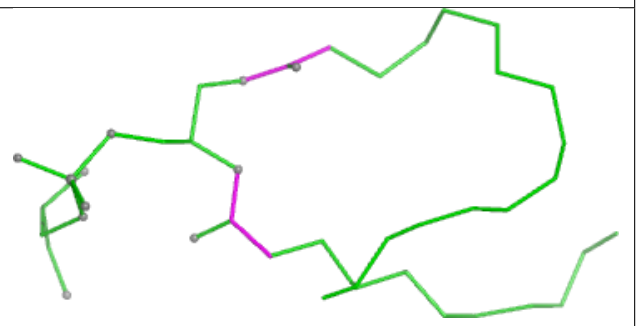

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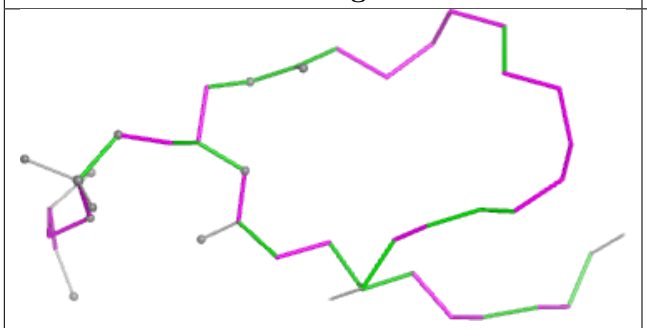
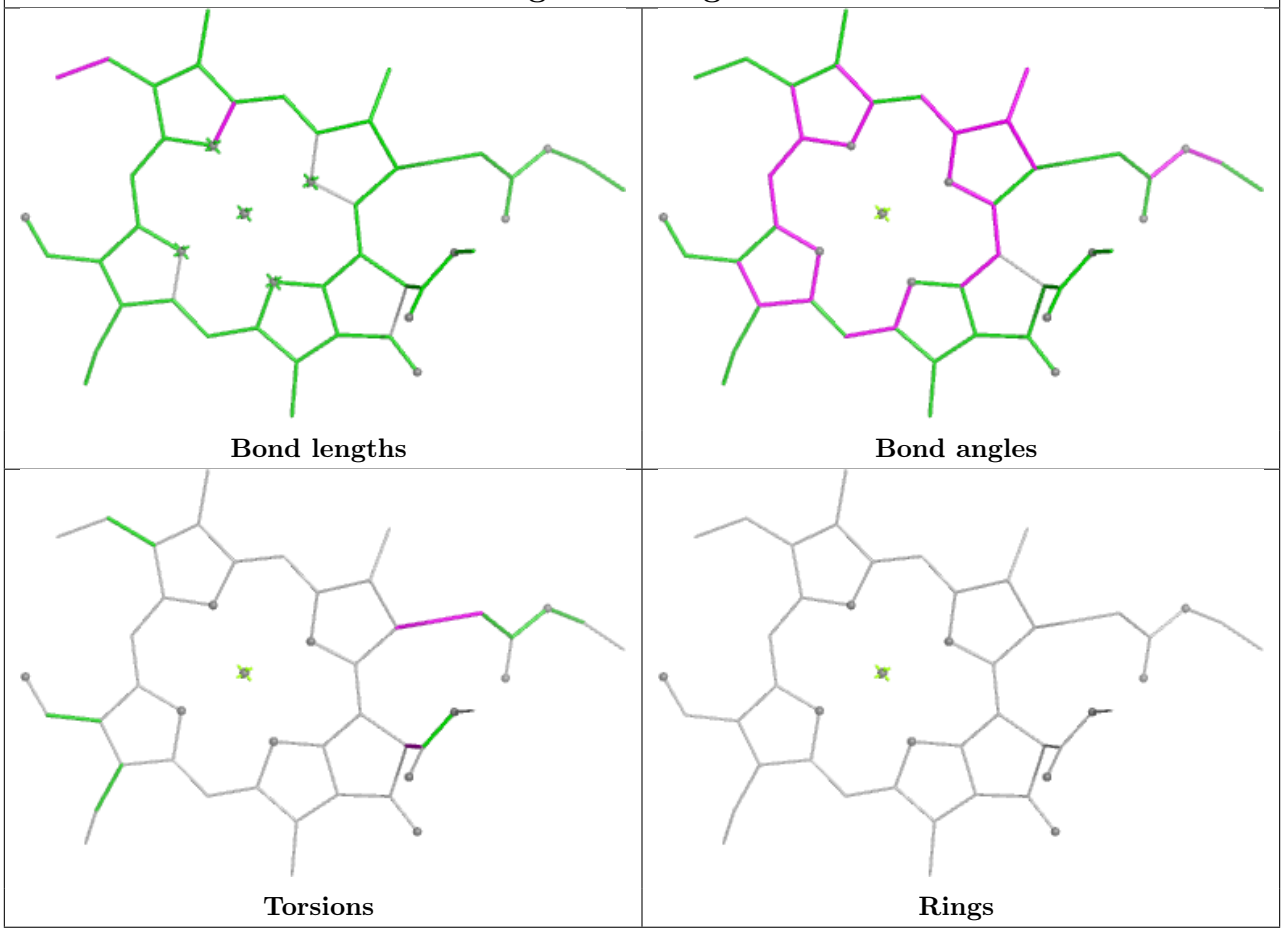


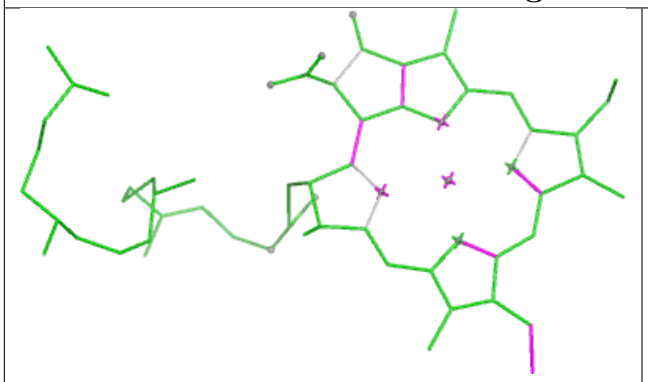
Torsions

Rings

Ligand CHL g 605



Ligand CLA B 613



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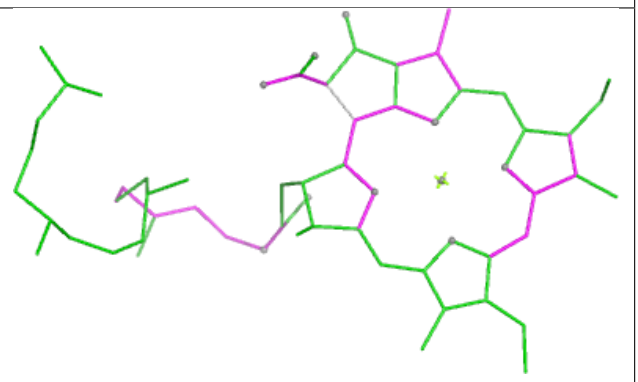

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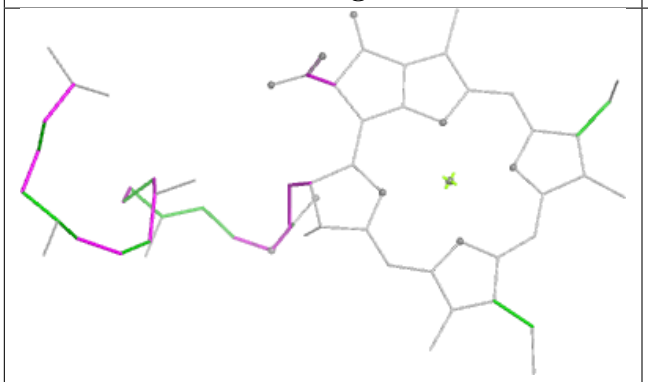

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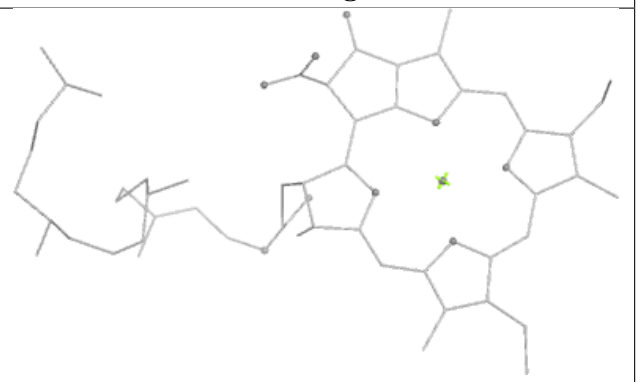

Rings

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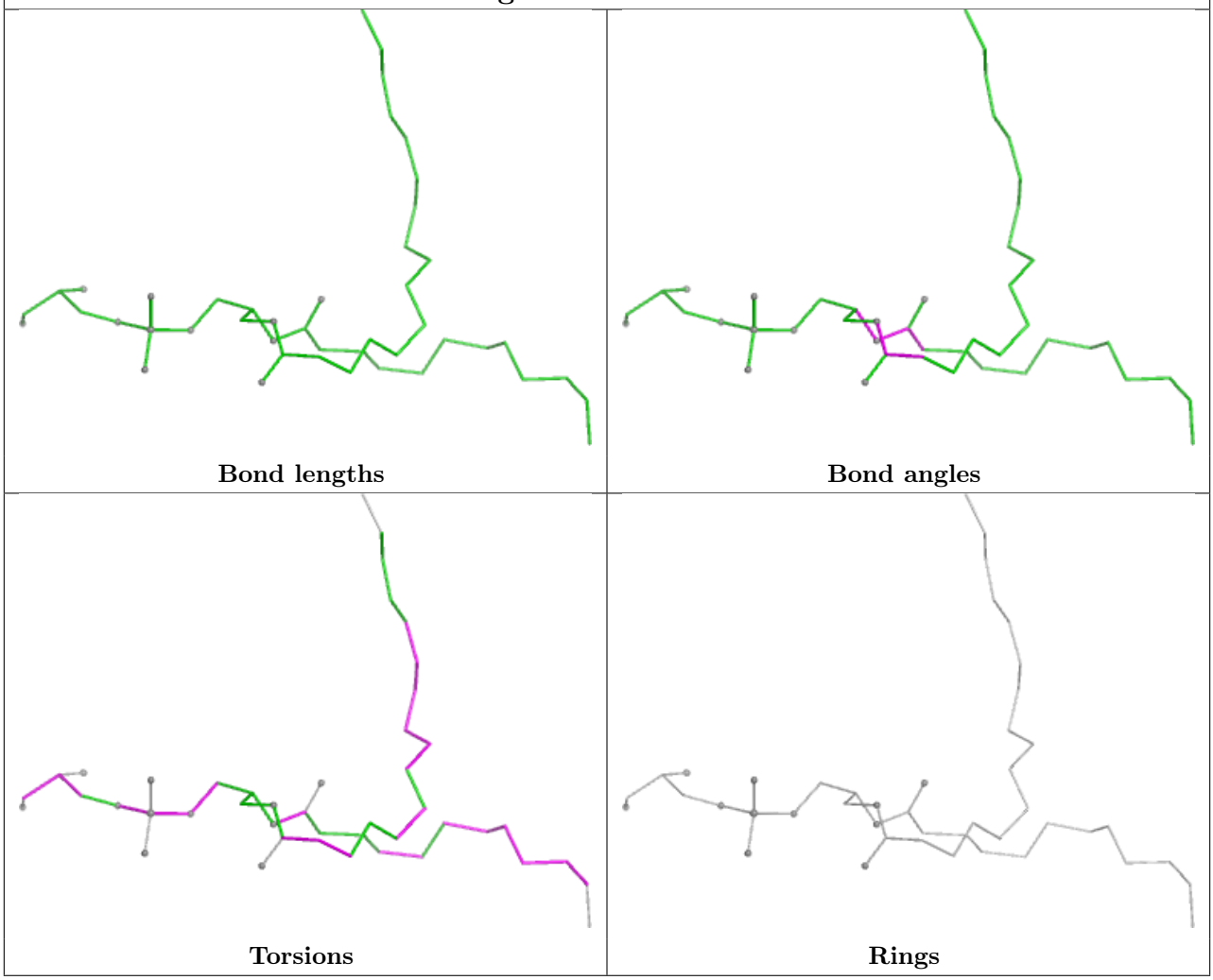

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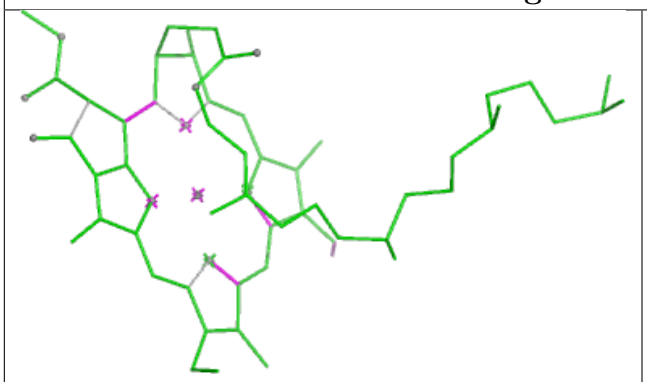

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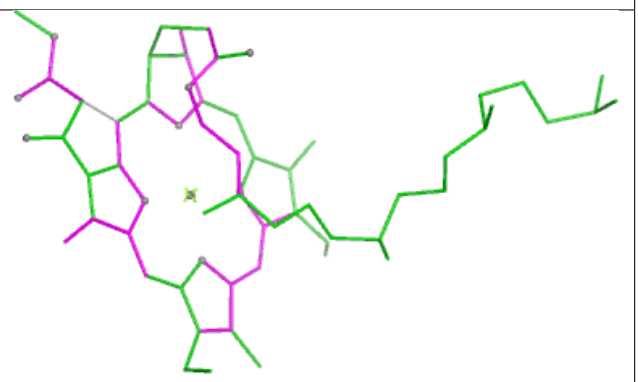

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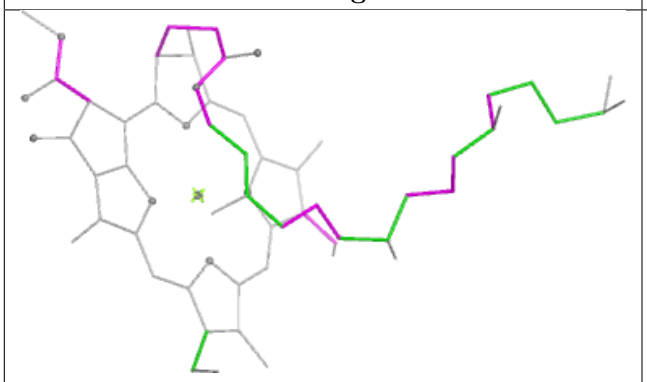

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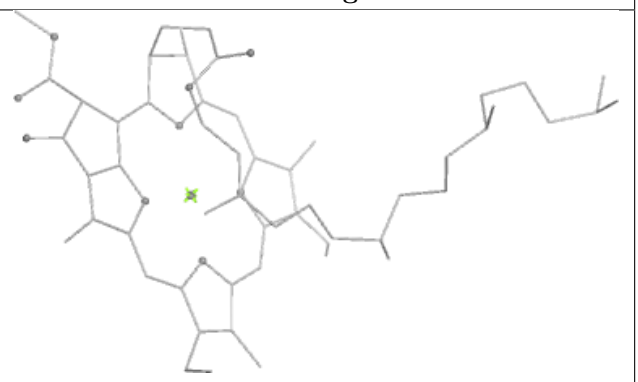
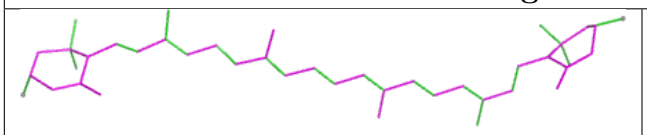


Rings

Ligand C7Z B1 620



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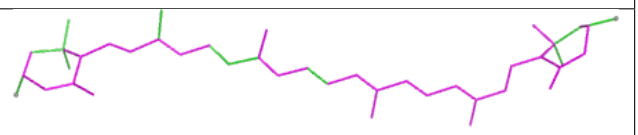

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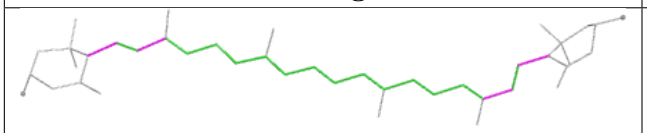

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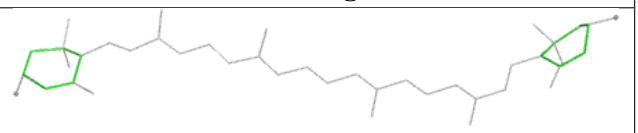
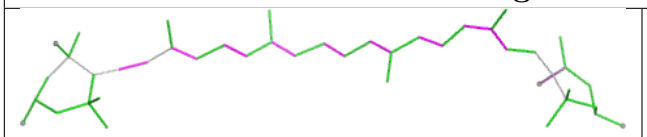


Rings

Ligand NEX G1 623



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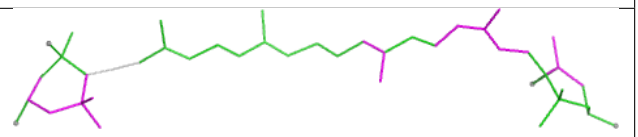
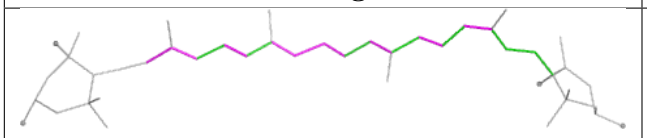


Bond angles



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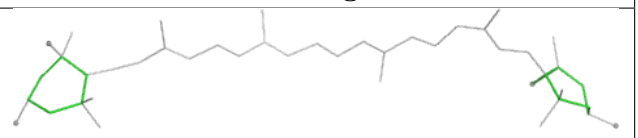
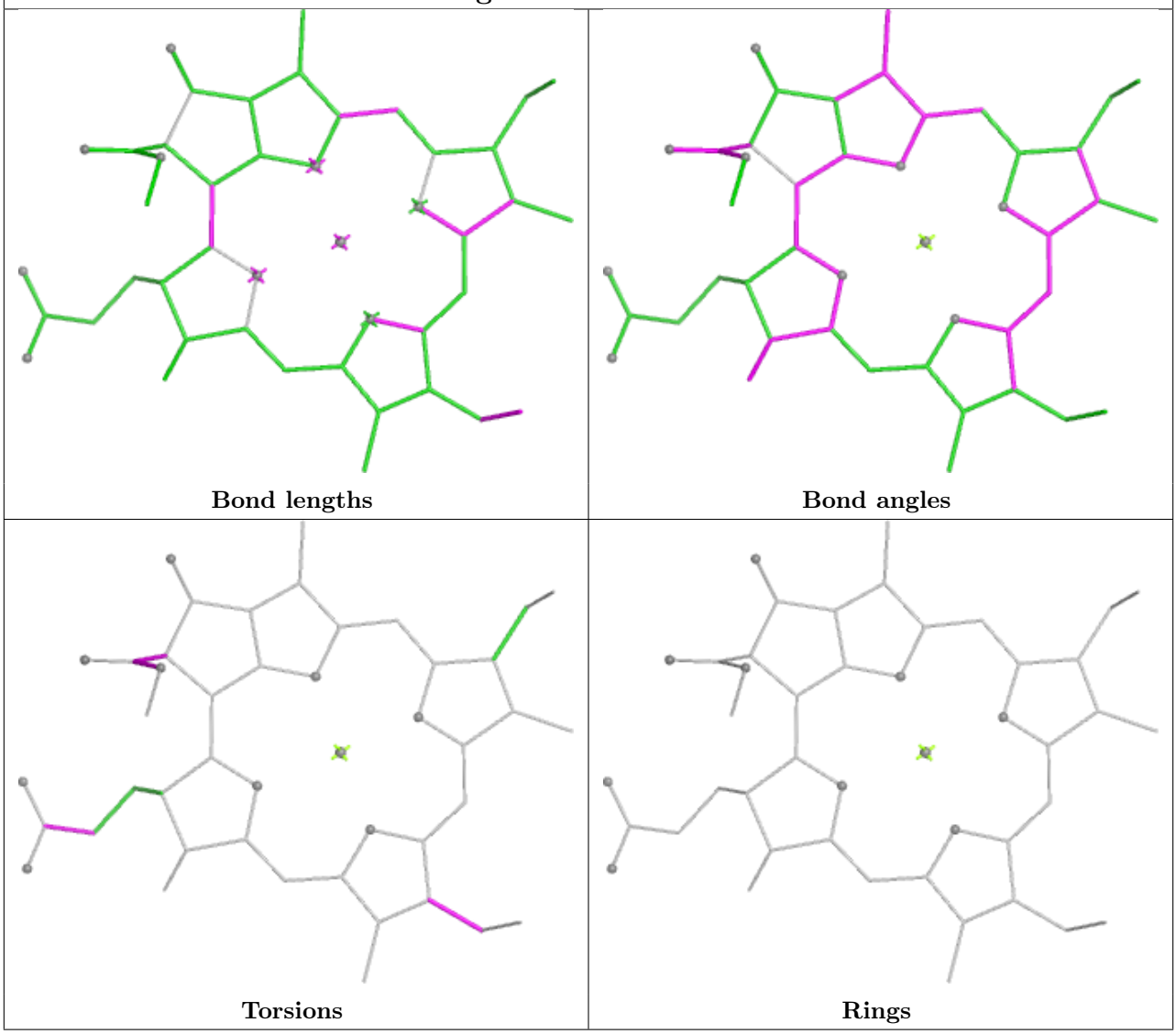
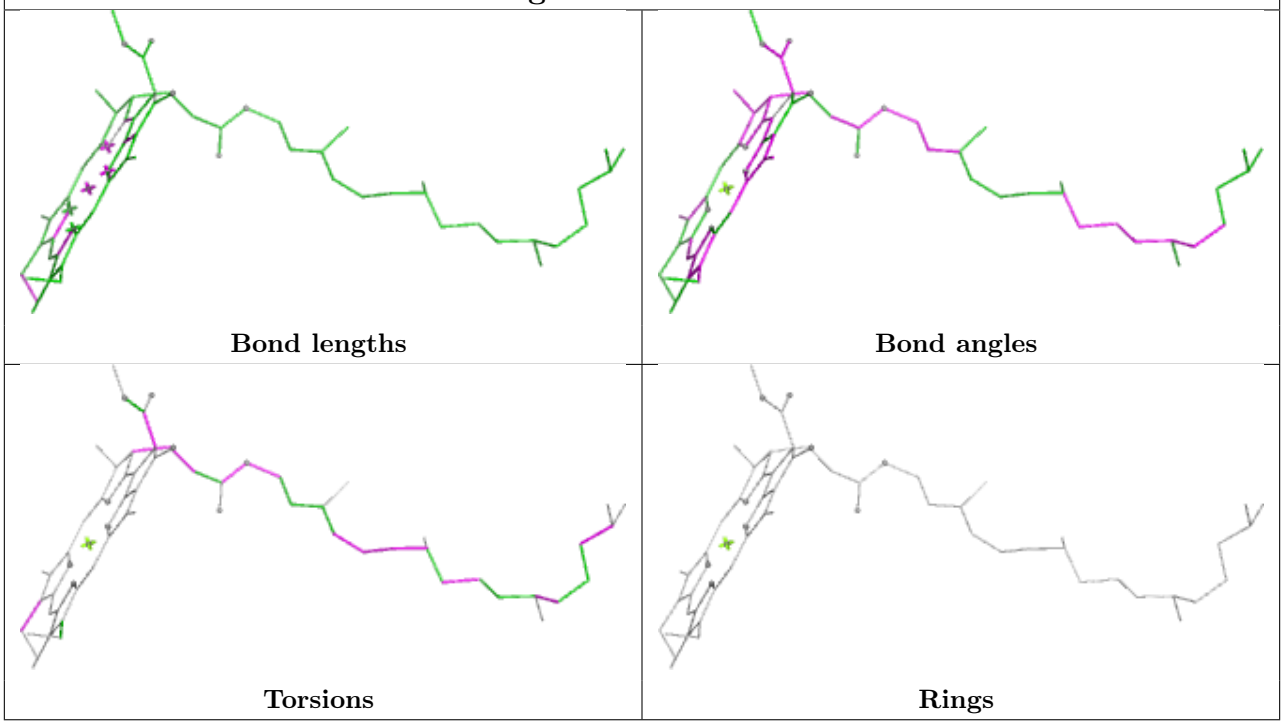


Rings

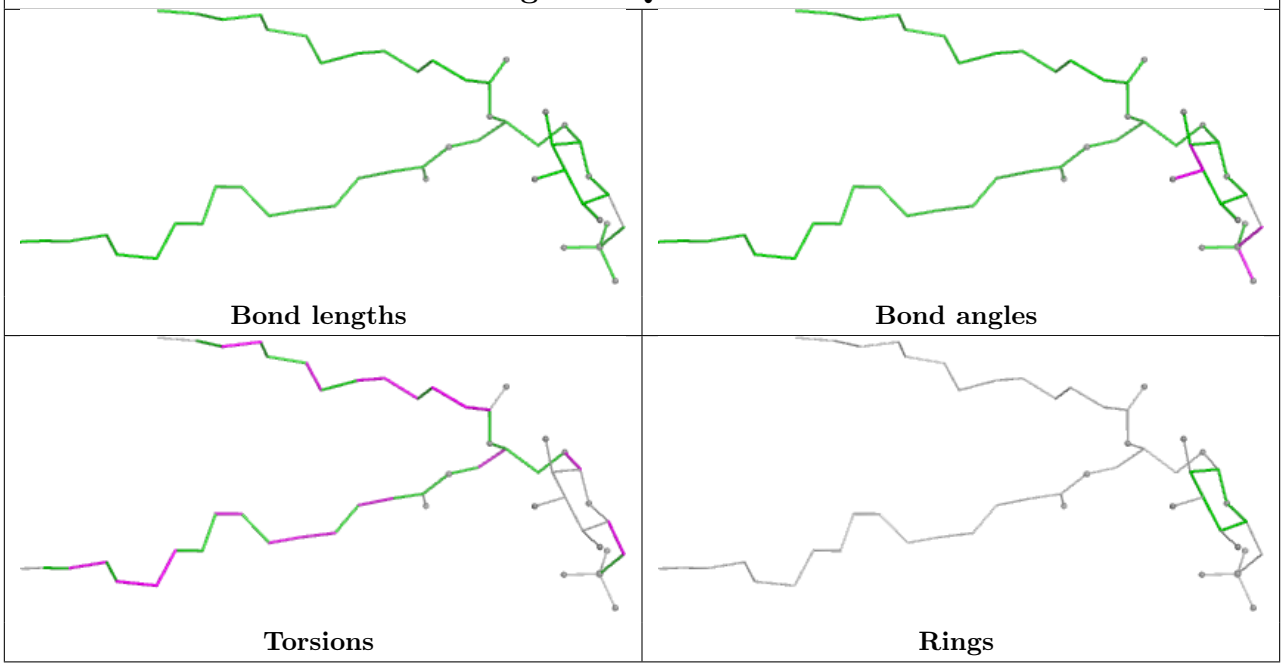
Ligand CLA n1 612



Ligand CLA b 605



Ligand SQD a1 412



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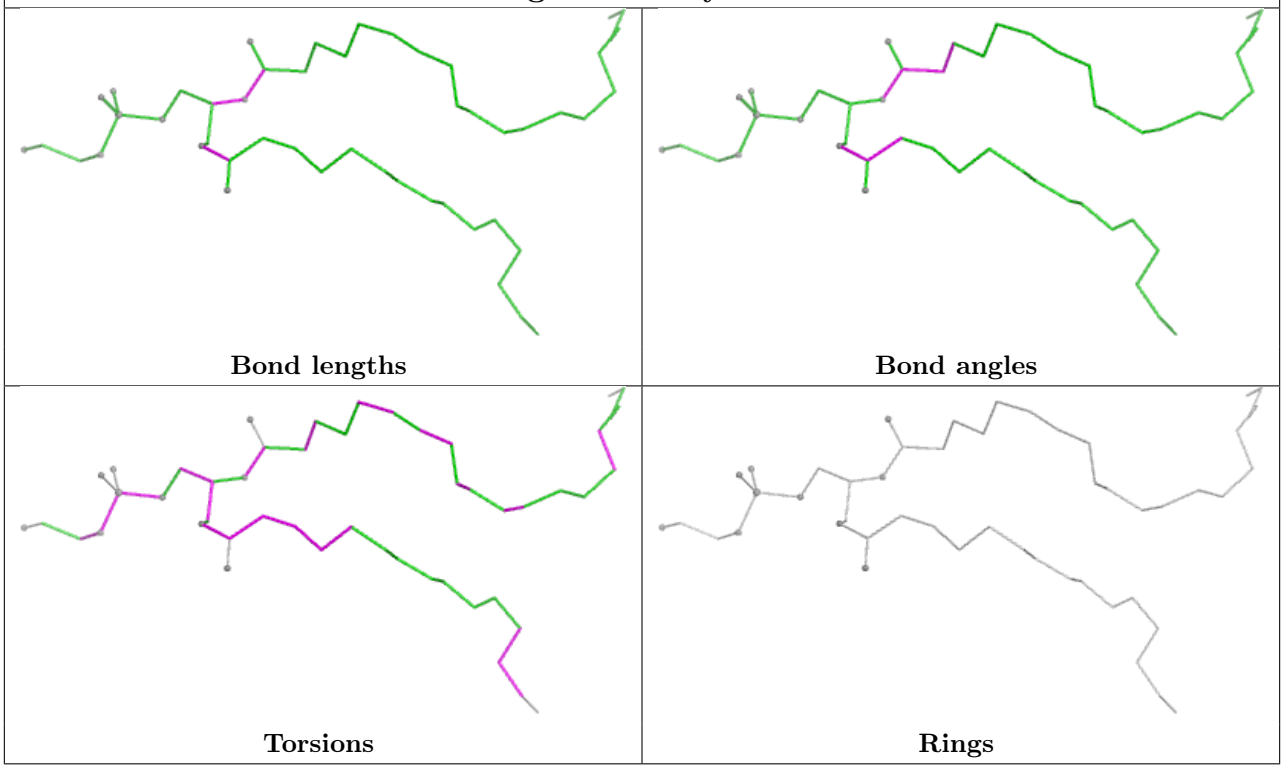

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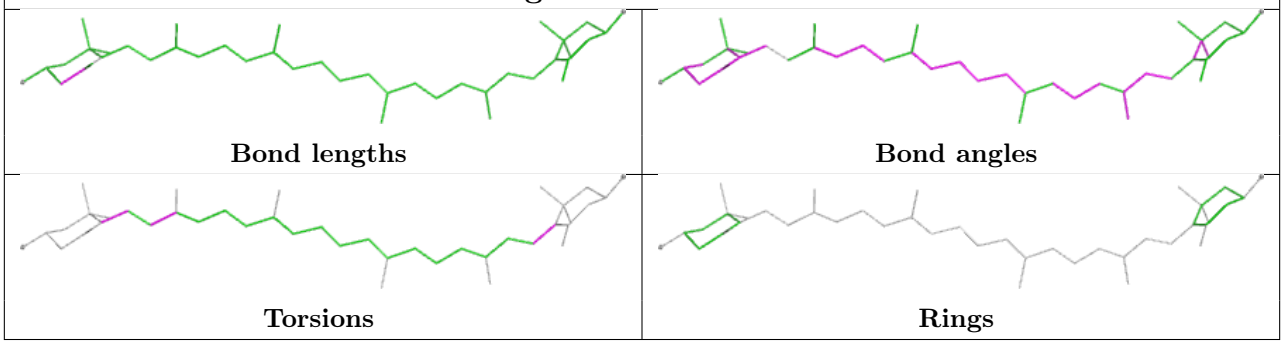
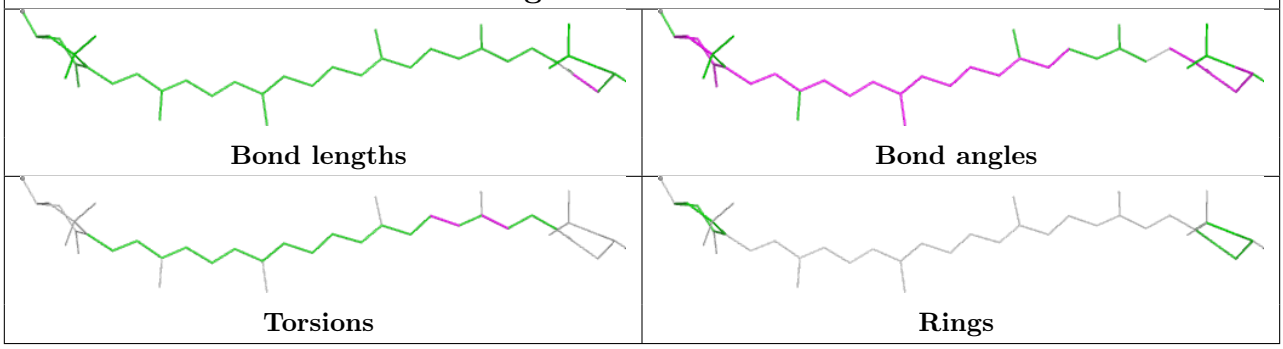
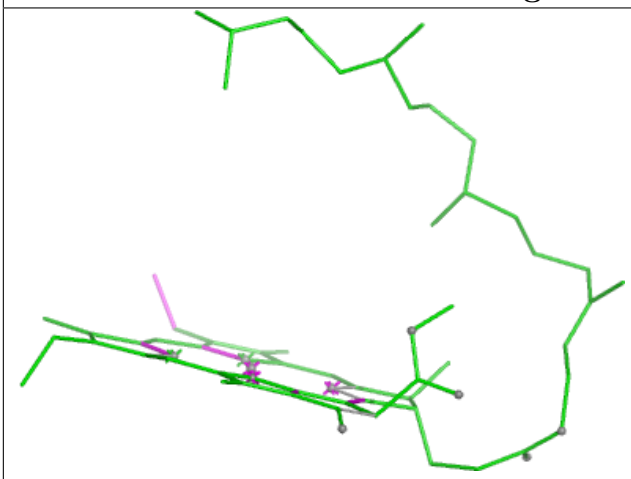


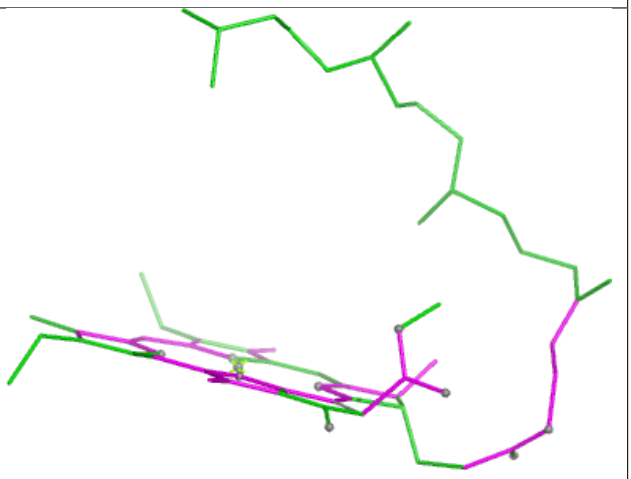
Ligand LUT G 620



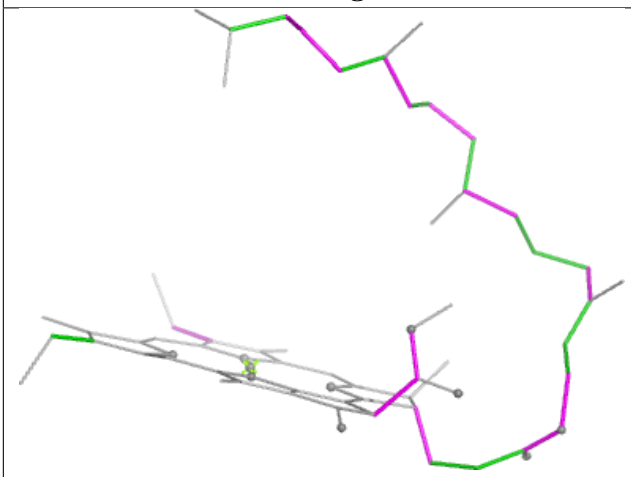
Ligand CLA Y 603



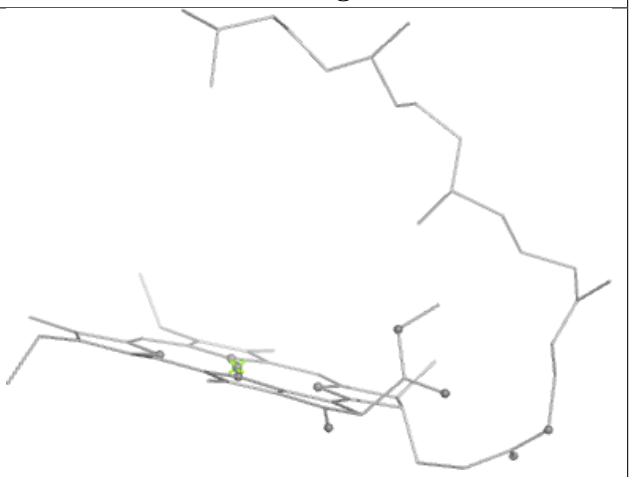
Bond lengths



Bond angles

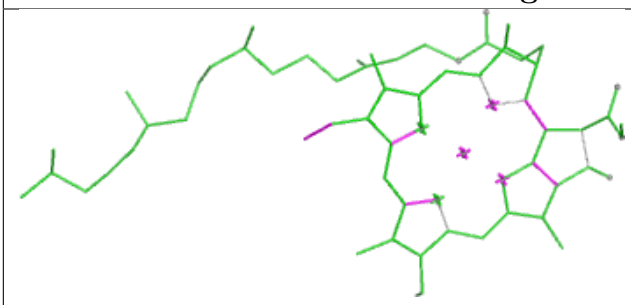


Torsions



Rings

Ligand CLA c1 501



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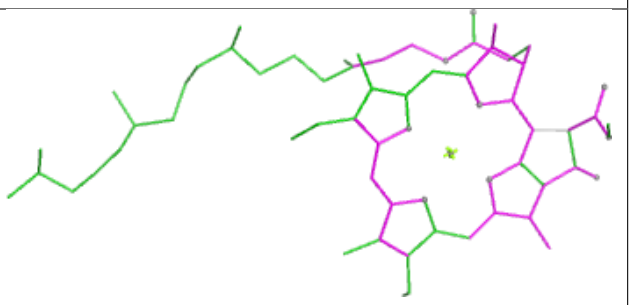
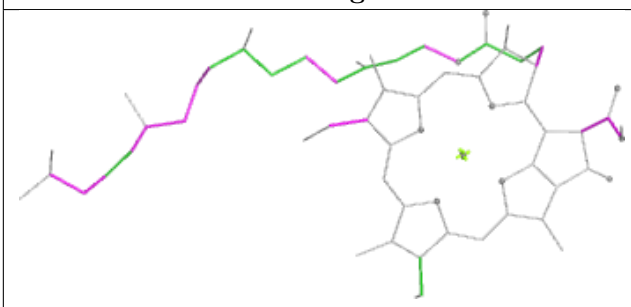


Bond angles



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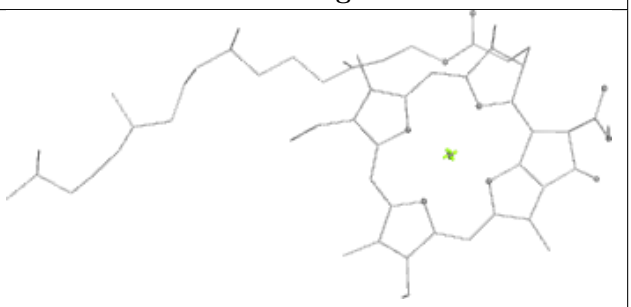
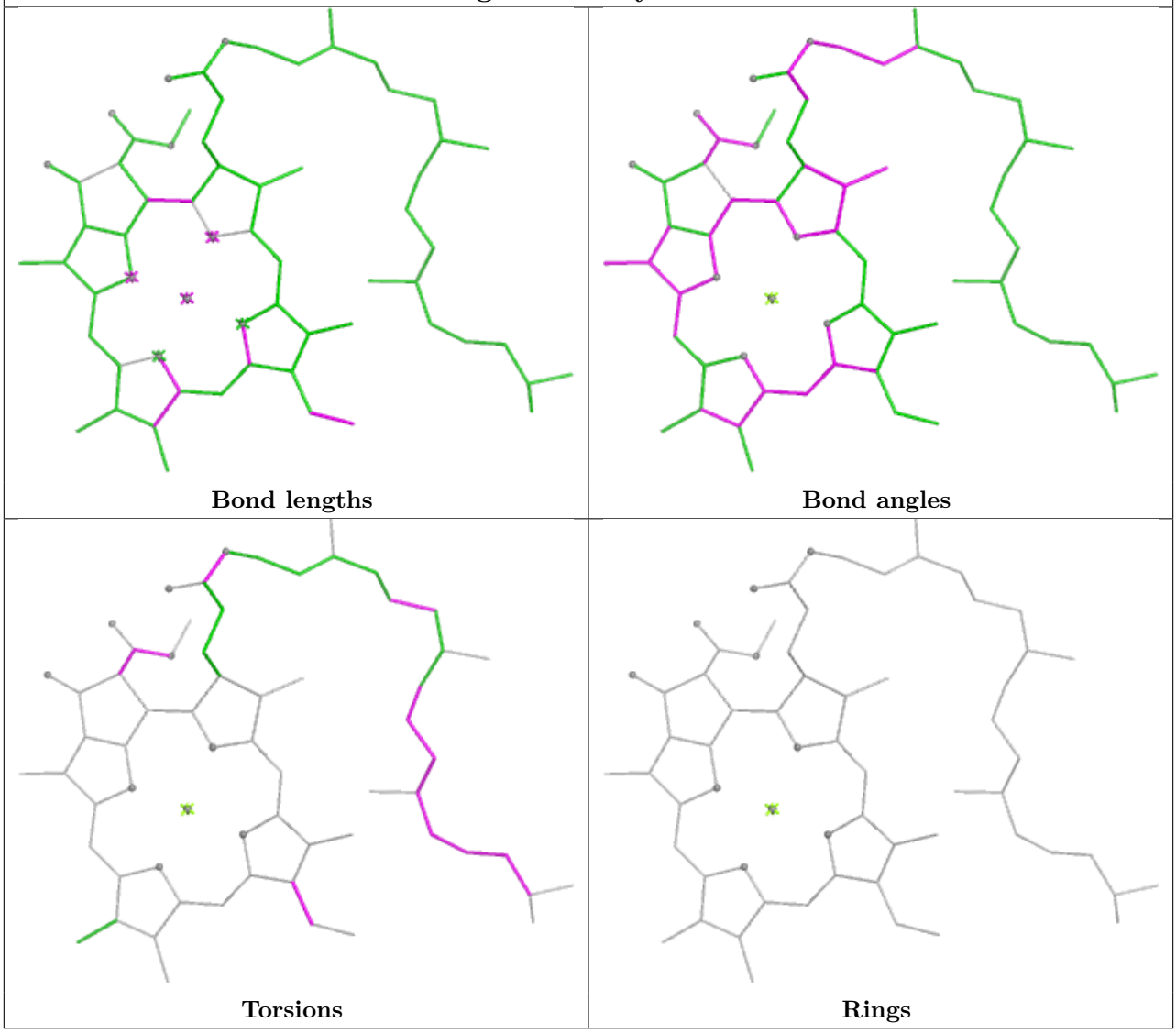
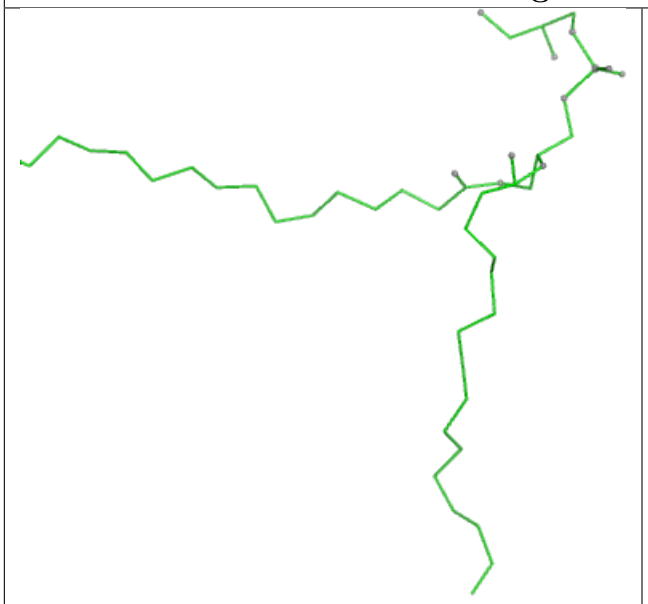


Rings

Ligand CLA y1 612



Ligand LHG l 101



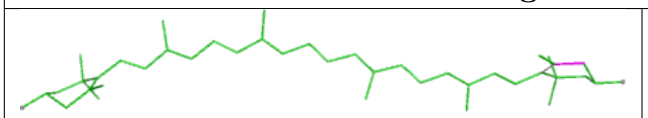
Bond lengths

Bond angles

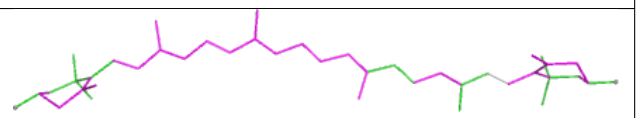
Torsions

Rings

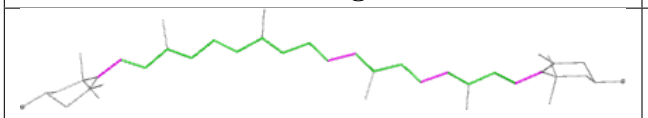
Ligand LUT n1 621



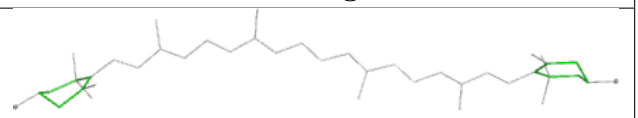
Bond lengths



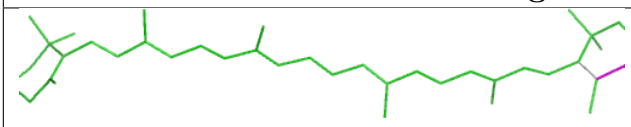
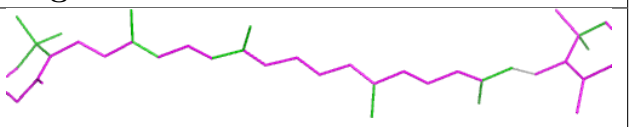
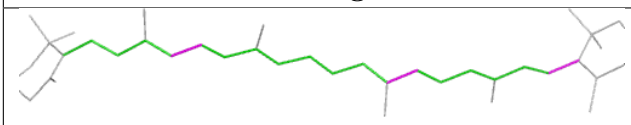
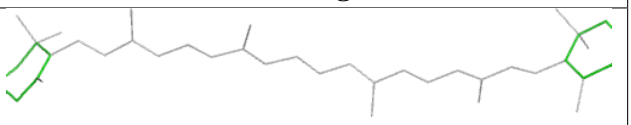
Bond angles



Torsions



Rings

Ligand LUT g 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

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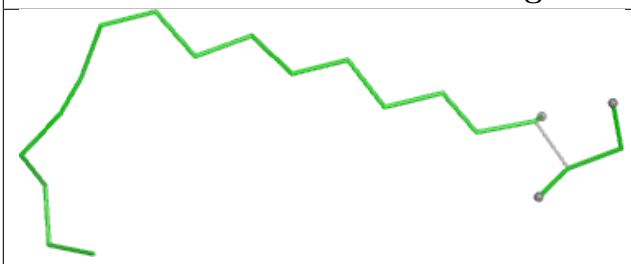
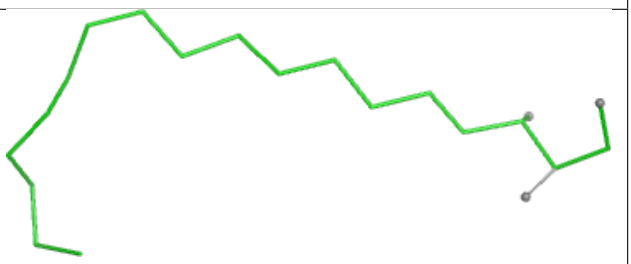
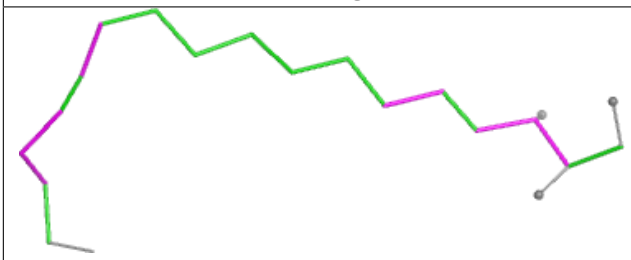
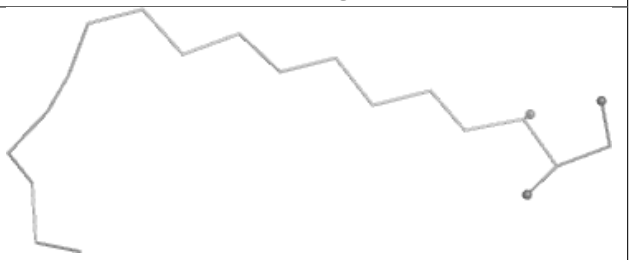
 Bond lengths	 Bond angles
 Torsions	 Rings

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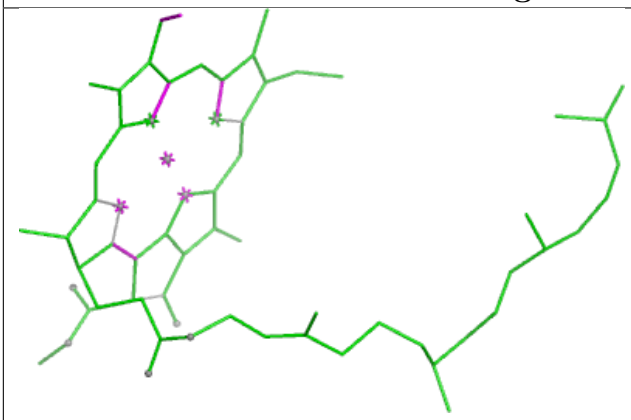
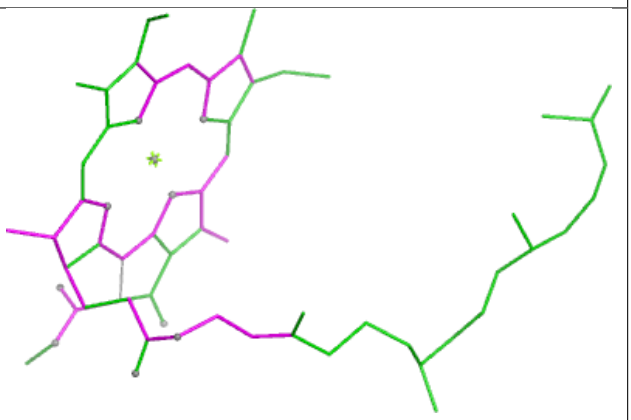
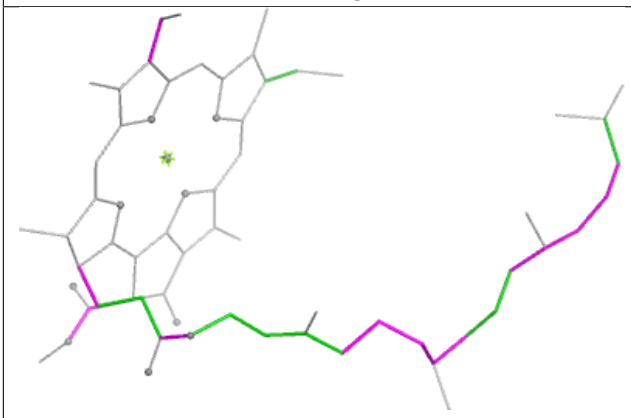
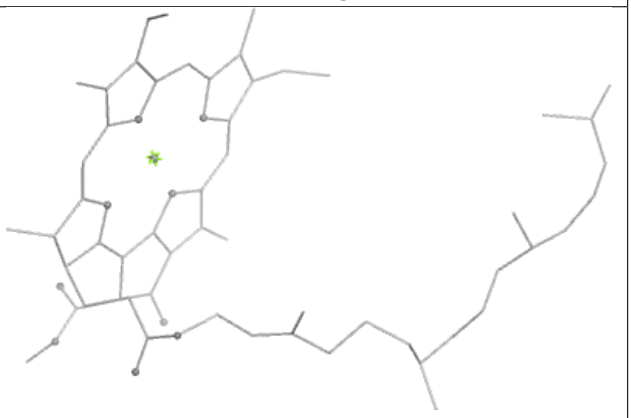
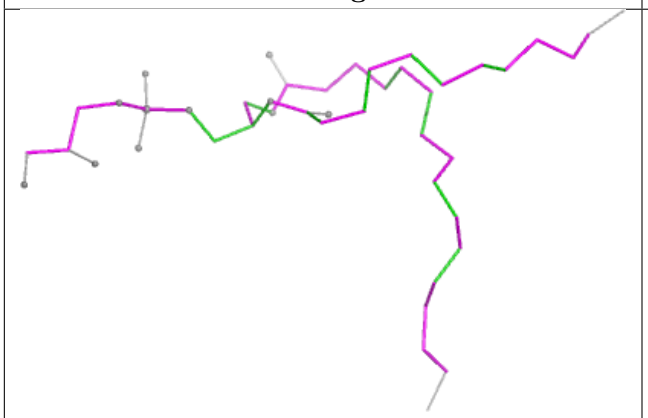
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG S1 624

Bond lengths

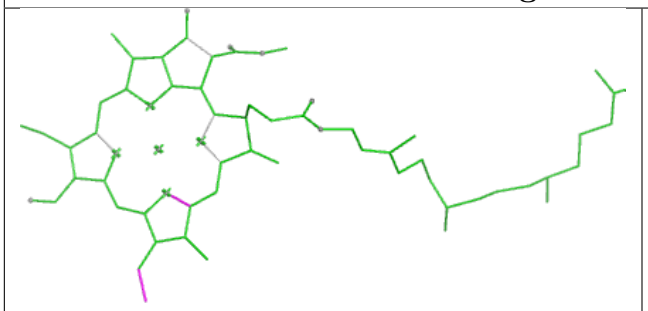
Bond angles



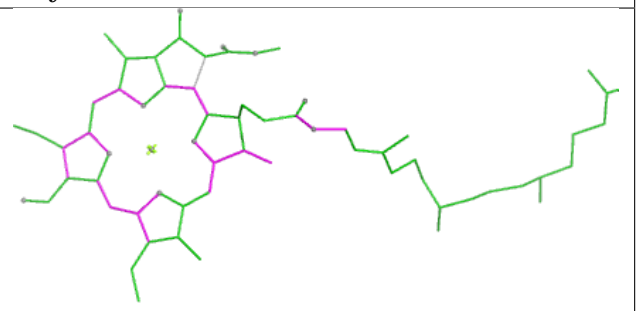
Torsions

Rings

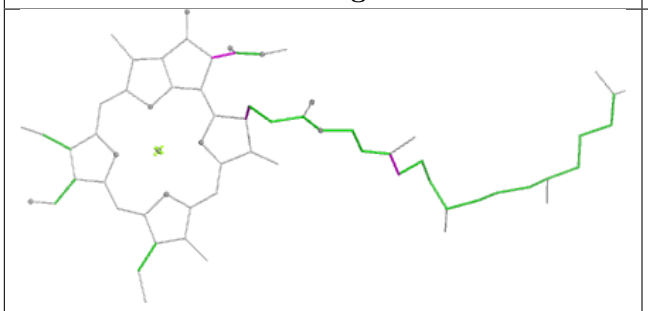
Ligand CHL y1 601



Bond lengths



Bond angles



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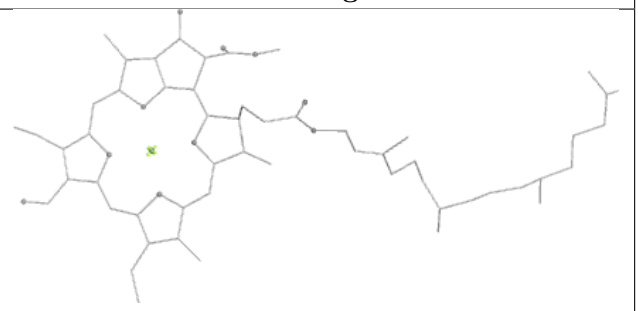
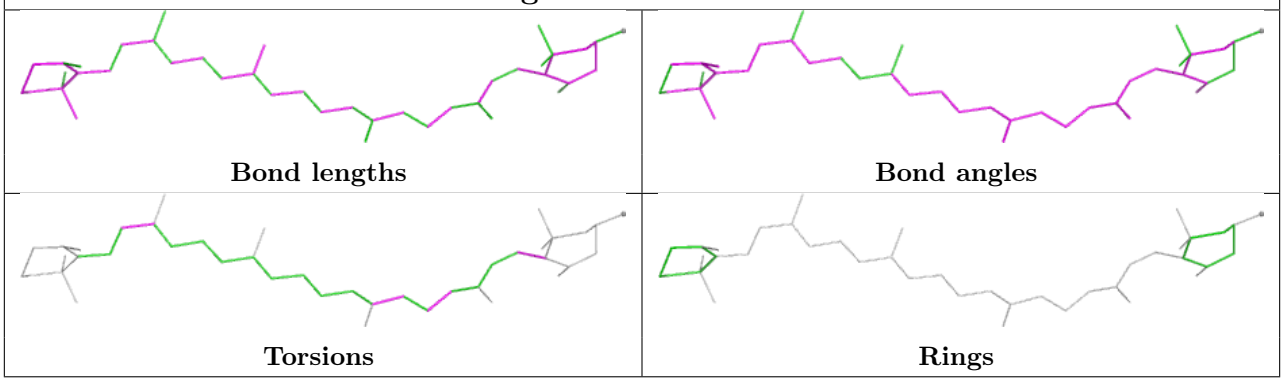
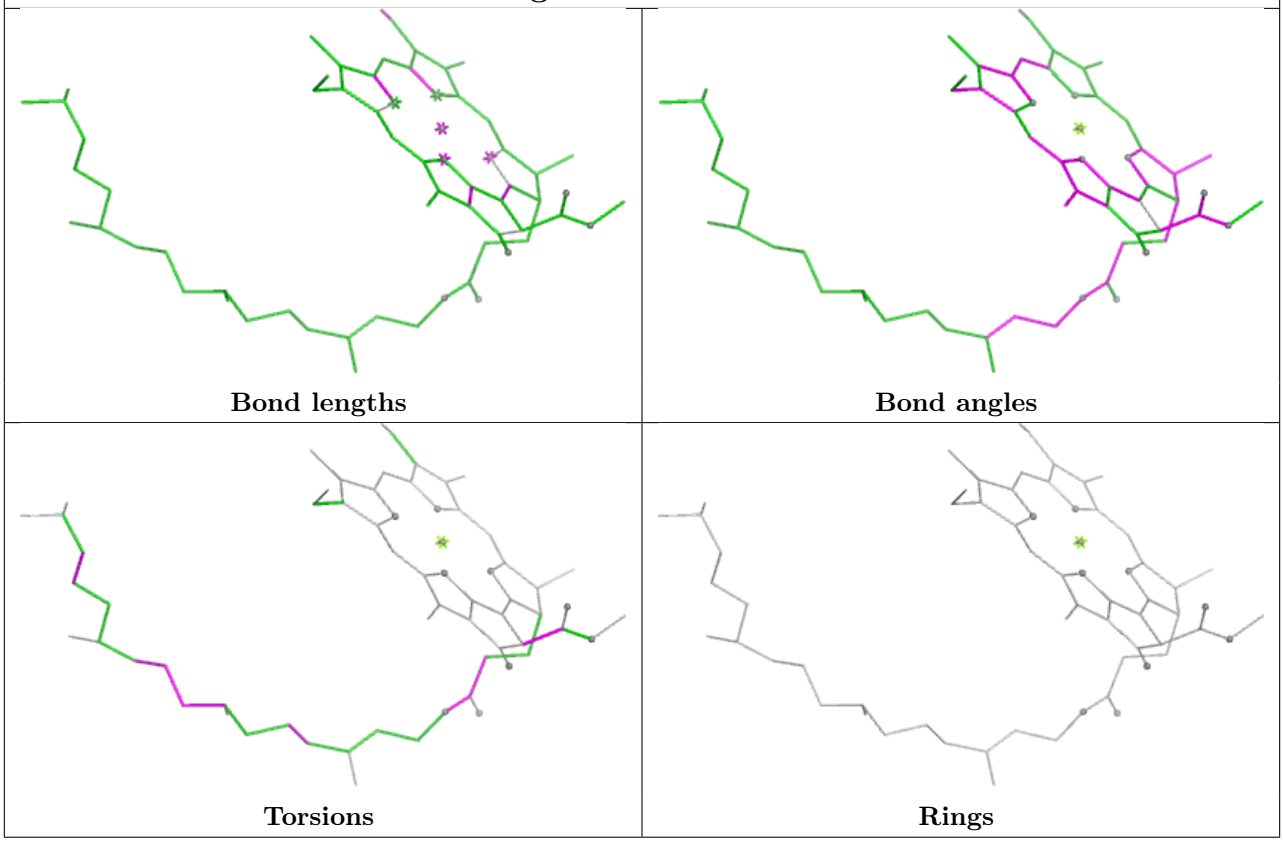


Rings

Ligand RRX H 101



Ligand CLA c 508



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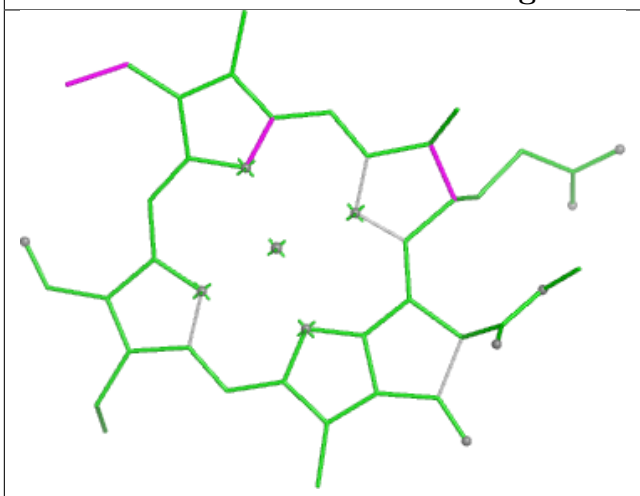
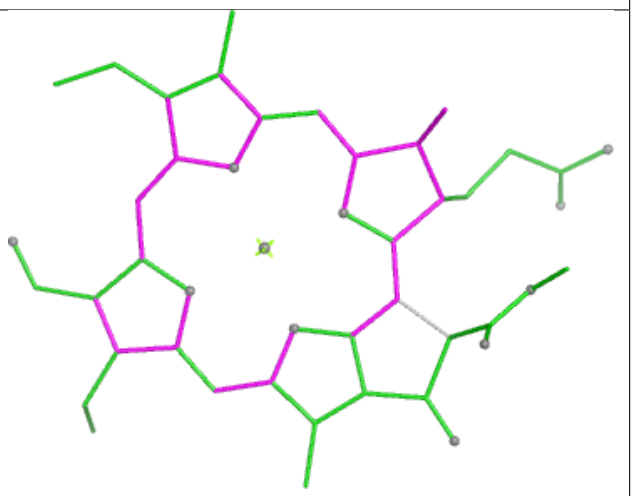
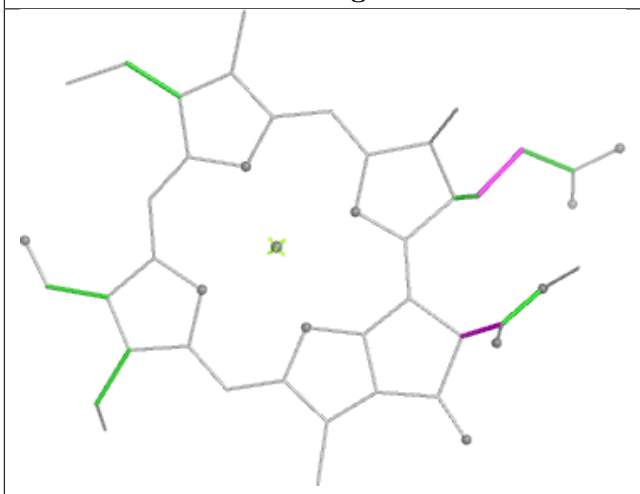
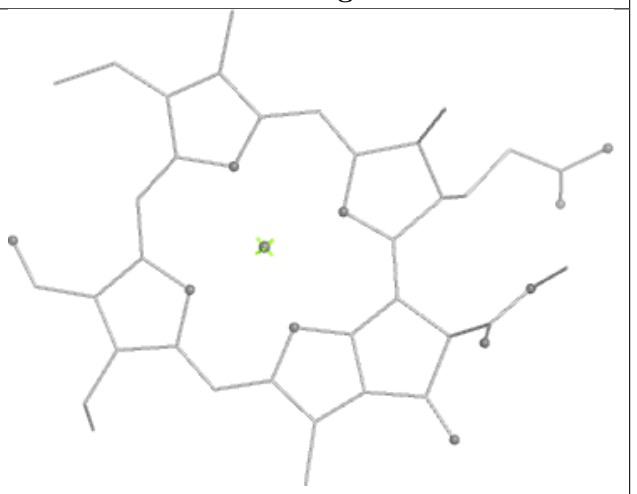
 Bond lengths	 Bond angles
 Torsions	 Rings

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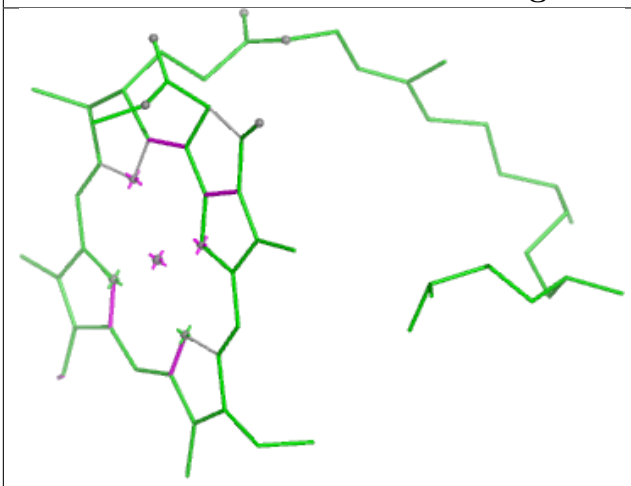
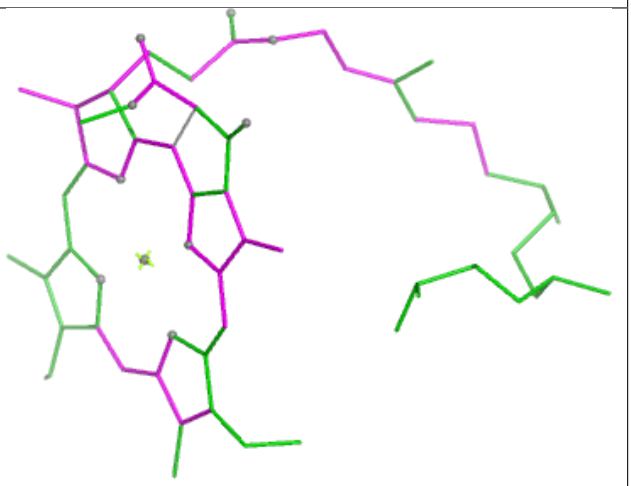
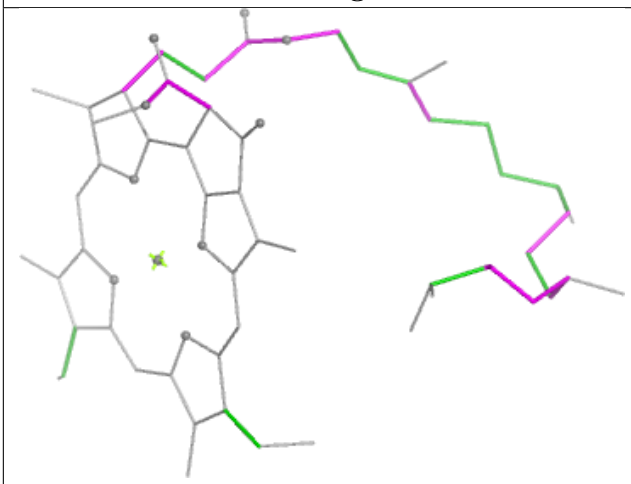
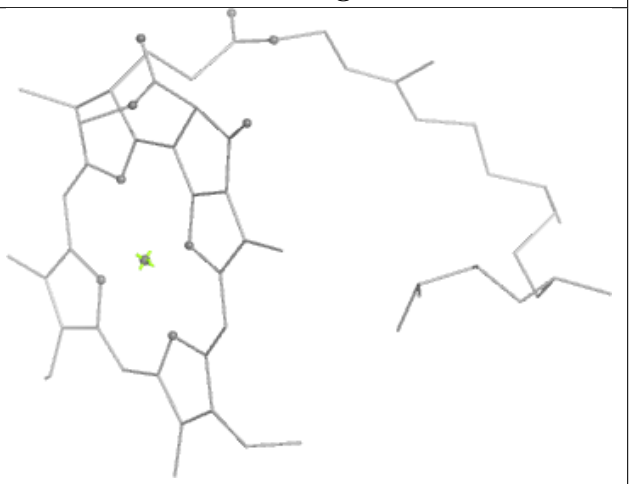
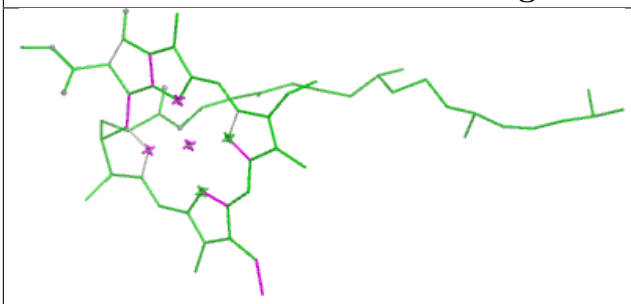
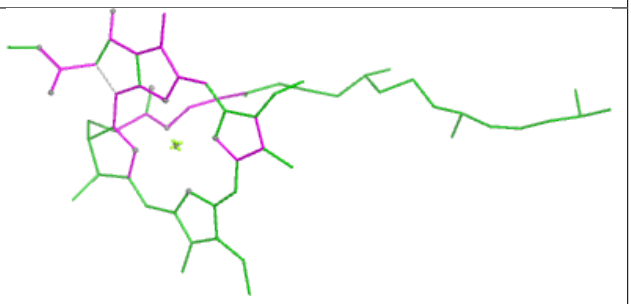
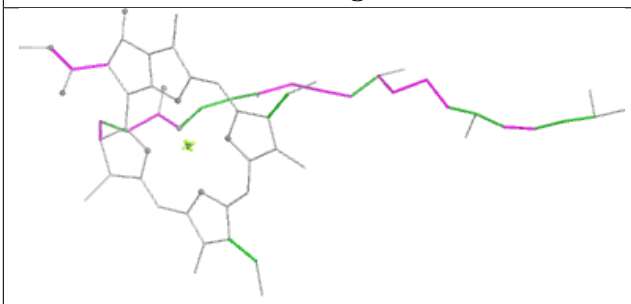
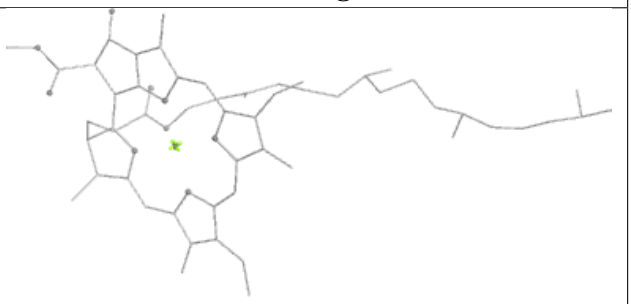
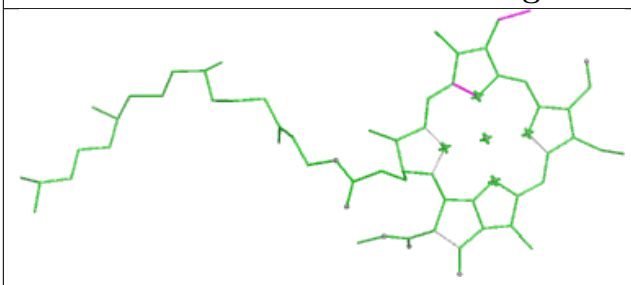
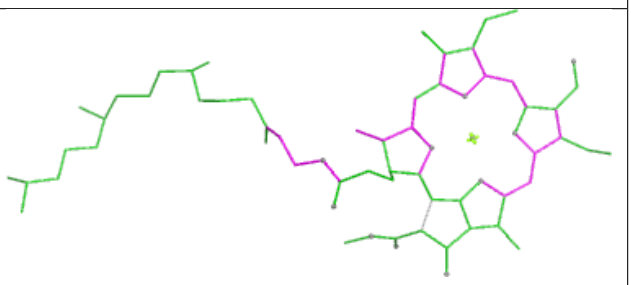
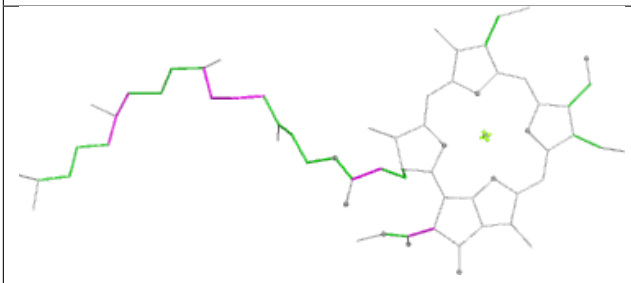
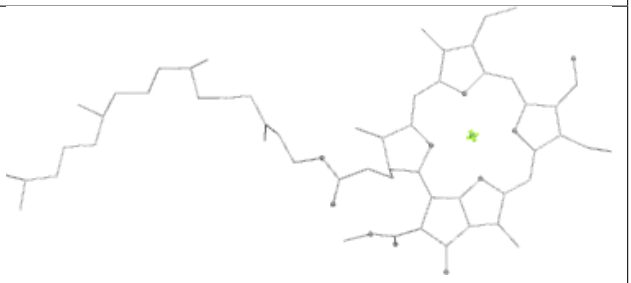
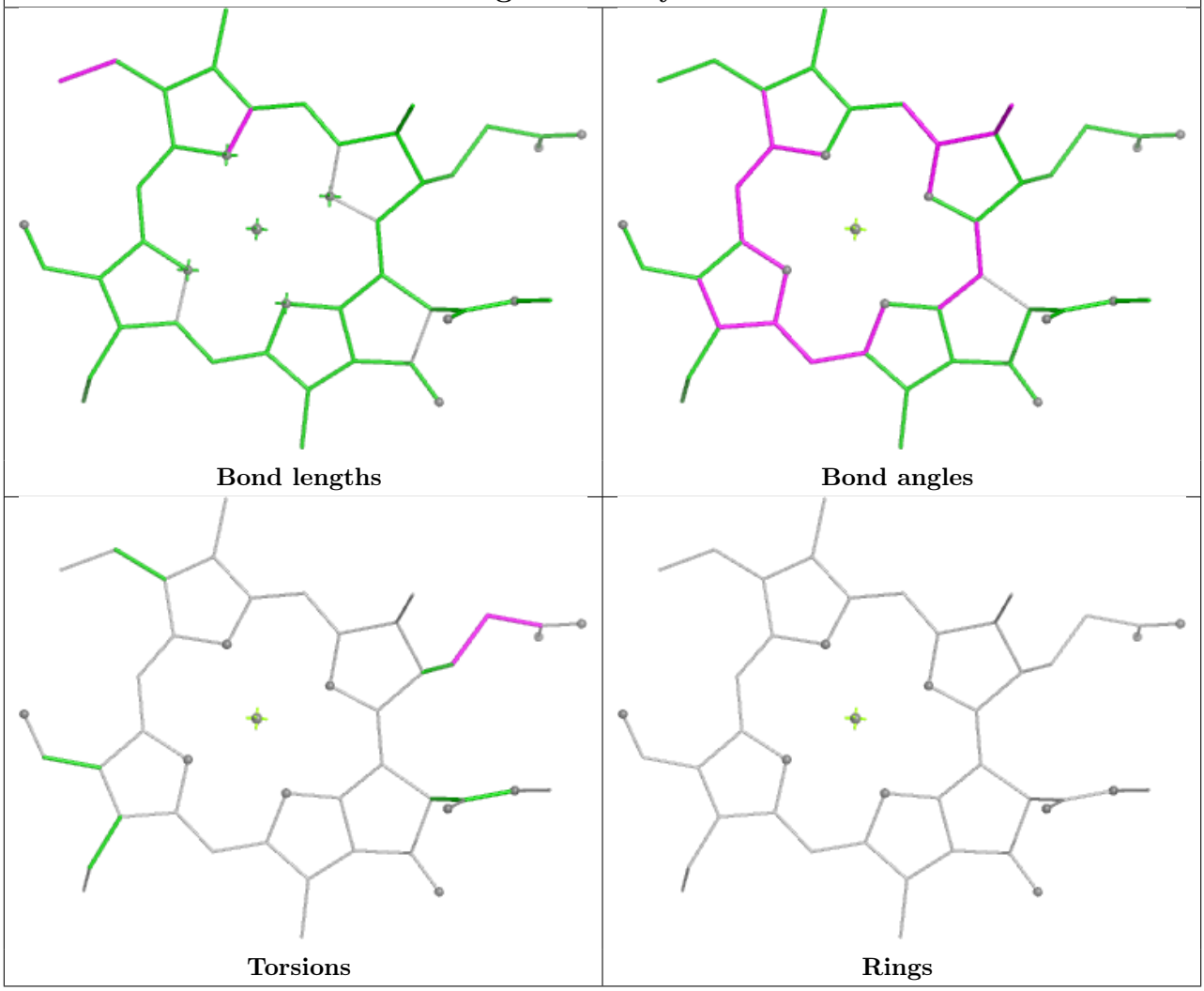
 Bond lengths	 Bond angles
 Torsions	 Rings

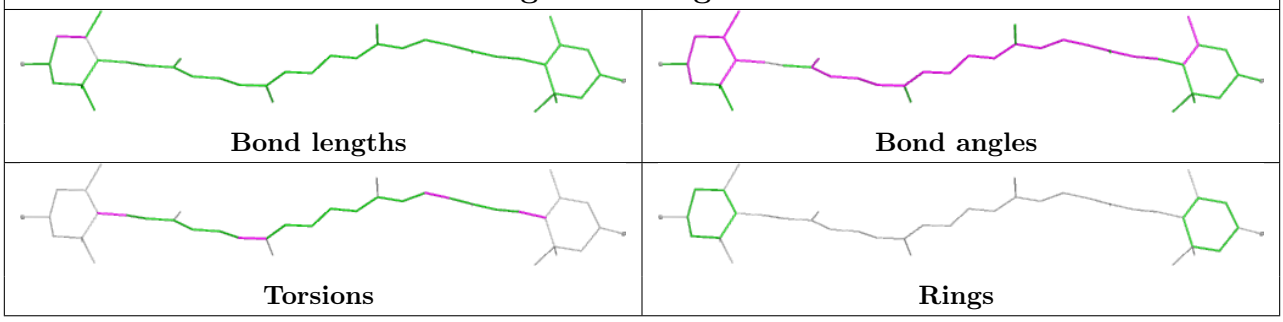
Ligand CLA b1 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL G 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL y 605



Ligand LUT g1 621



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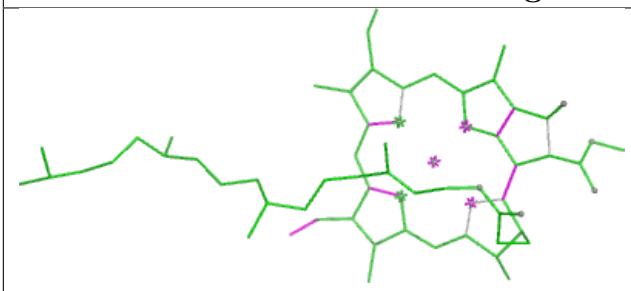
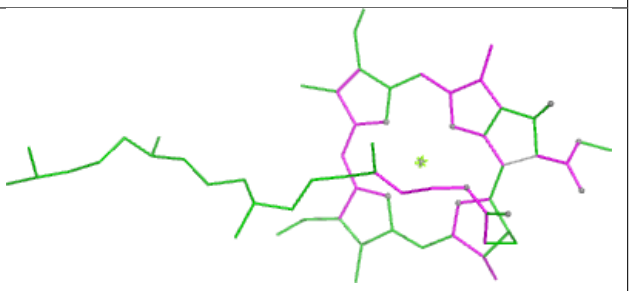
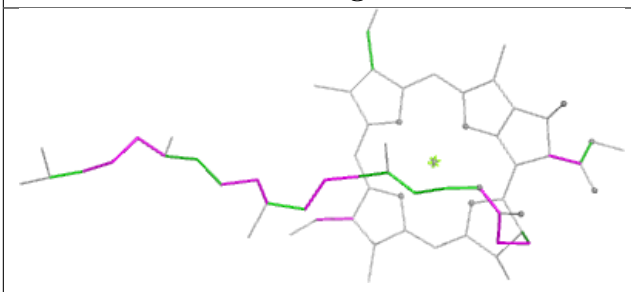
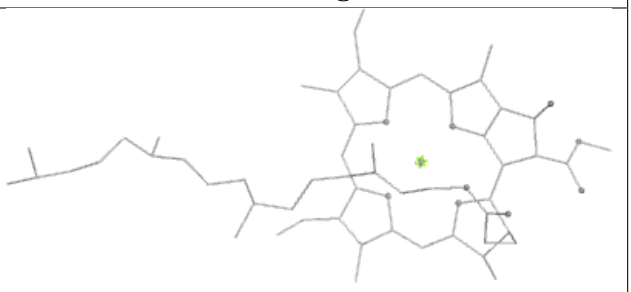
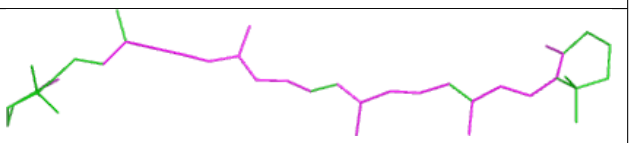
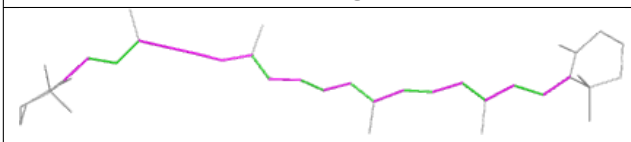
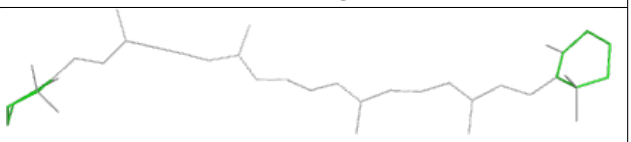
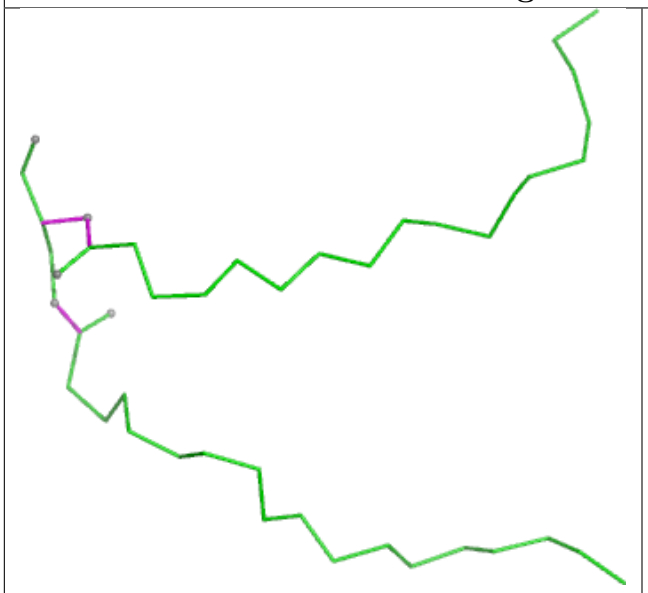
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR C 514	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGA c1 524



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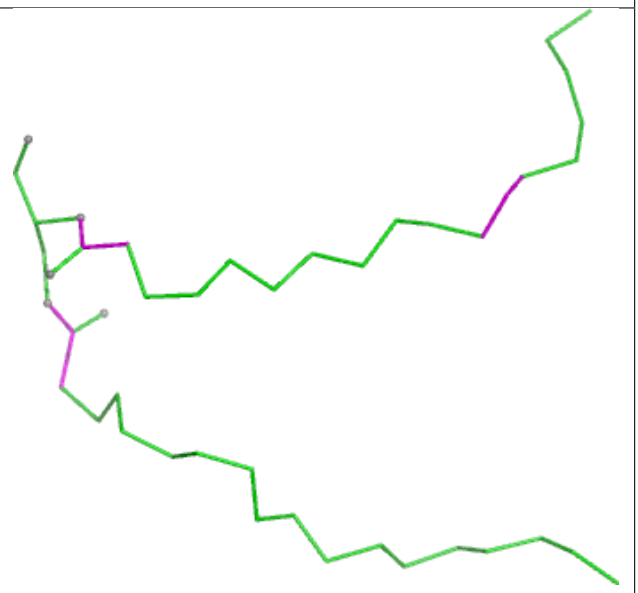

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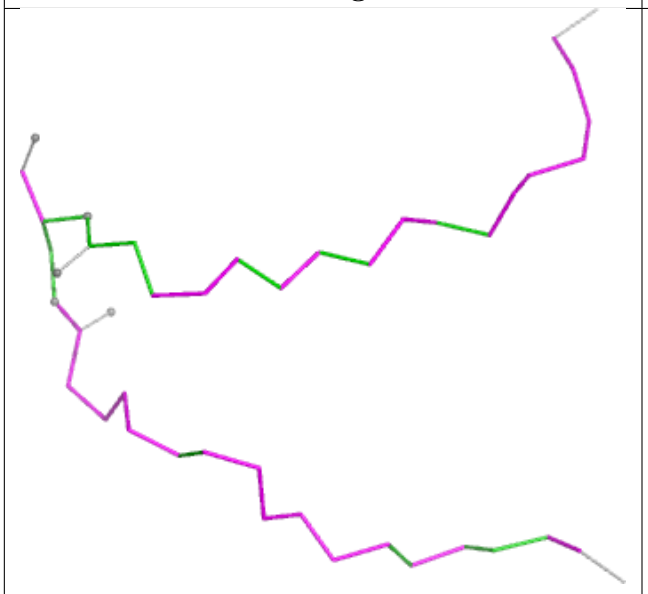
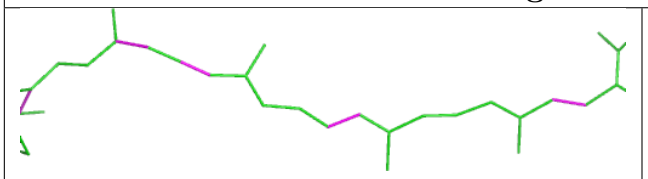


Torsions

Rings

Ligand BCR b 618



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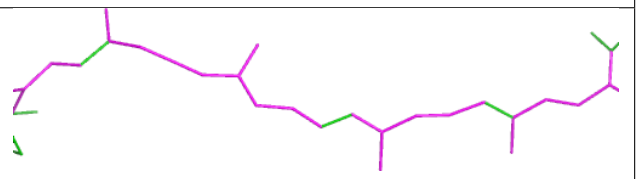

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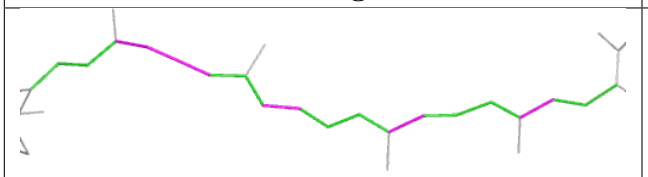

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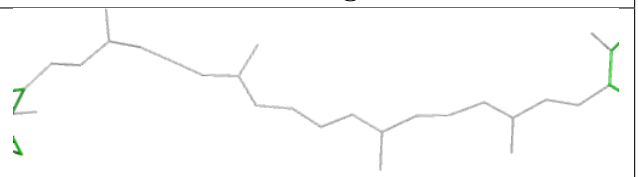
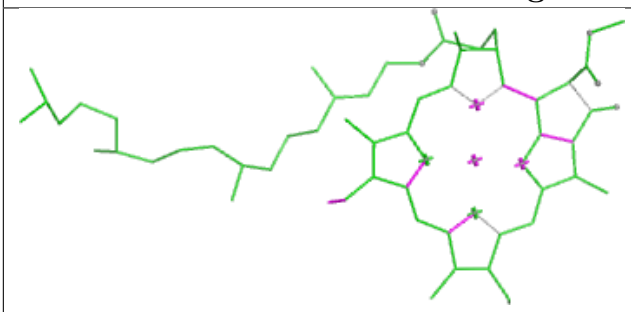


Rings

Ligand CLA b 604



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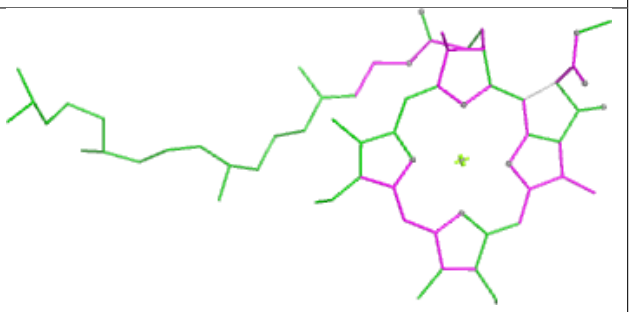

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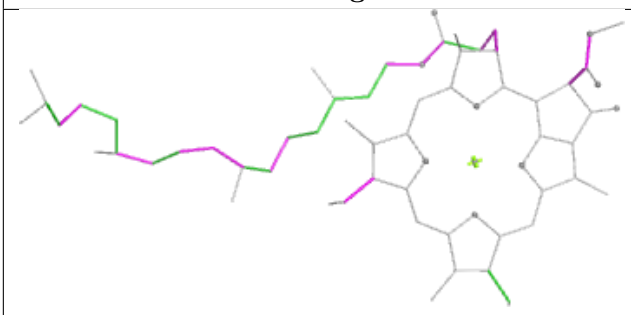

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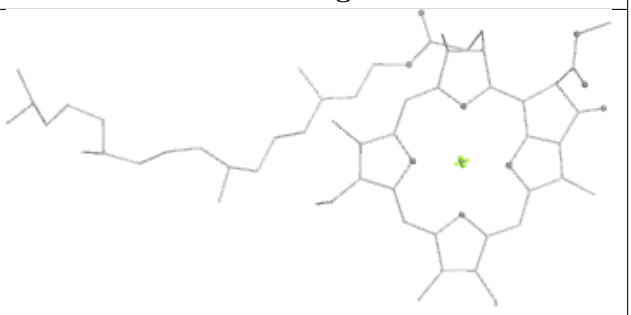
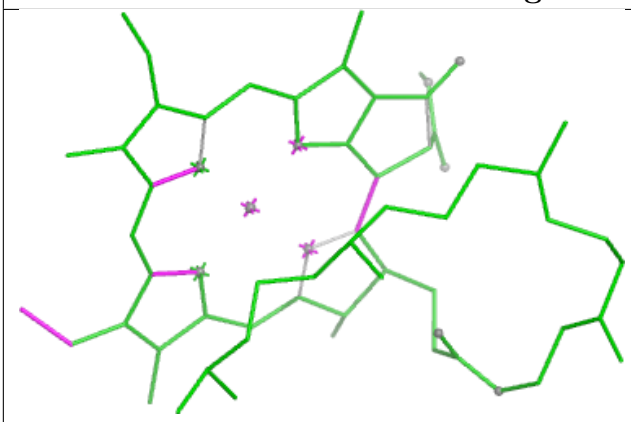


Rings

Ligand CLA B 602



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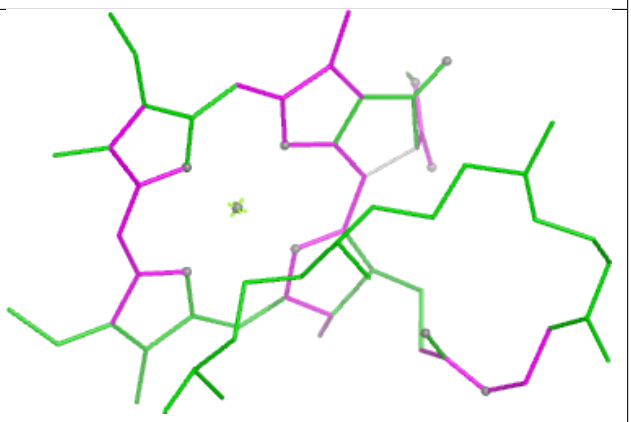

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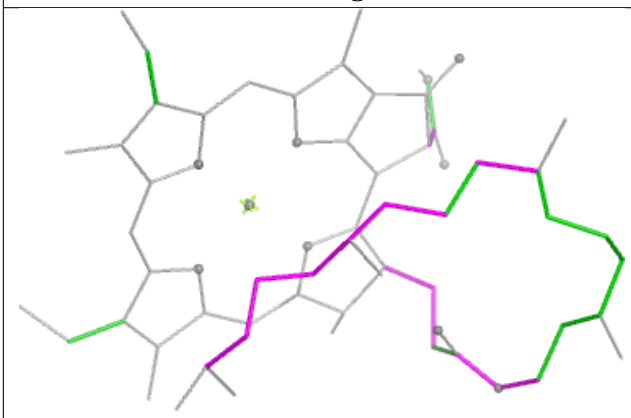

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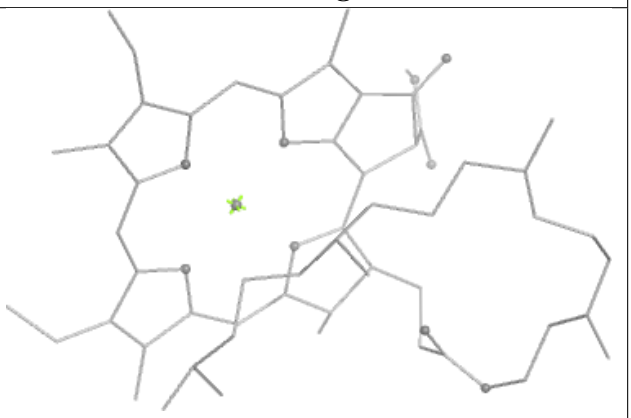

Rings

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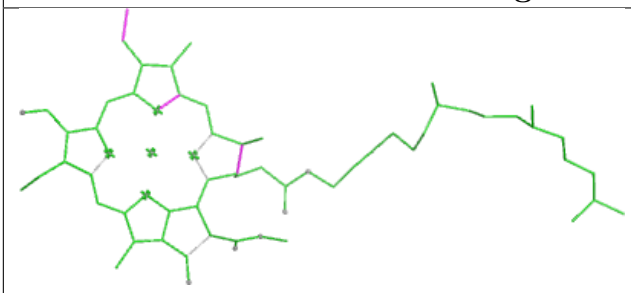

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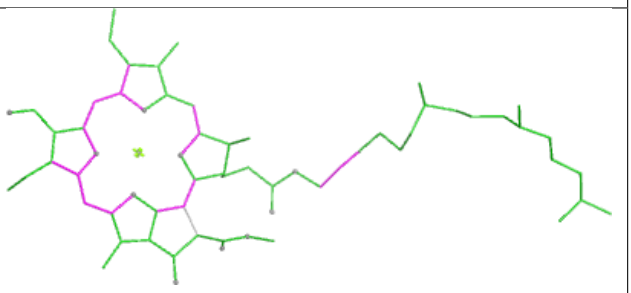

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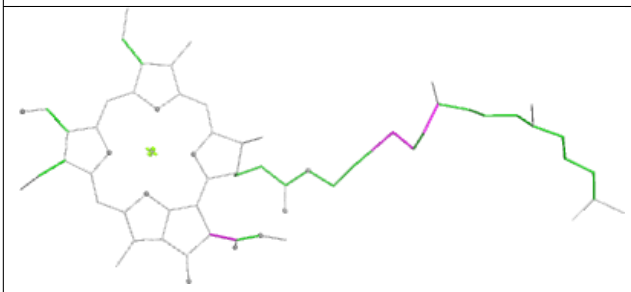

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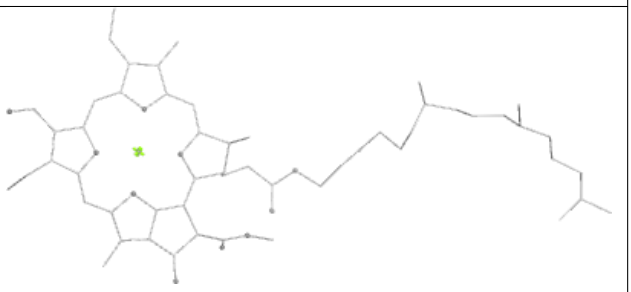

Rings

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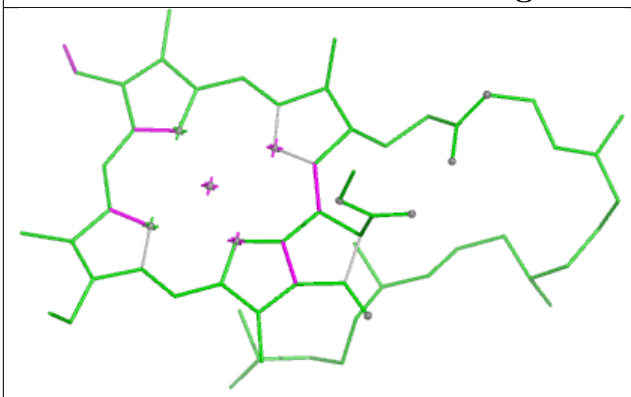

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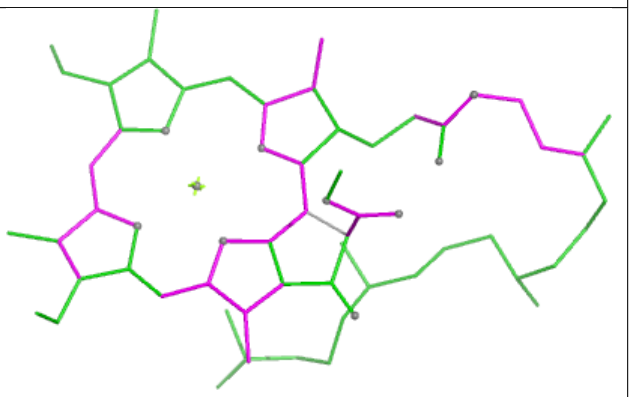

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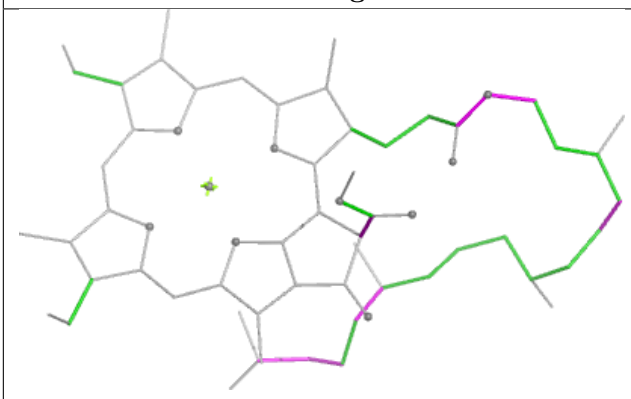

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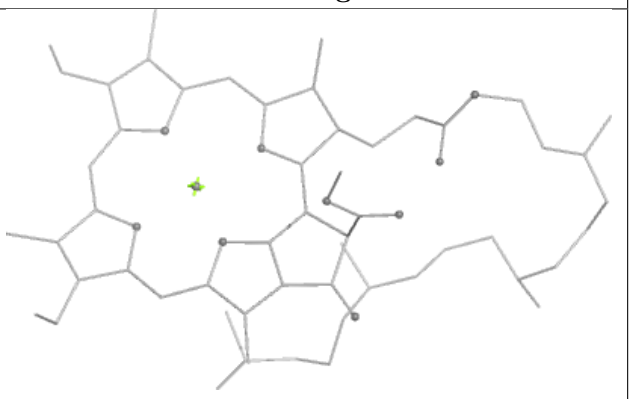

Rings

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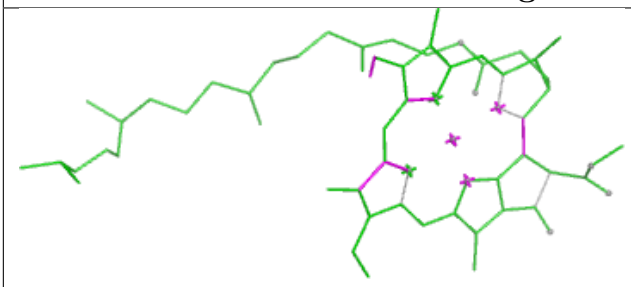

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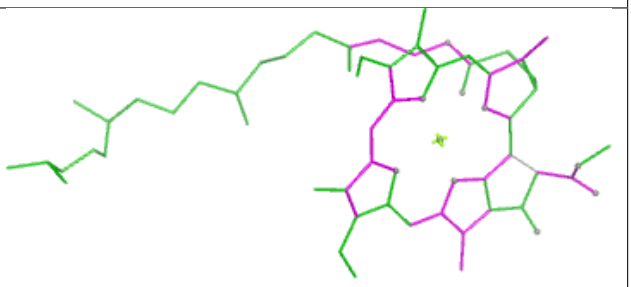

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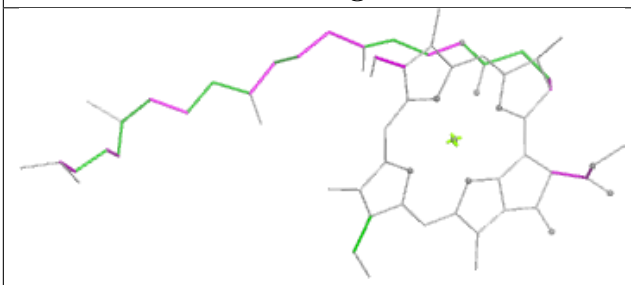

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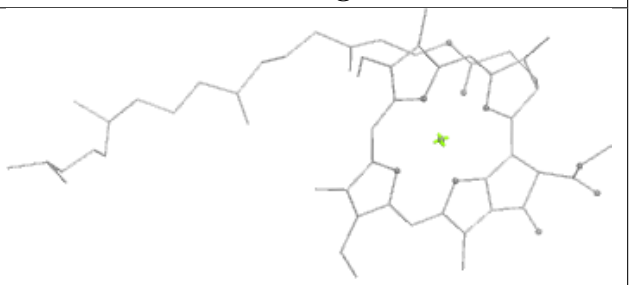
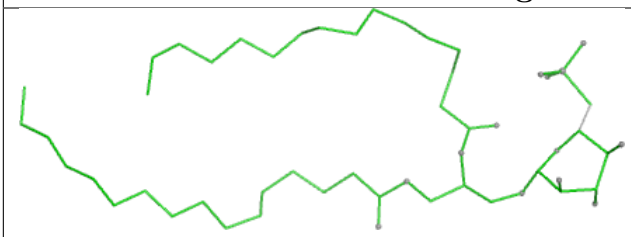


Rings

Ligand SQD B1 626



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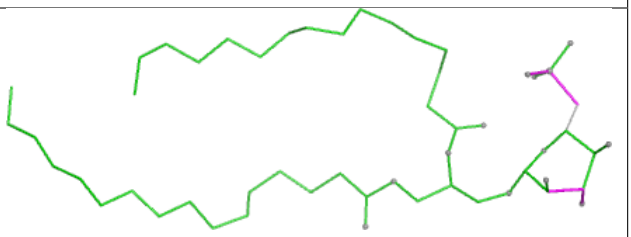

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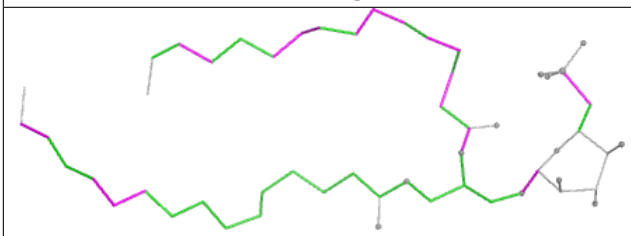

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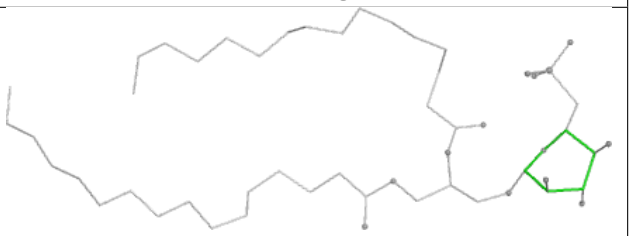
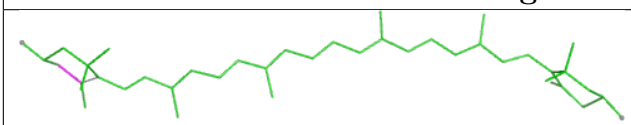


Rings

Ligand LUT g1 620



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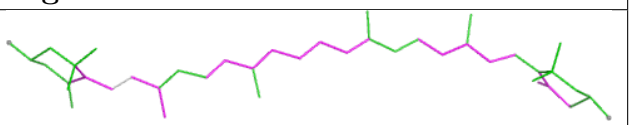

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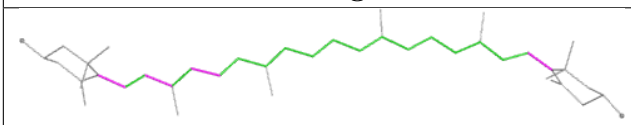

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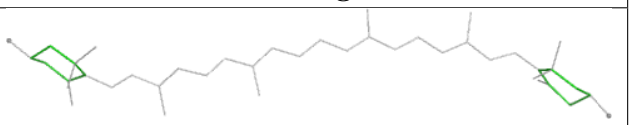
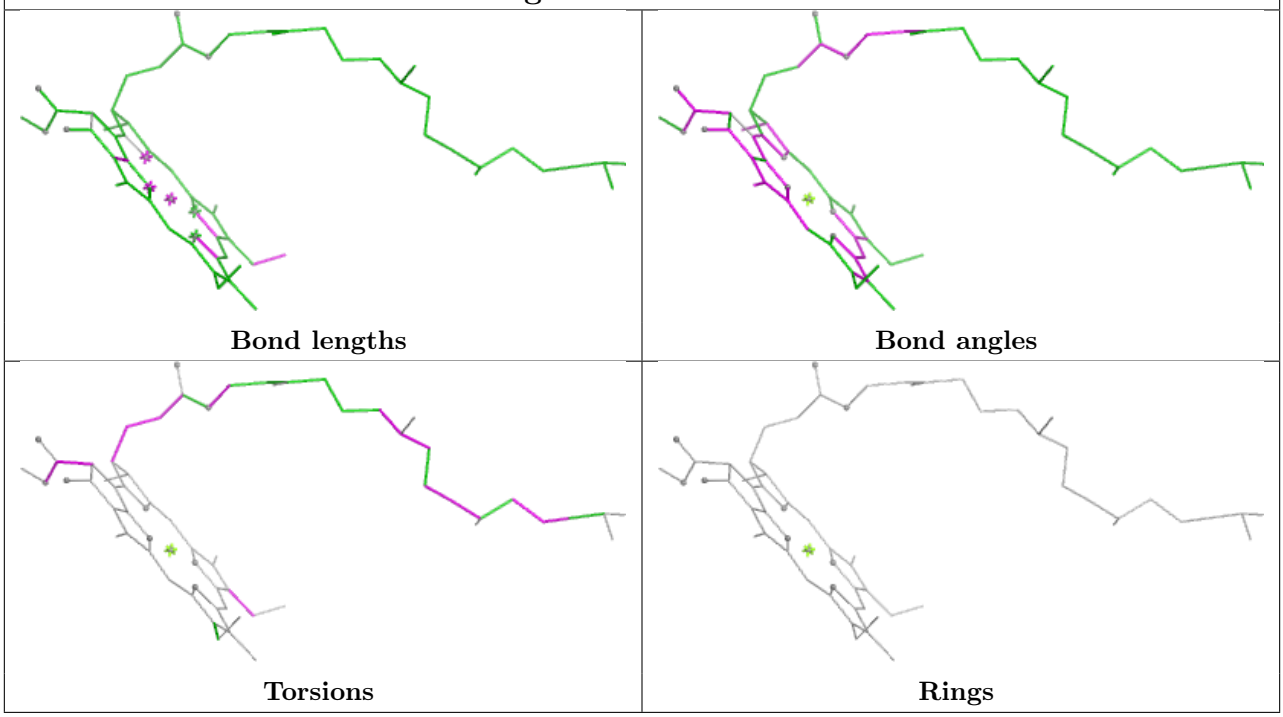


Rings

Ligand CLA N 604



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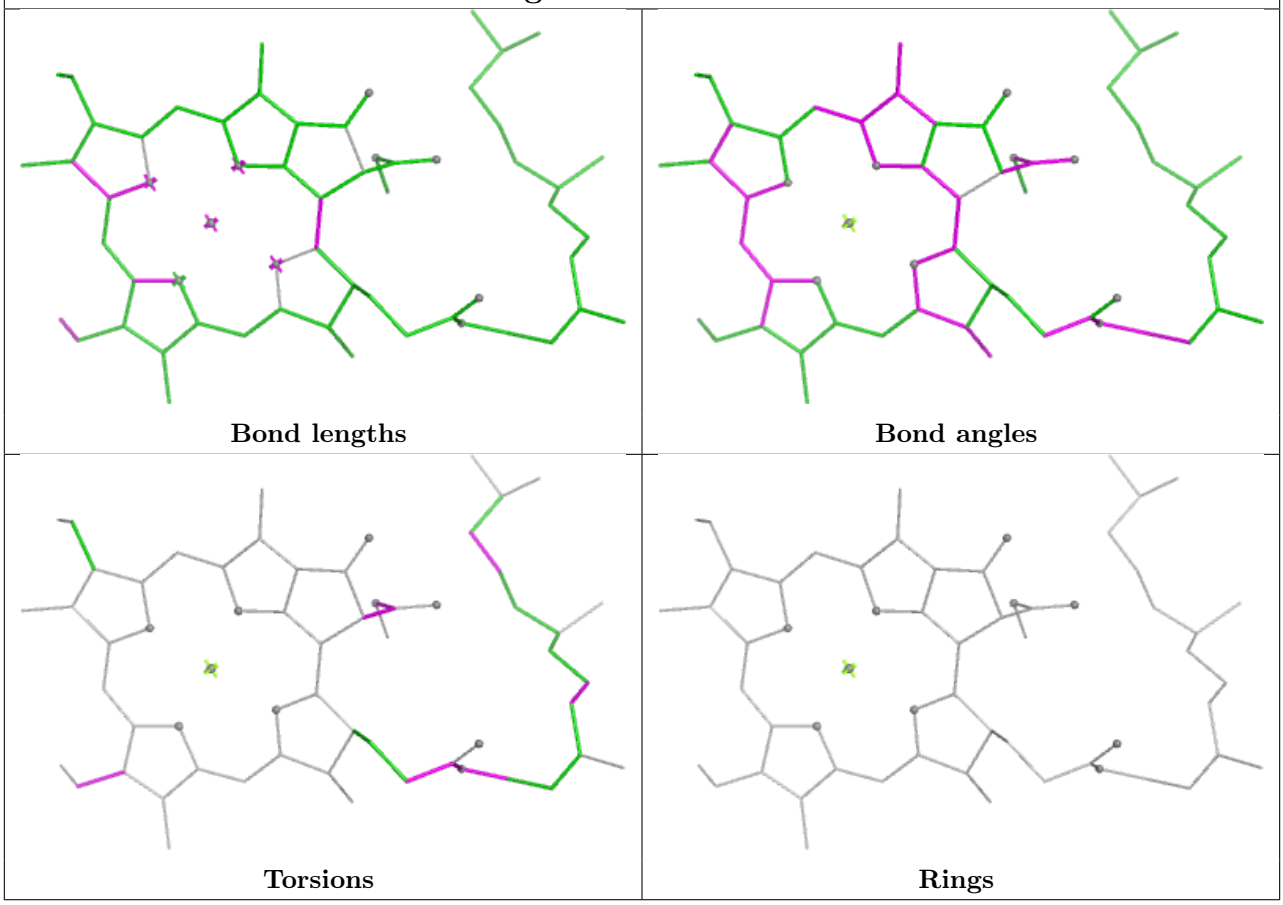

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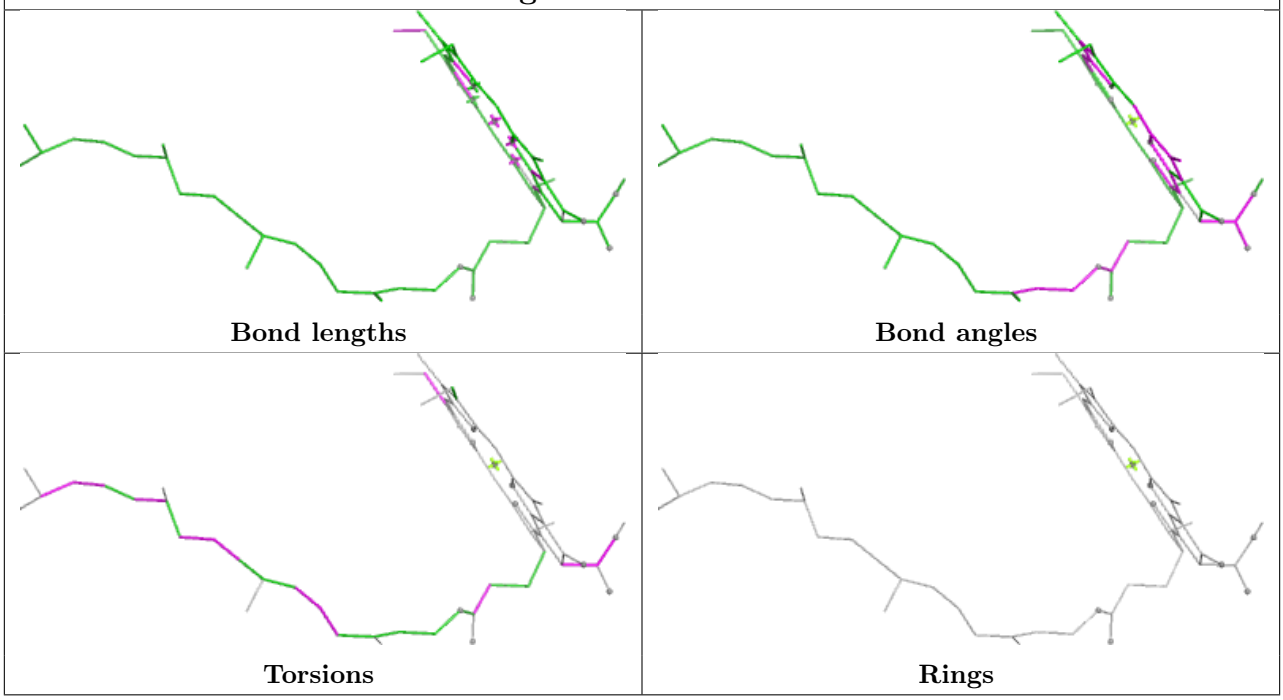

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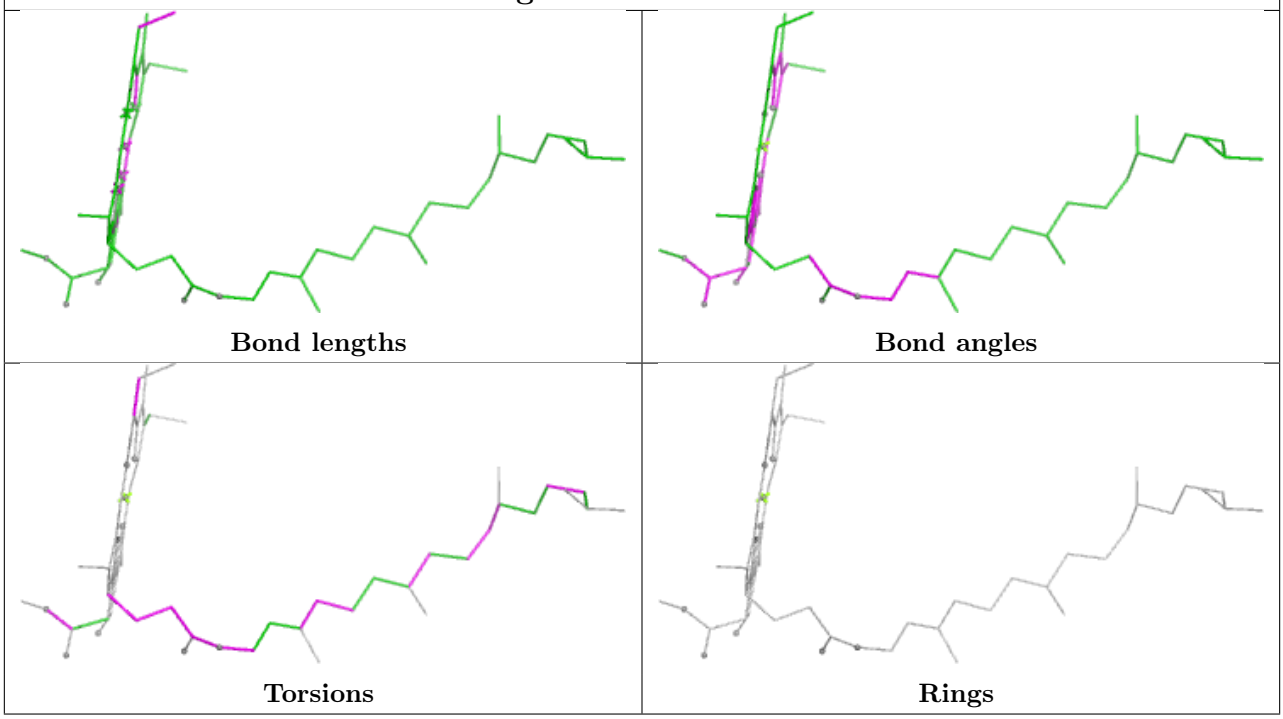

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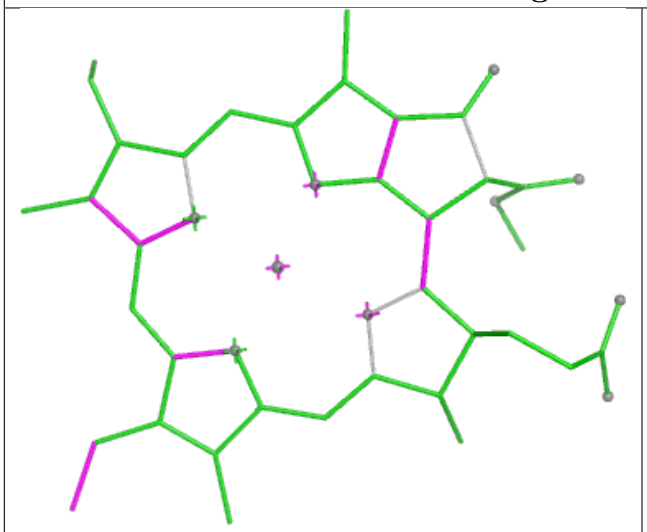

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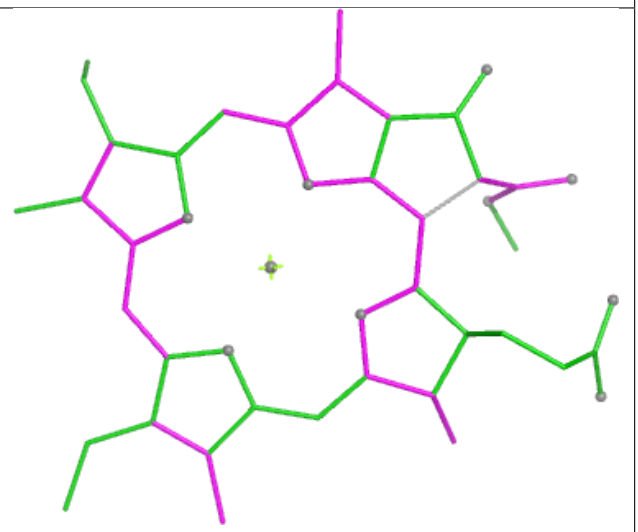

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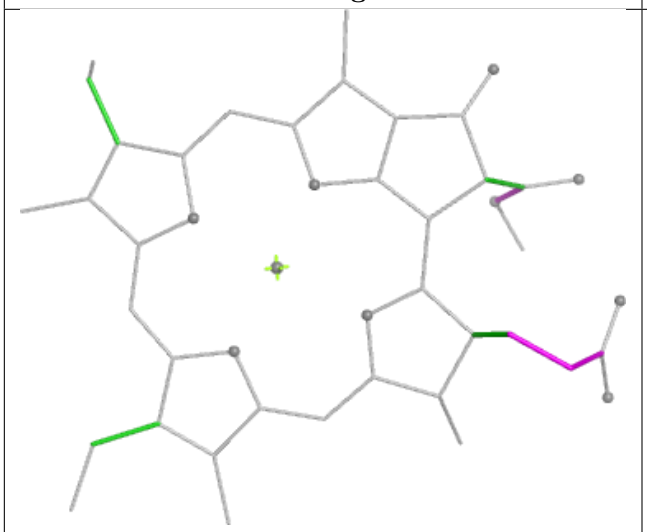

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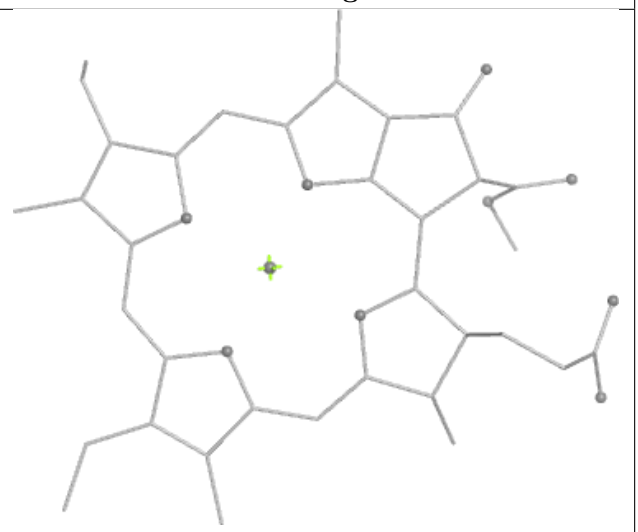

Rings

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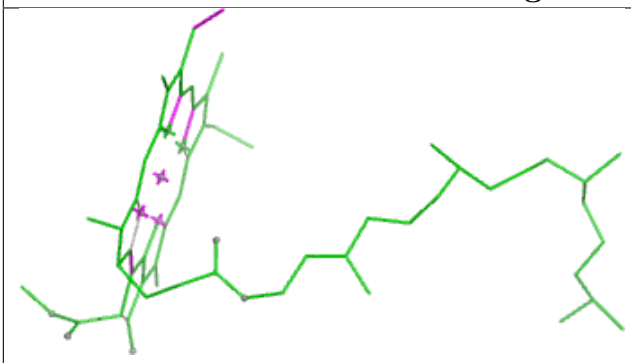
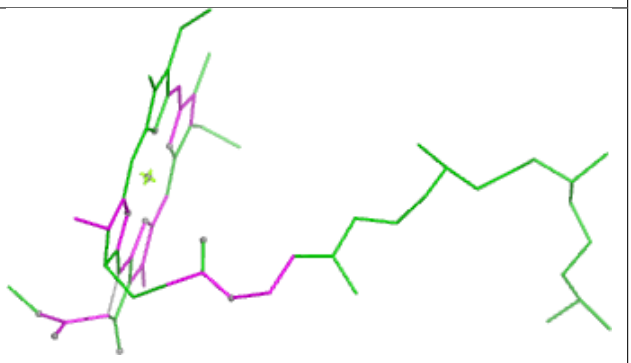
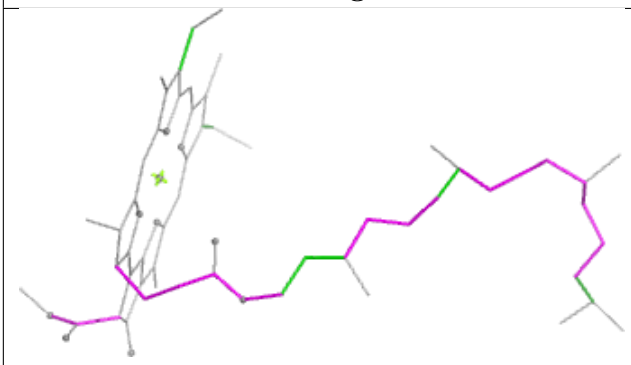
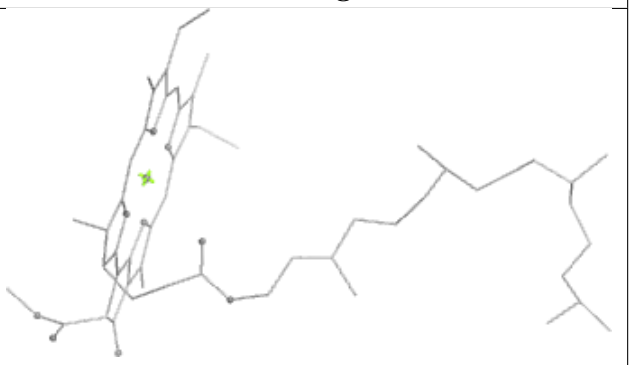
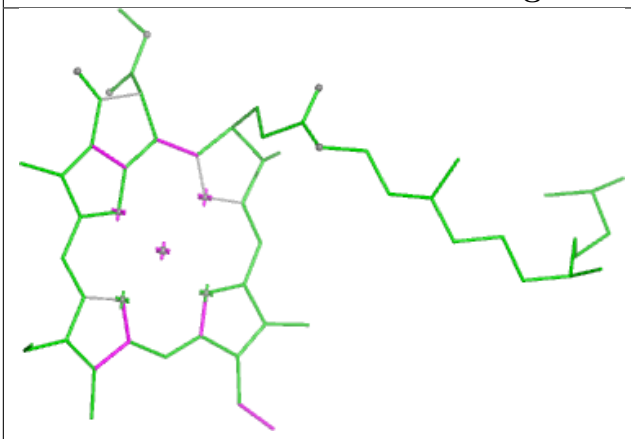
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 410



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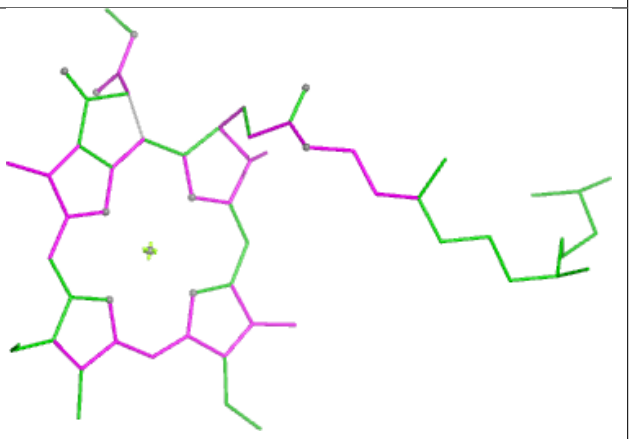

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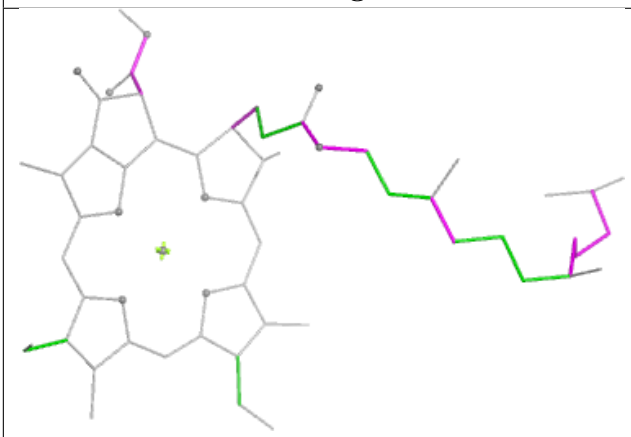
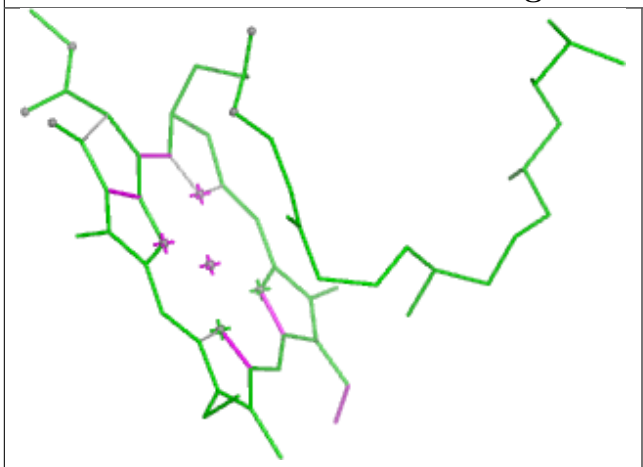
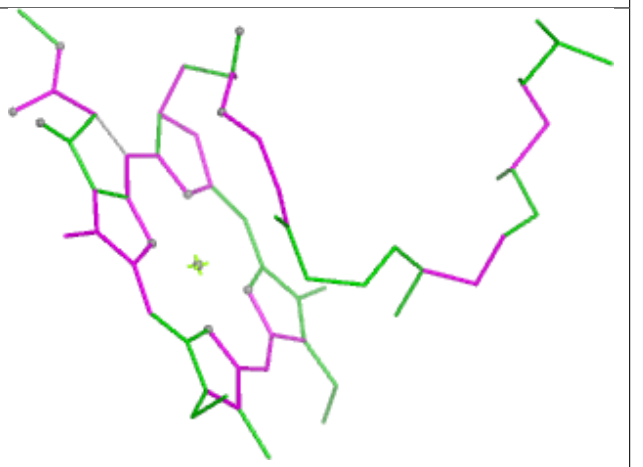
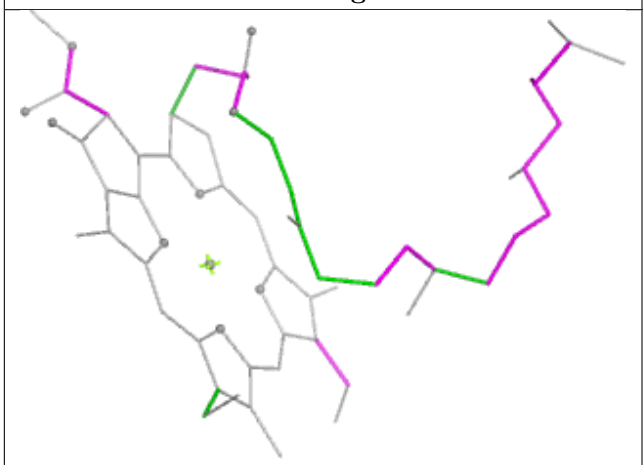
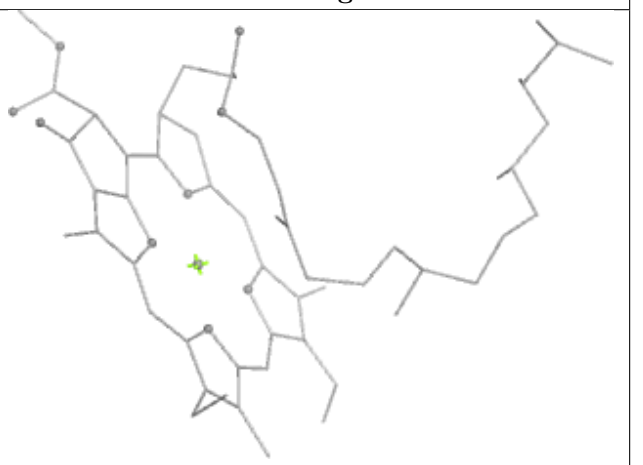
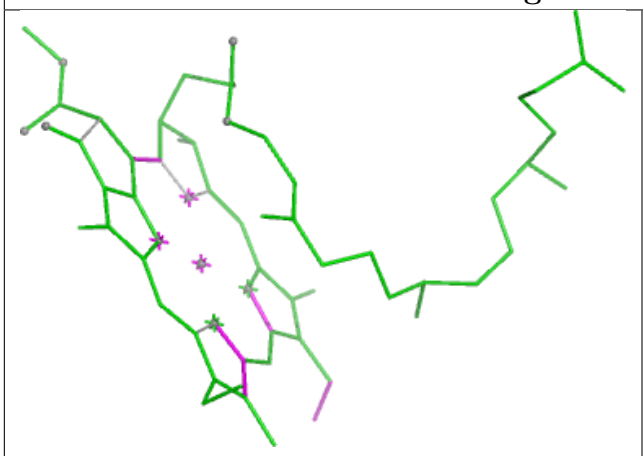
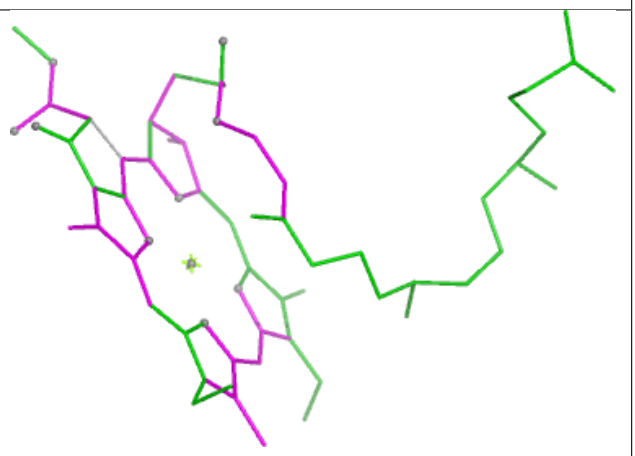
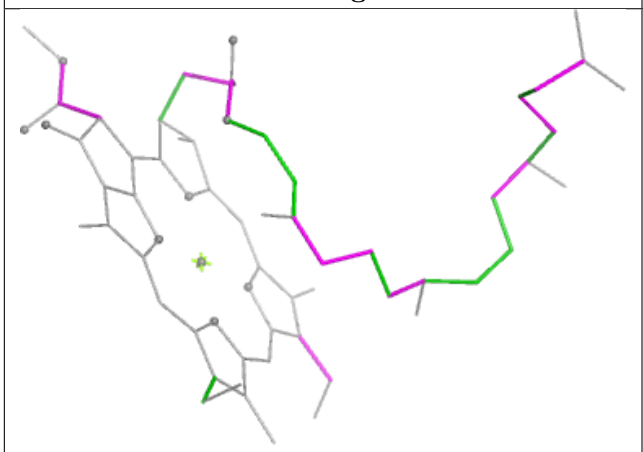


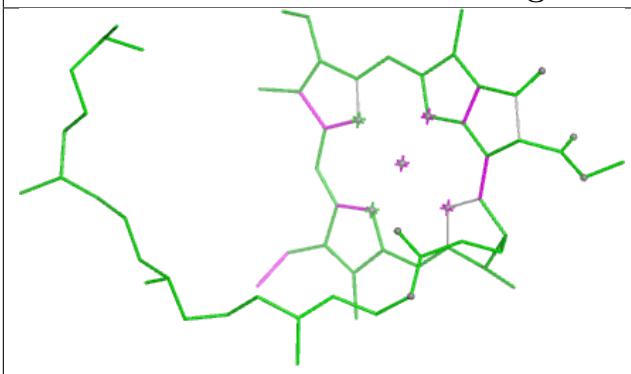
Torsions

Rings

Ligand CLA Y 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 613	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA n 610



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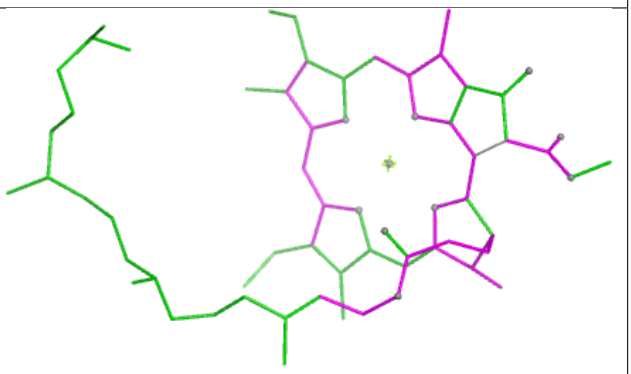

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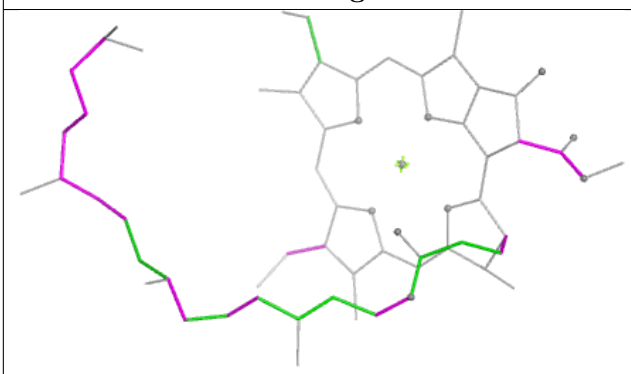

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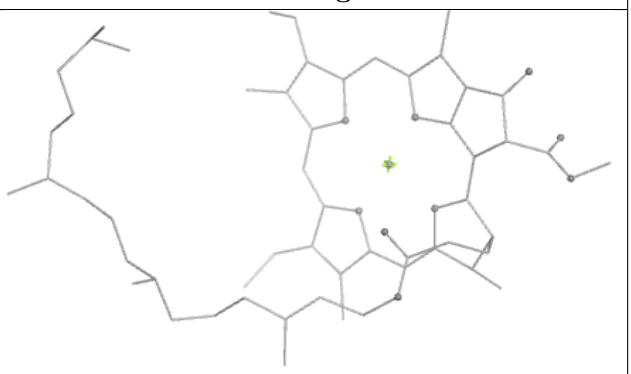
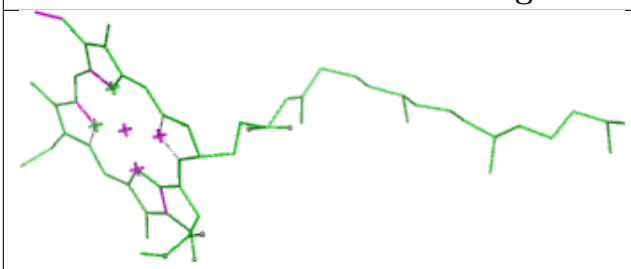


Rings

Ligand CLA C1 502



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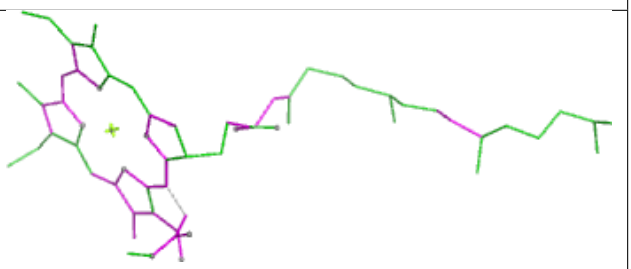

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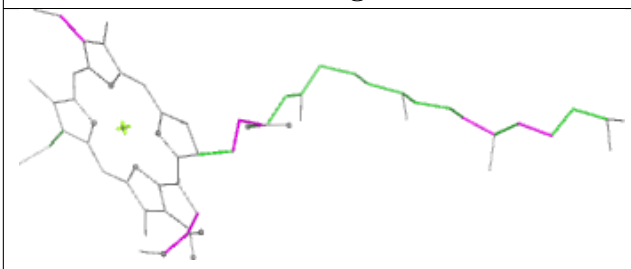

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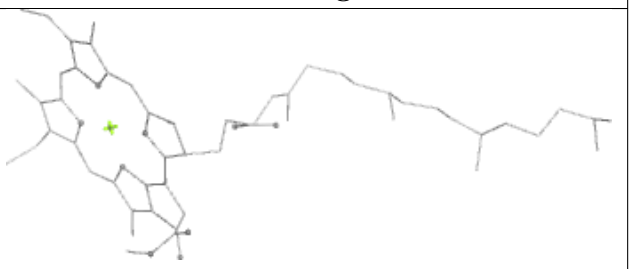

Rings

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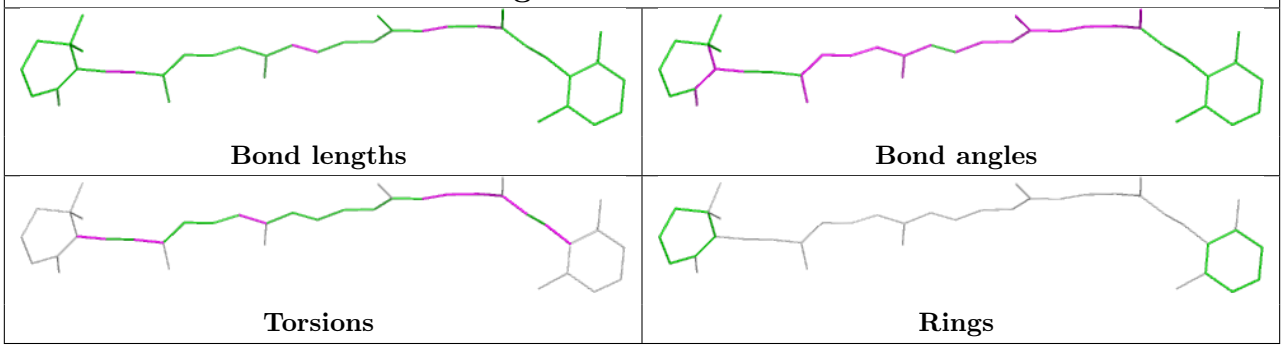

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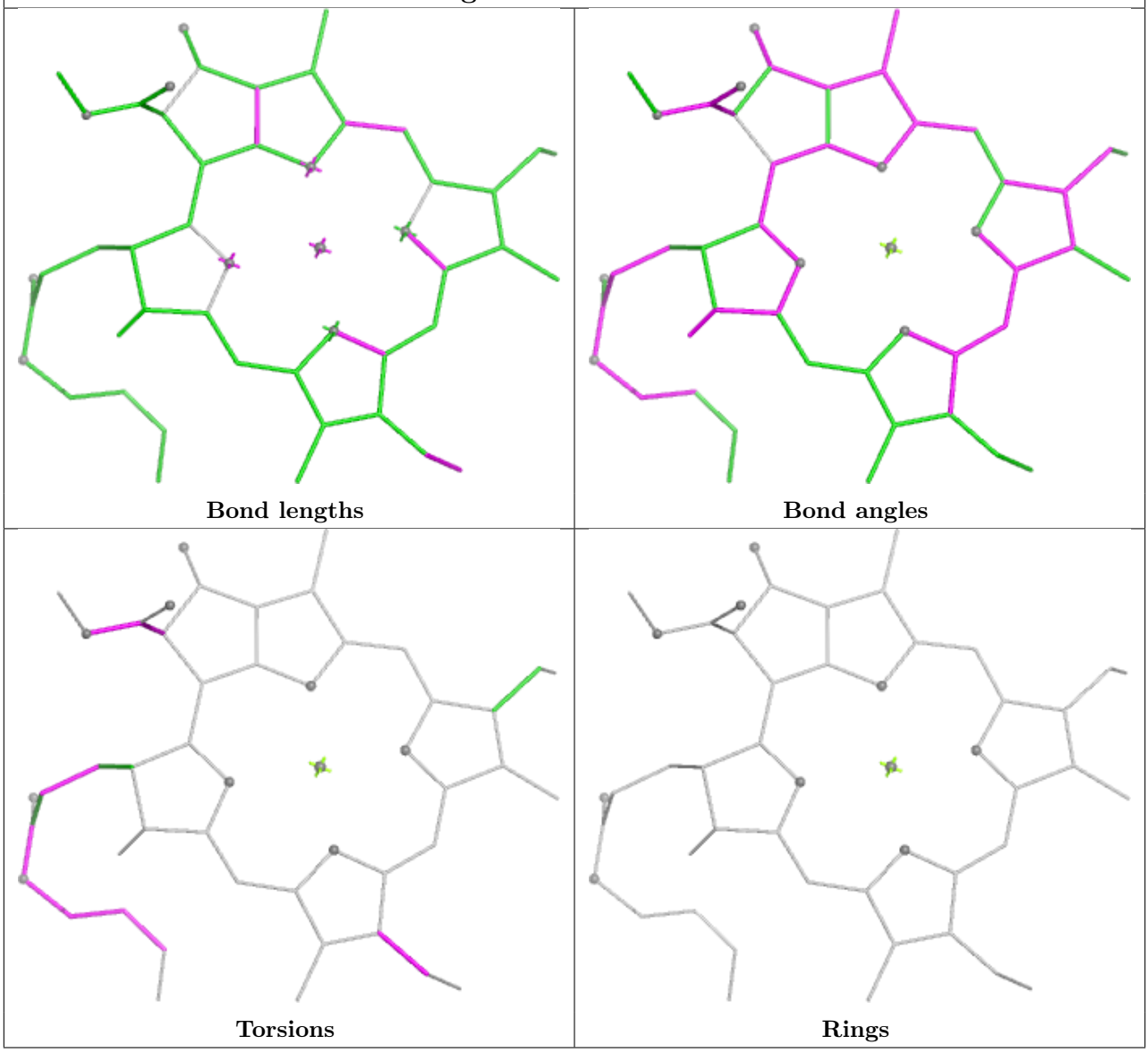

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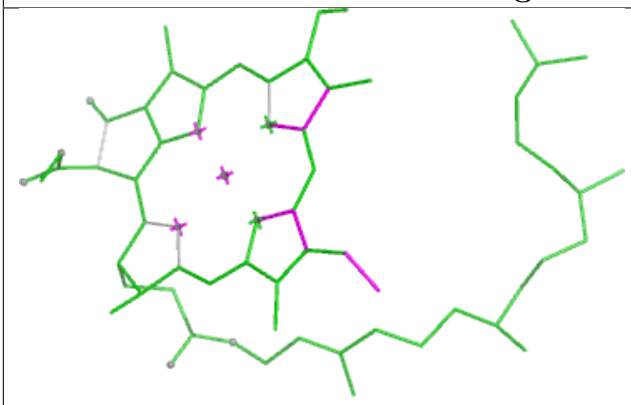
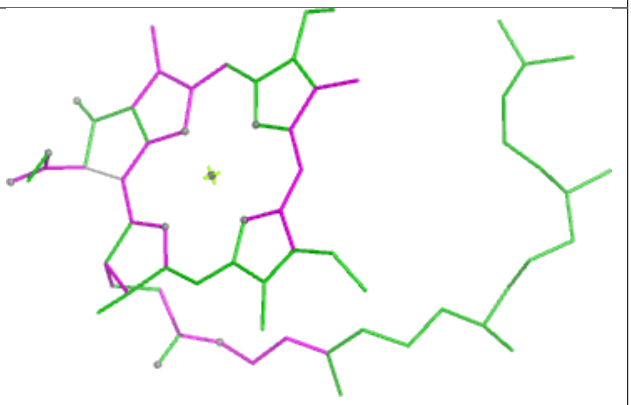
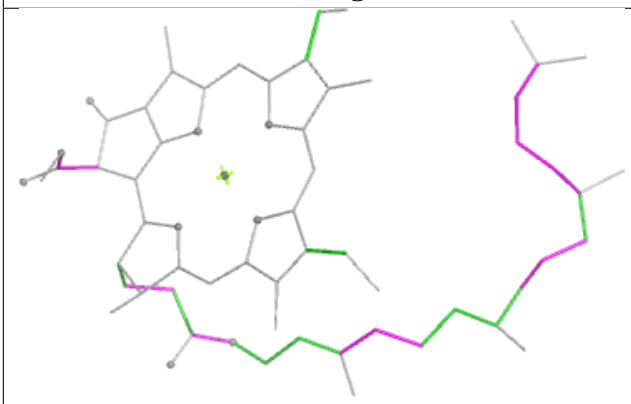
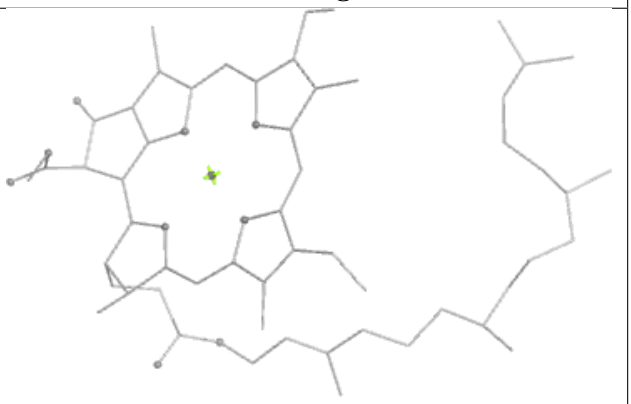
 Bond lengths	 Bond angles
 Torsions	 Rings

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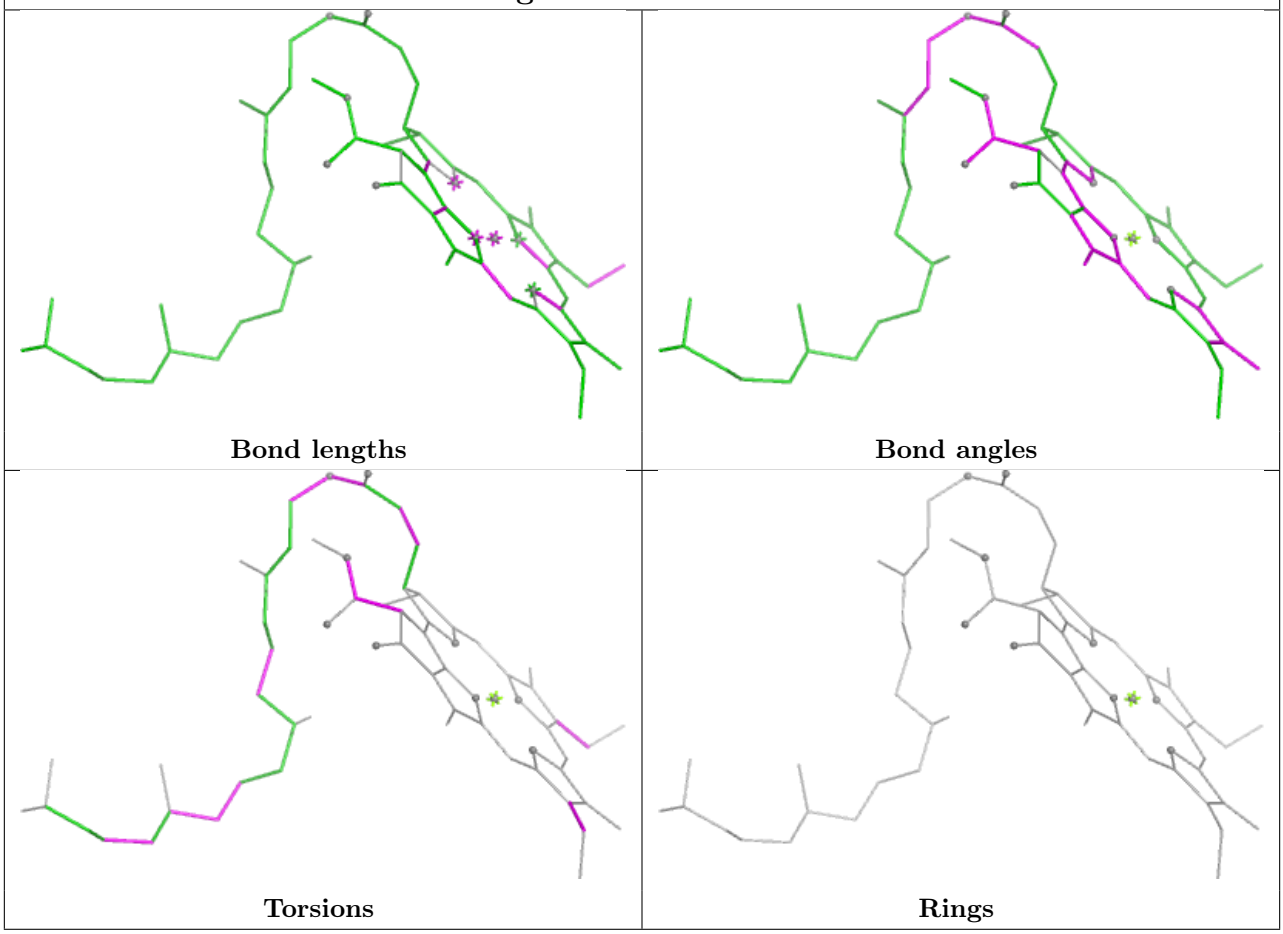

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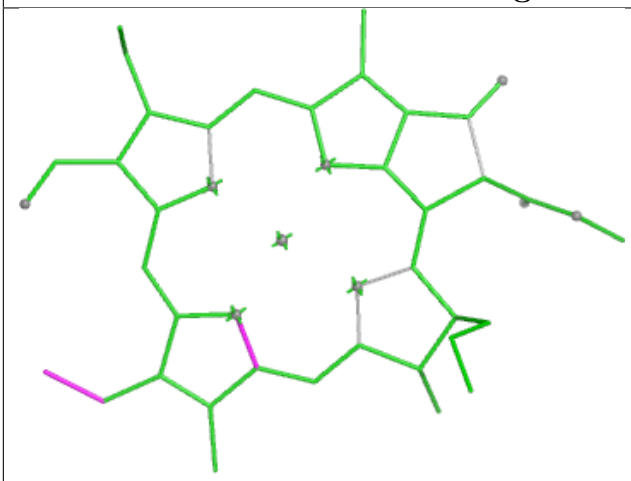
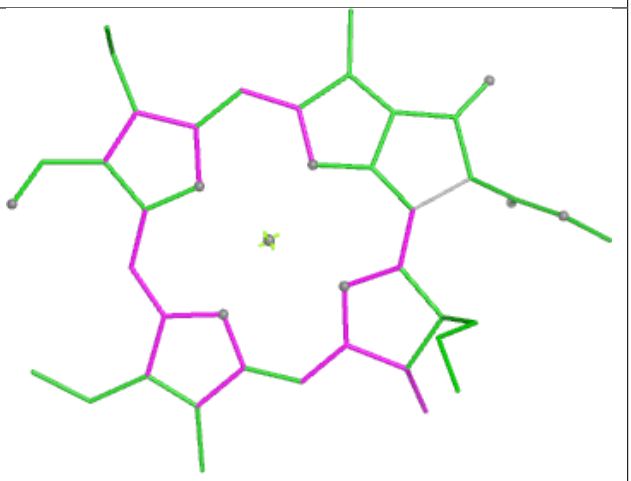
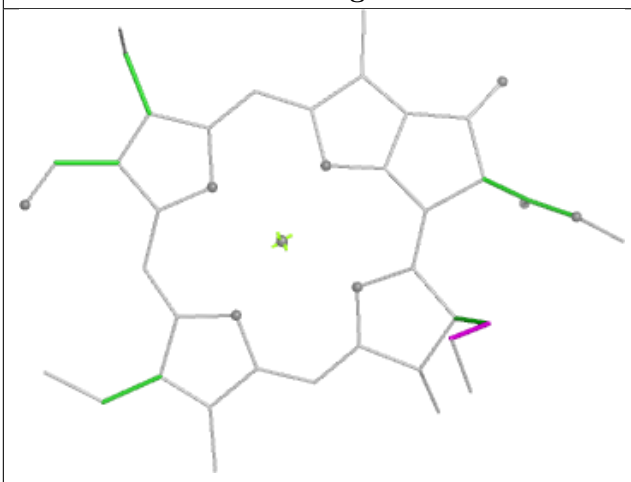
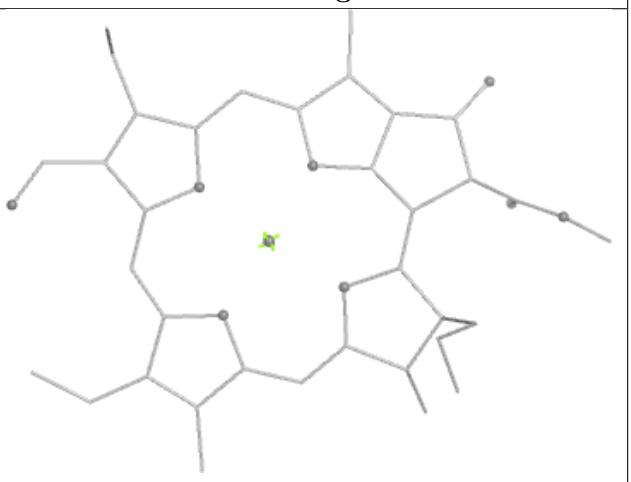
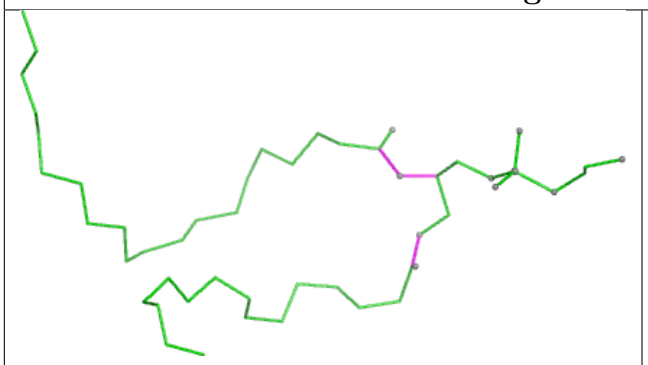
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PTY Y 626



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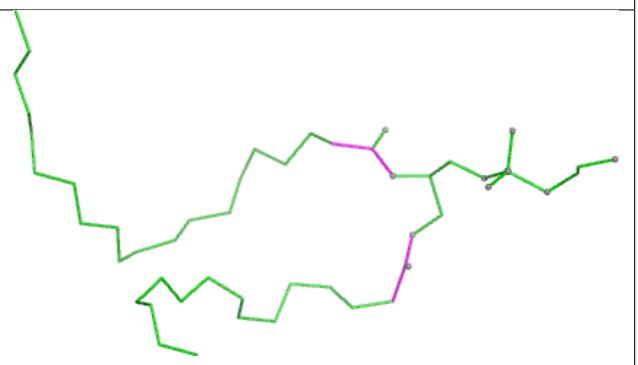

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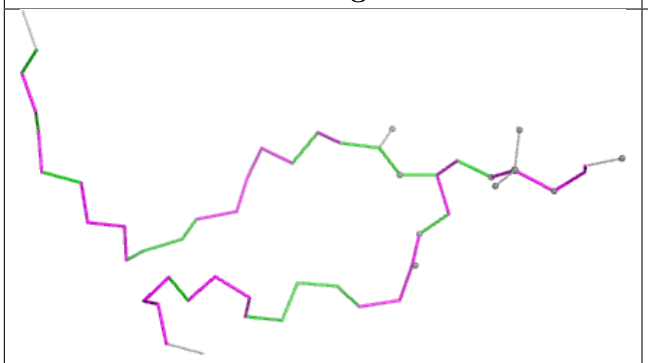

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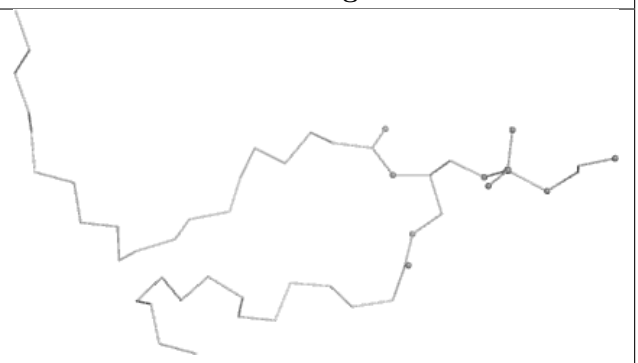
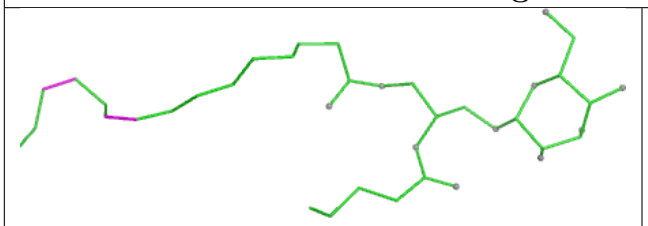


Rings

Ligand LMG w1 201



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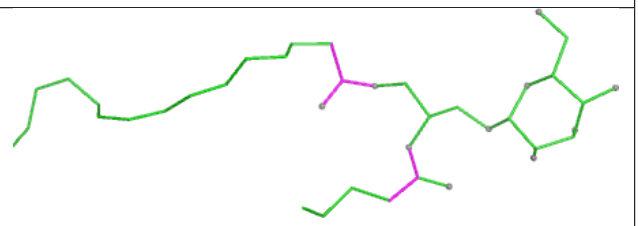

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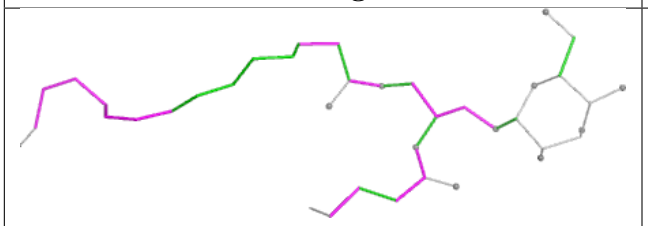

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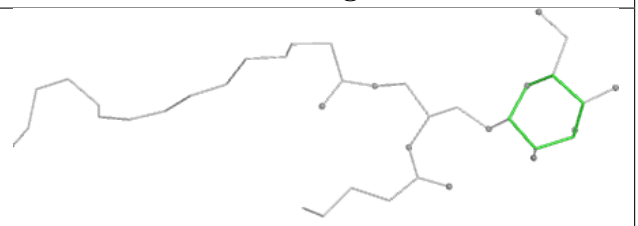
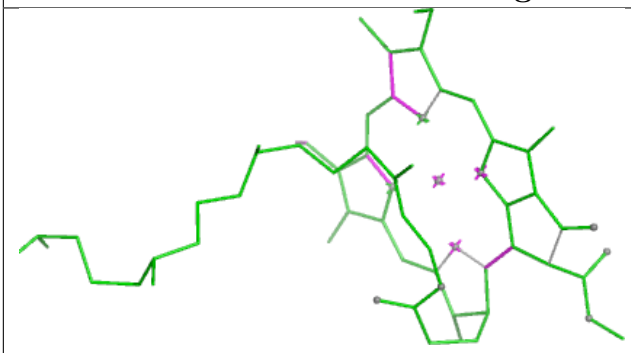


Rings

Ligand CLA N1 613



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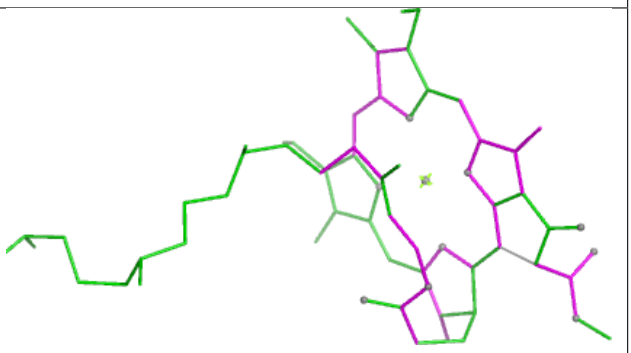

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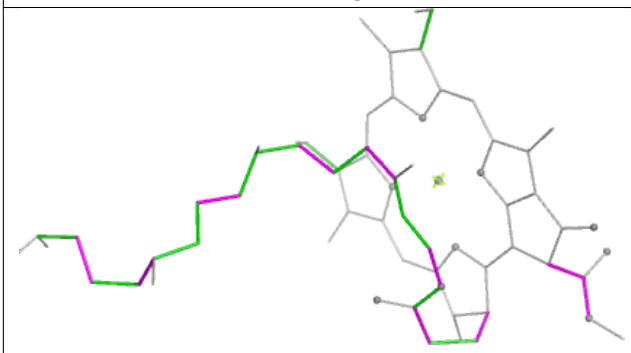
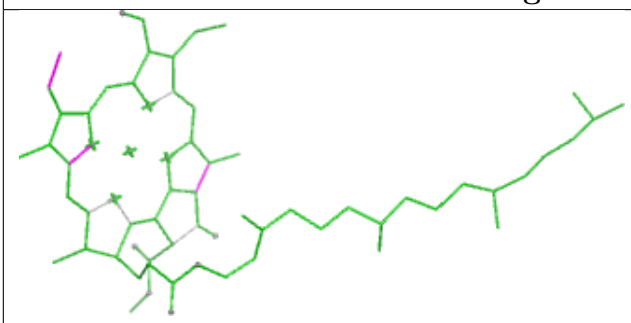


Torsions

Rings

Ligand CHL Y 609



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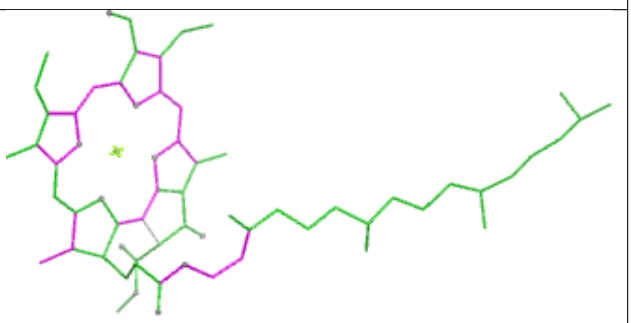

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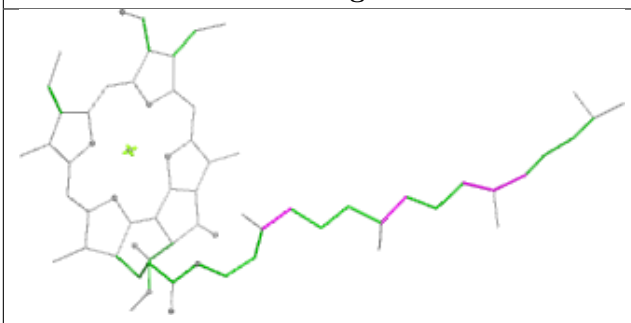

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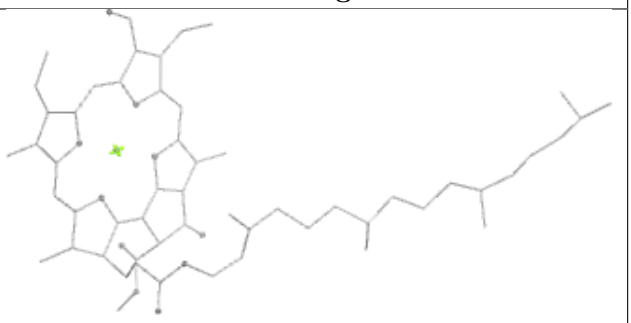
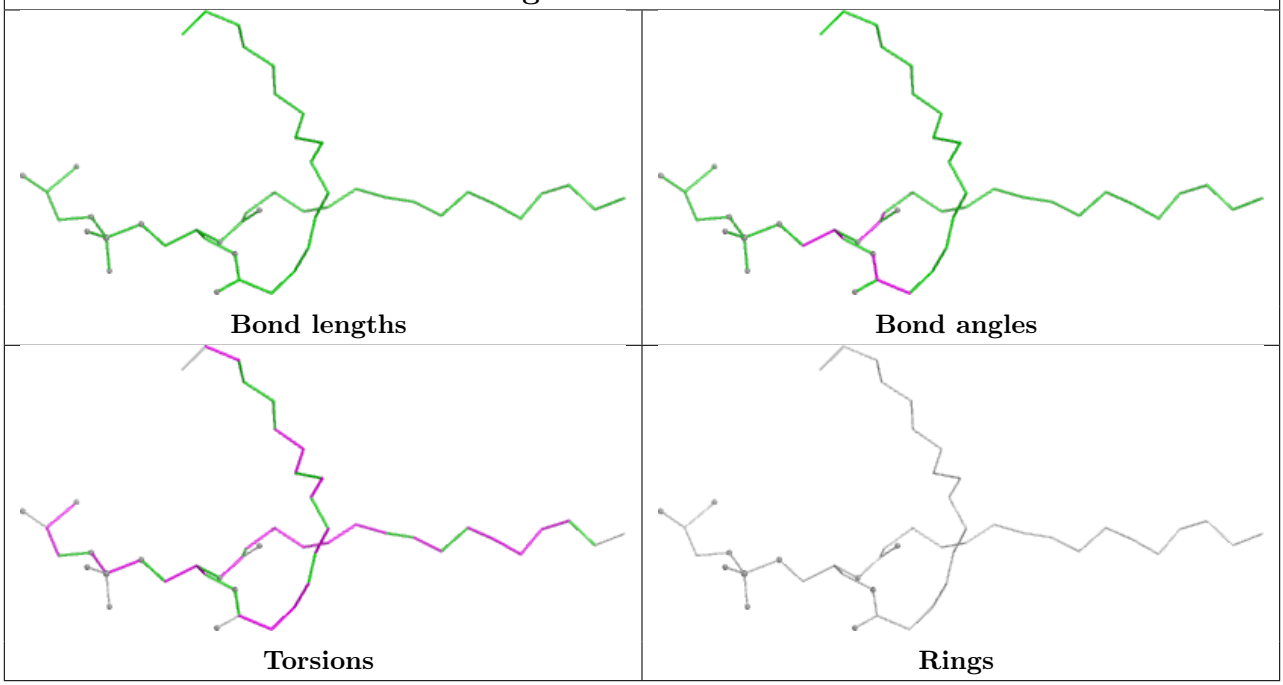
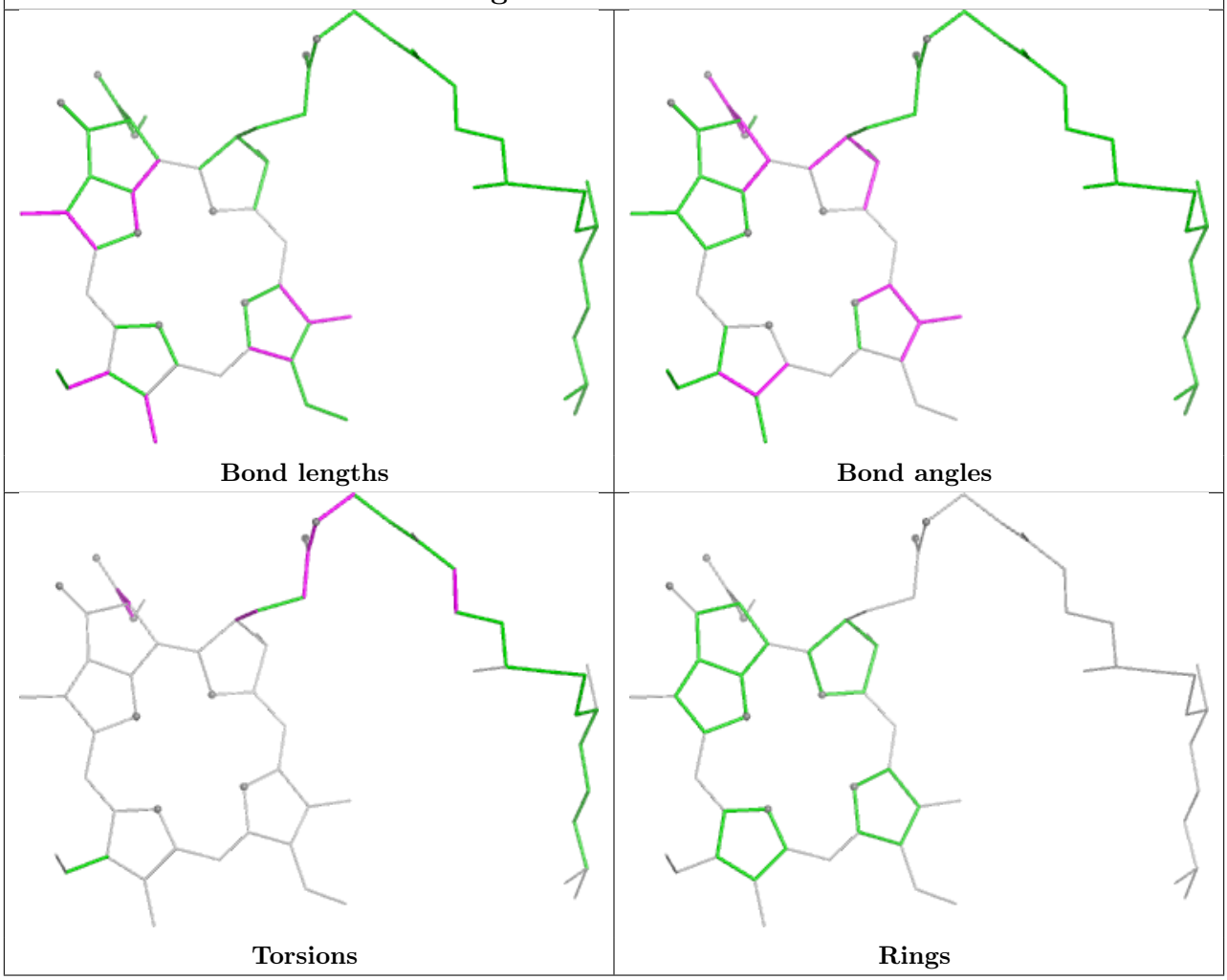


Rings

Ligand LHG G 624



Ligand PHO A1 409



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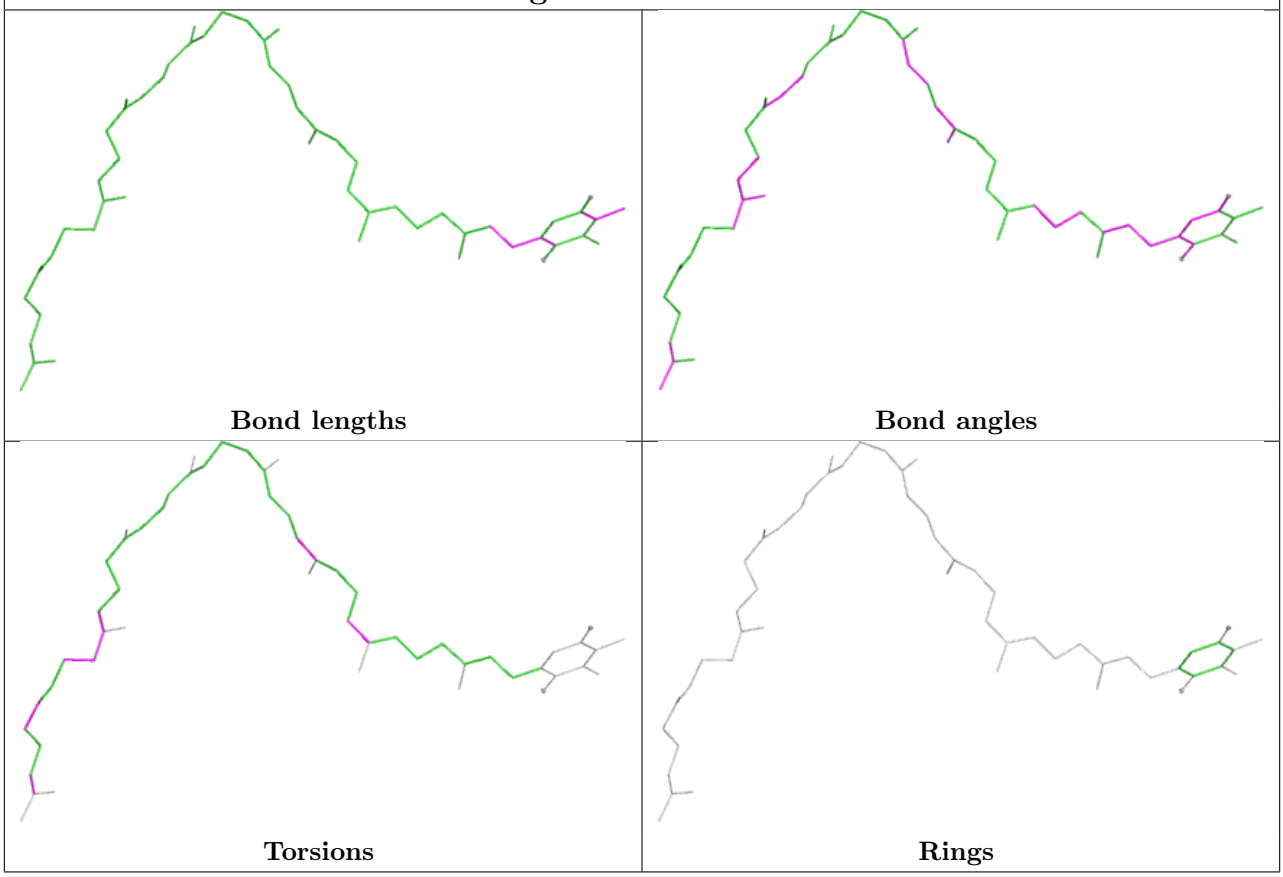

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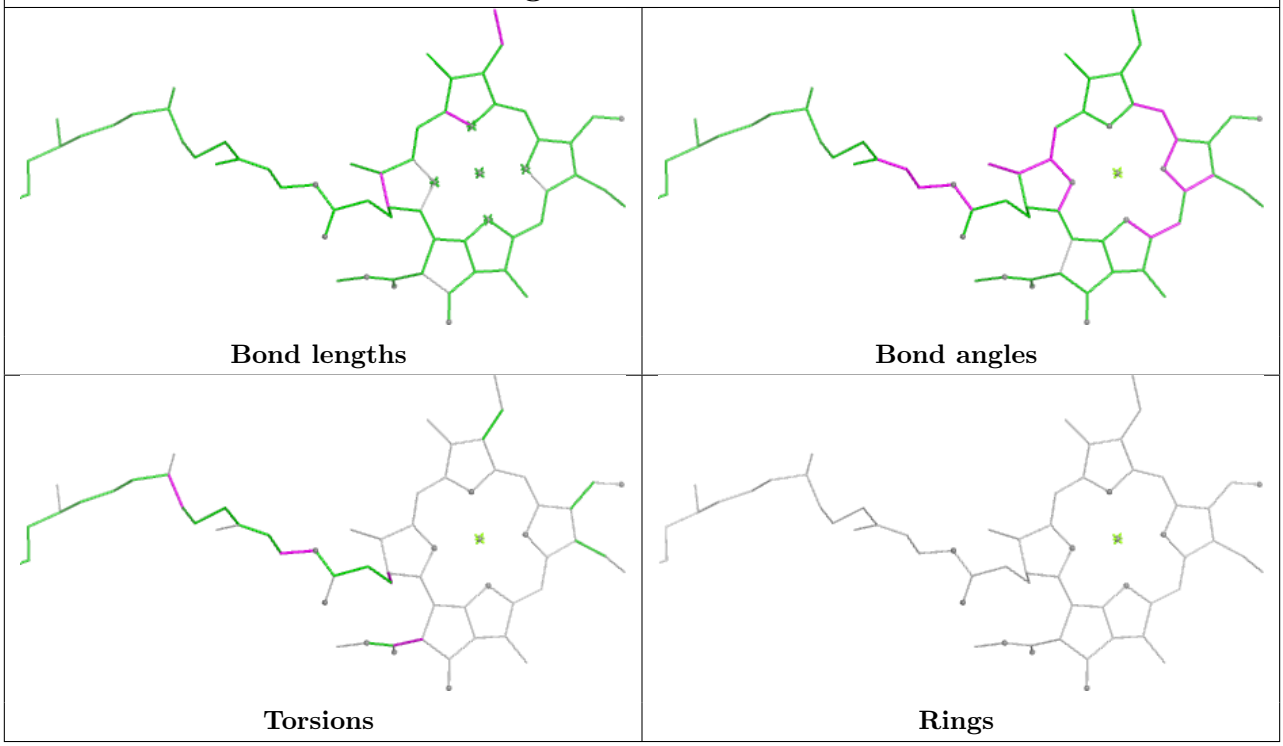
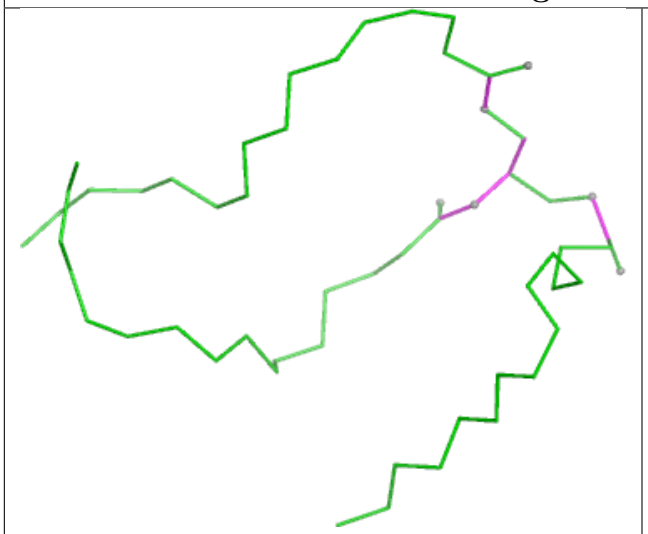


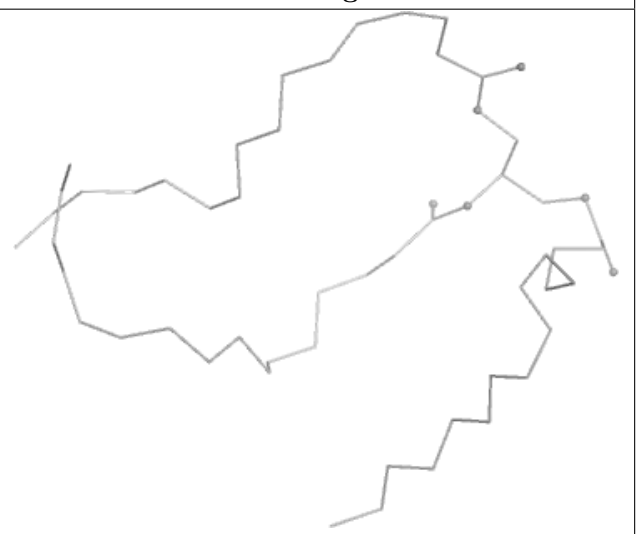
Ligand 4RF k 101



Bond lengths

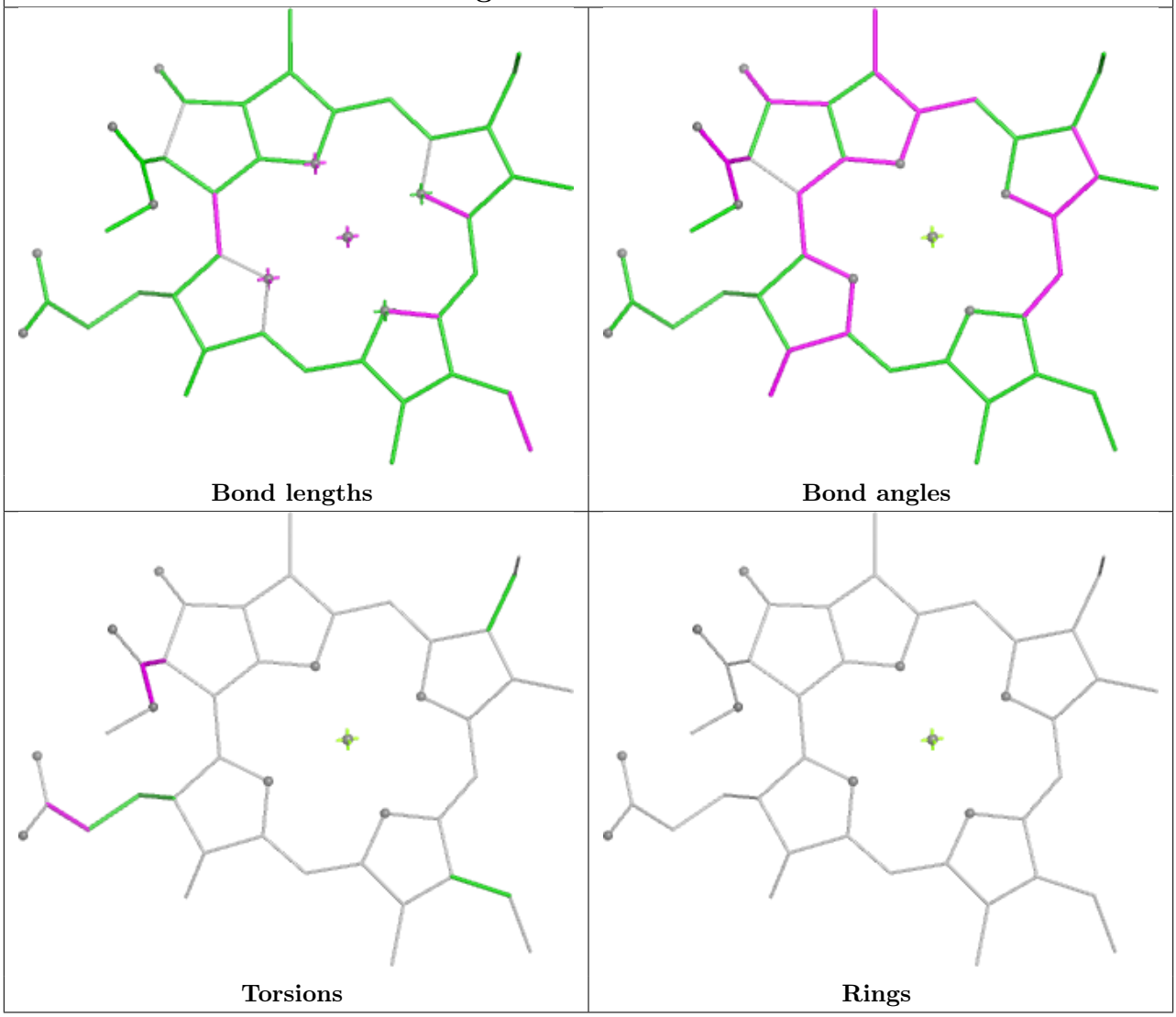
Bond angles

Torsions

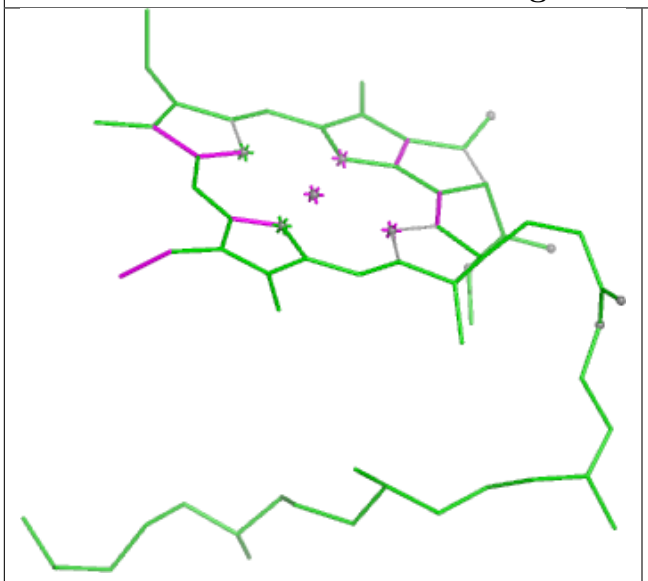


Rings

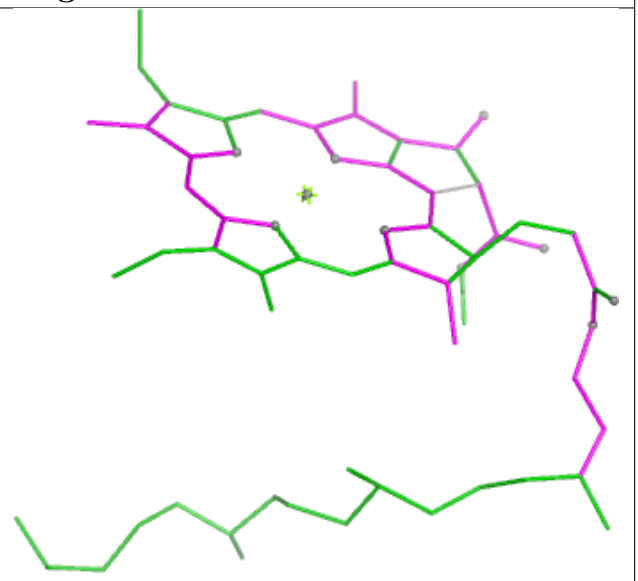
Ligand CLA S1 612



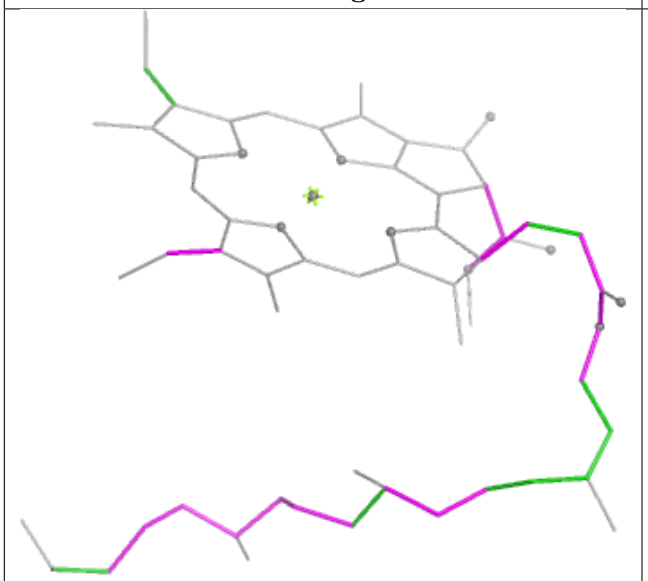
Ligand CLA g 603



Bond lengths



Bond angles



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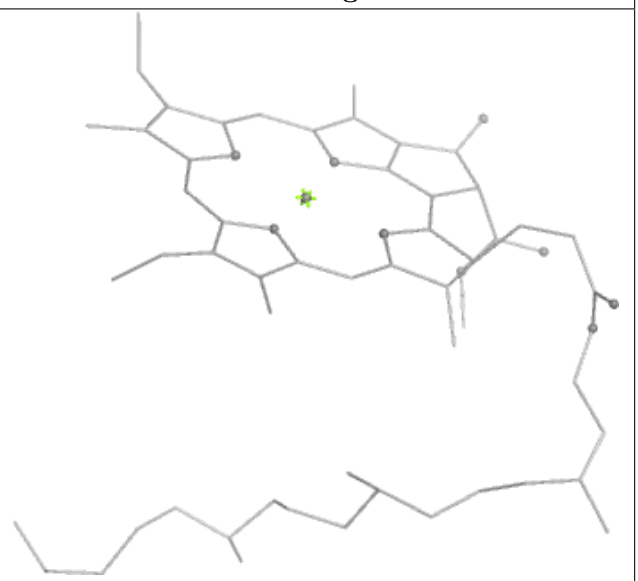

Rings

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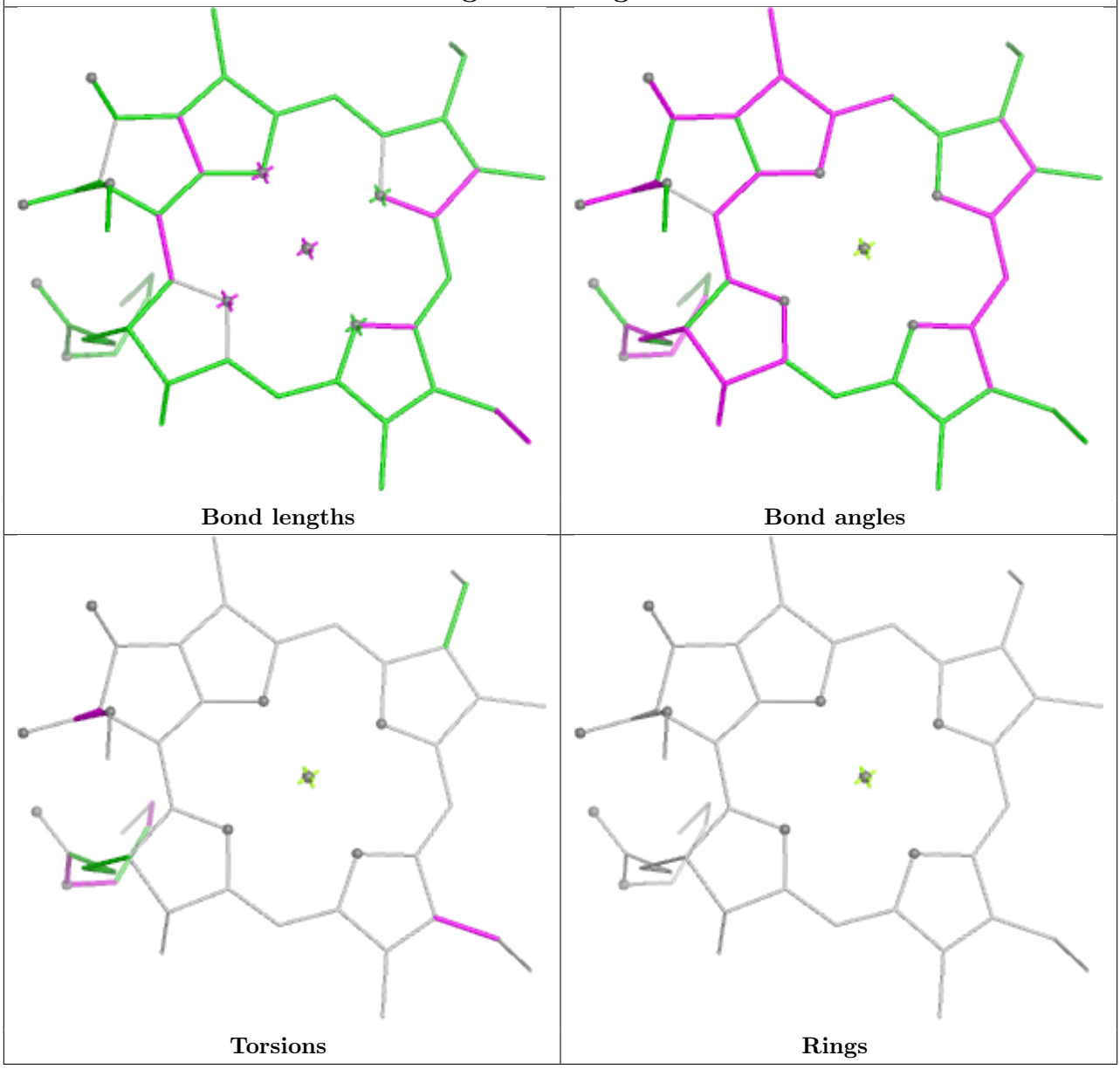

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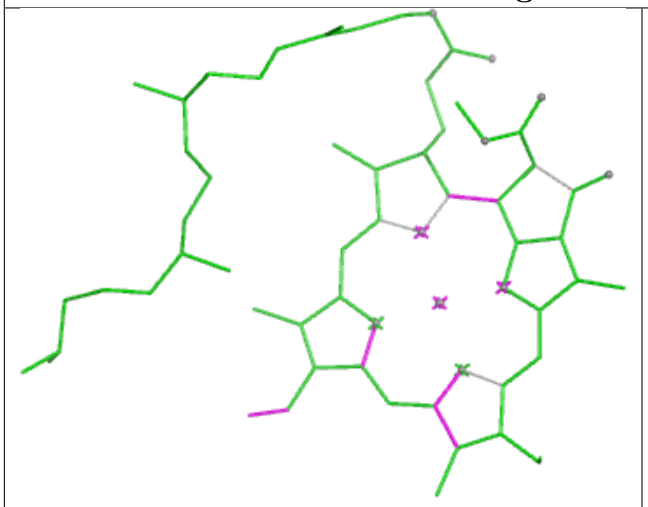

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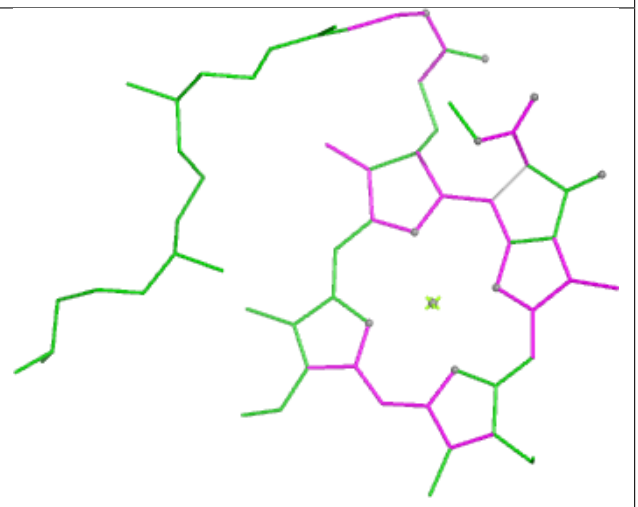
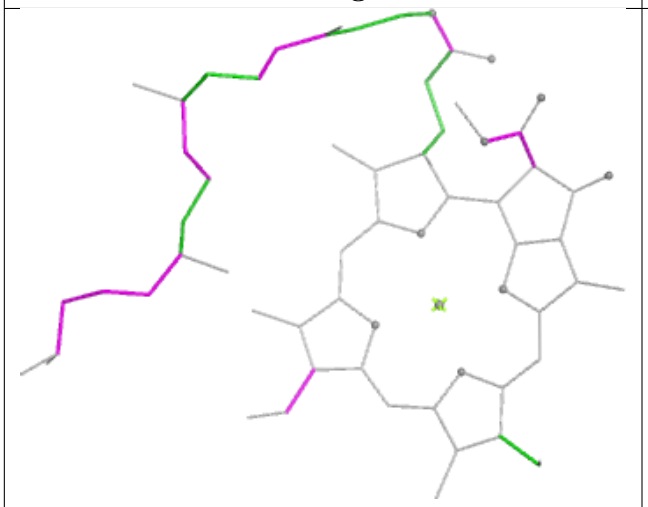
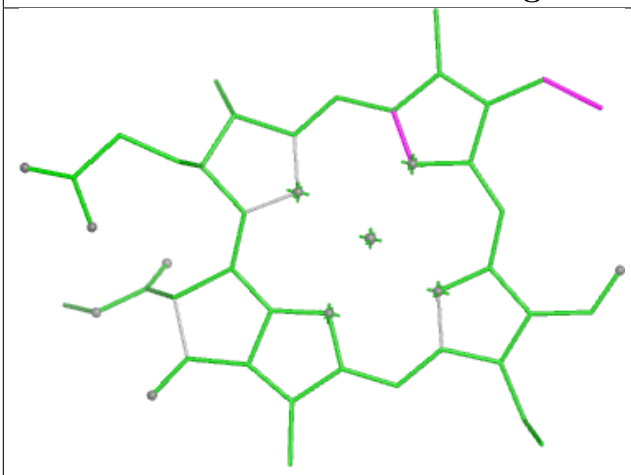
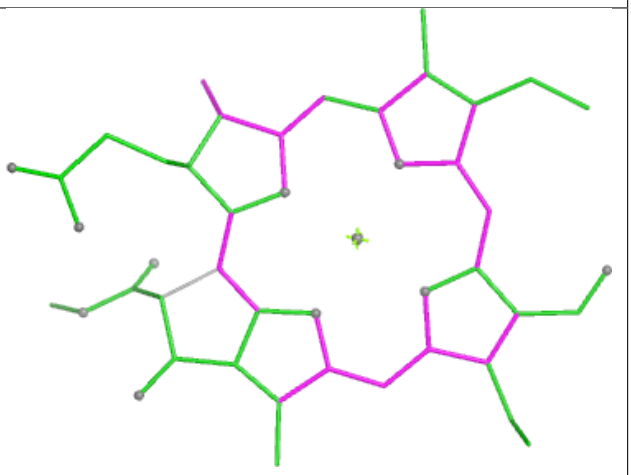
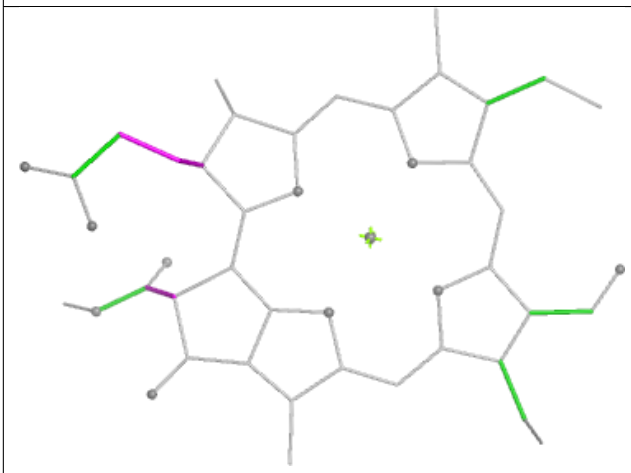
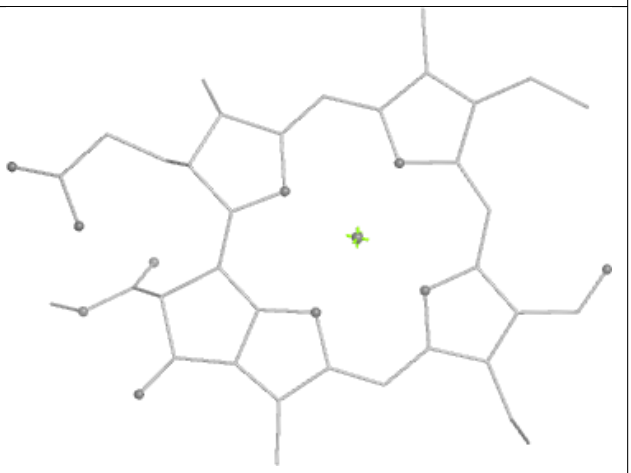


Bond angles

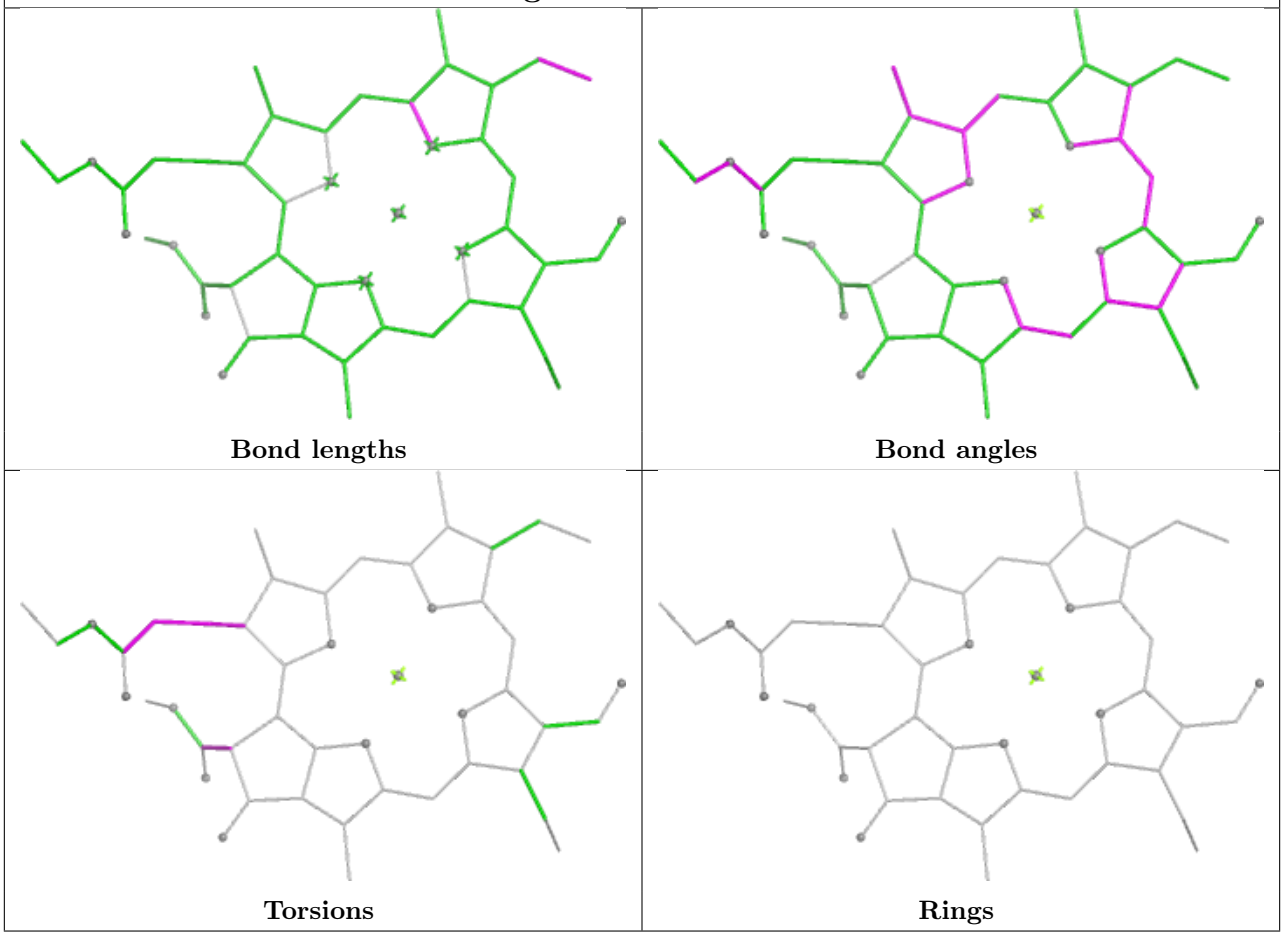


Torsions

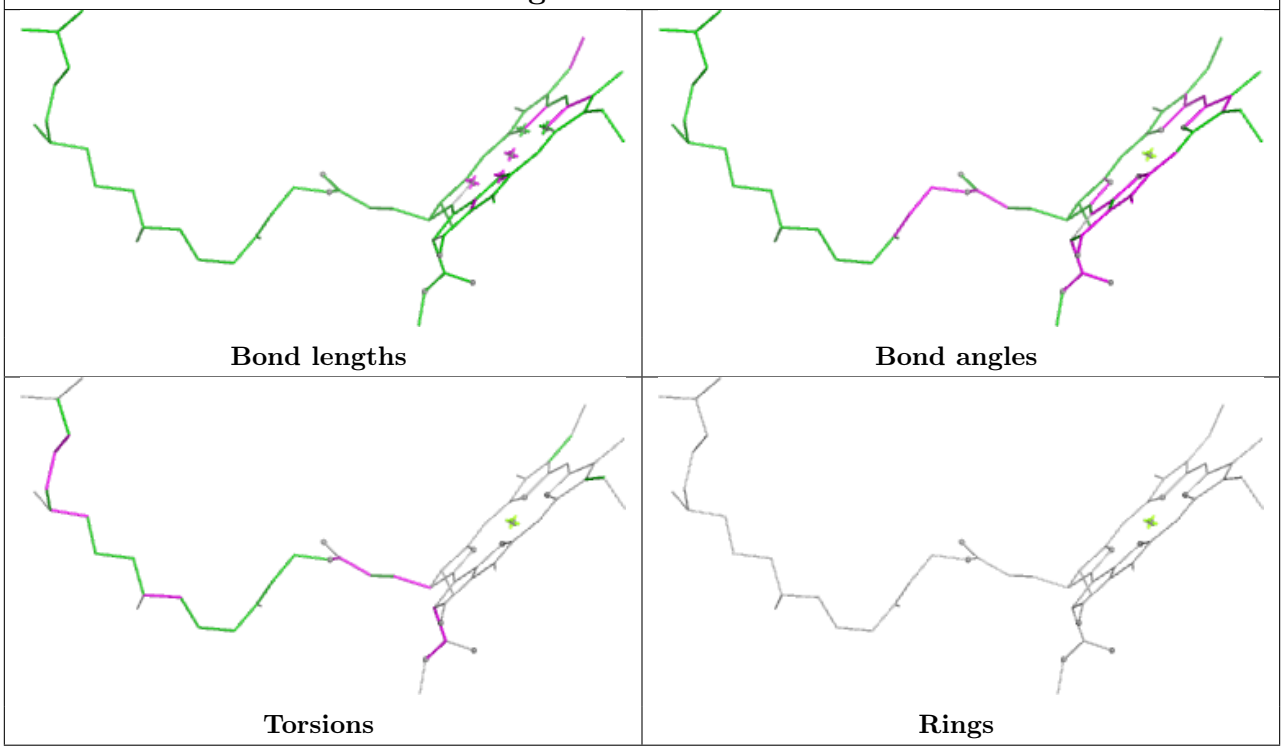
Rings

Ligand CHL Y 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL G 605



Ligand CLA d 402



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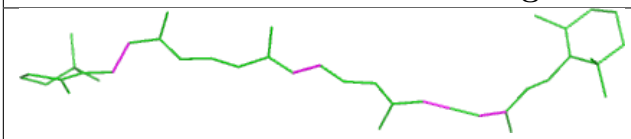
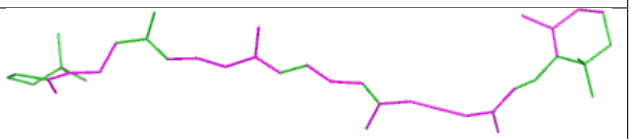


Bond lengths



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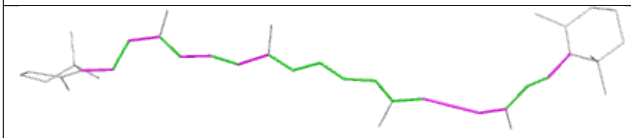

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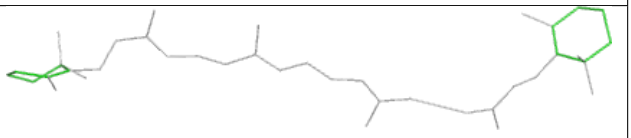
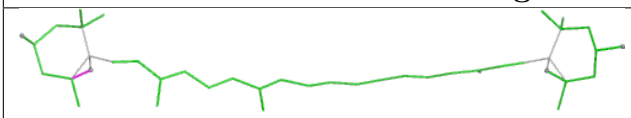


Rings

Ligand XAT G1 622



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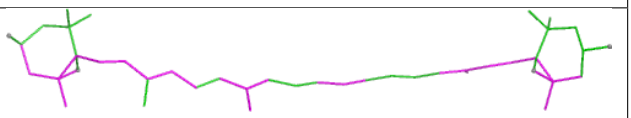

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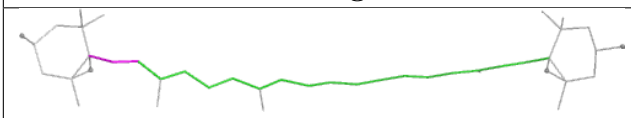

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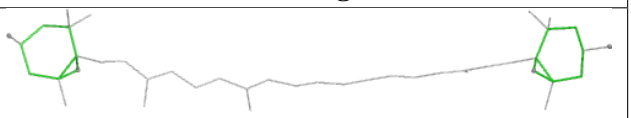
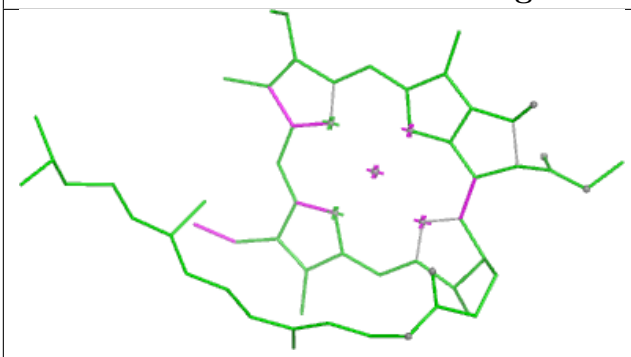


Rings

Ligand CLA R1 608



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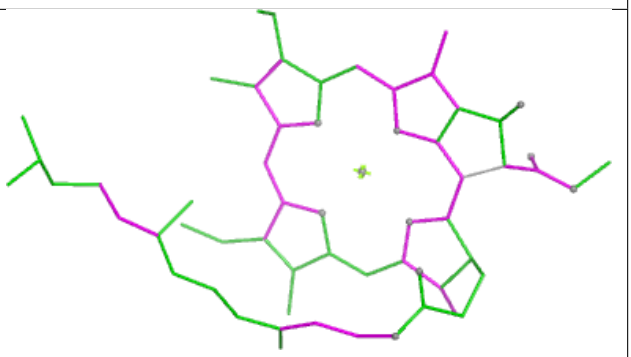

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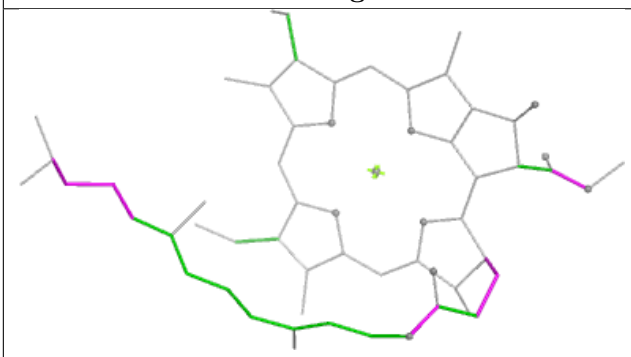

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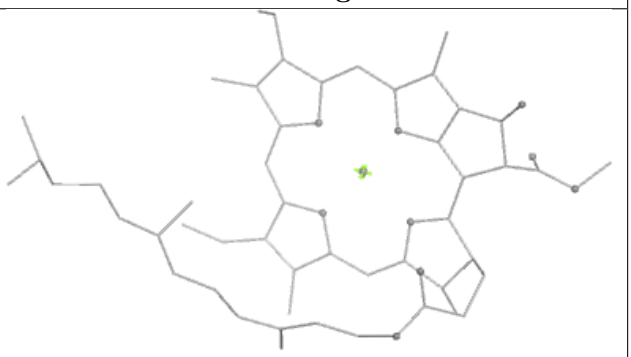
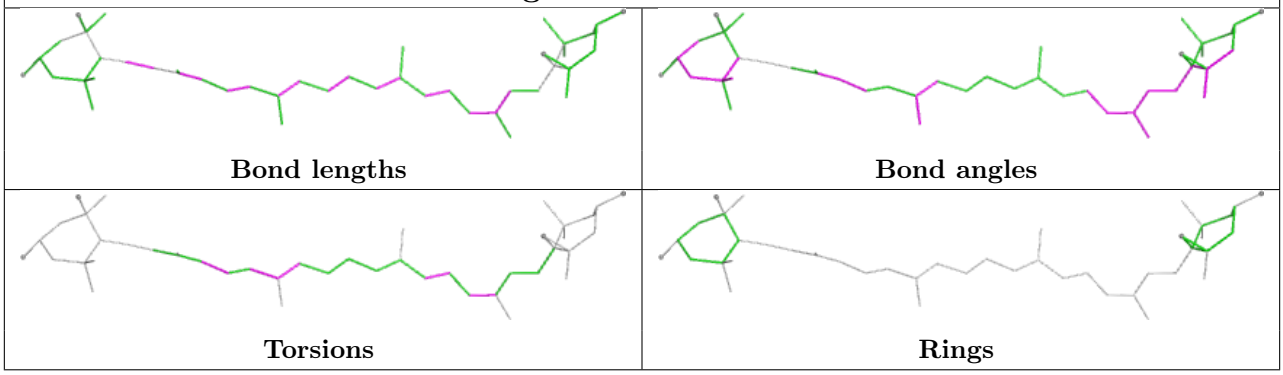
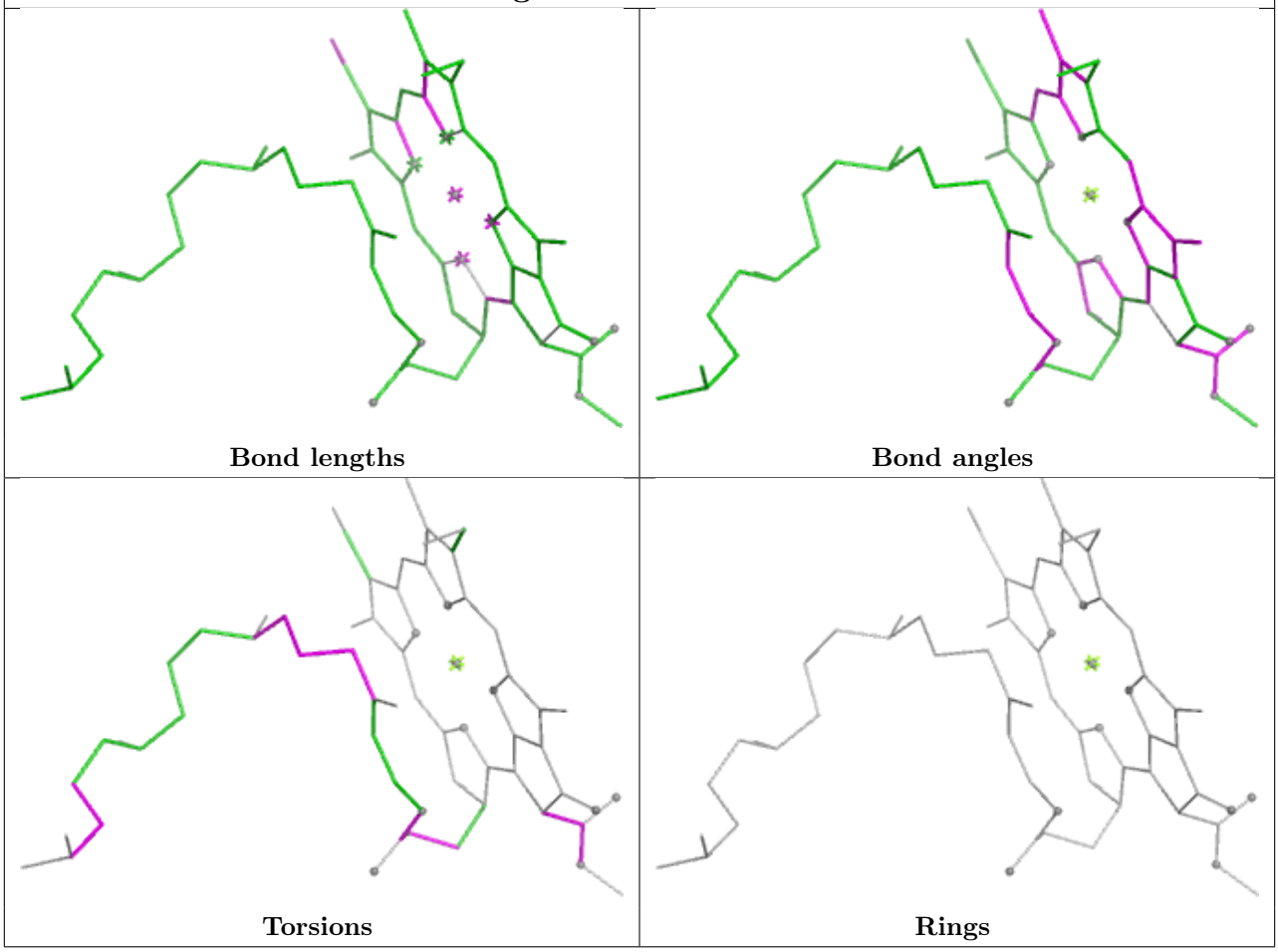


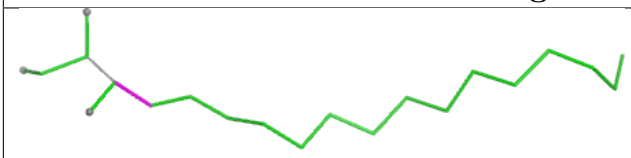
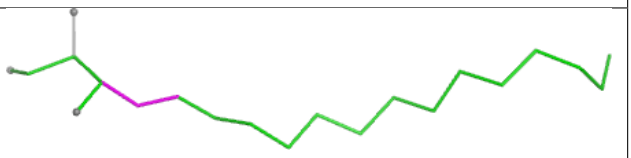
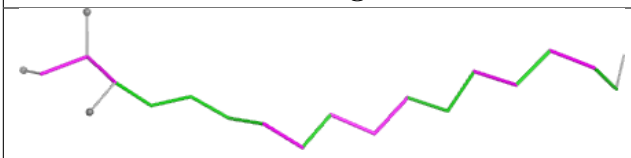
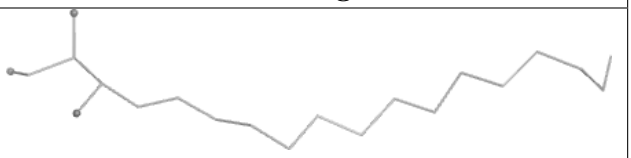
Rings

Ligand NEX Y 623



Ligand CLA G1 613



Ligand SPH a 414	
 Bond lengths	 Bond angles
 Torsions	 Rings

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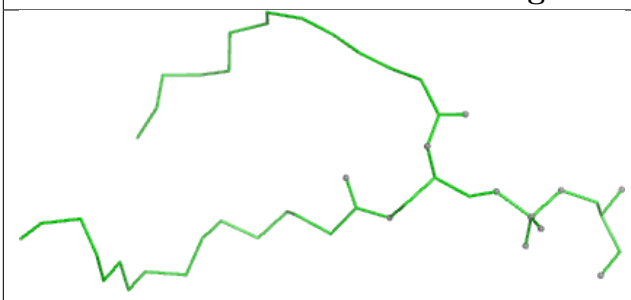
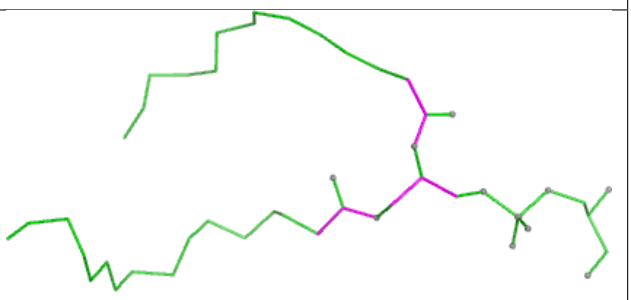
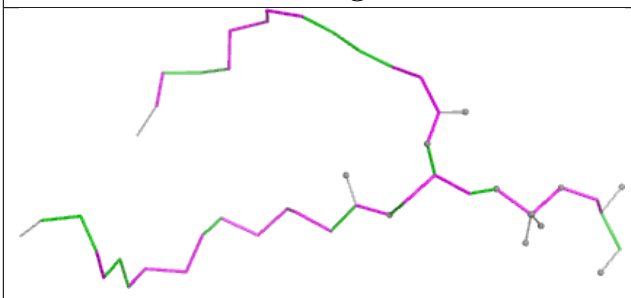
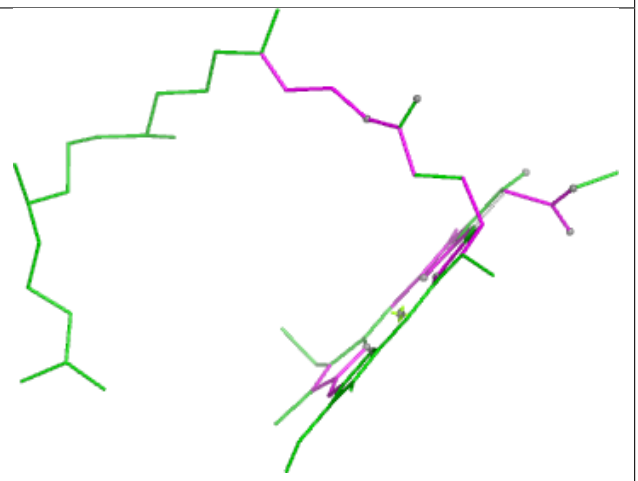
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA b 612

Bond lengths



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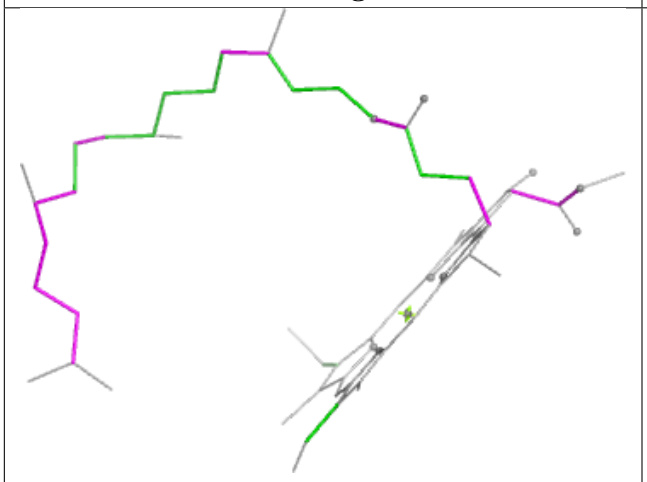
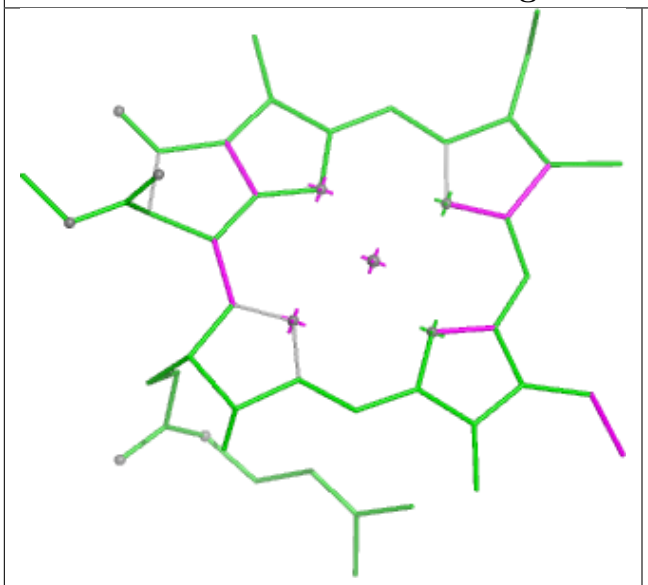


Torsions

Rings

Ligand CLA S1 617



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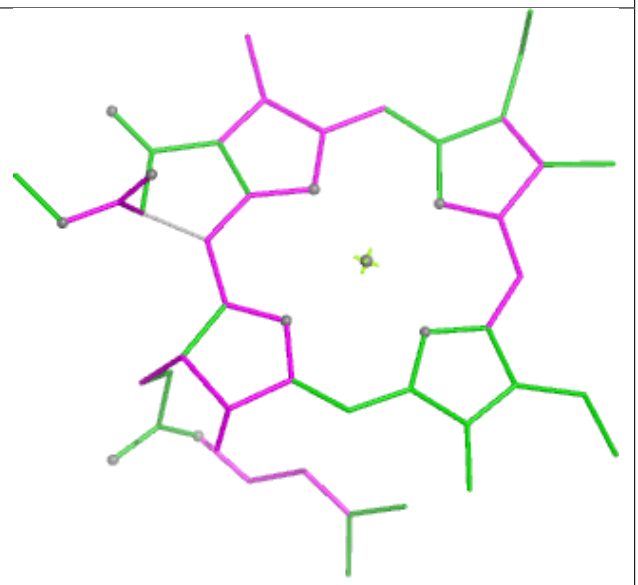

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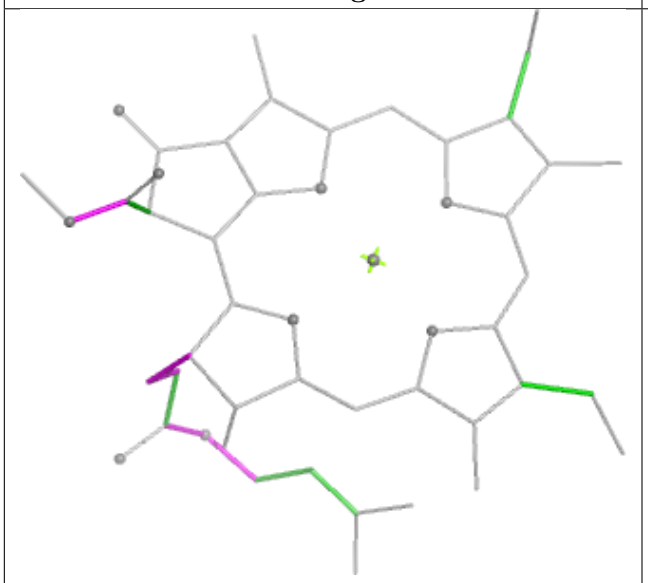

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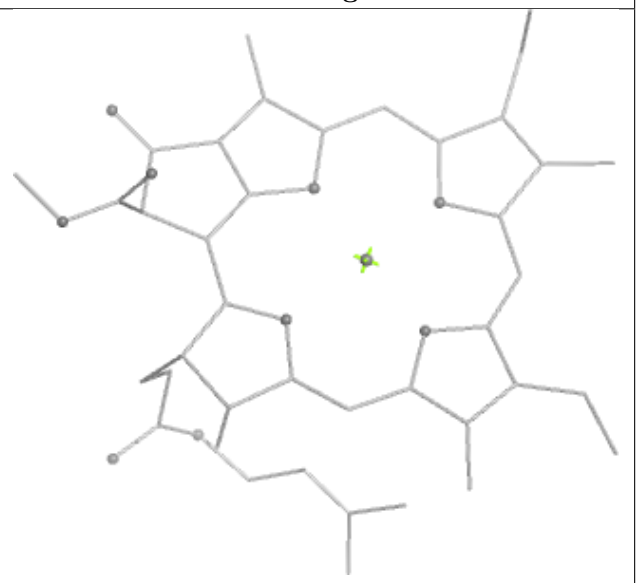

Rings

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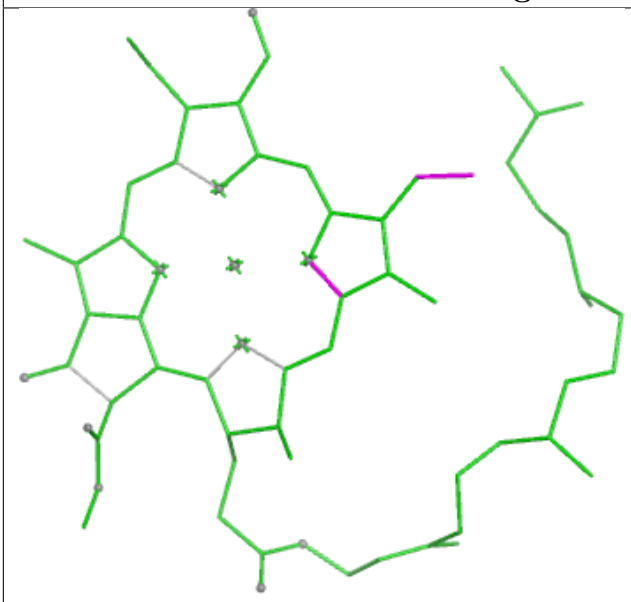
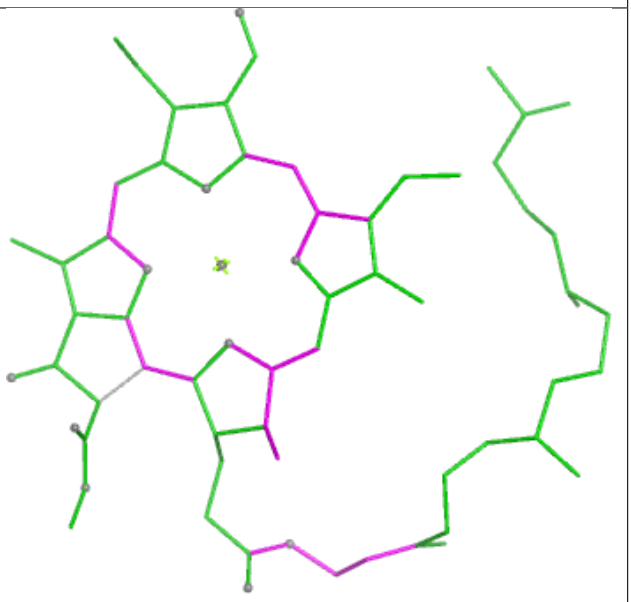
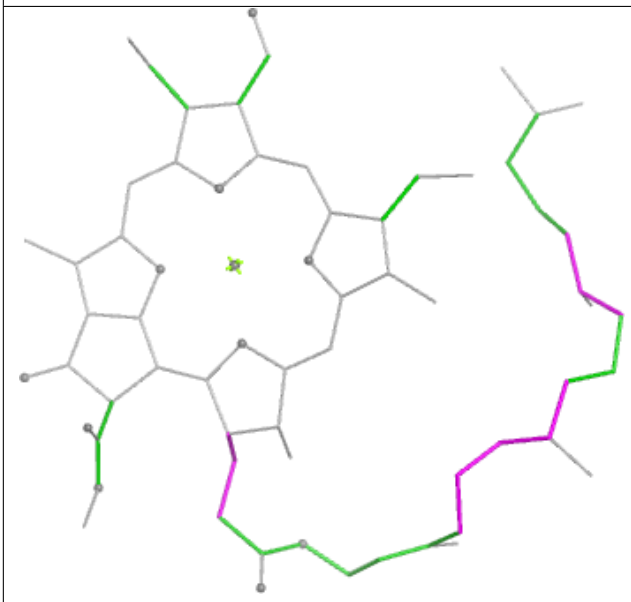
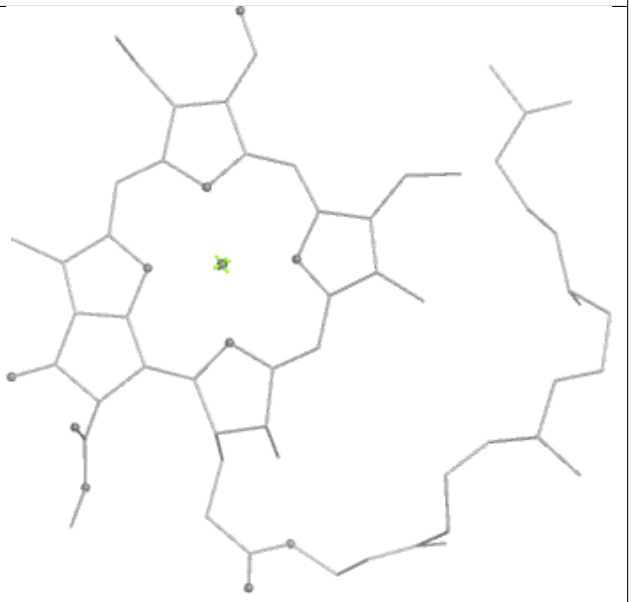
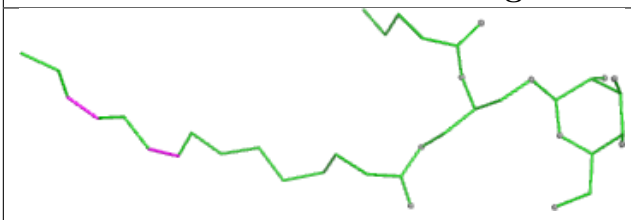
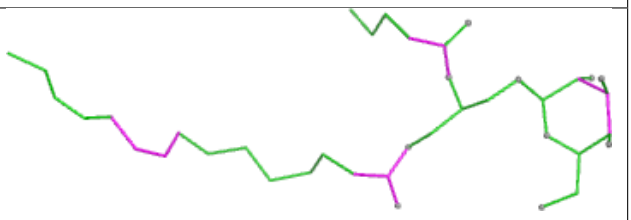
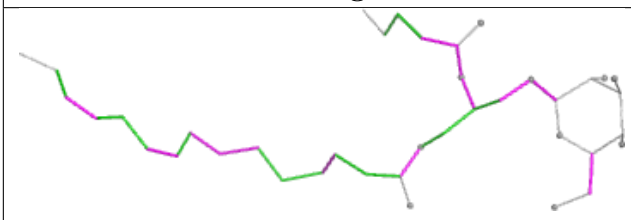
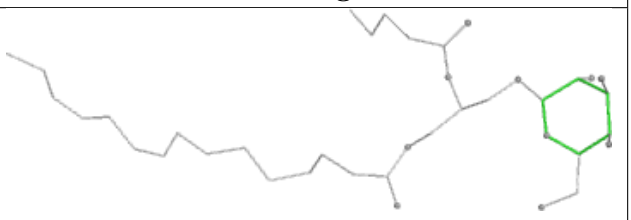
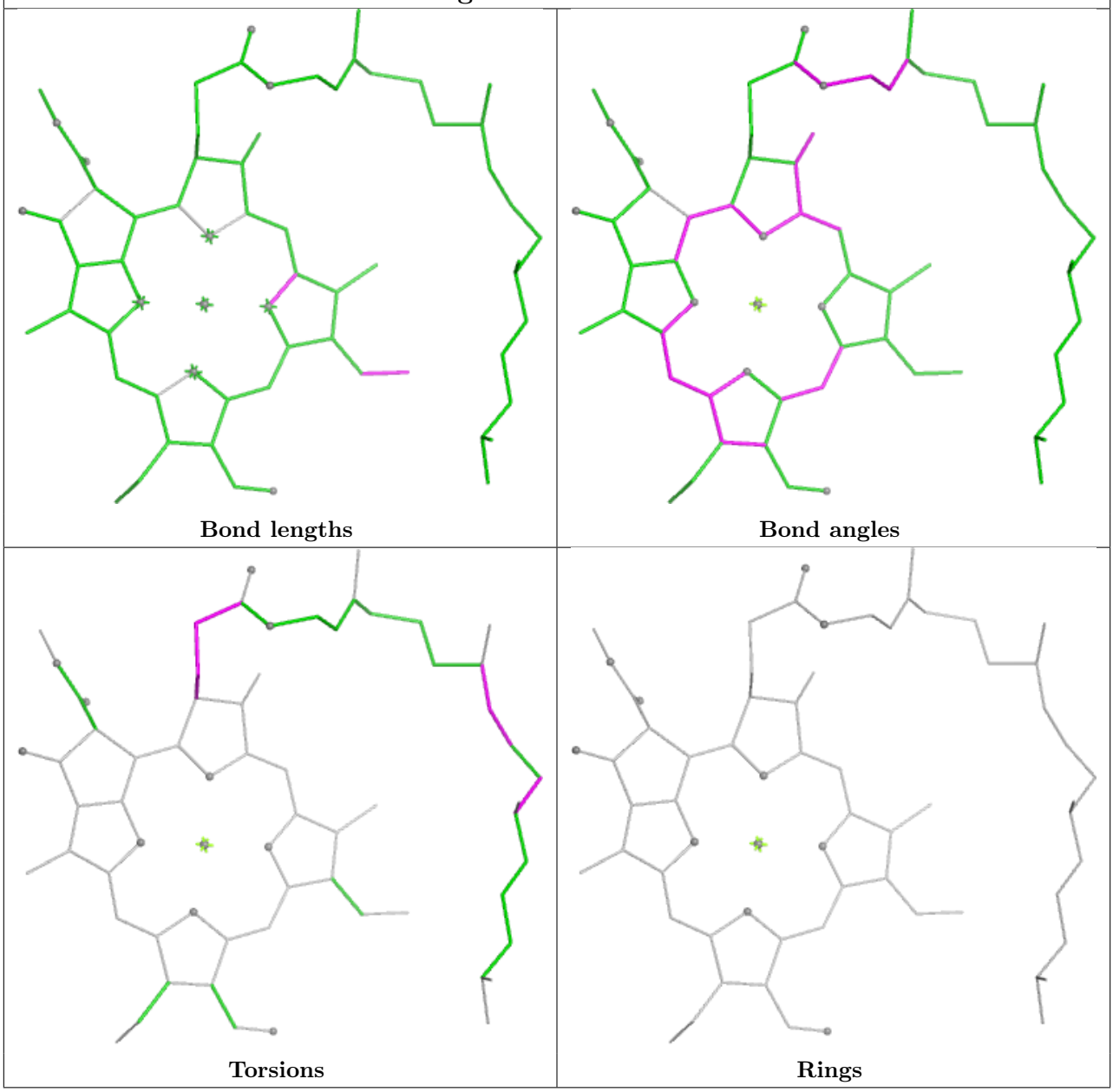
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG W1 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL n 607



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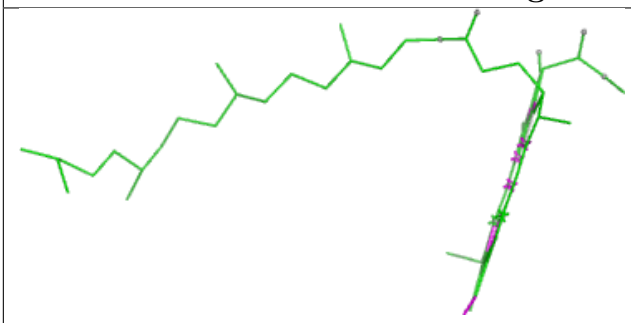
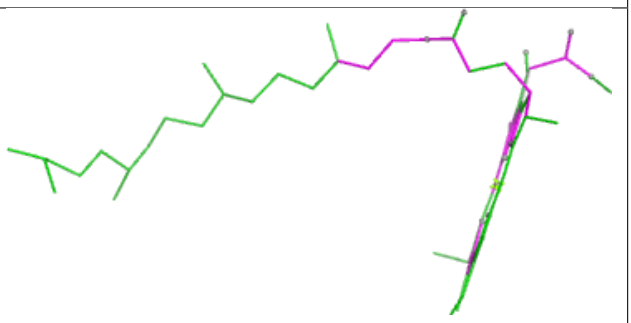
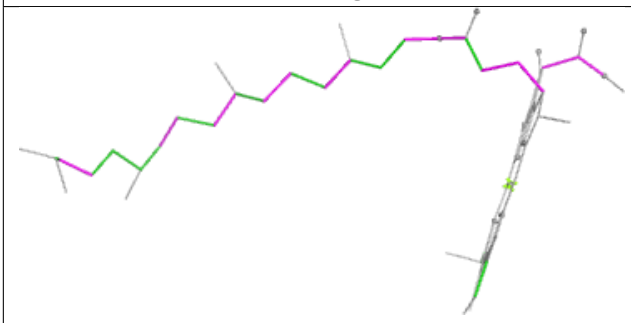
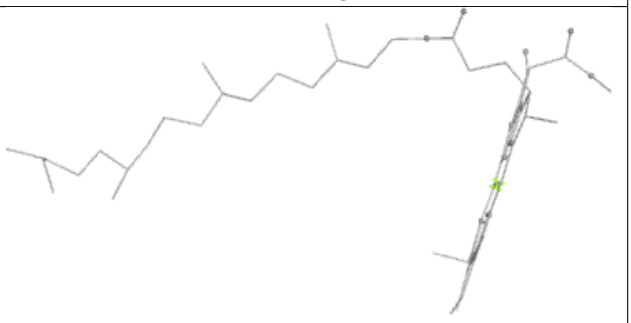
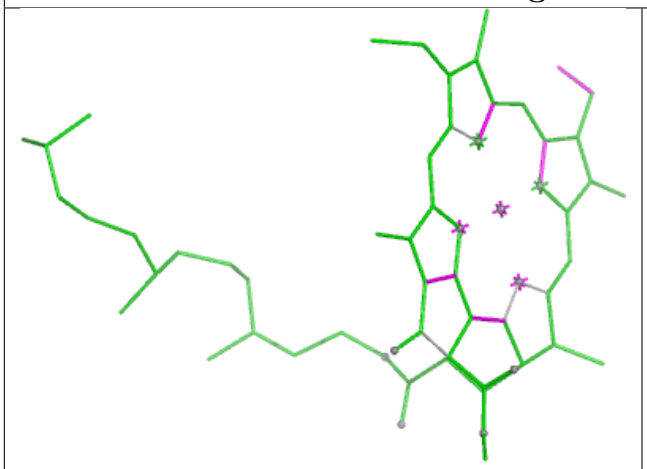
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 609



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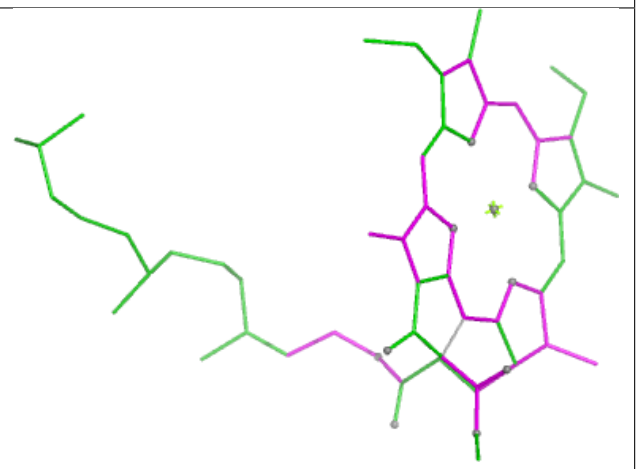
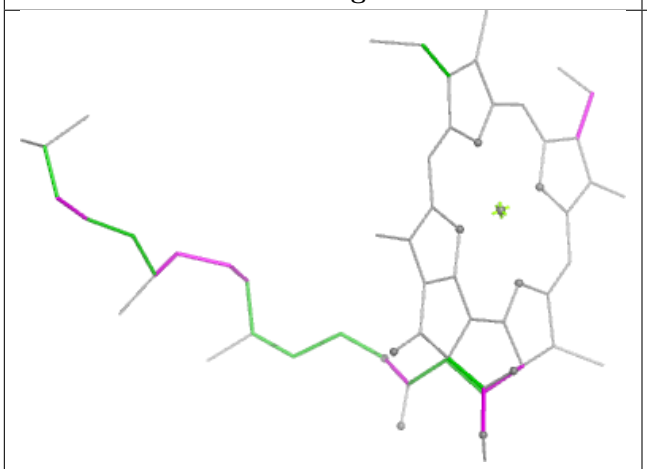


Bond angles



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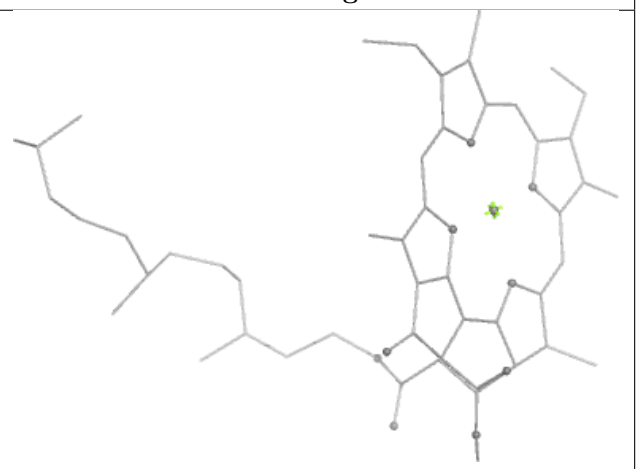
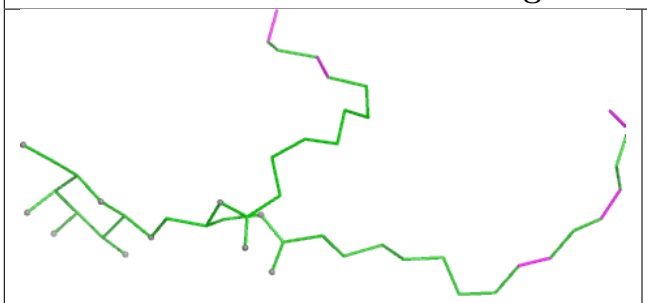


Rings

Ligand LMG h 102



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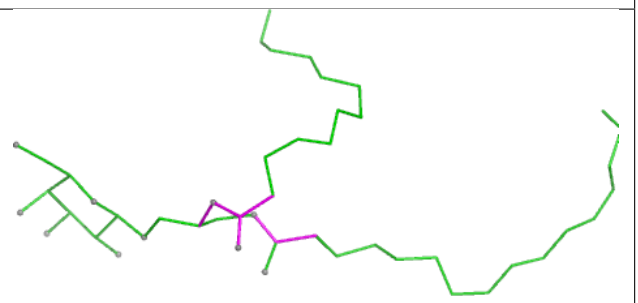
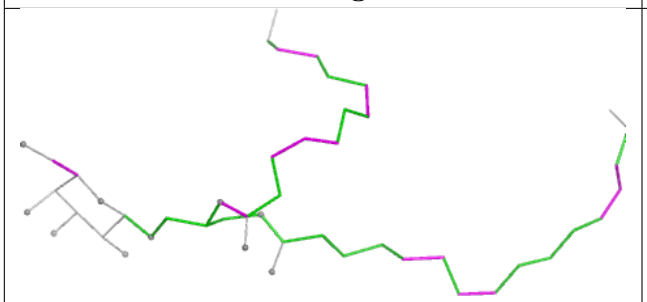


Bond angles



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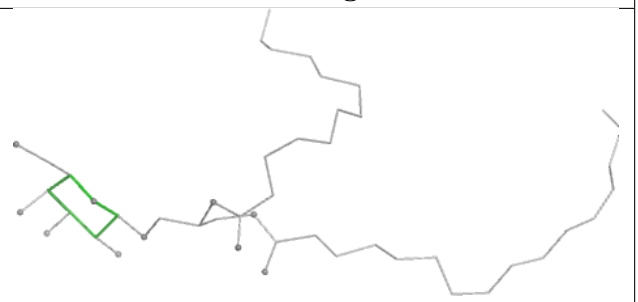
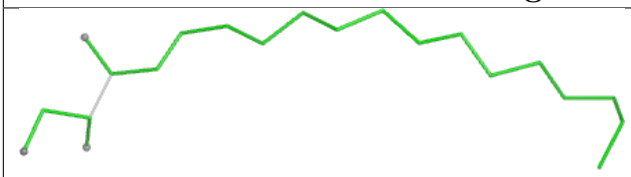
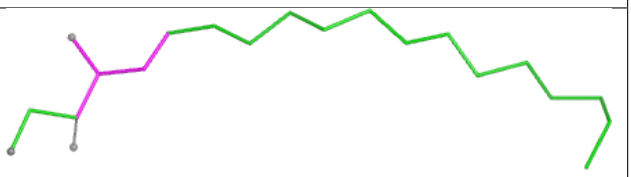
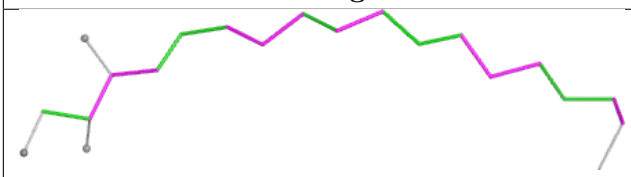
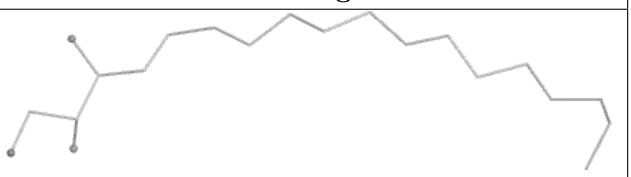


Rings

Ligand SPH A 414	
 Bond lengths	 Bond angles
 Torsions	 Rings

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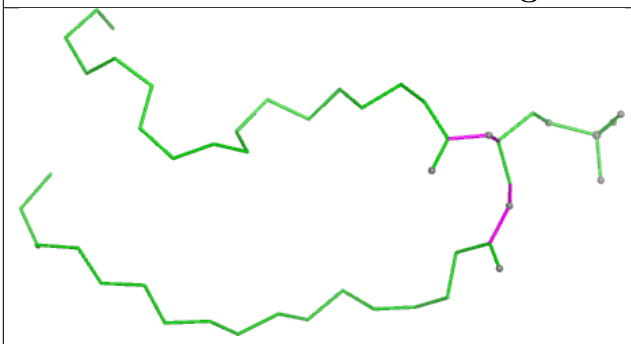
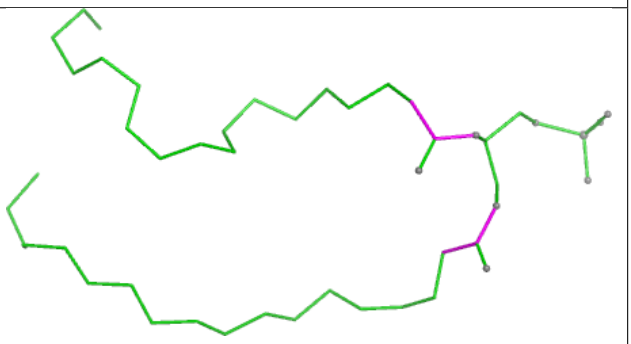
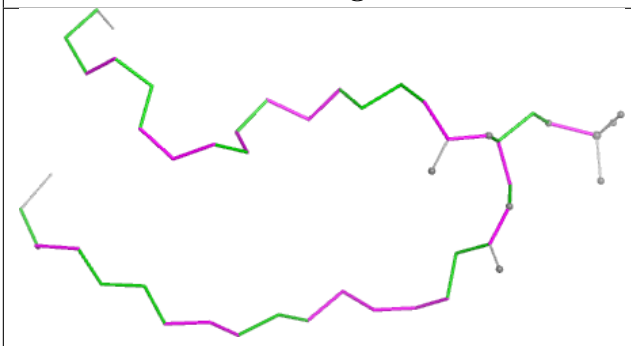
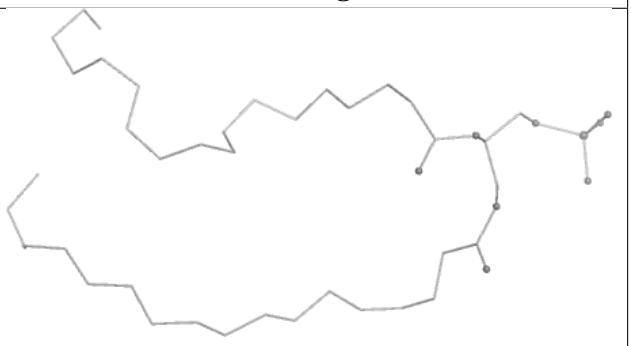
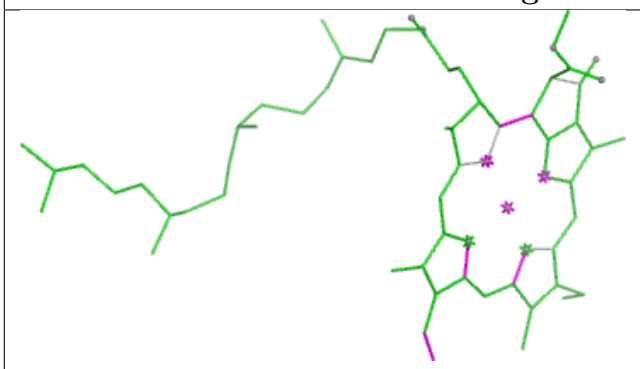
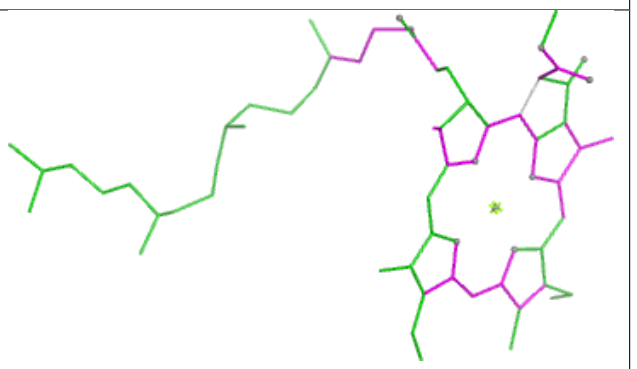
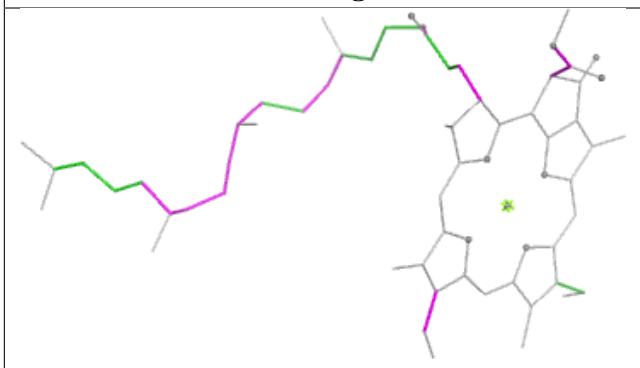
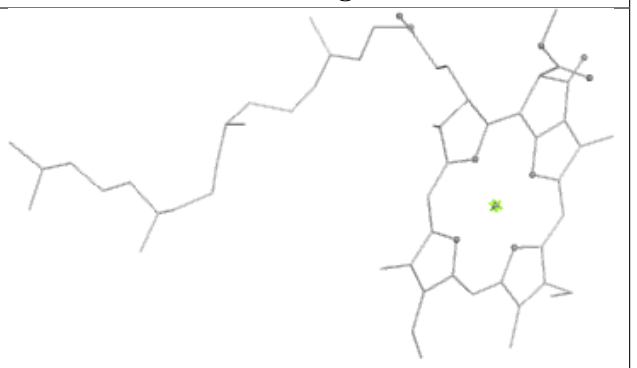
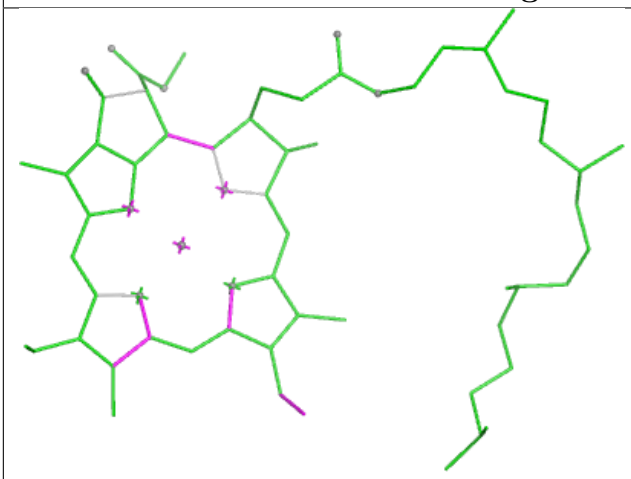
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c1 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s1 603



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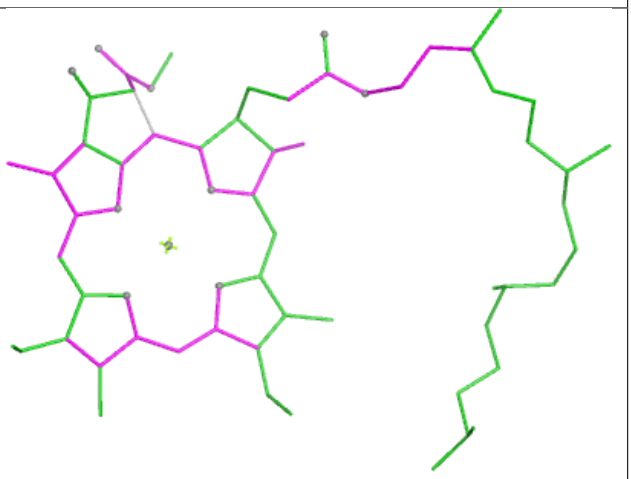

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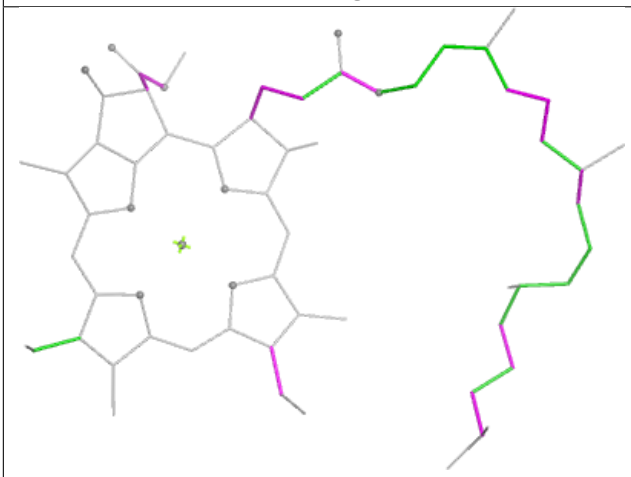

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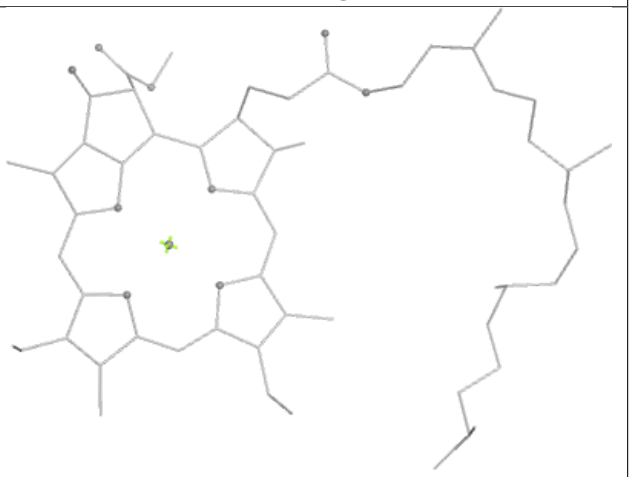
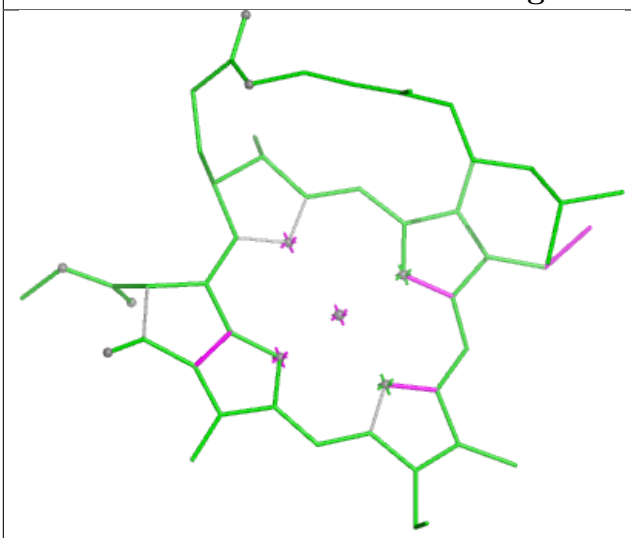


Rings

Ligand CLA S 614



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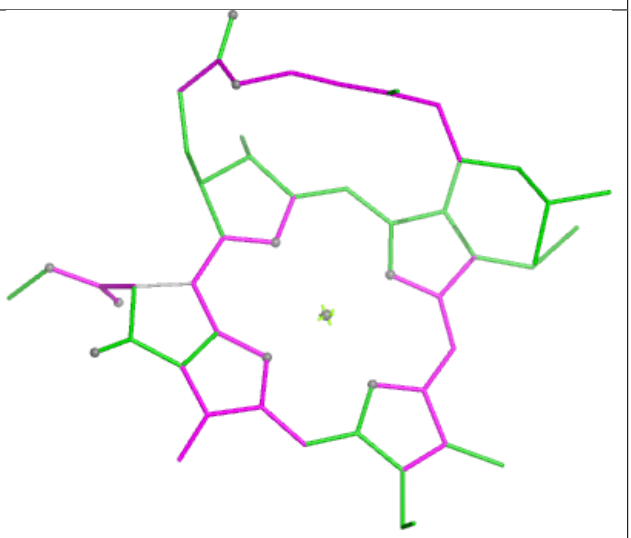

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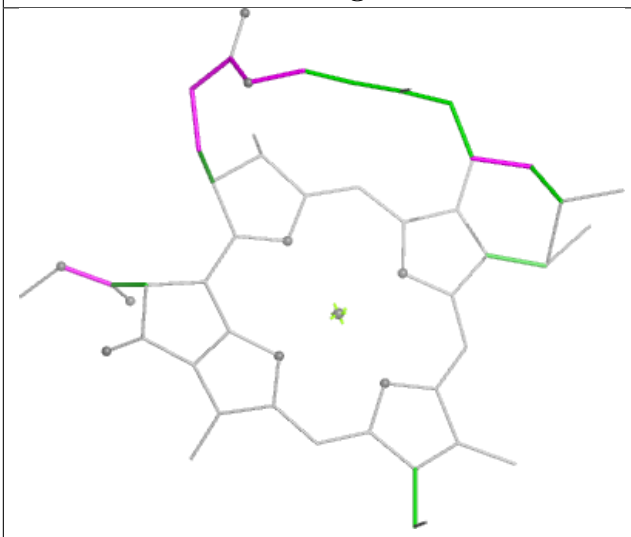

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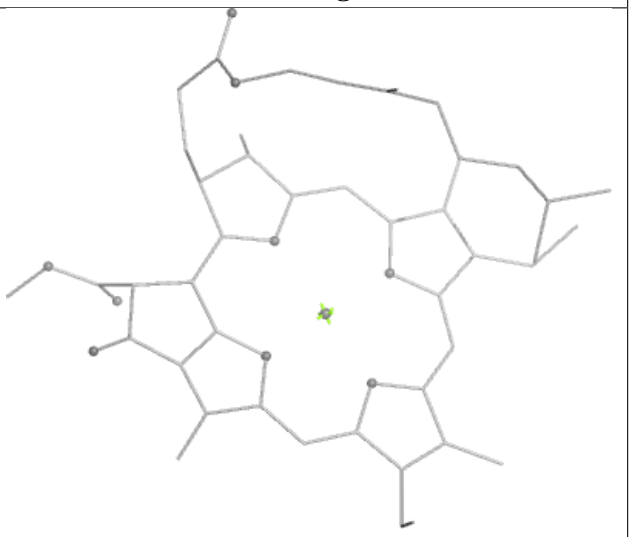
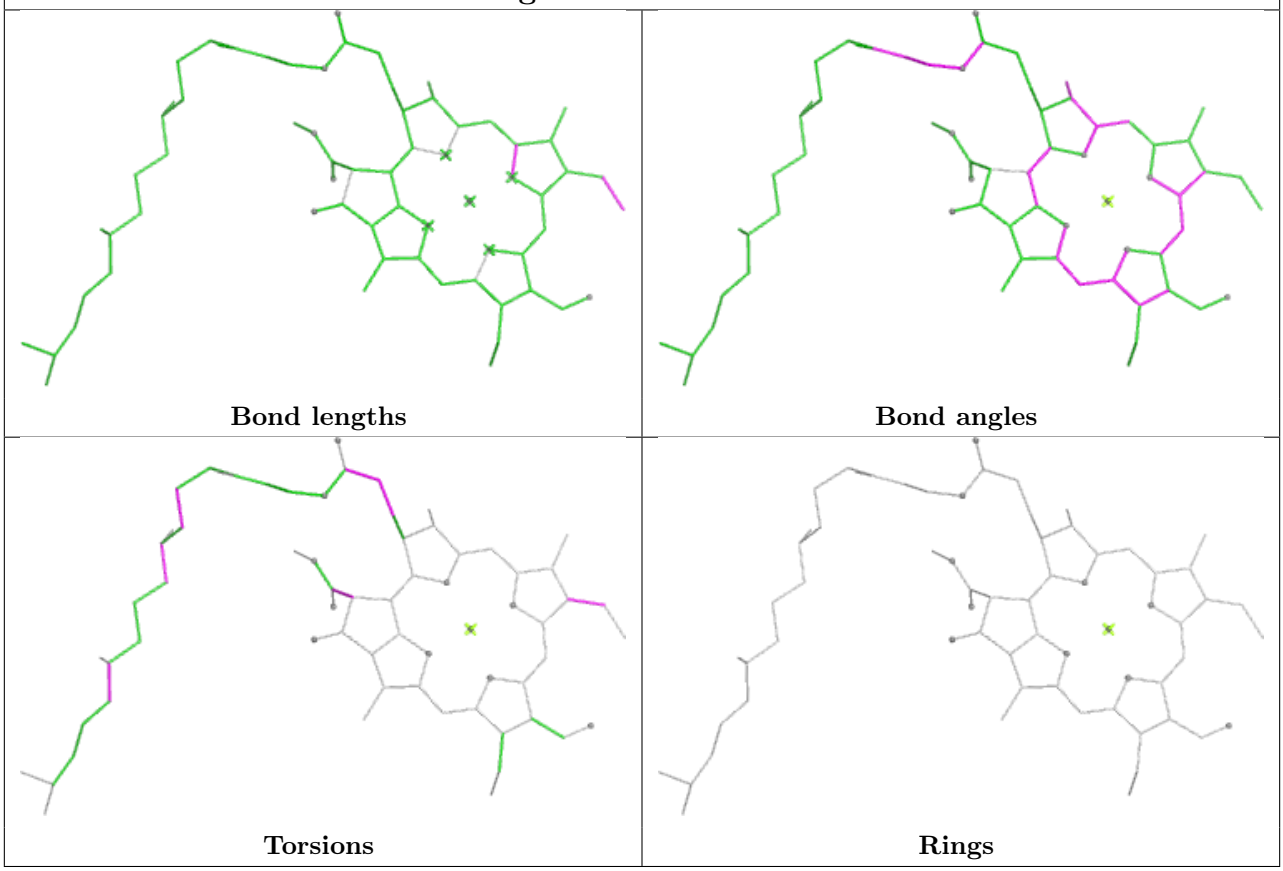
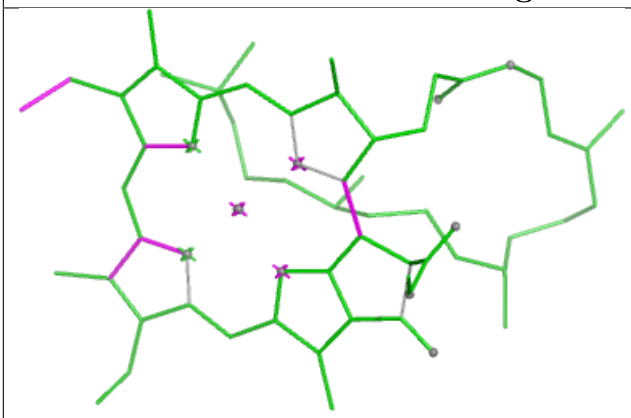
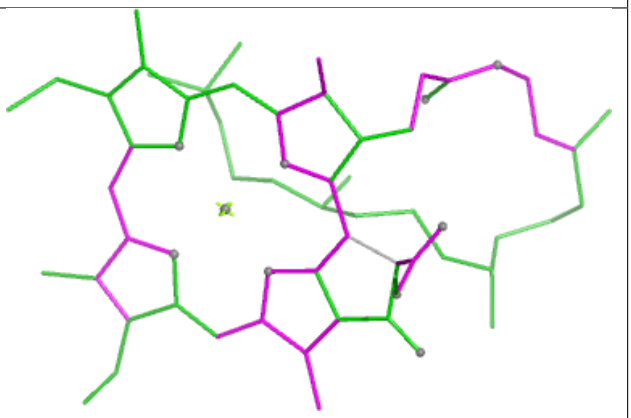
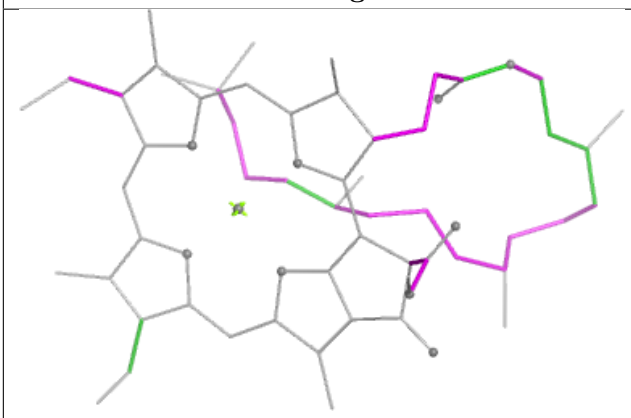
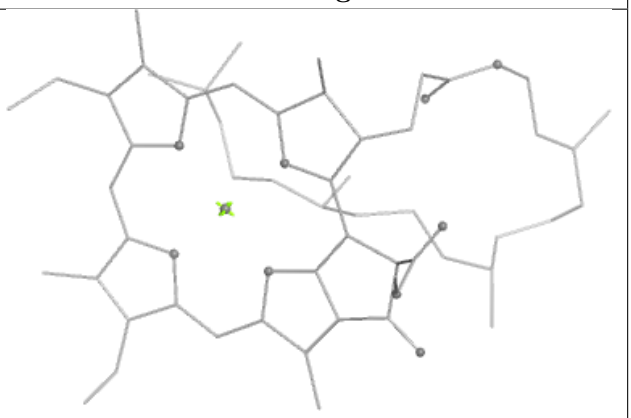


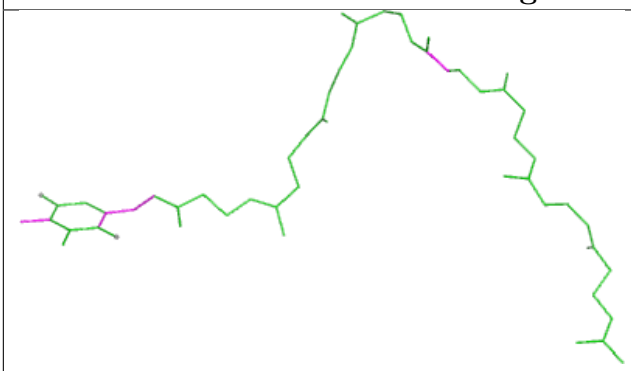
Rings

Ligand CHL n1 606



Ligand CLA B1 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 D1 405



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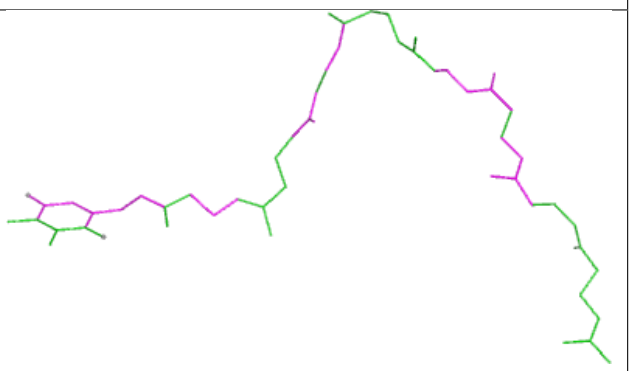

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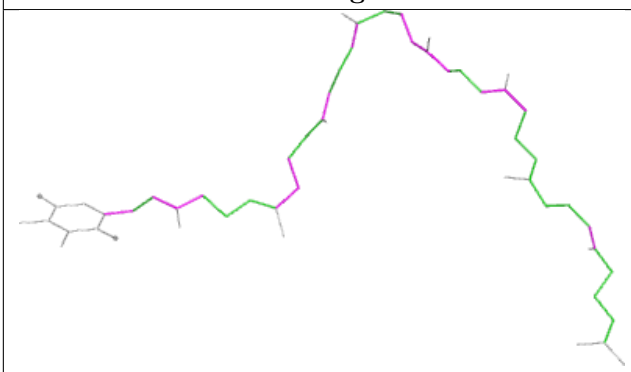

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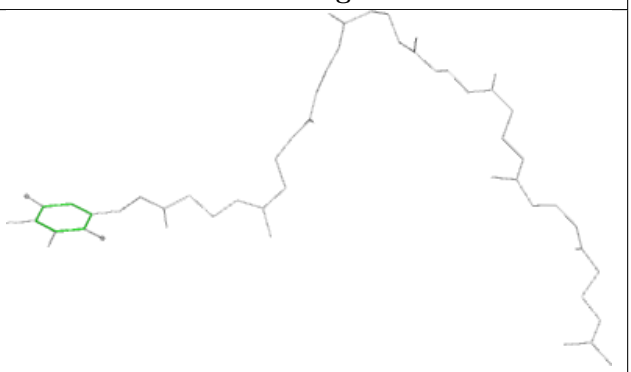
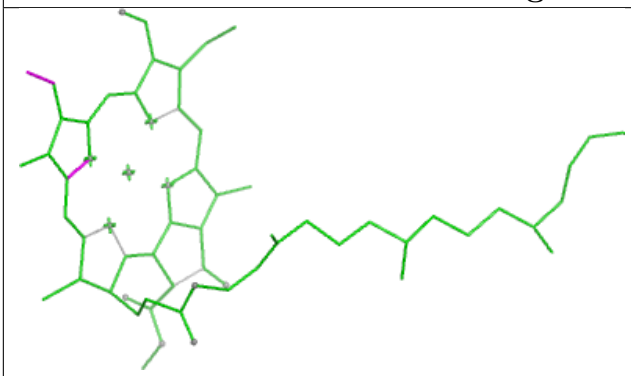


Rings

Ligand CHL n 609



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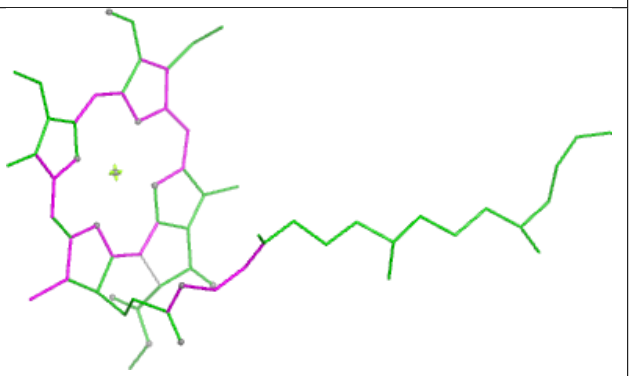
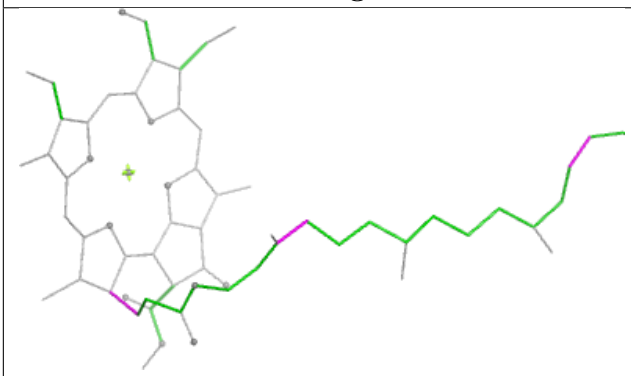


Bond angles



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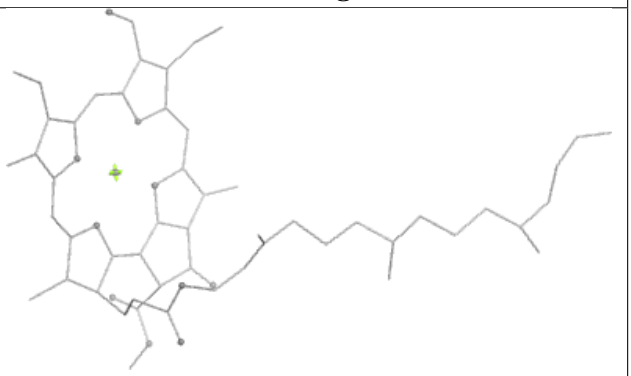
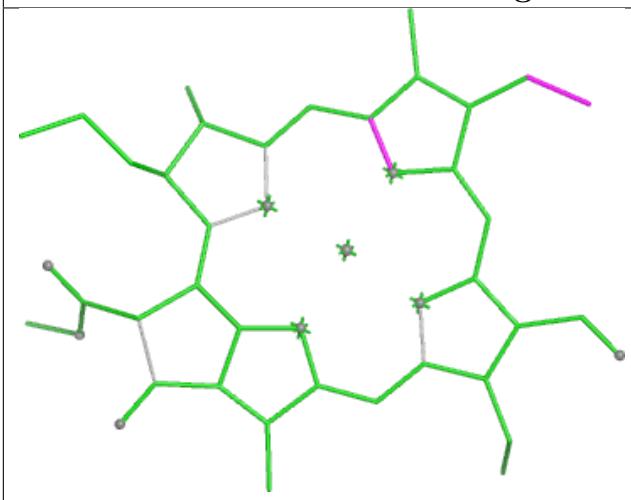
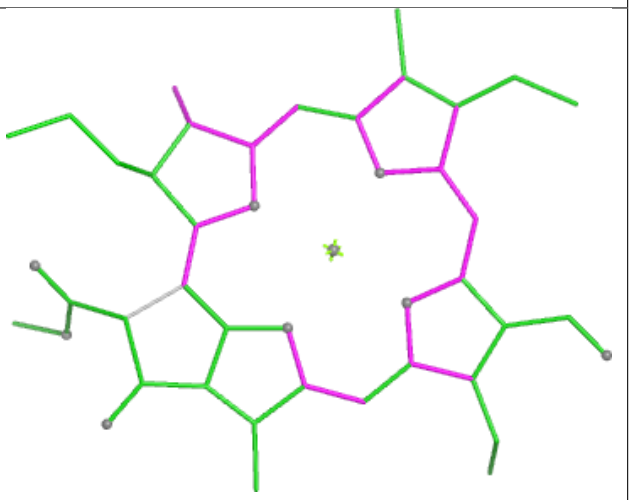
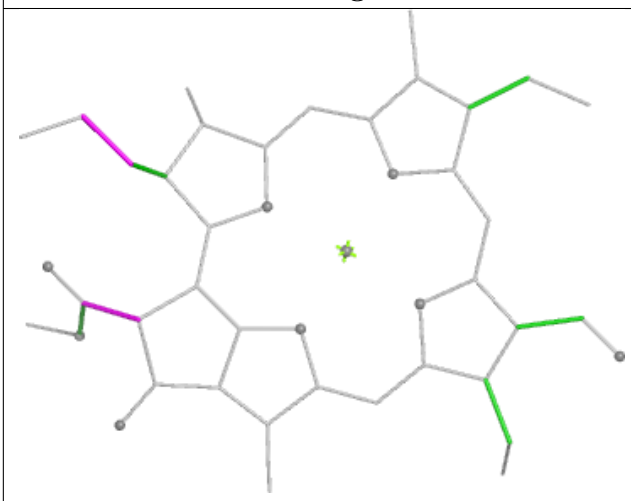
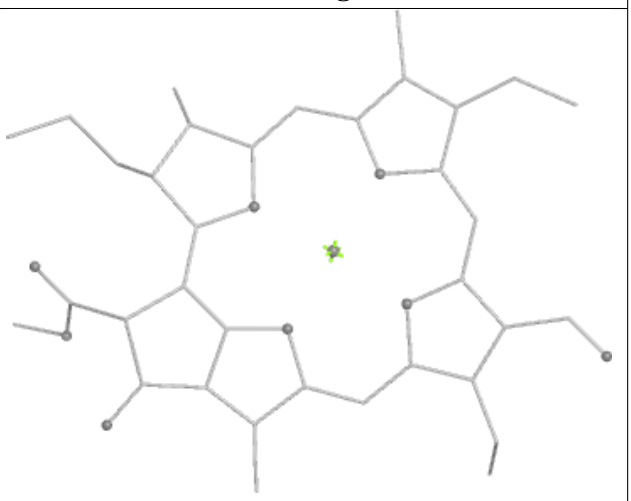


Rings

Ligand CHL R1 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

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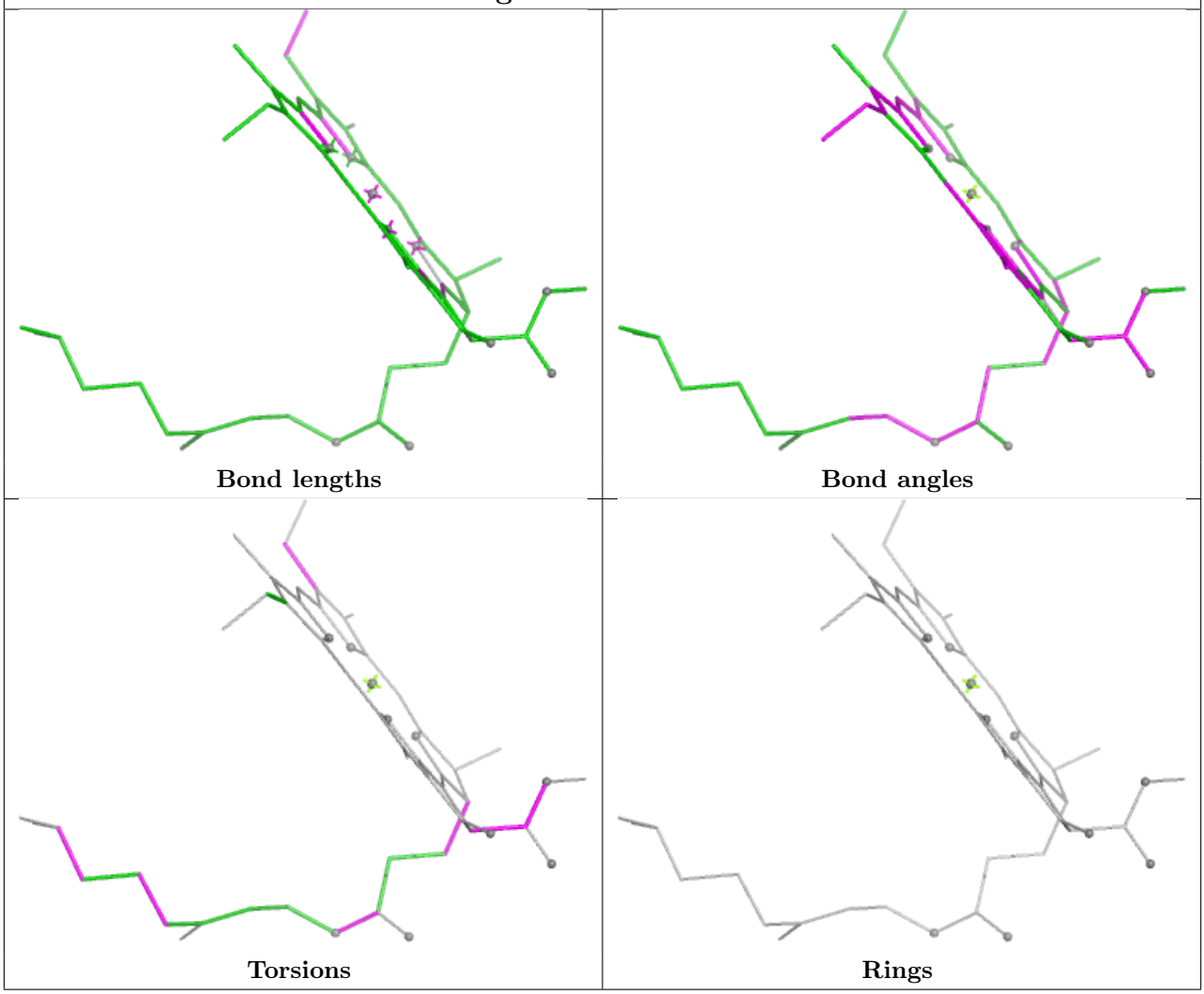
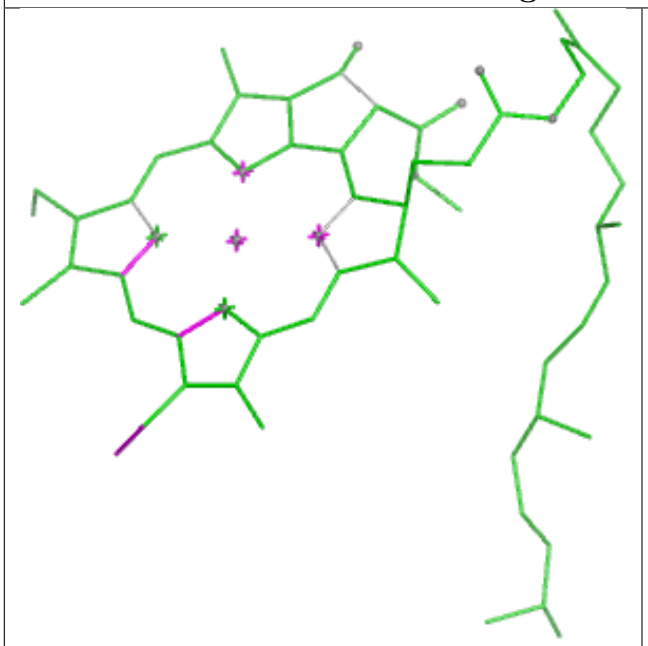


Ligand CLA b1 617



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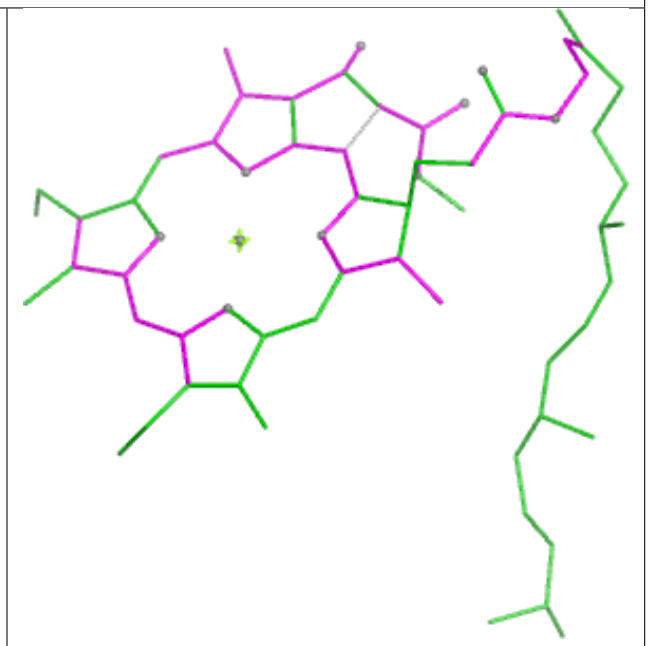
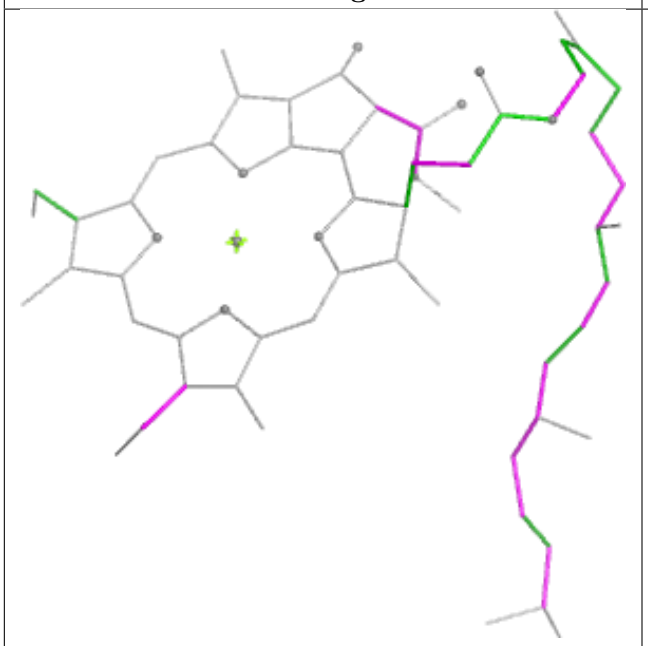
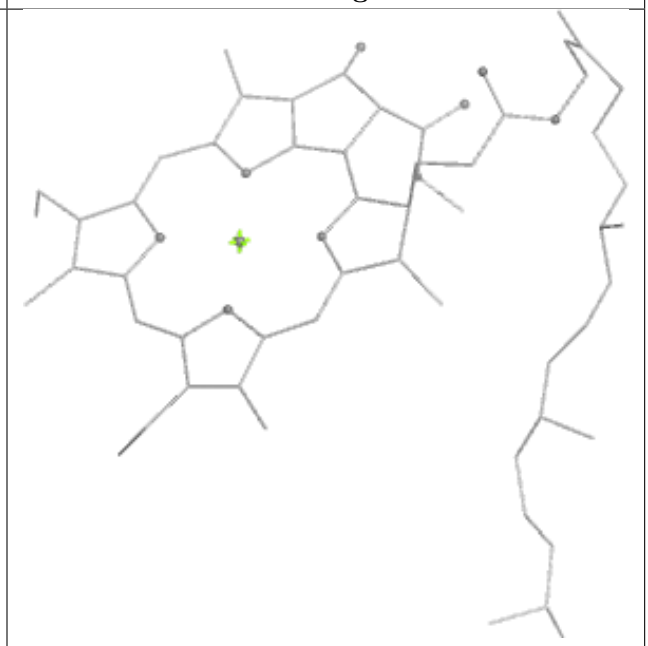


Bond angles

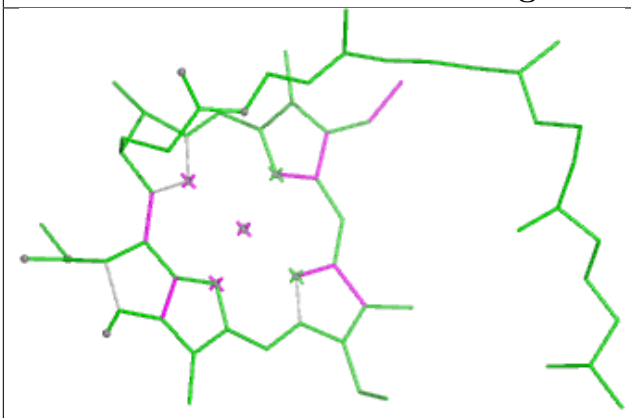


Torsions



Rings

Ligand CLA y1 602



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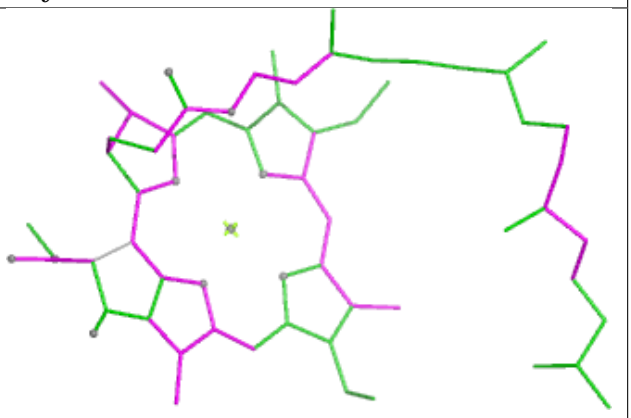
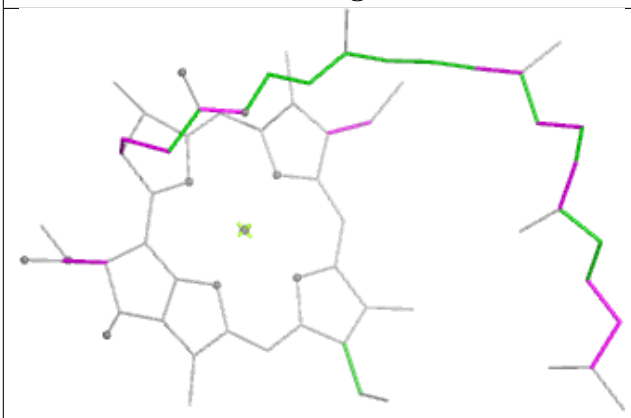


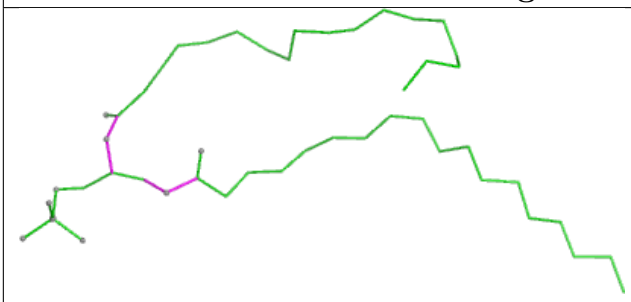
Bond angles



Torsions

Rings

Ligand 3PH T1 101



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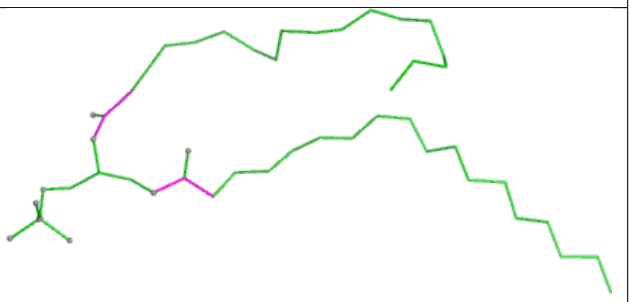

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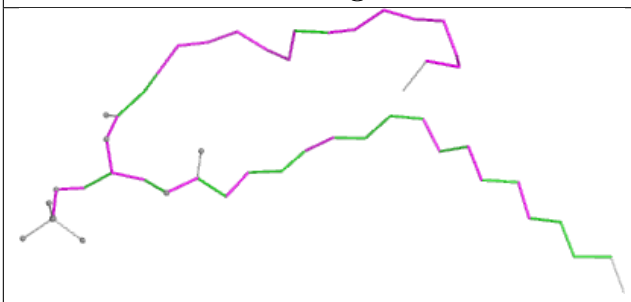

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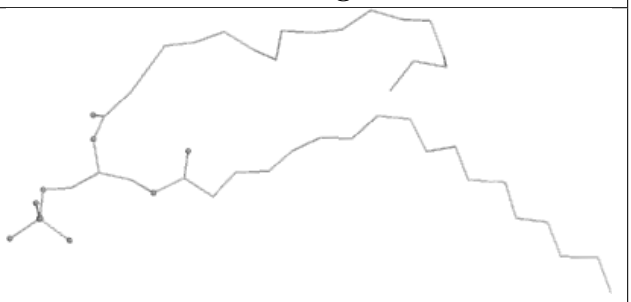
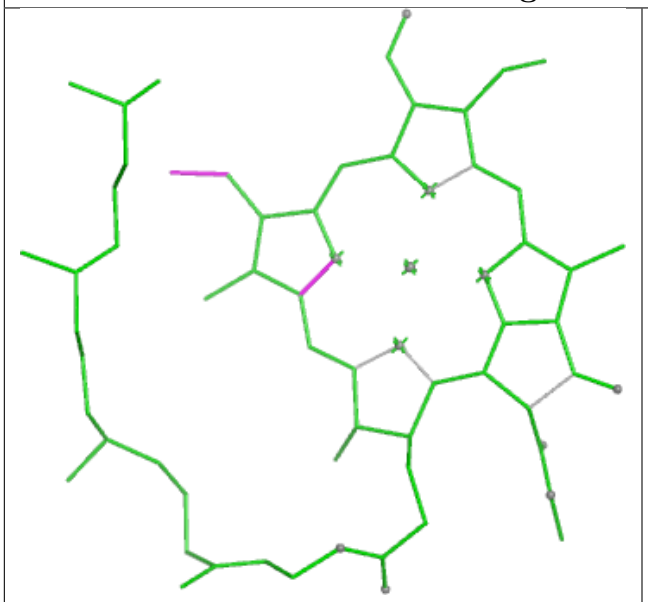


Rings

Ligand CHL g1 607



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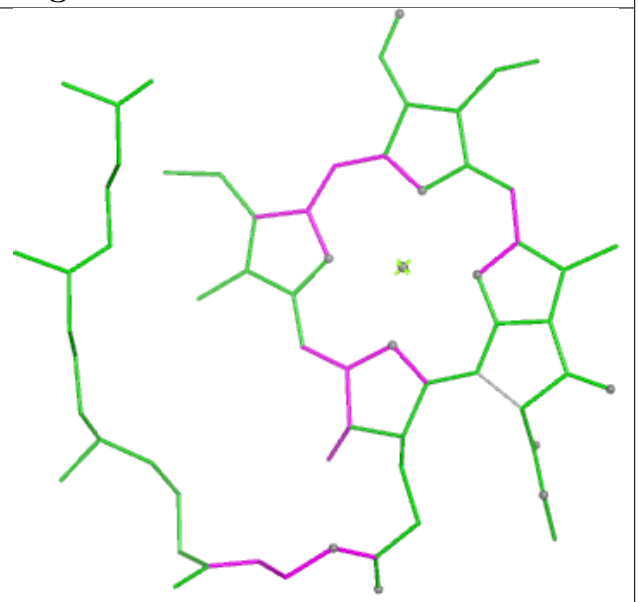

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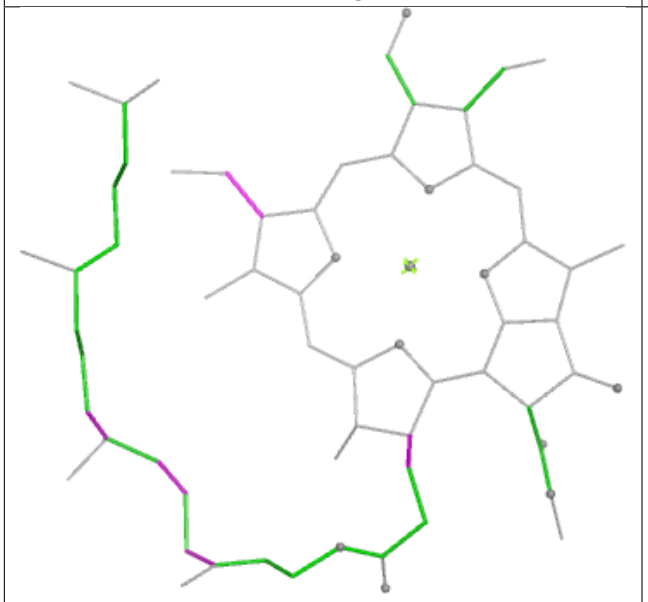

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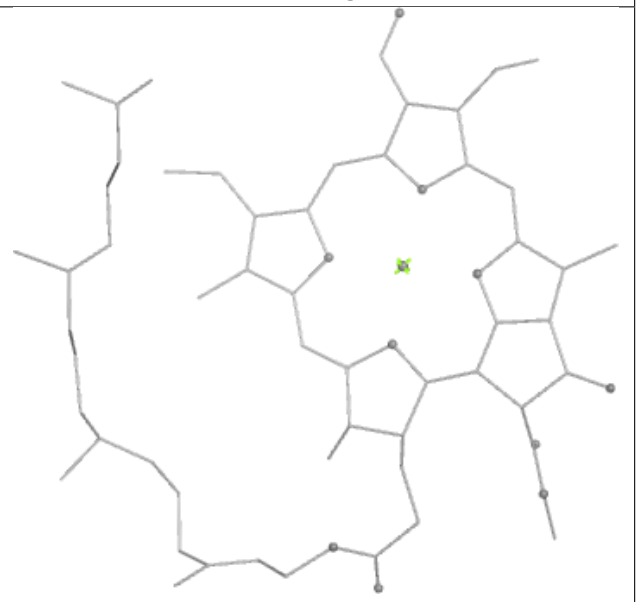
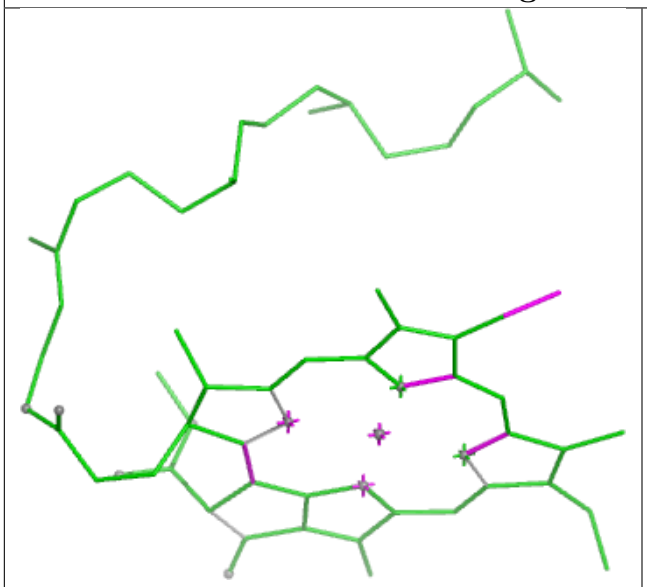


Rings

Ligand CLA n1 603



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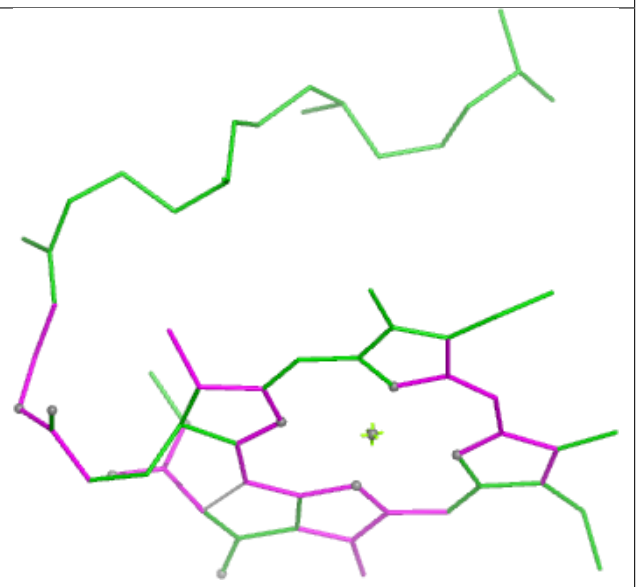

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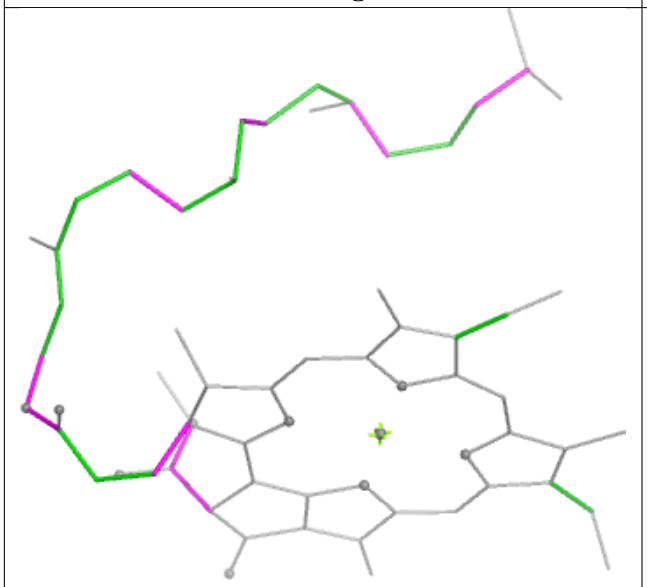

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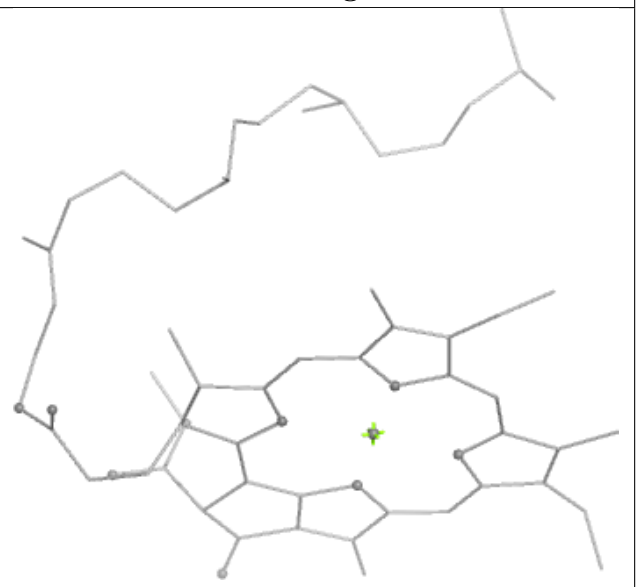
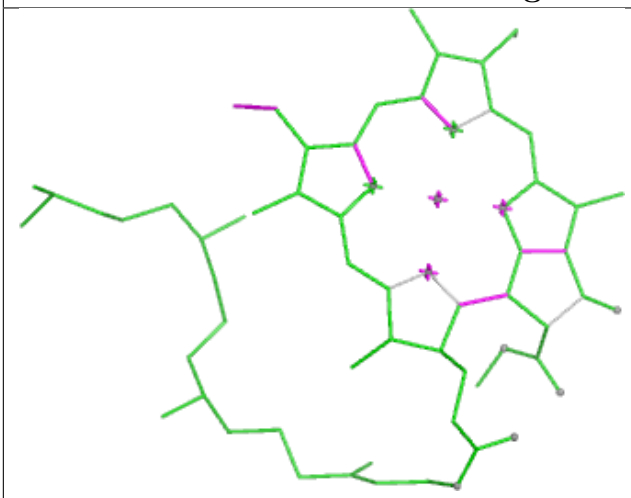


Rings

Ligand CLA Y 612



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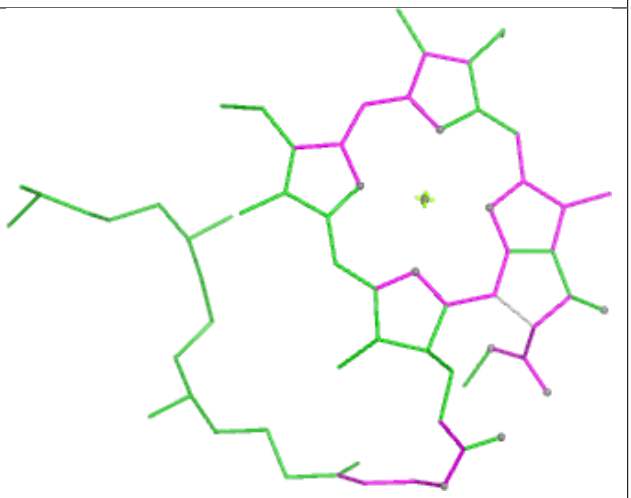
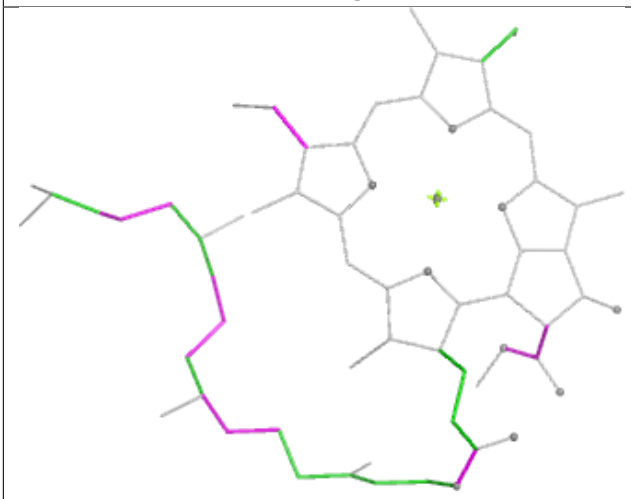


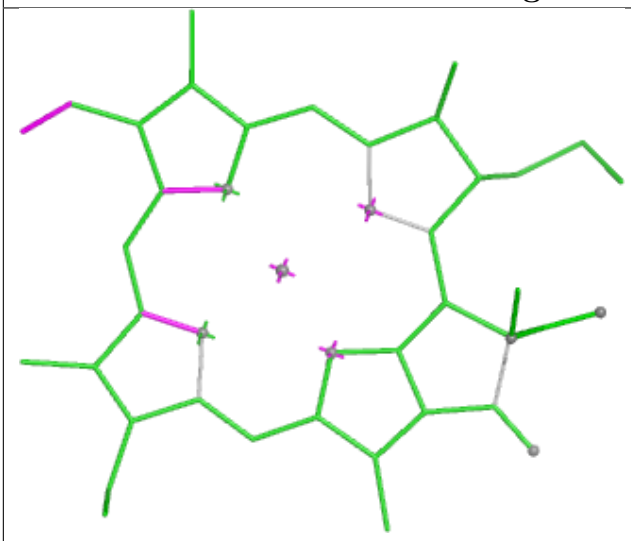
Bond angles



Torsions

Rings

Ligand CLA G 612



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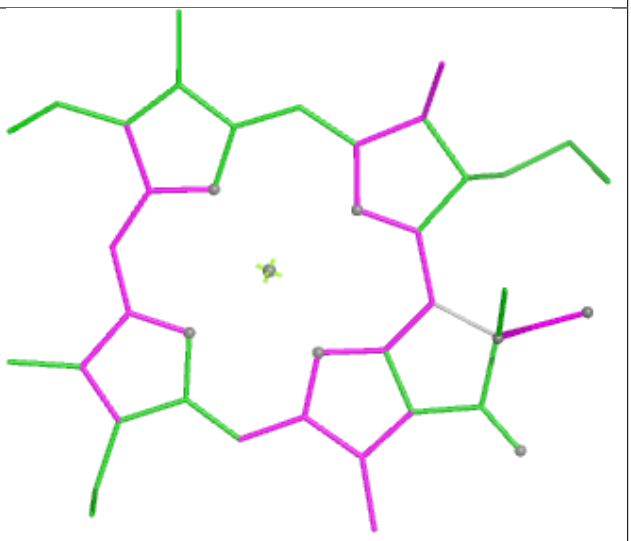
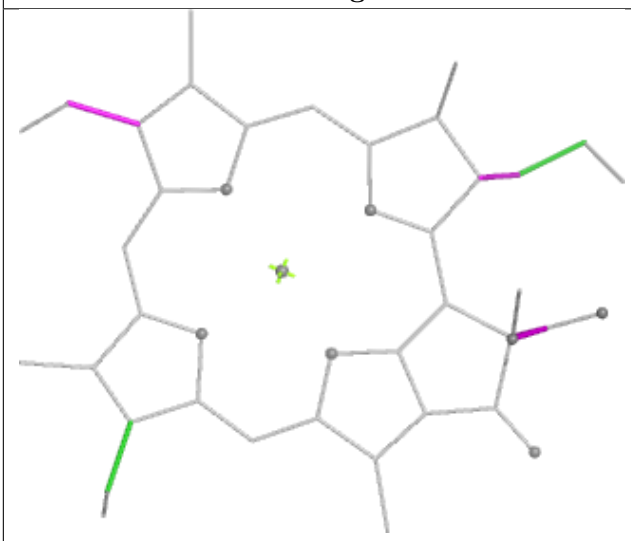
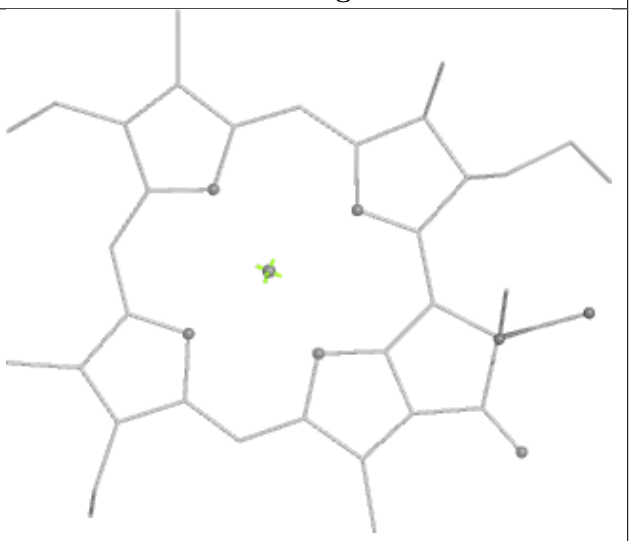


Bond angles

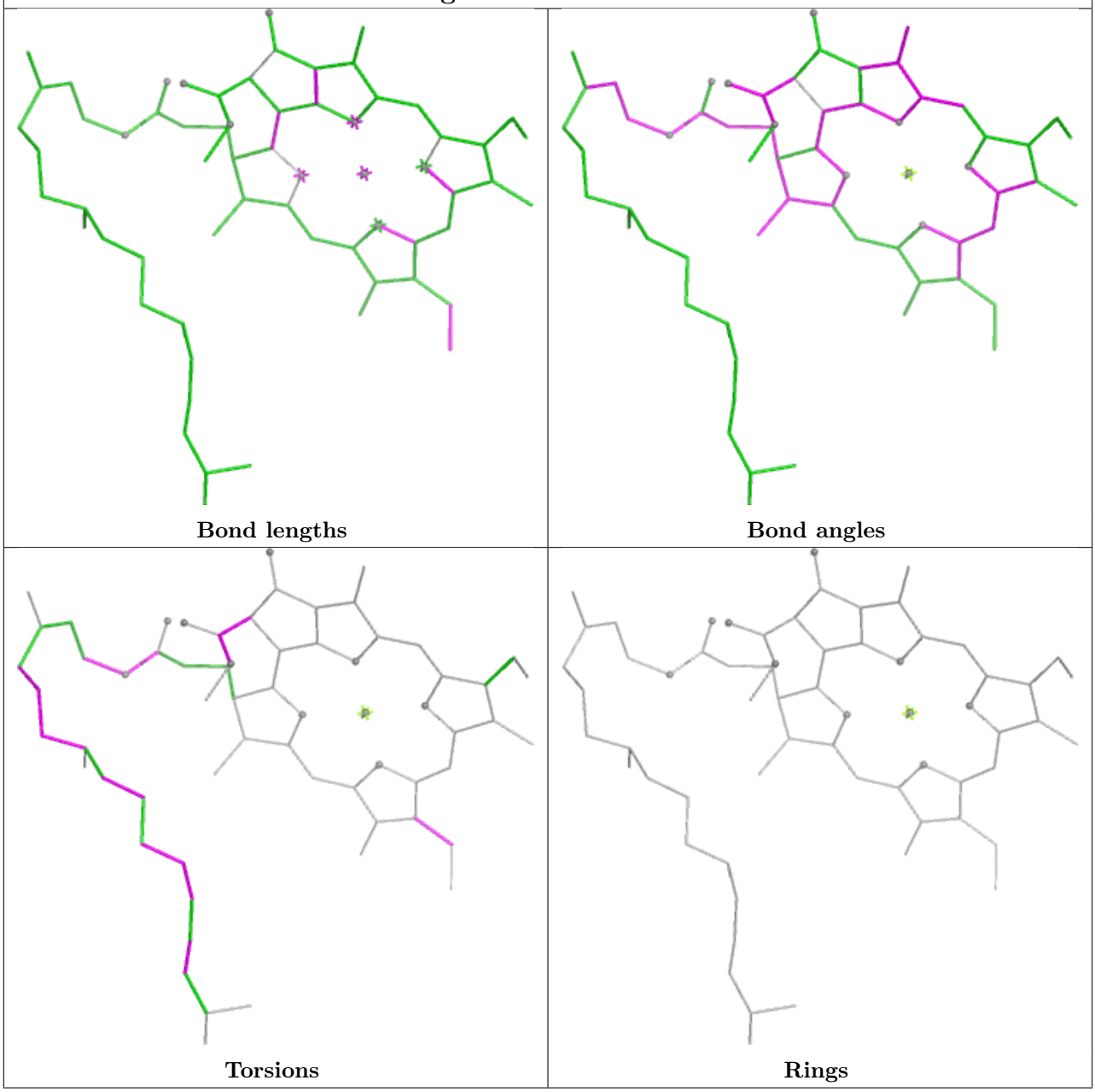


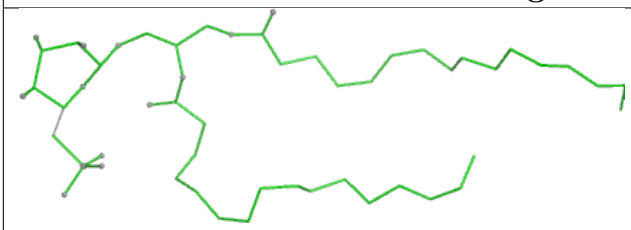
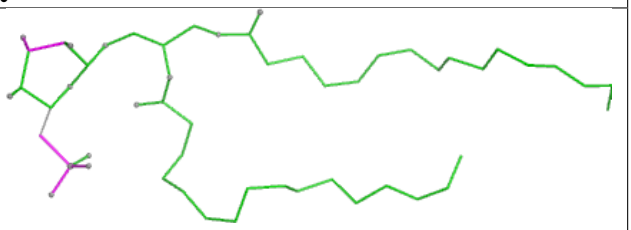
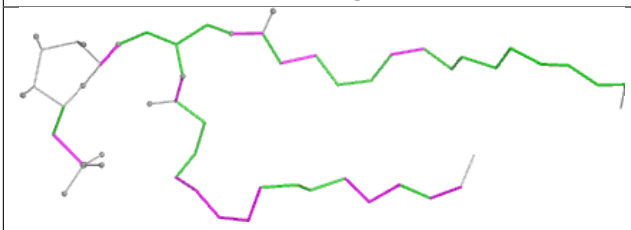
Torsions



Rings

Ligand CLA B1 617



Ligand SQD b 626	
 Bond lengths	 Bond angles
 Torsions	Rings

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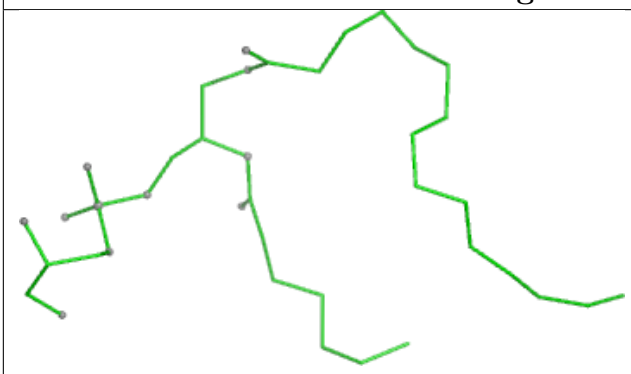
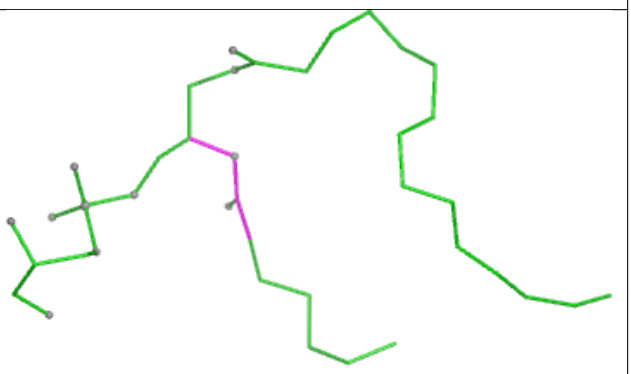
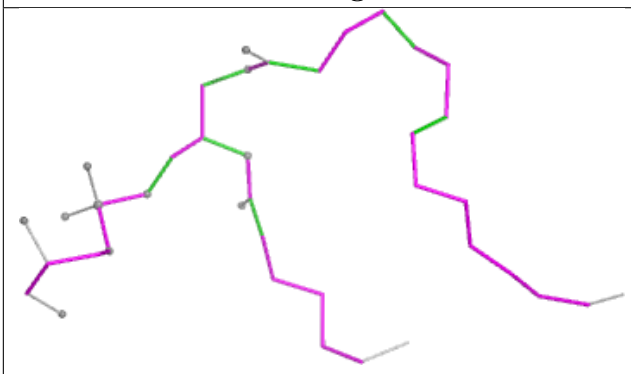
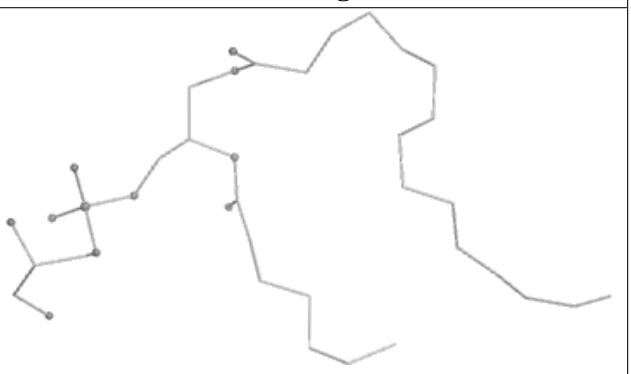
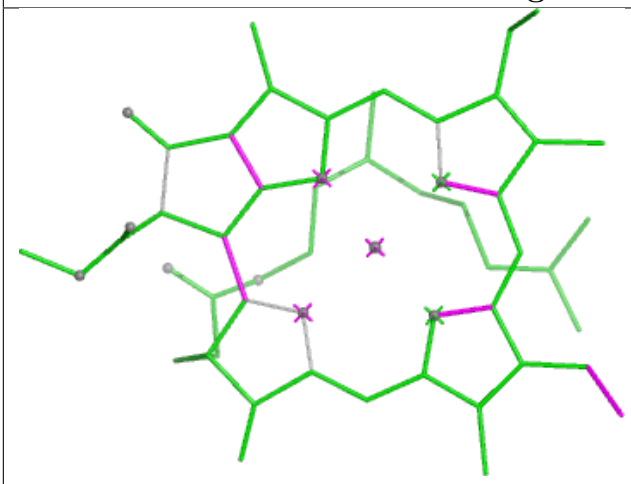
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 613



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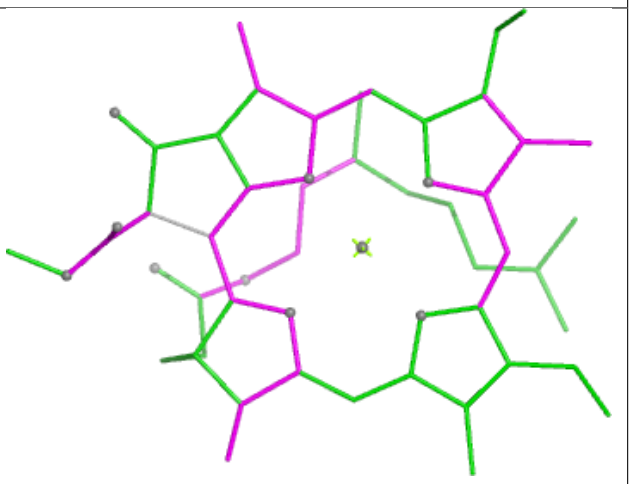

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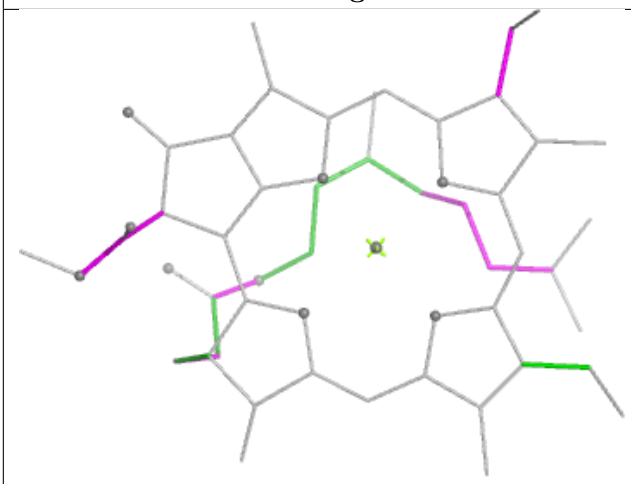

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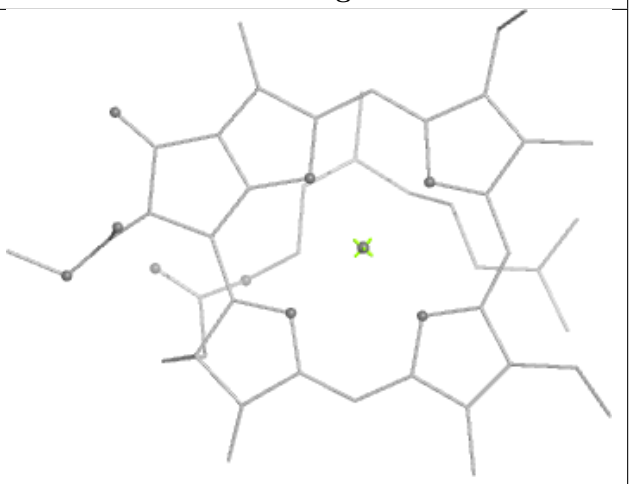
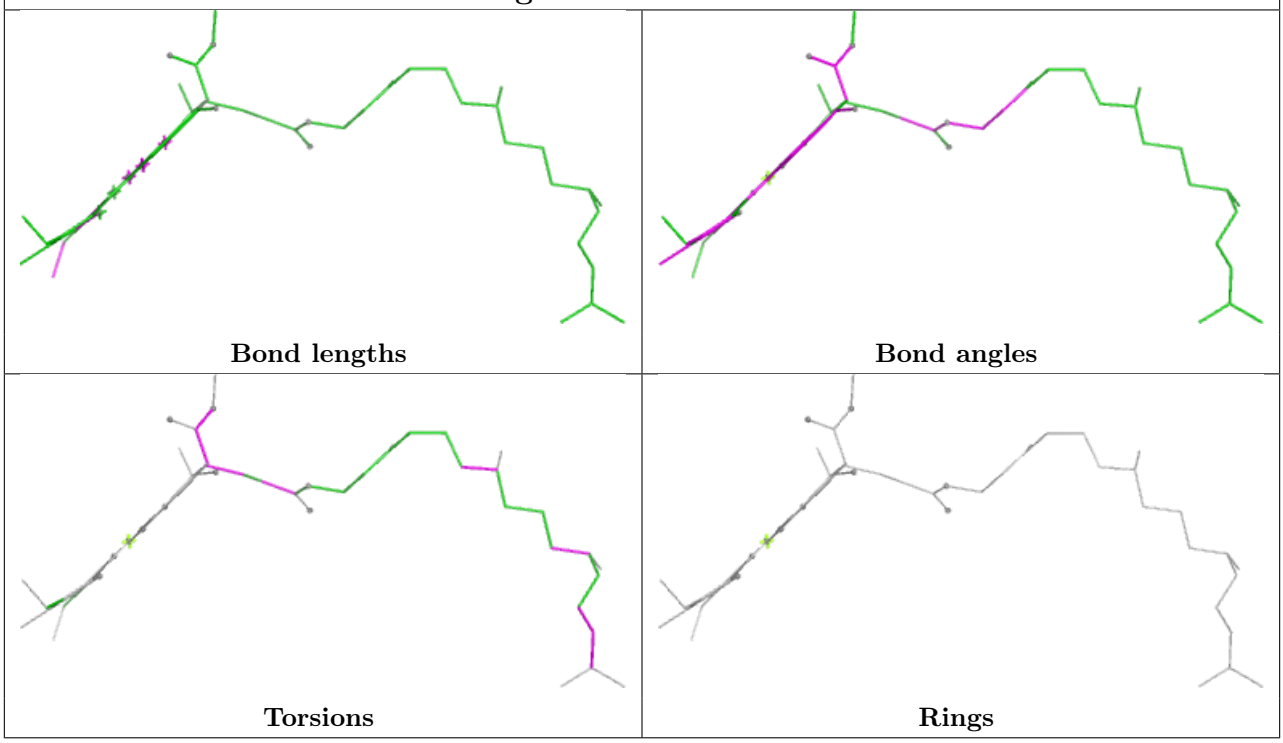


Rings

Ligand CLA D1 402



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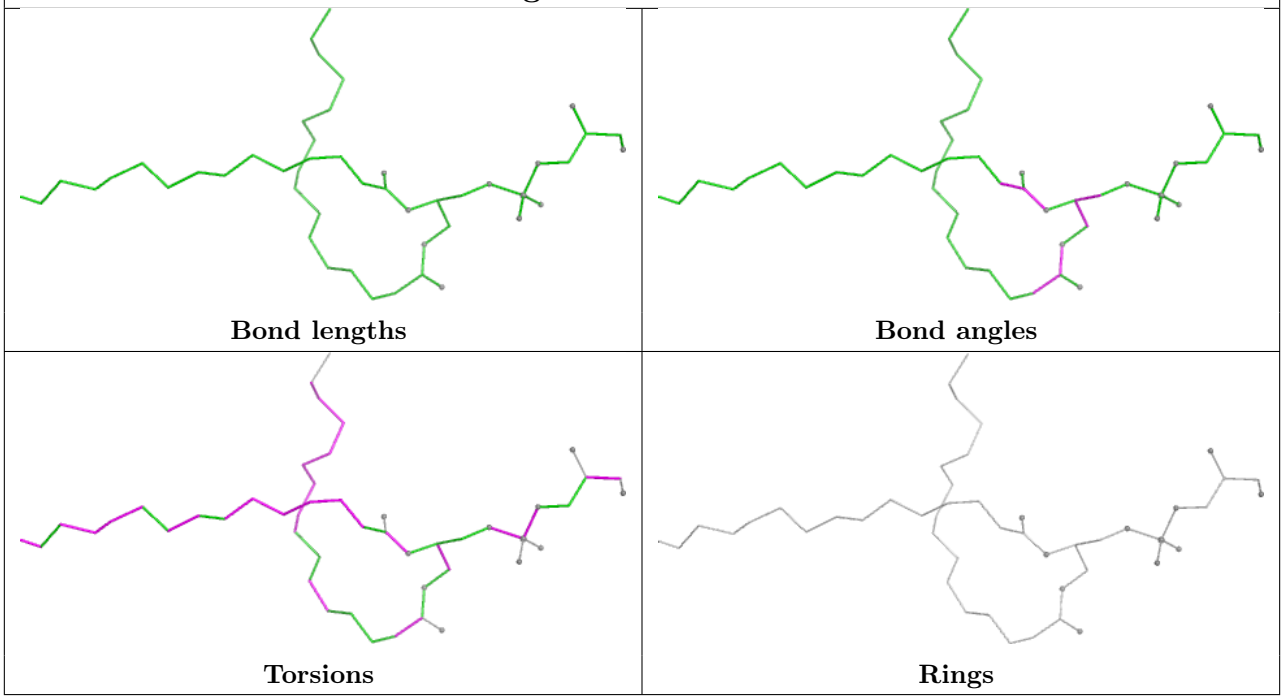
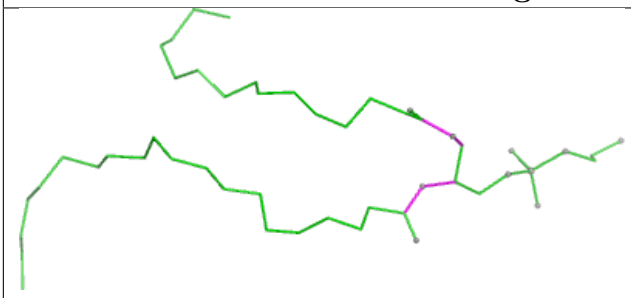


Ligand PTY Y1 626



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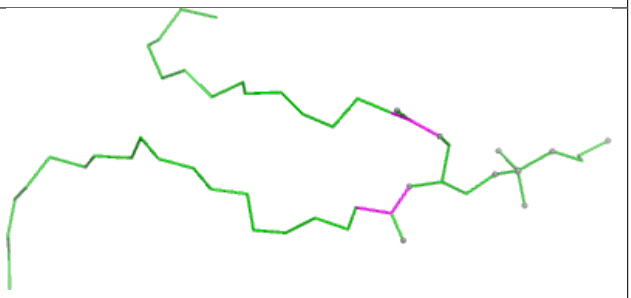

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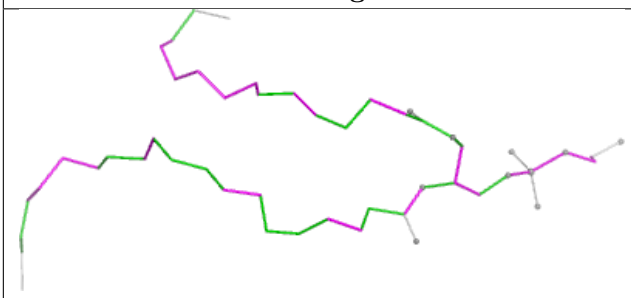

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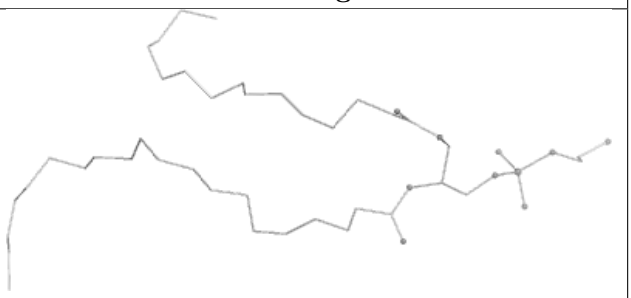
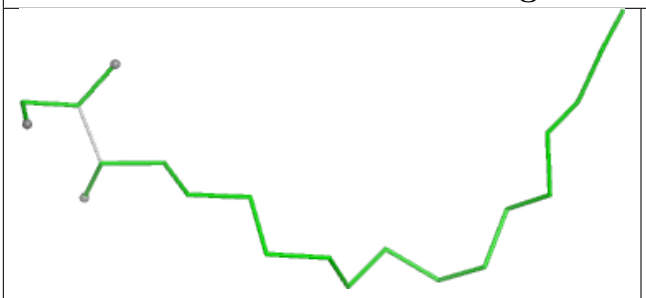


Rings

Ligand SPH y1 625



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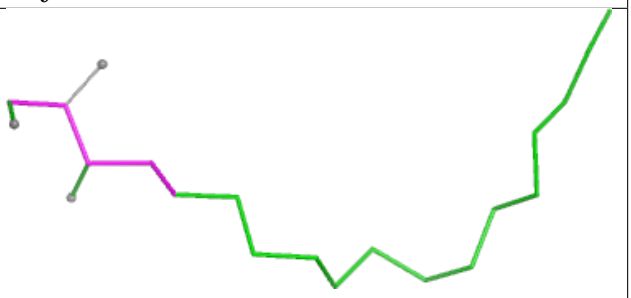

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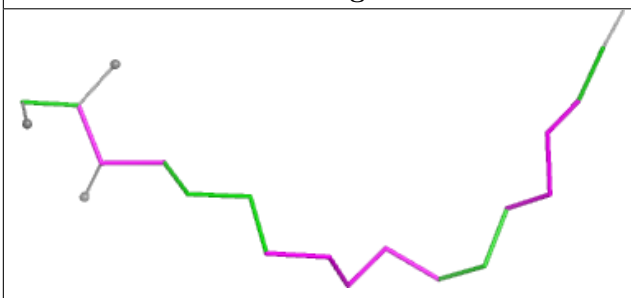

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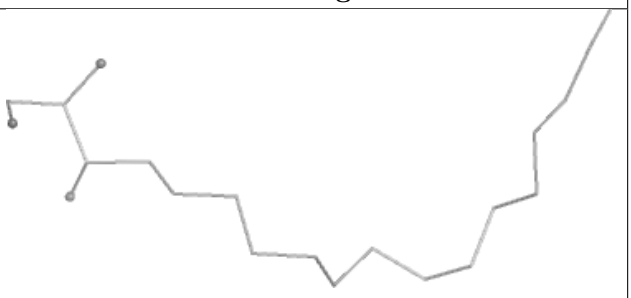
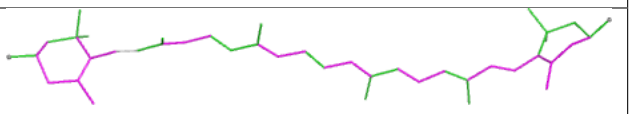


Rings

Ligand LUT N 621

Bond lengths



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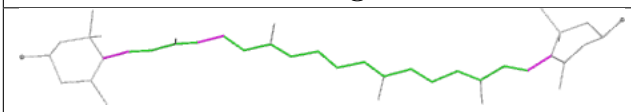

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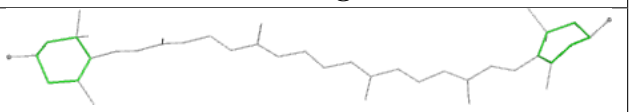
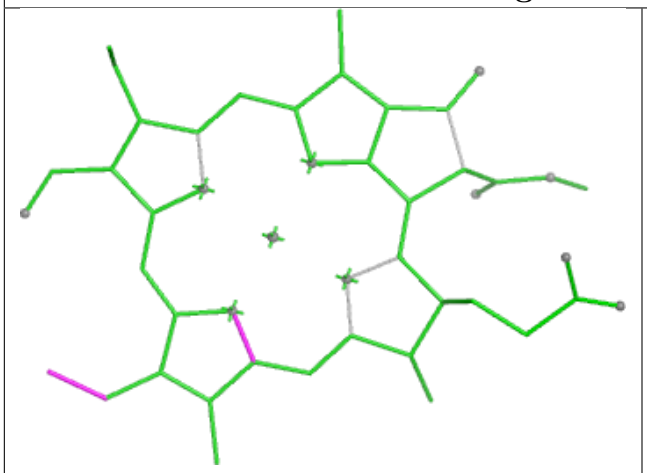


Rings

Ligand CHL Y1 605



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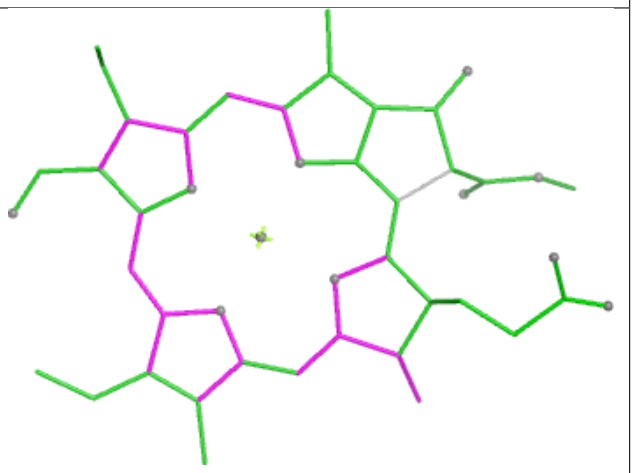

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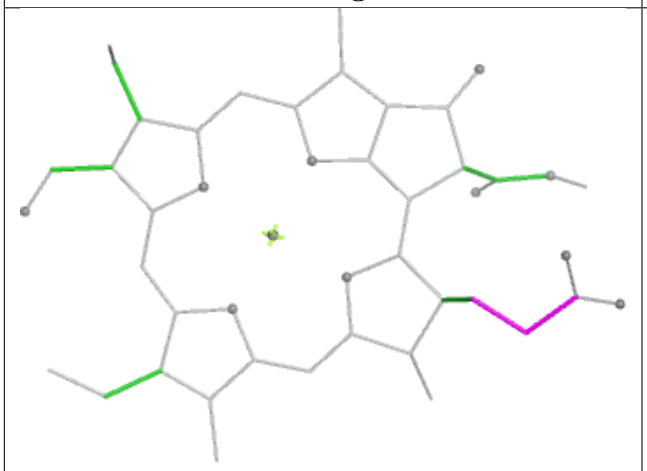

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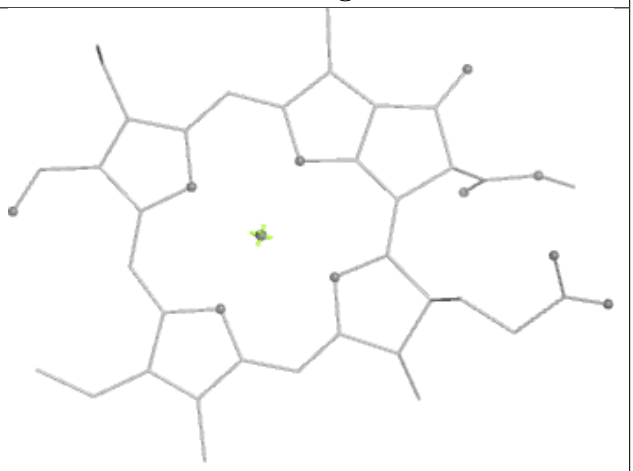
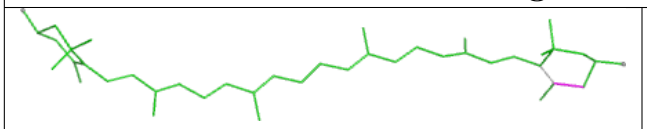
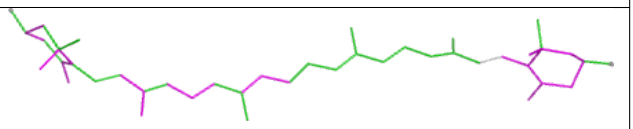


Rings

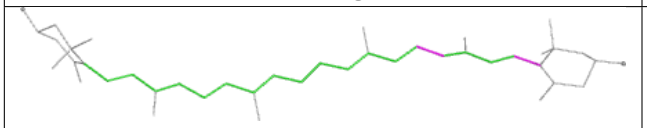
Ligand LUT n 621



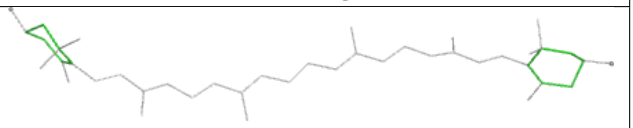
Bond lengths



Bond angles

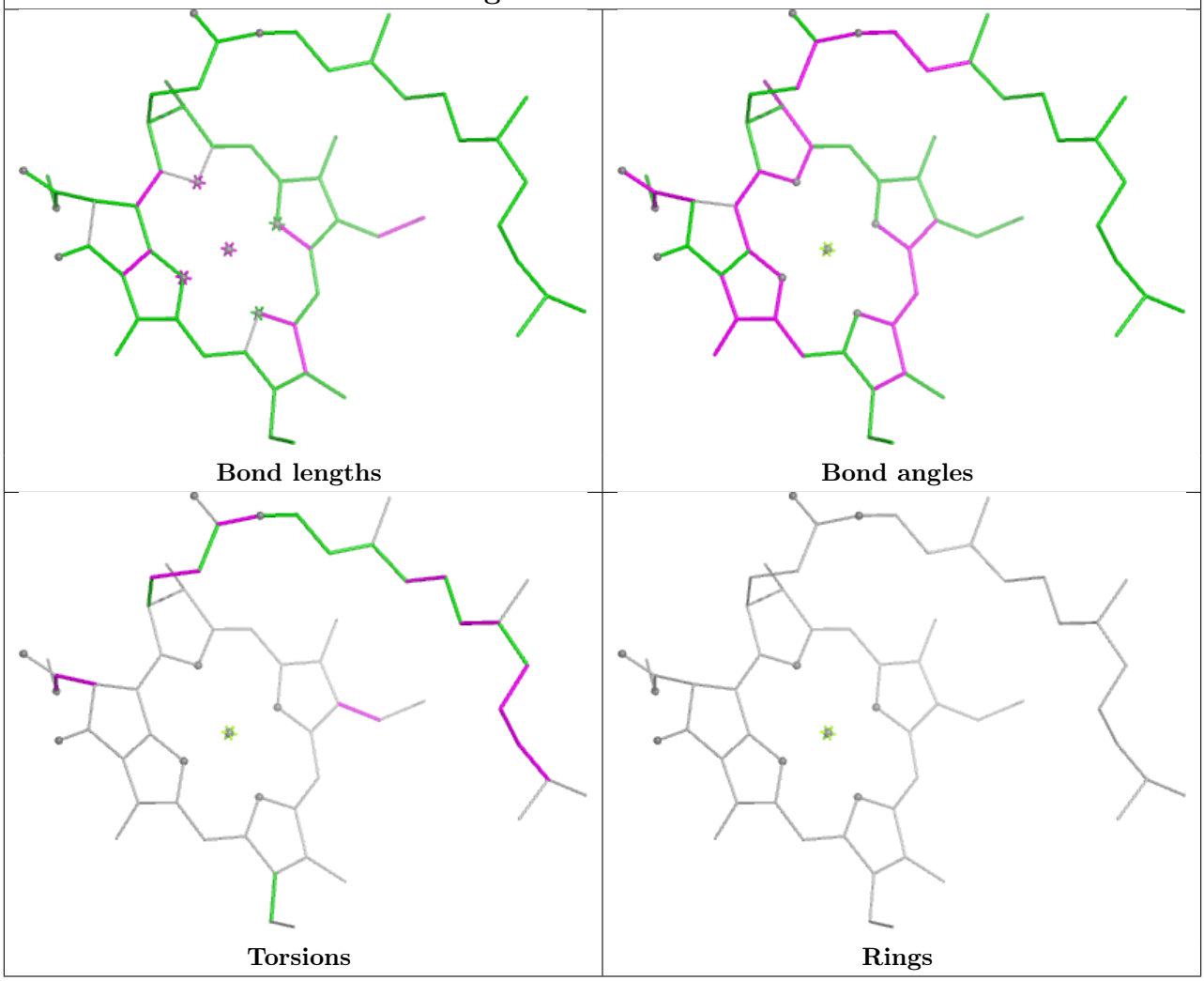


Torsions

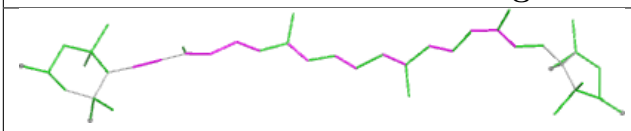
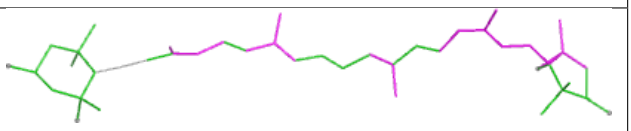
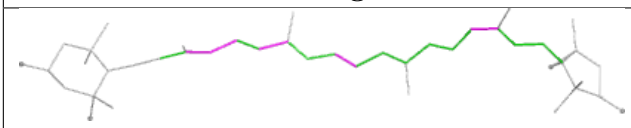
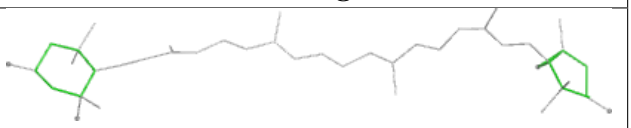


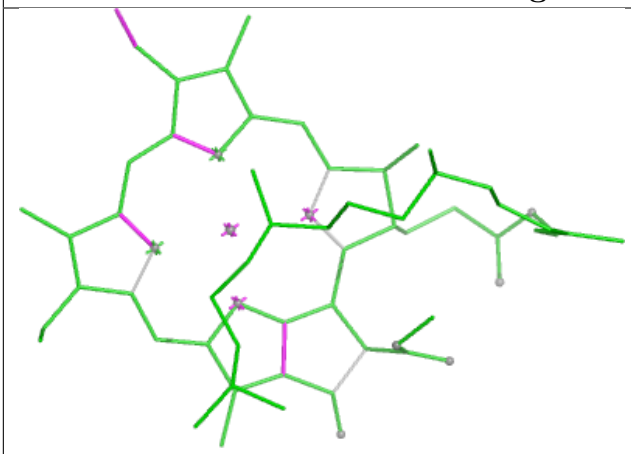
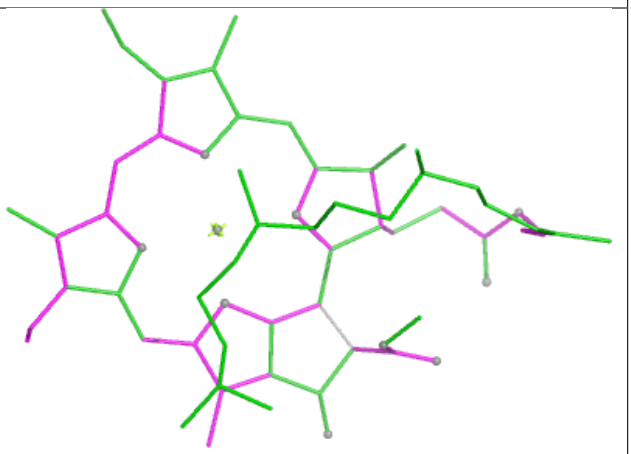
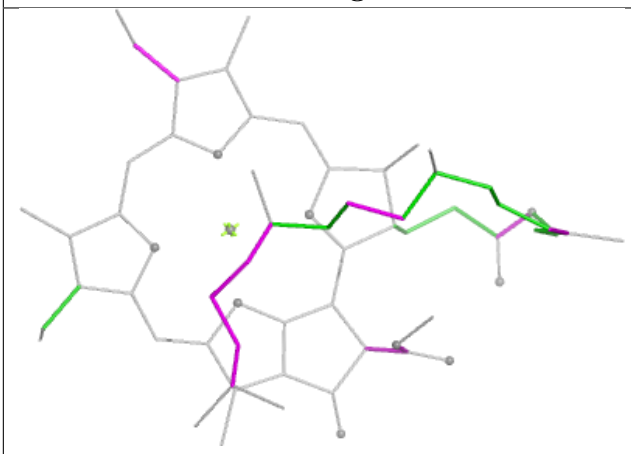
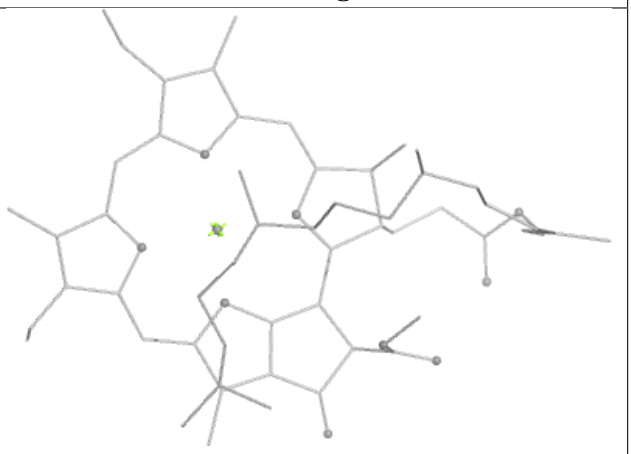
Rings

Ligand CLA R1 602



Ligand BCR A1 411

Ligand NEX Y1 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

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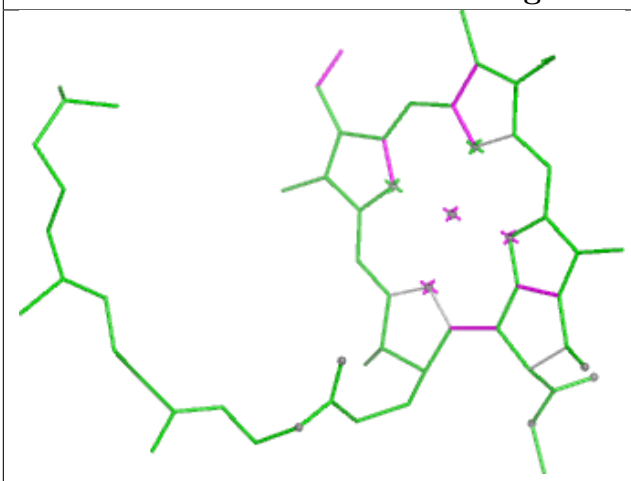	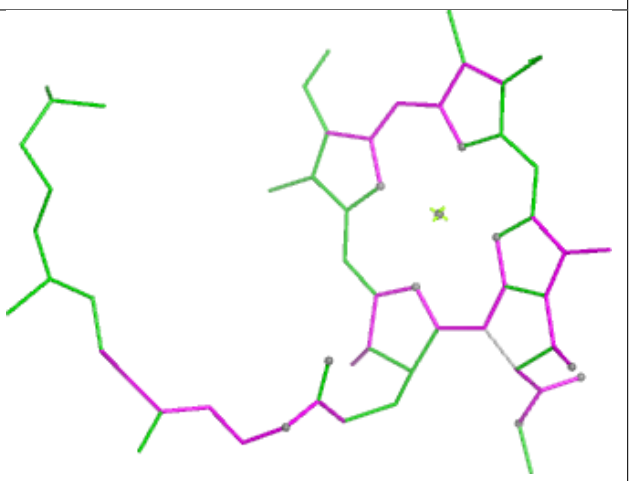
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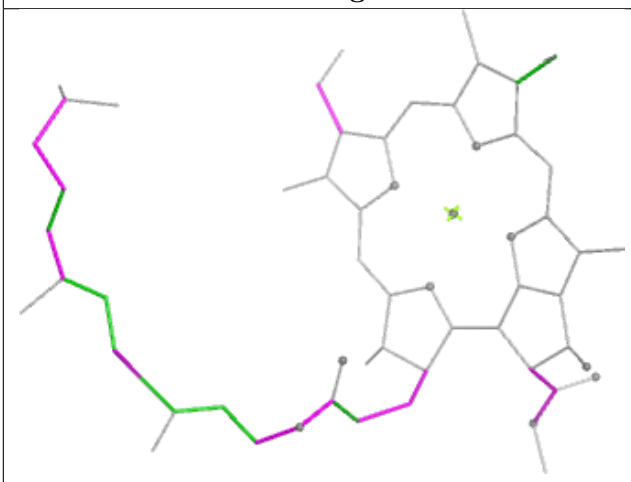
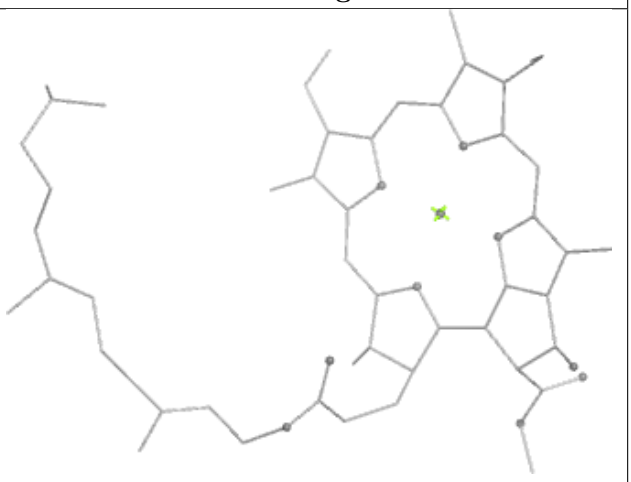
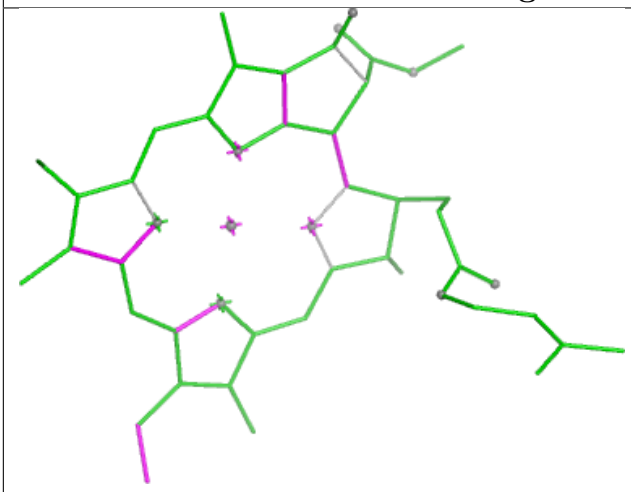
	
Torsions	**Rings**

Ligand CLA y1 608



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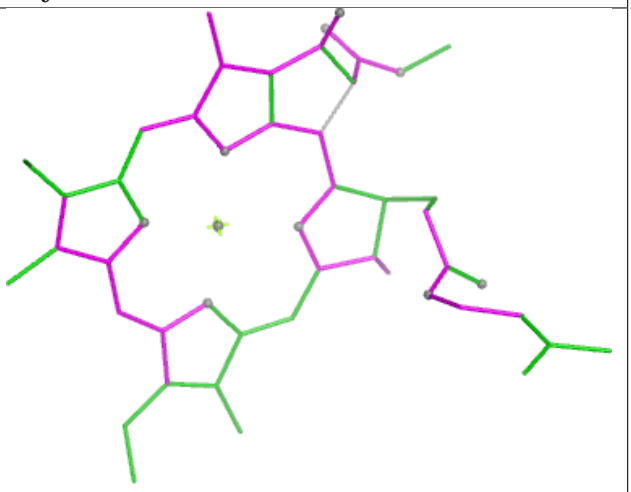
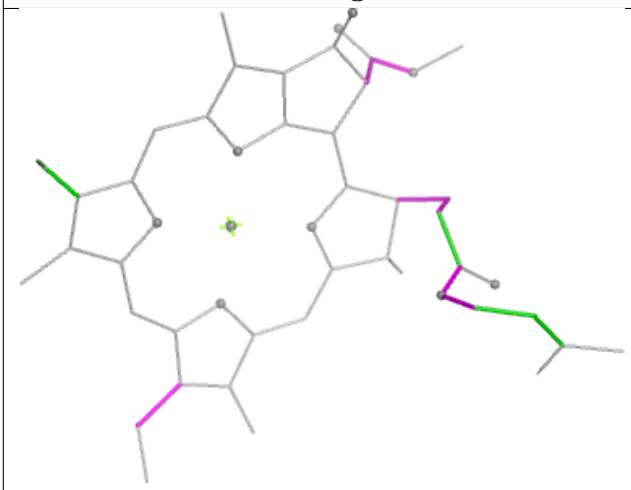


Bond angles



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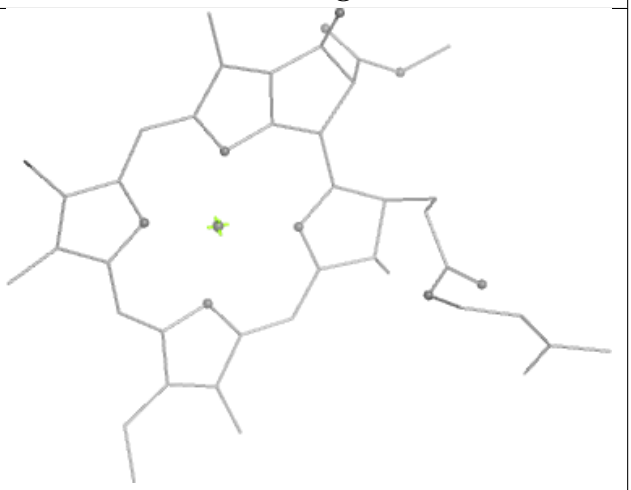
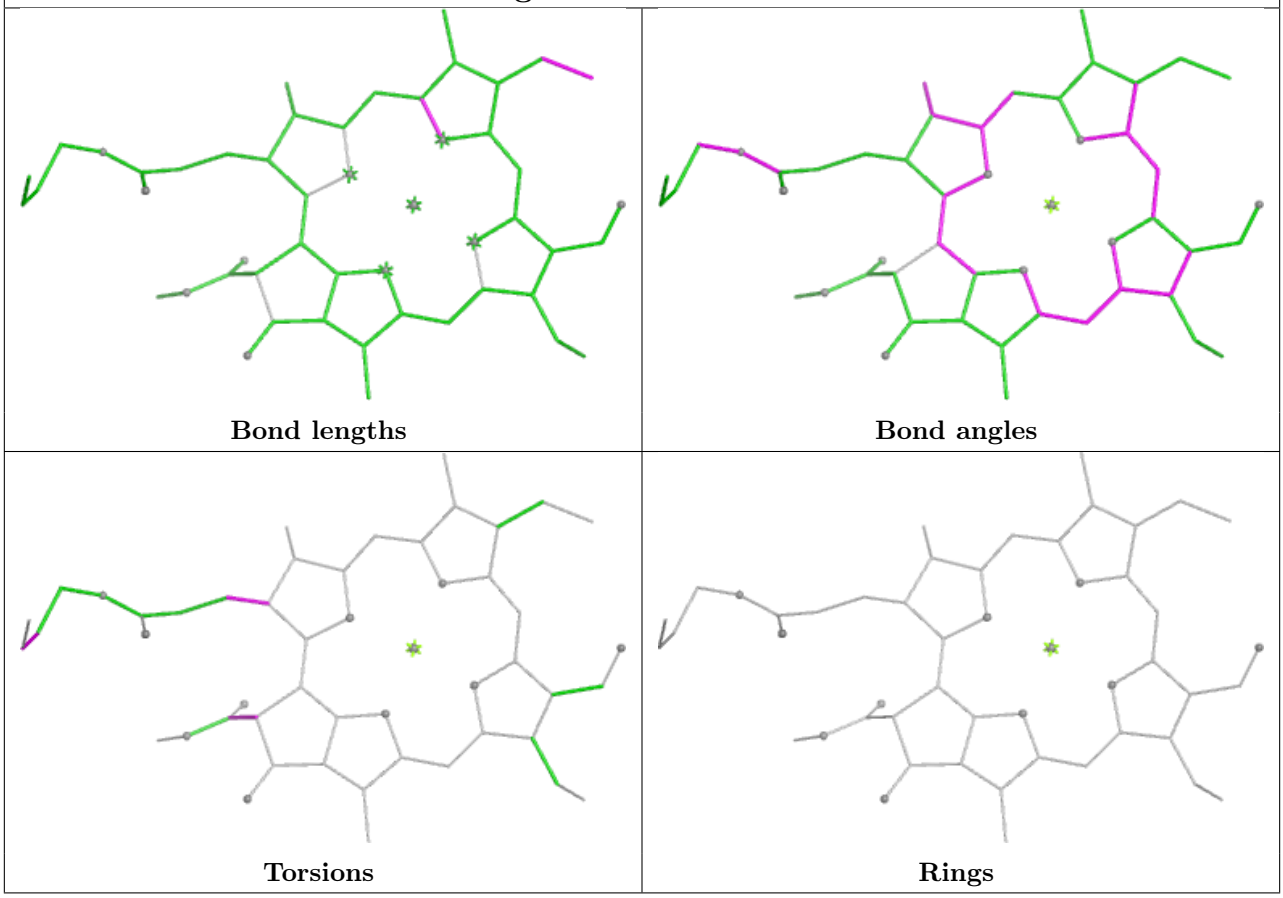
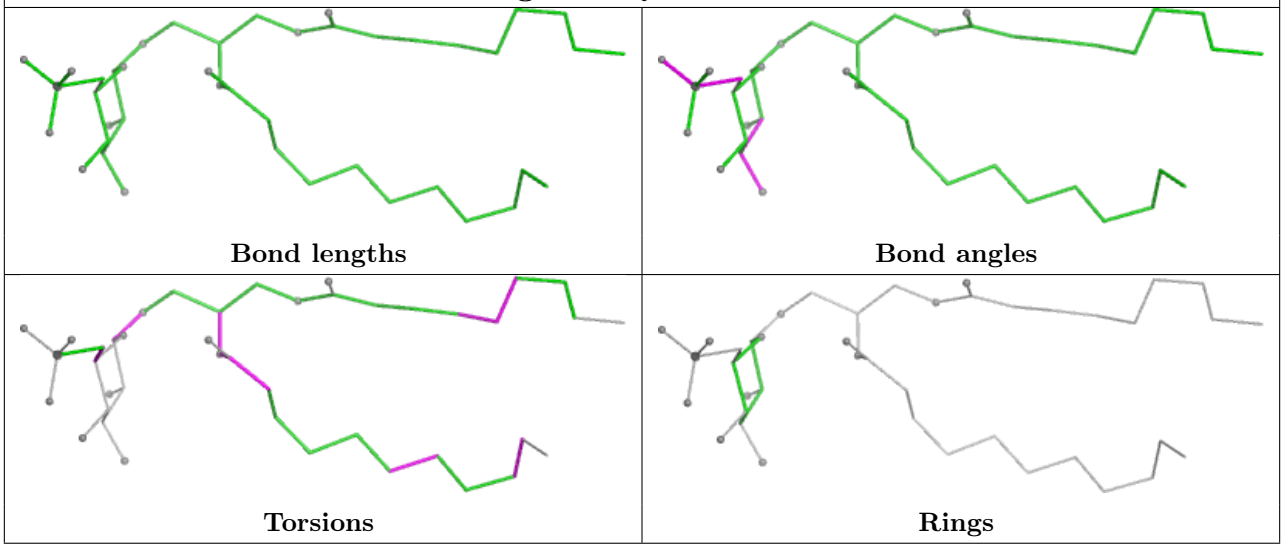


Rings

Ligand CHL G1 606



Ligand SQD B1 621



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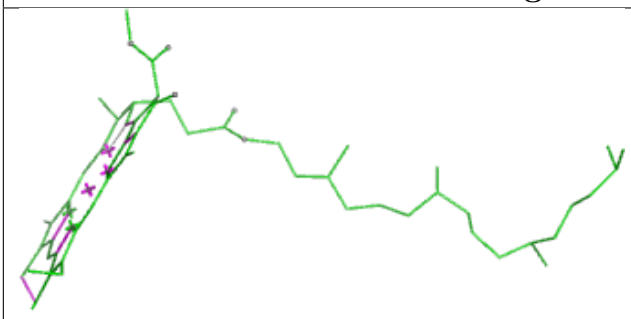
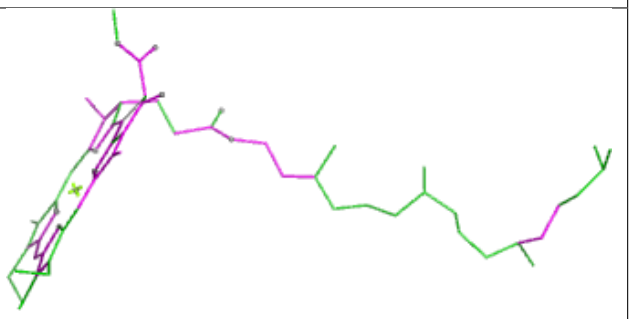
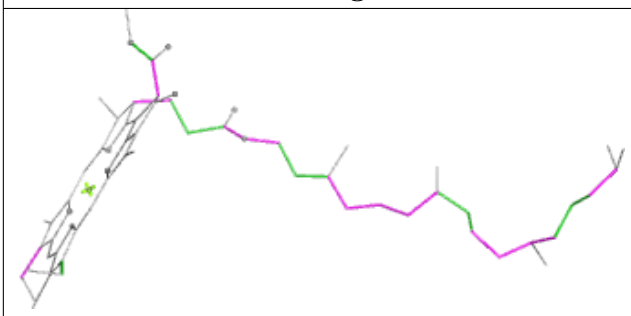
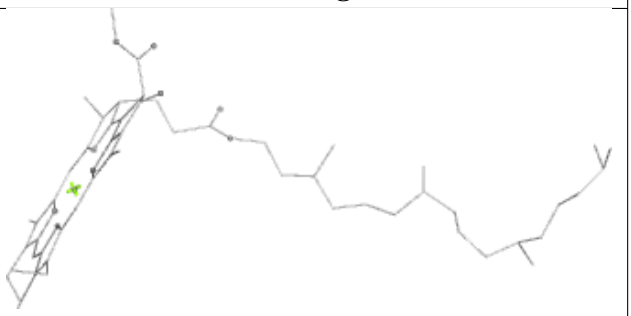
 Bond lengths	 Bond angles
 Torsions	 Rings

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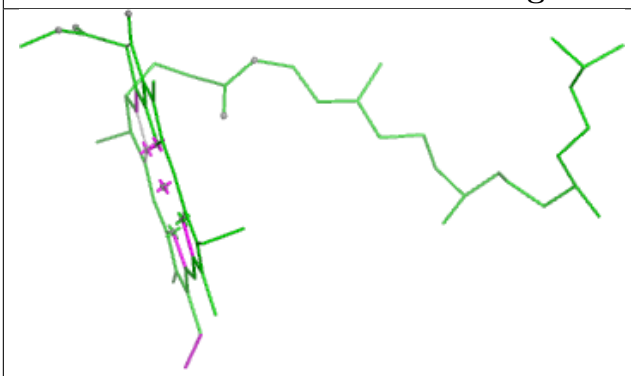
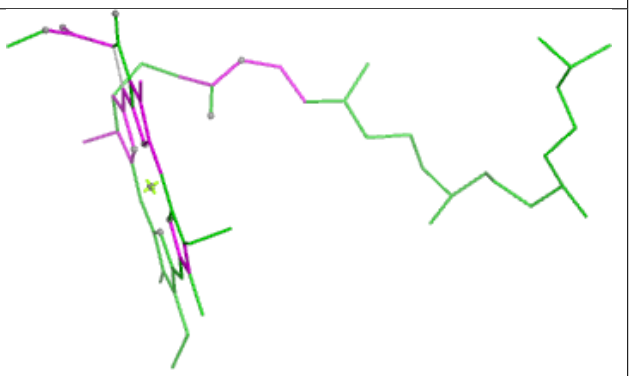
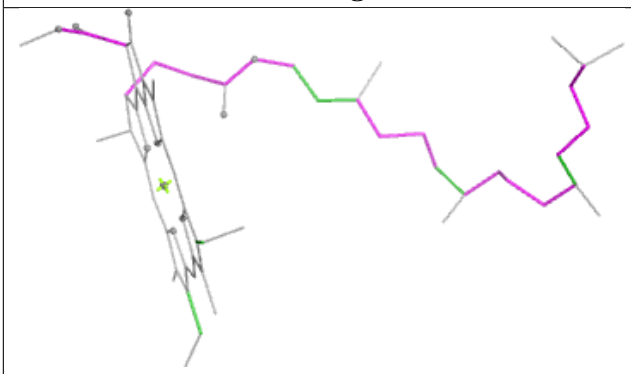
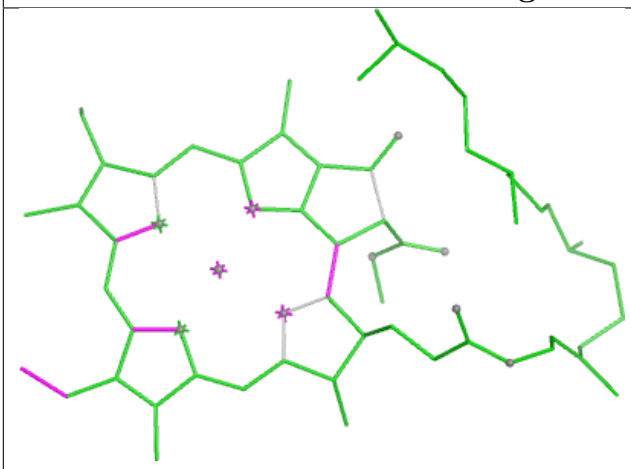
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA b1 611



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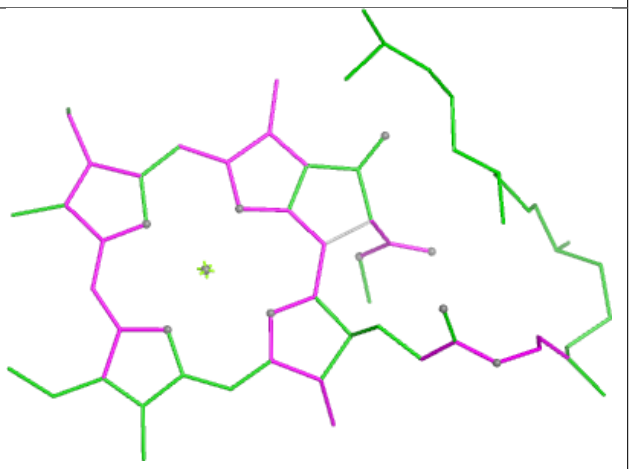

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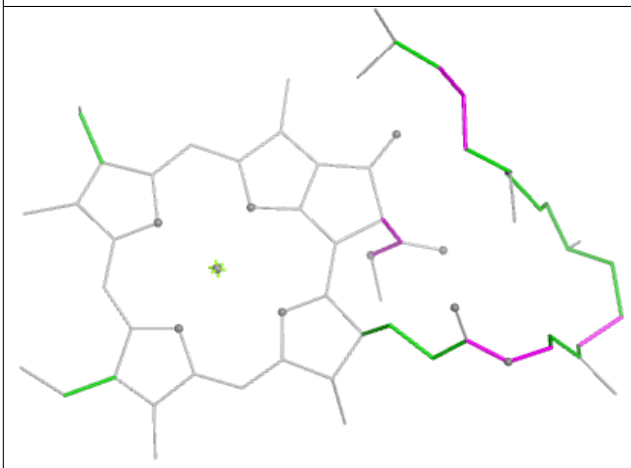

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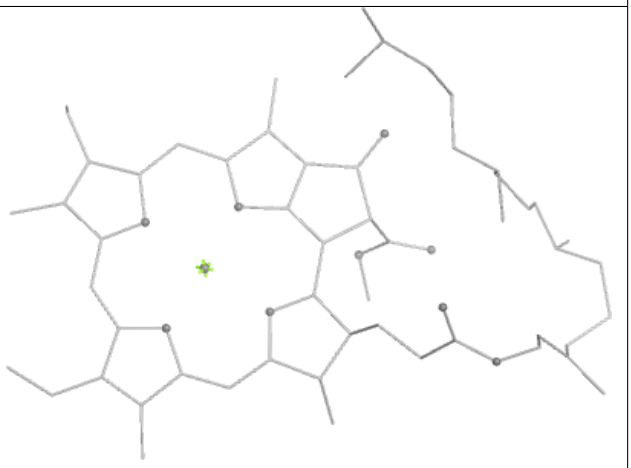
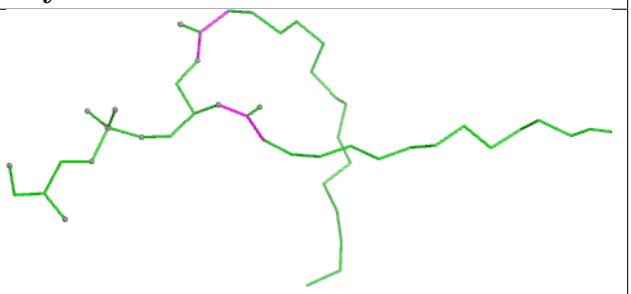


Rings

Ligand LHG y1 624

Bond lengths

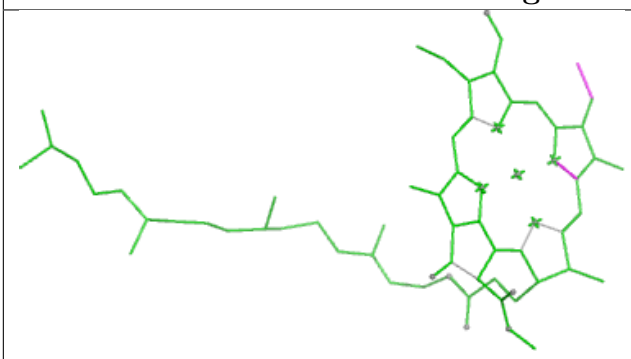


Bond angles

Torsions

Rings

Ligand CHL G 609



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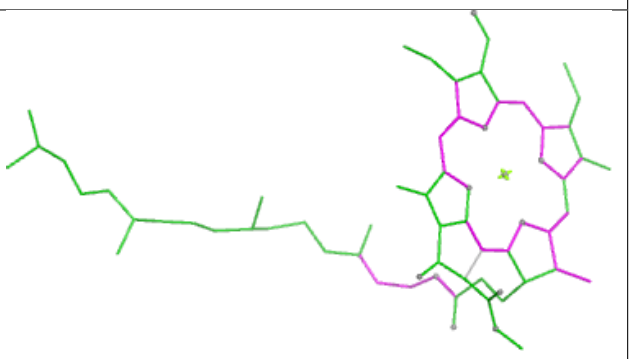

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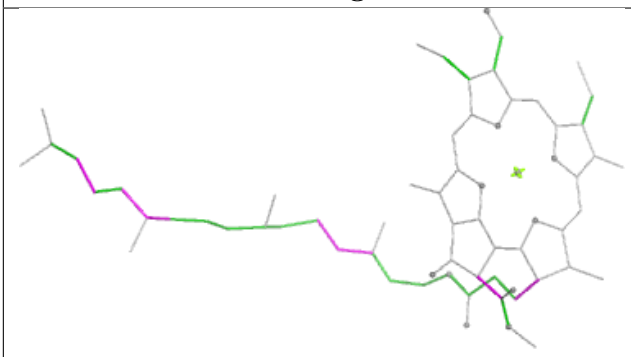

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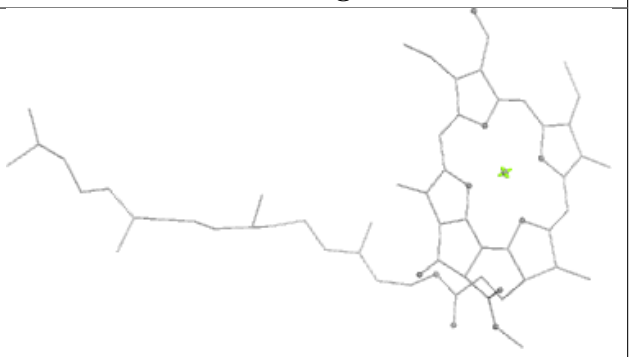
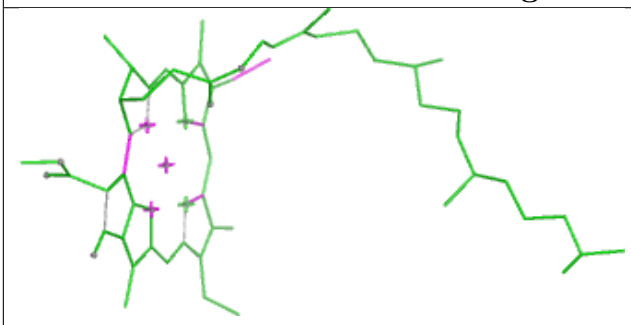


Rings

Ligand CLA s1 610



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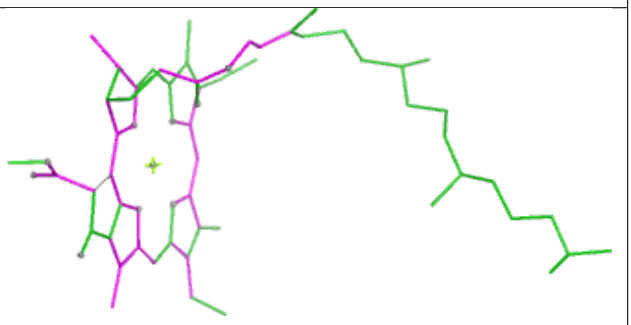

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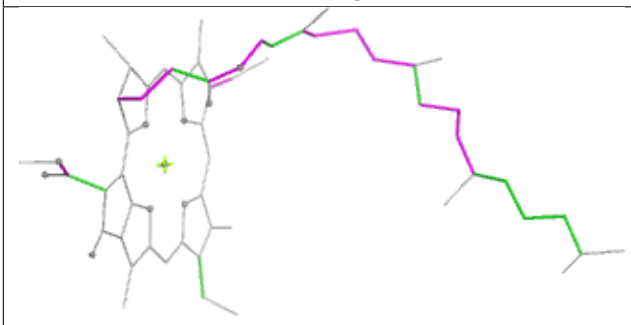
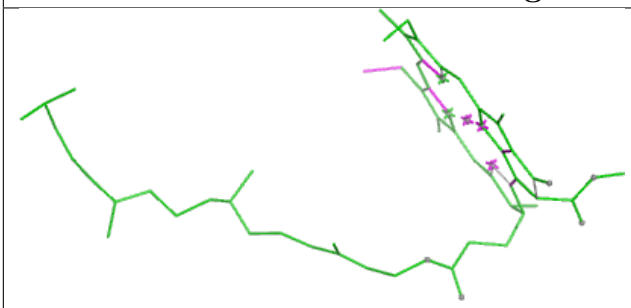


Torsions

Rings

Ligand CLA C 504



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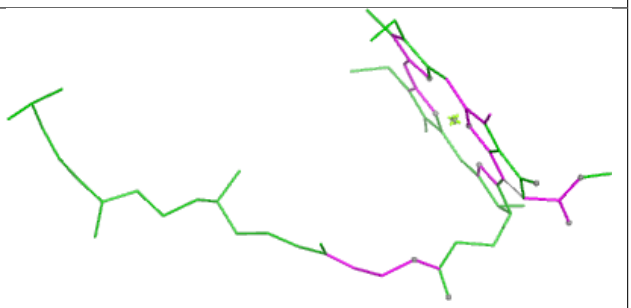

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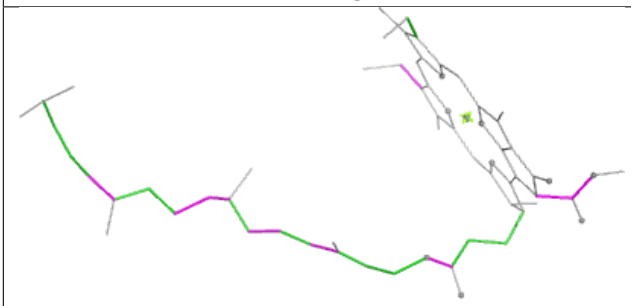
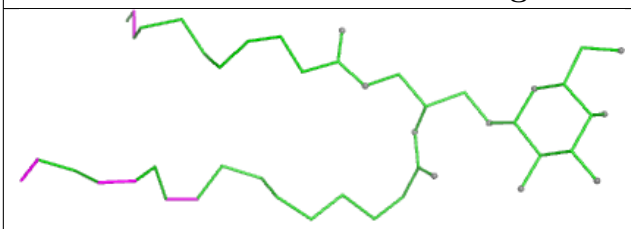


Torsions

Rings

Ligand LMG D1 411



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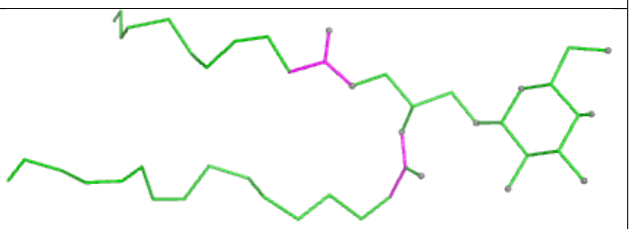

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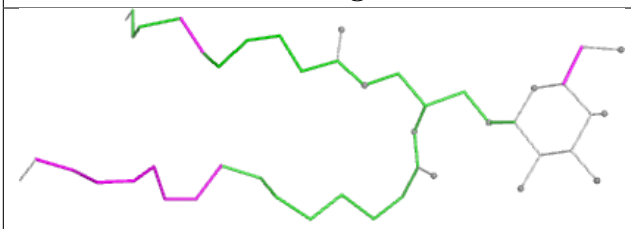

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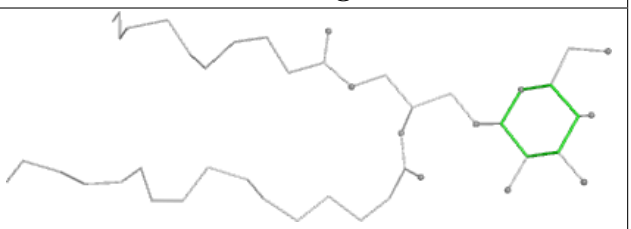
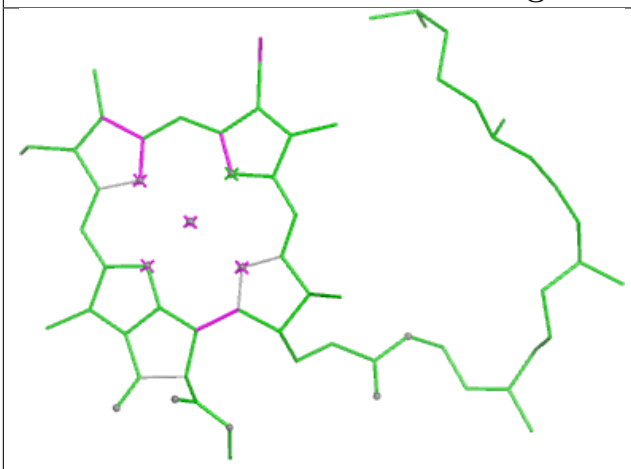


Rings

Ligand CLA S 603



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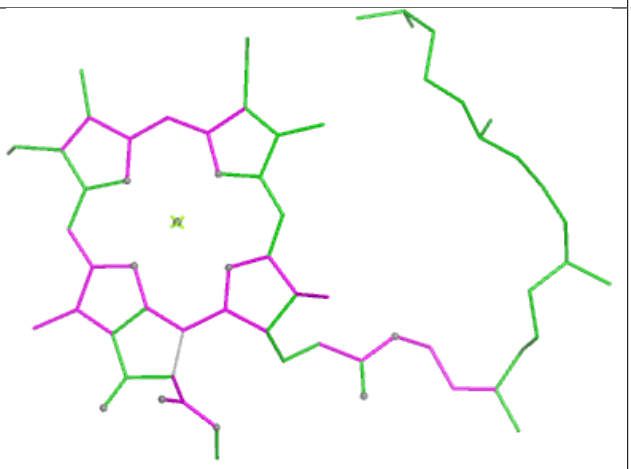

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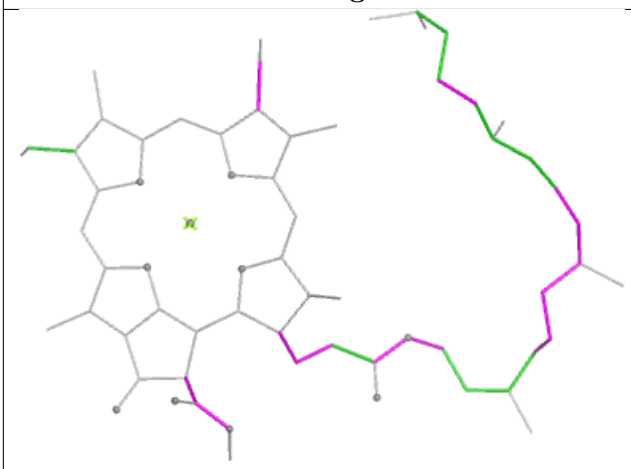

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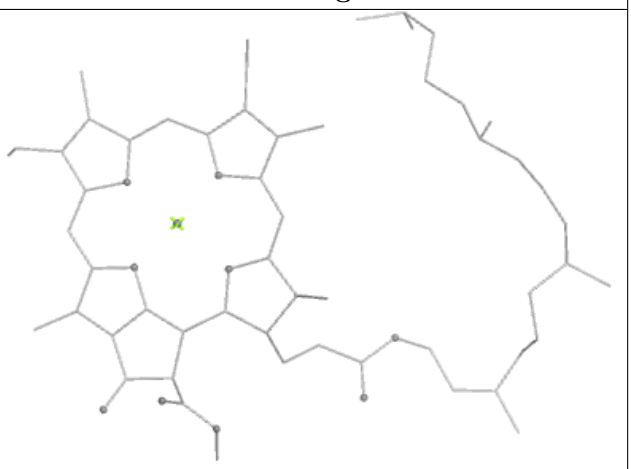
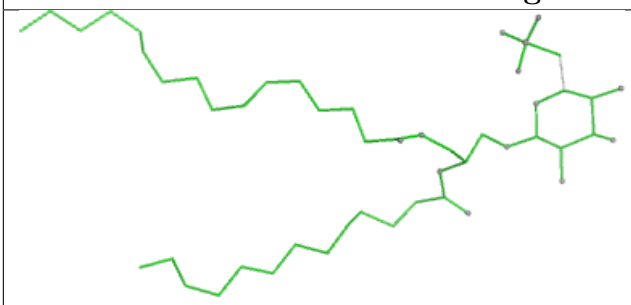


Rings

Ligand SQD A 412



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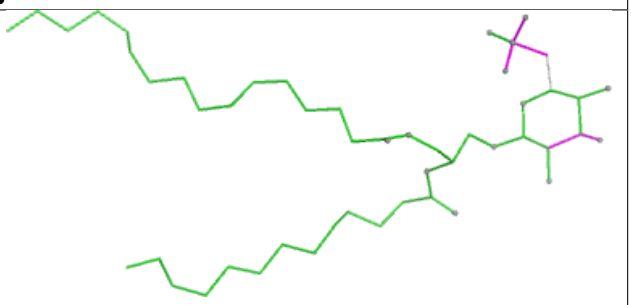

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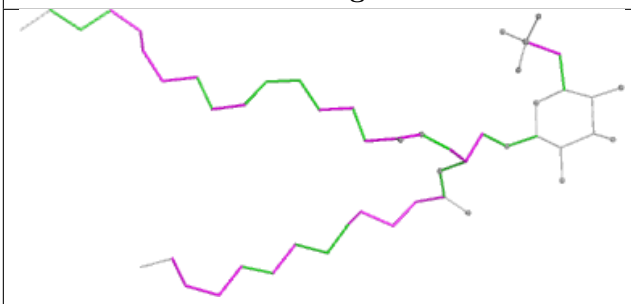
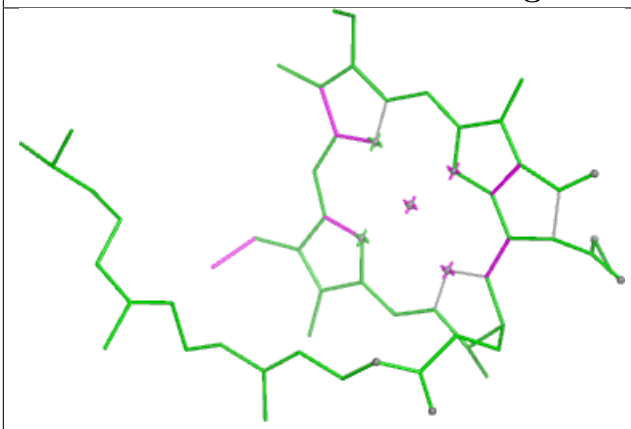
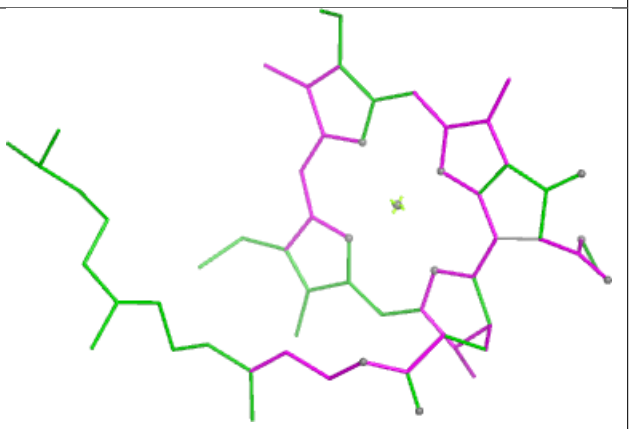
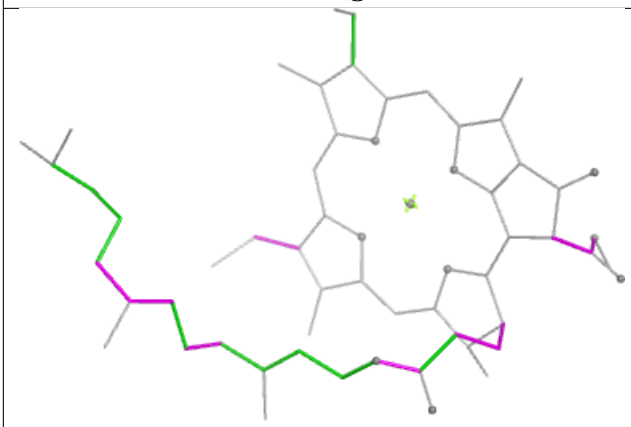


Torsions

Rings

Ligand CLA R 602	
 Bond lengths	 Bond angles
 Torsions	Rings

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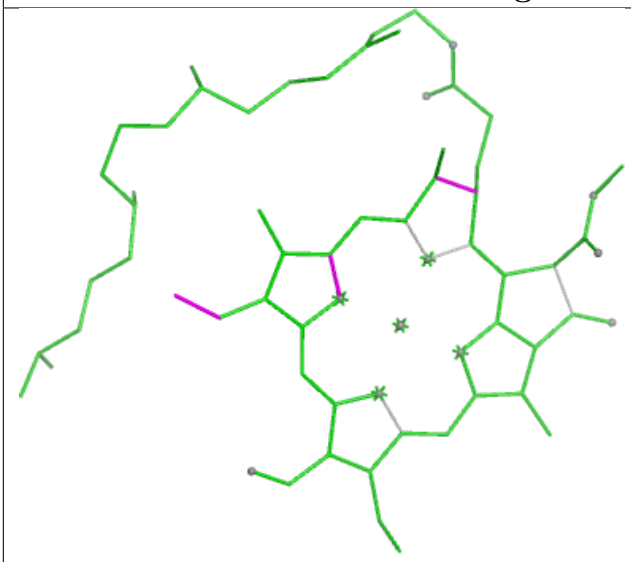
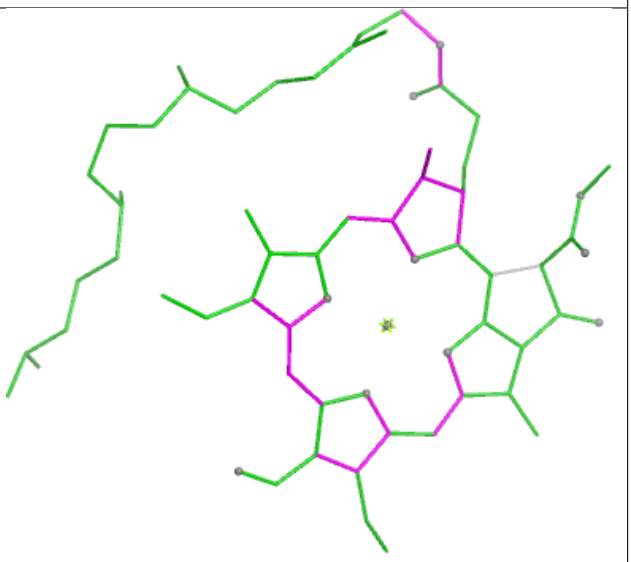
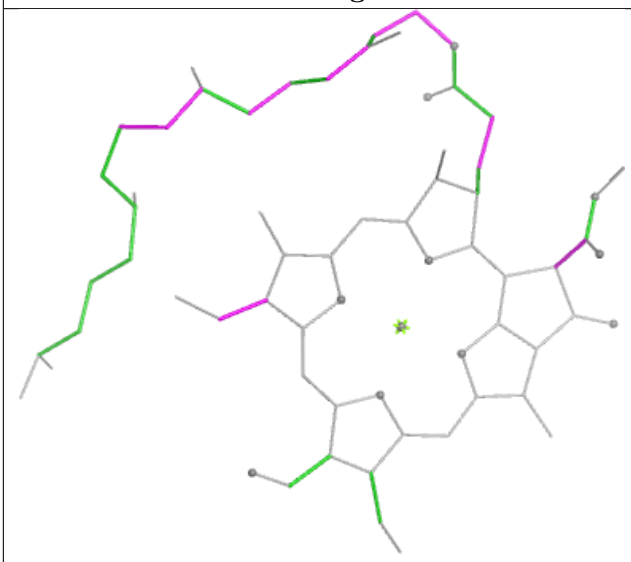
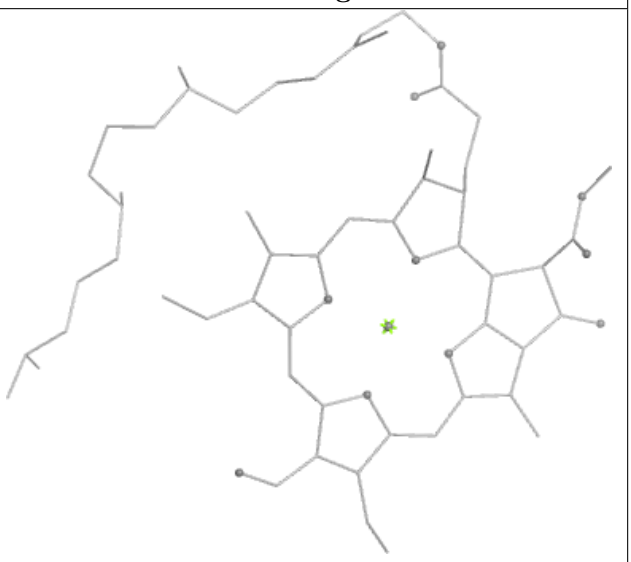
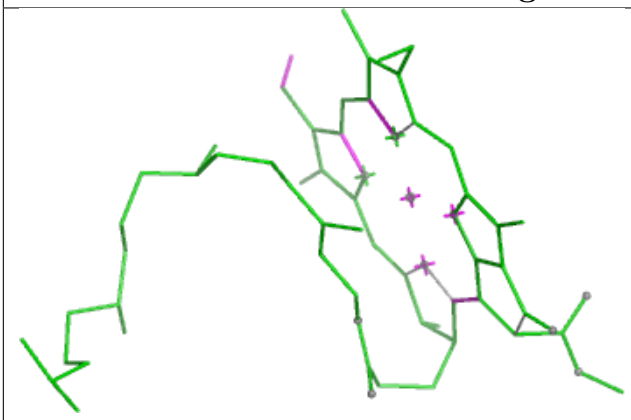
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA y1 613



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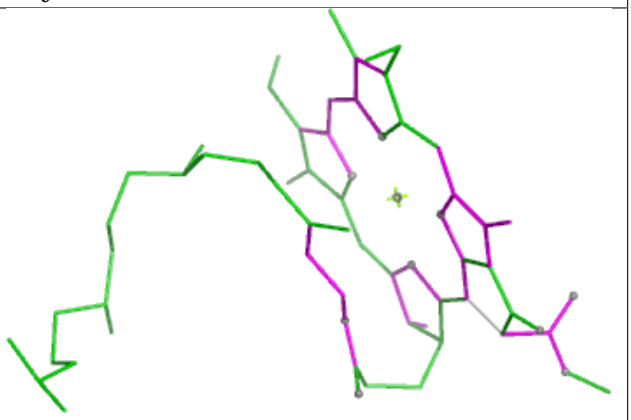

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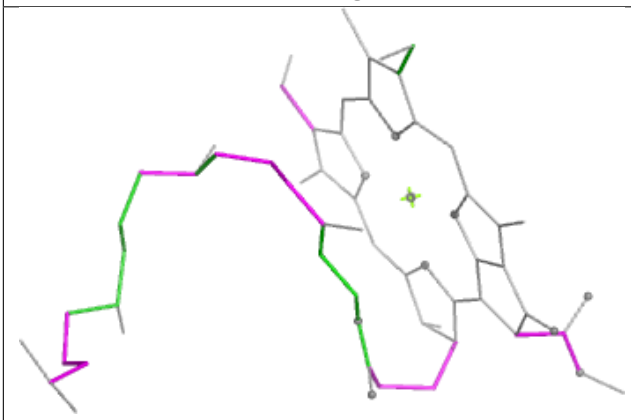

Torsions

Rings

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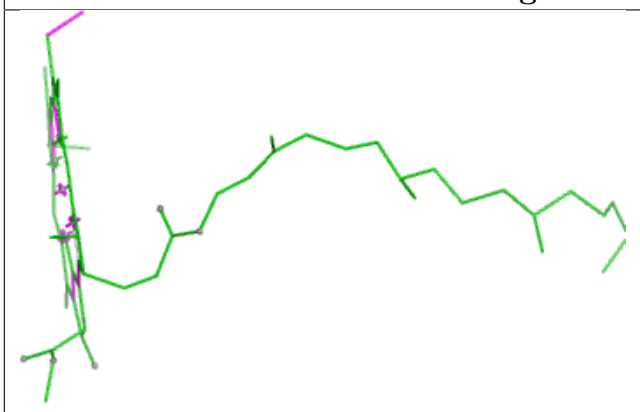
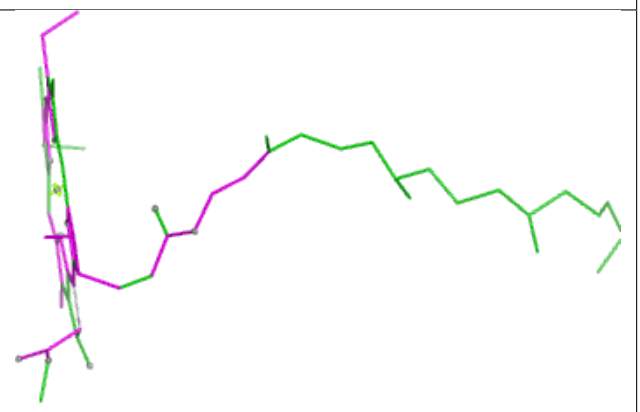
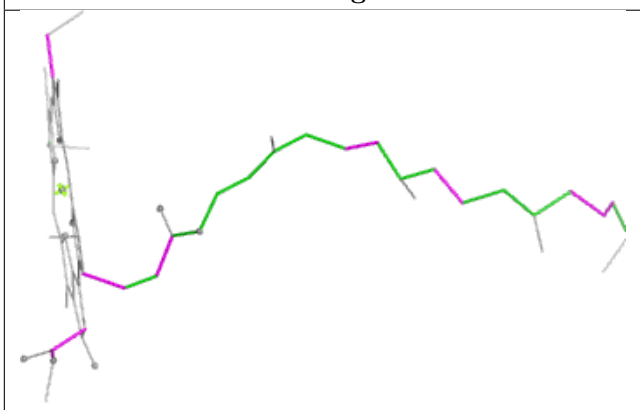
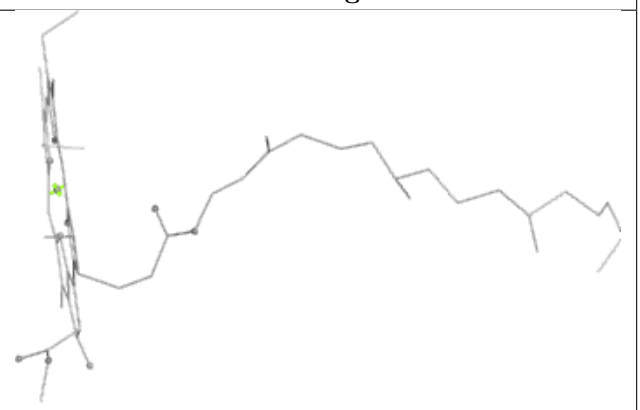
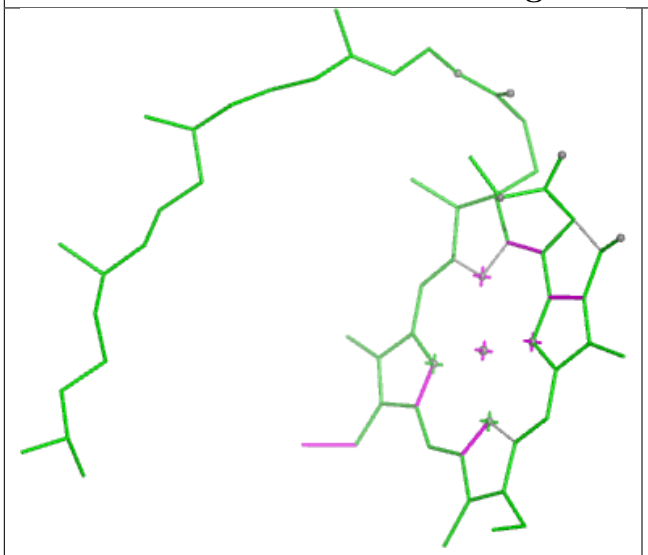
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 507



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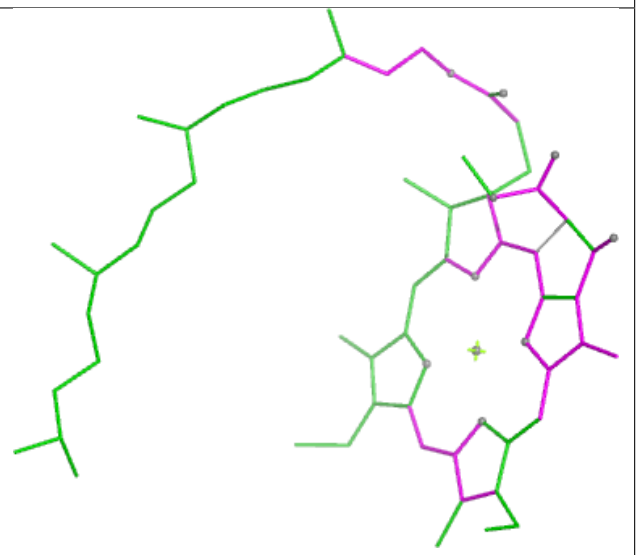

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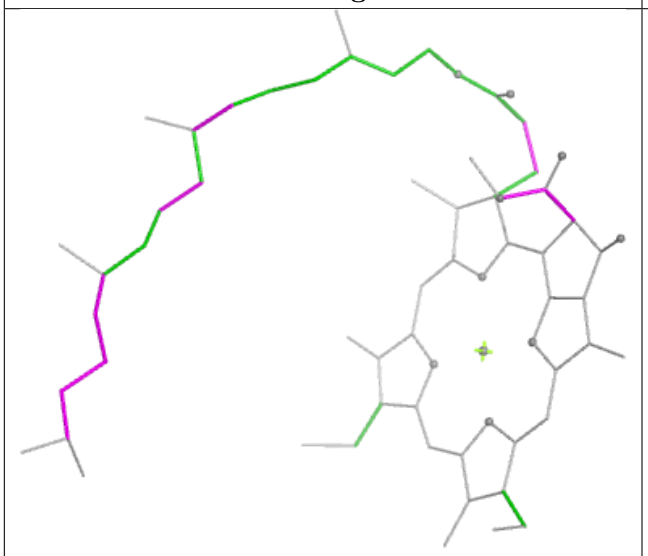
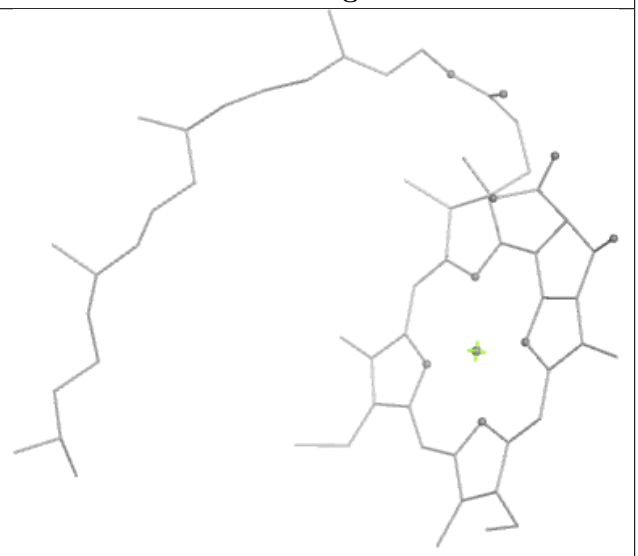
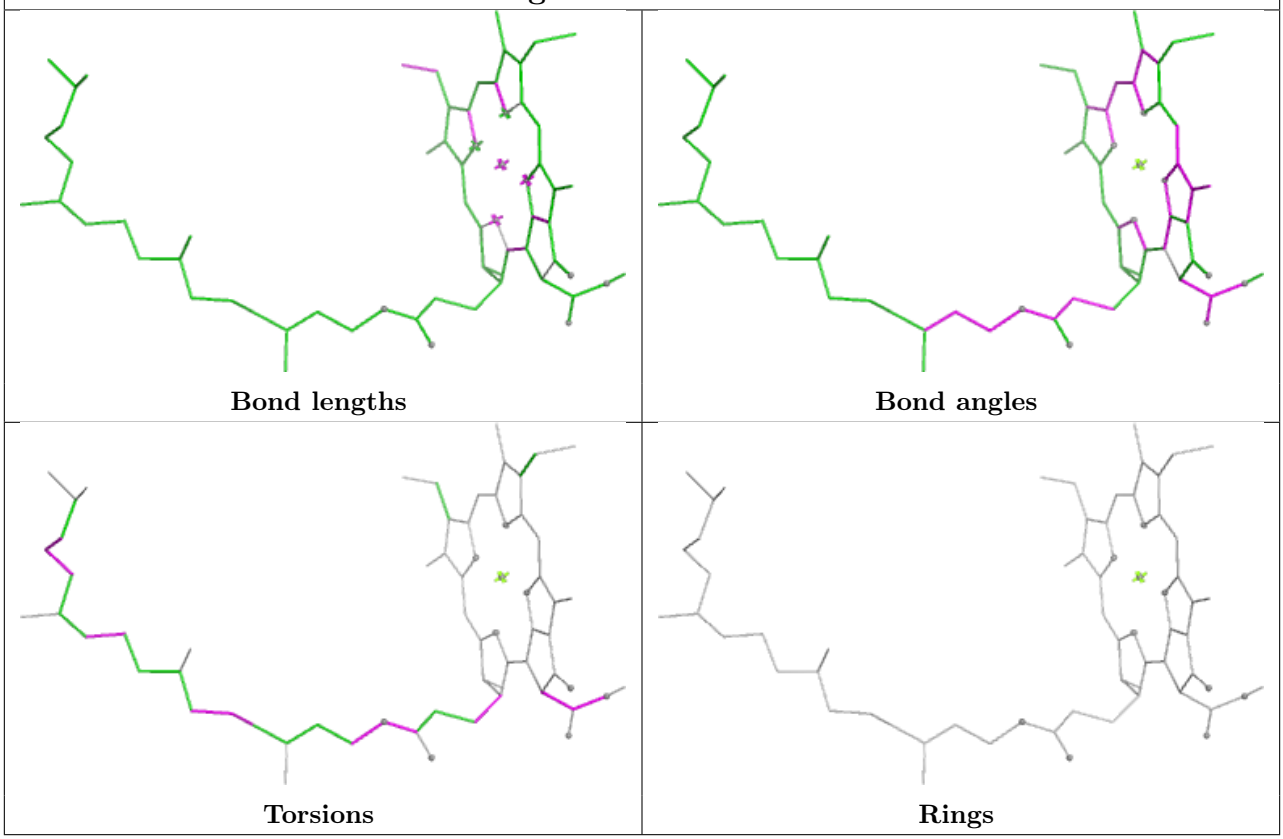


Torsions



Rings

Ligand CLA b 610



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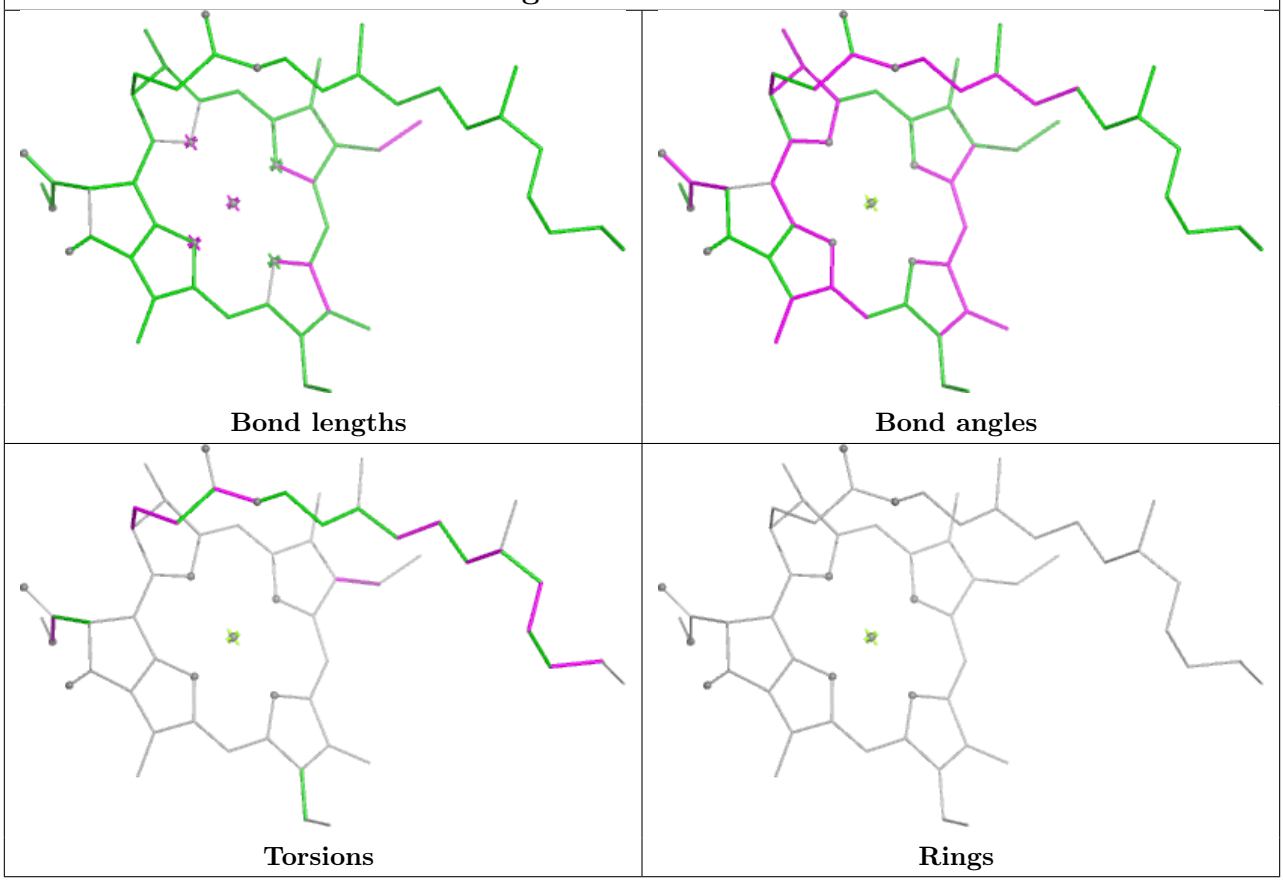

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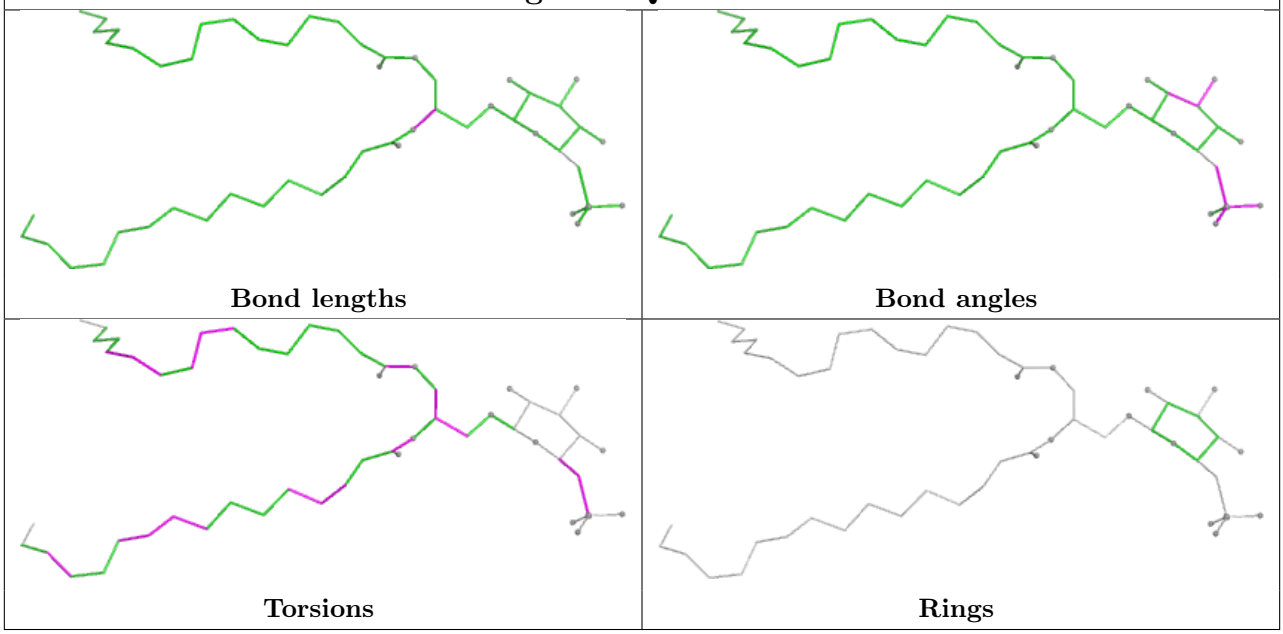
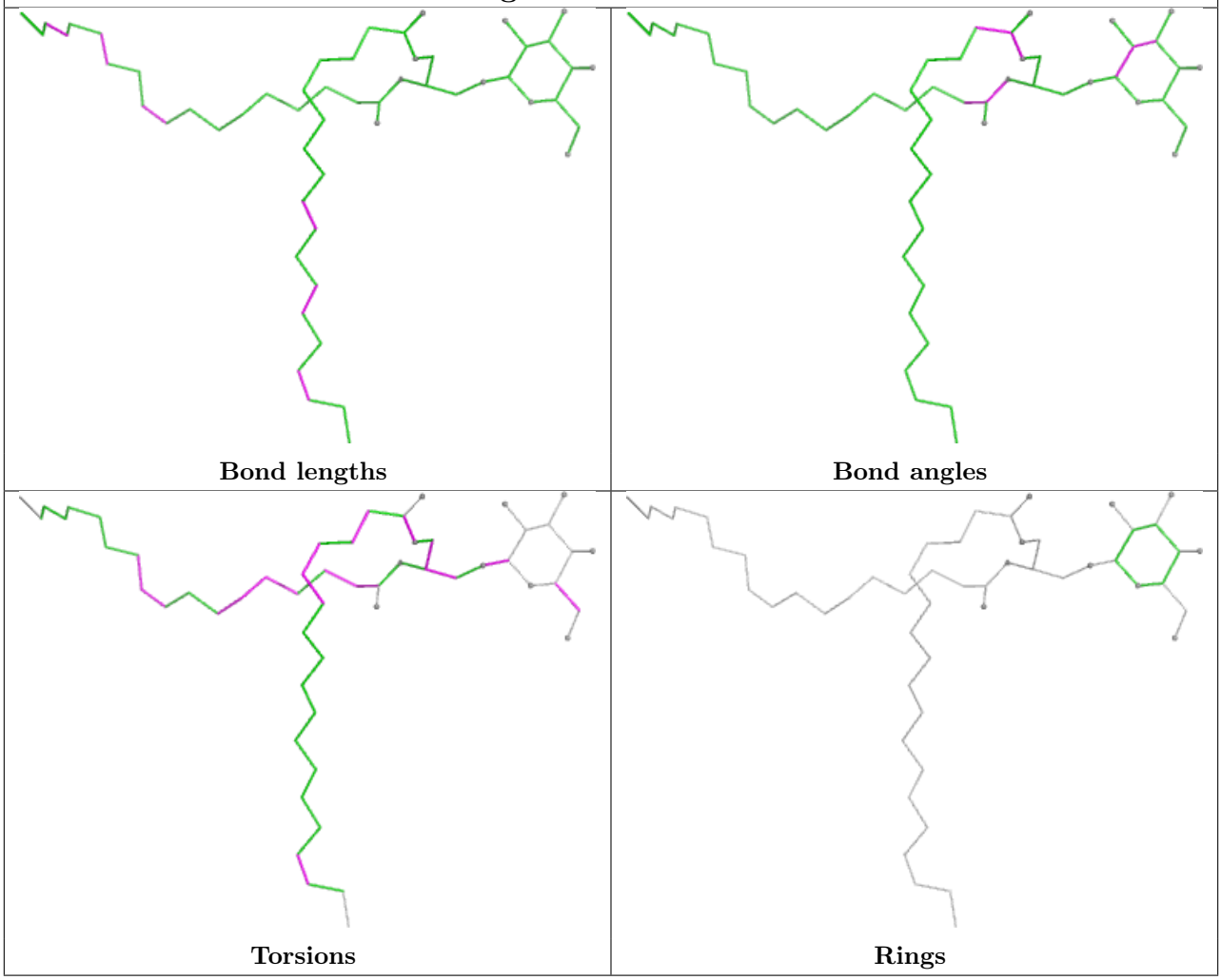
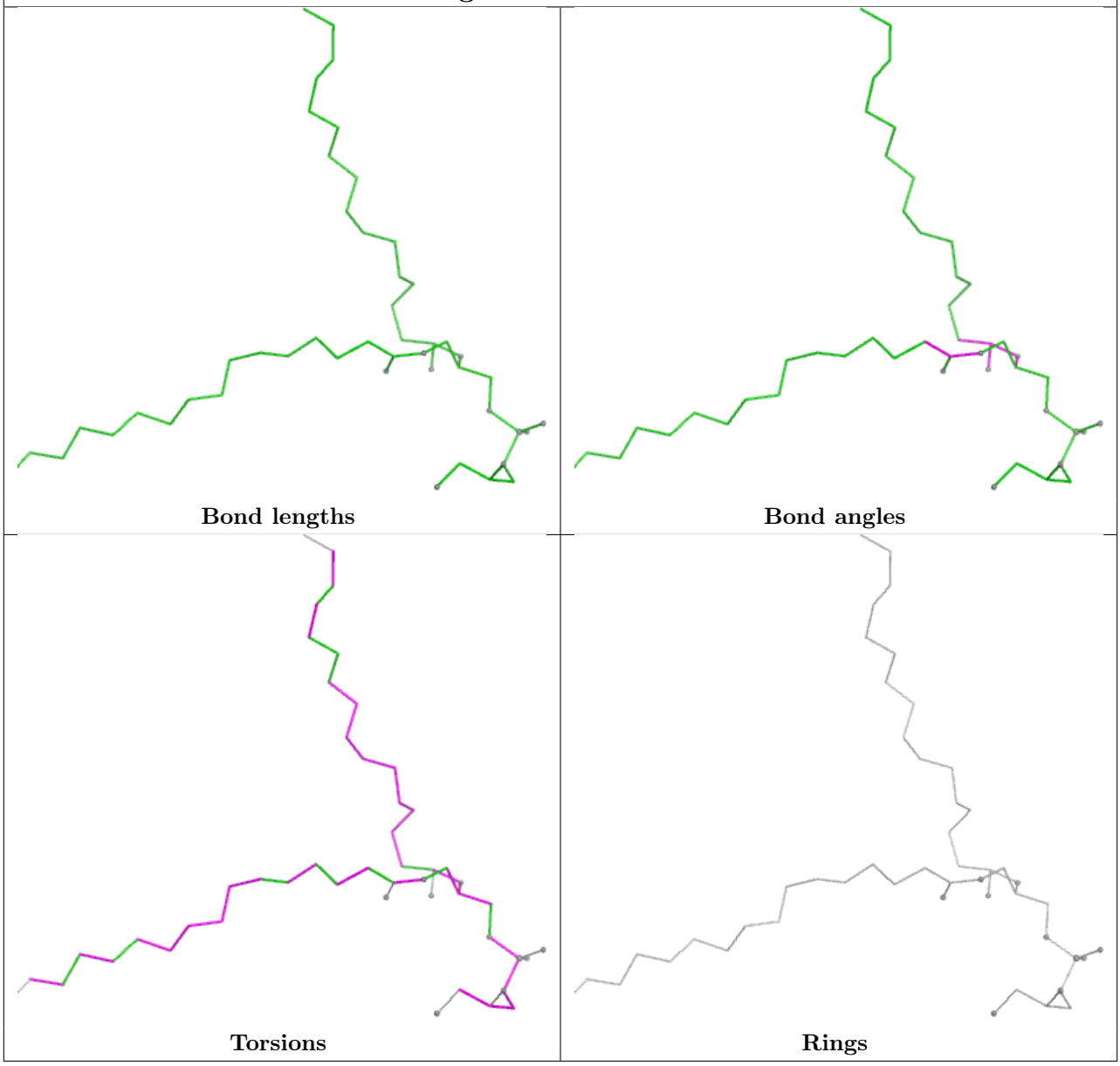


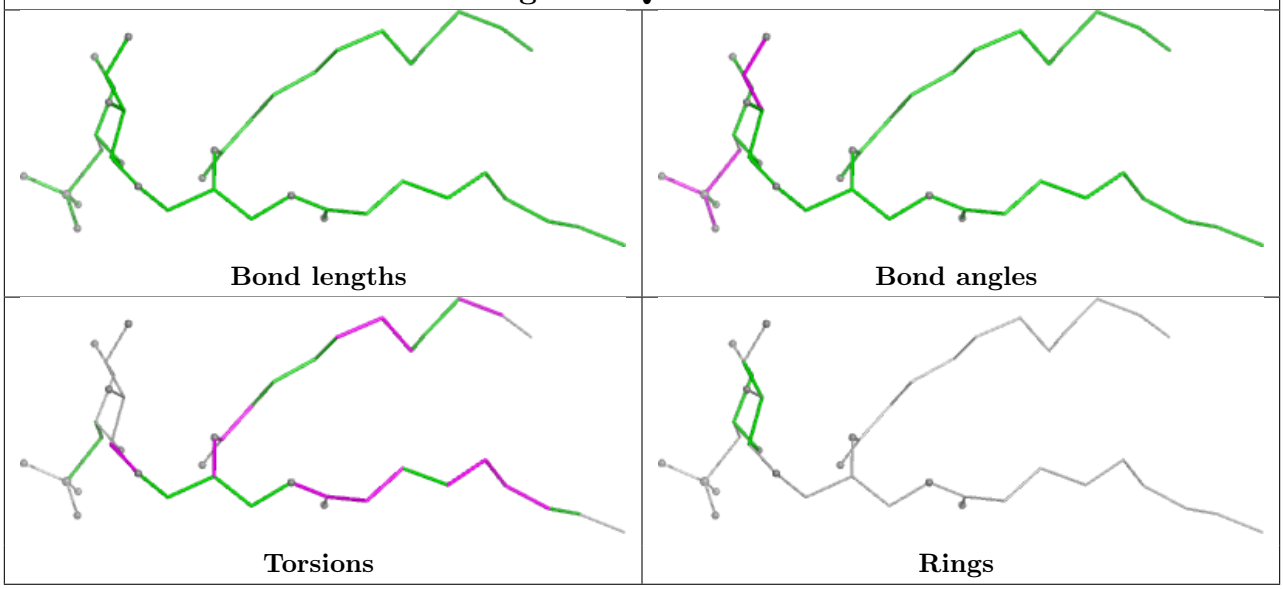
Ligand LMG c 523



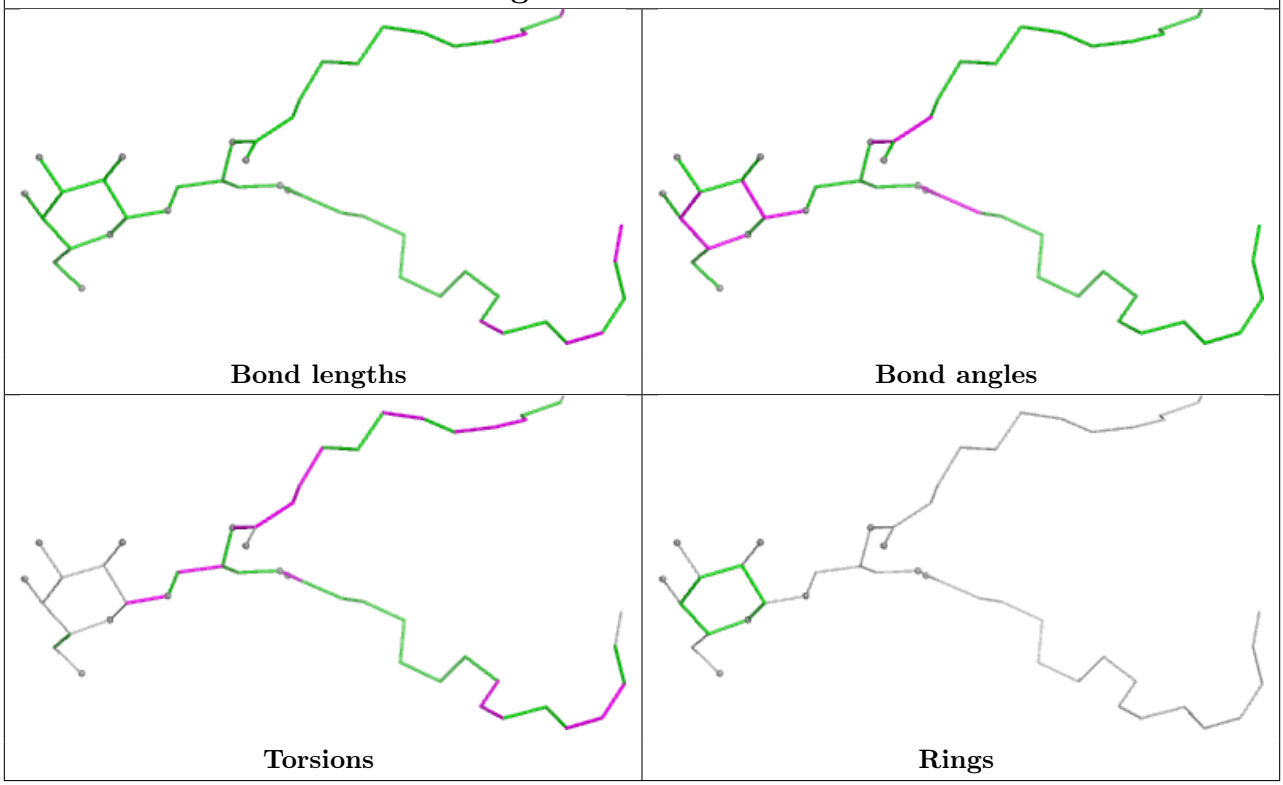
Ligand LHG L 101



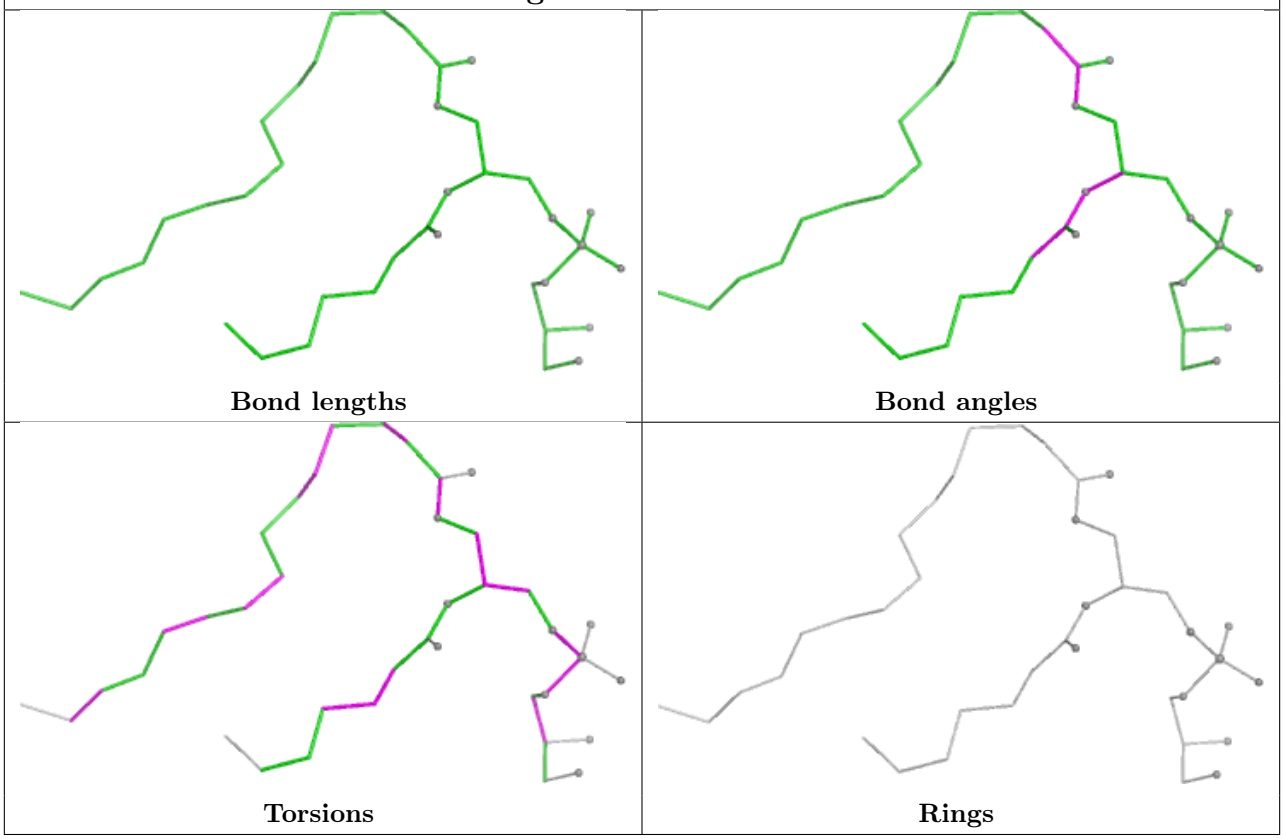
Ligand SQD b1 621



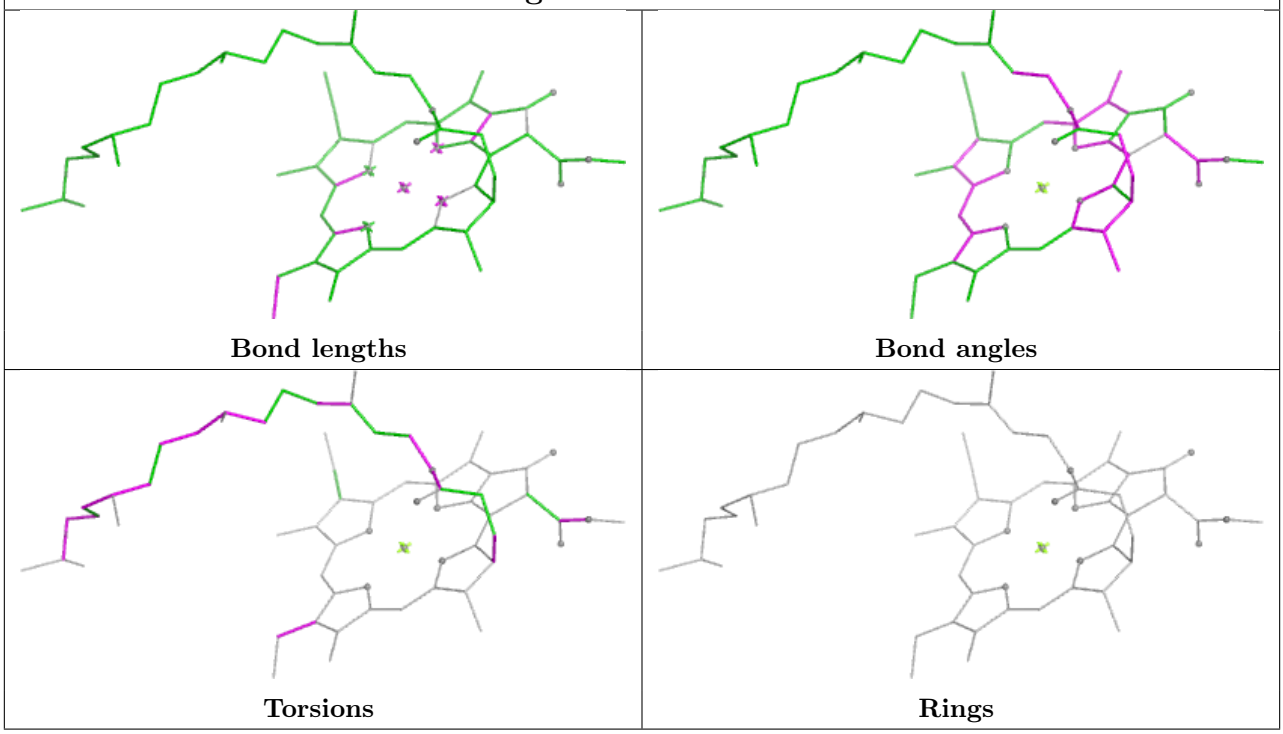
Ligand LMG A1 413



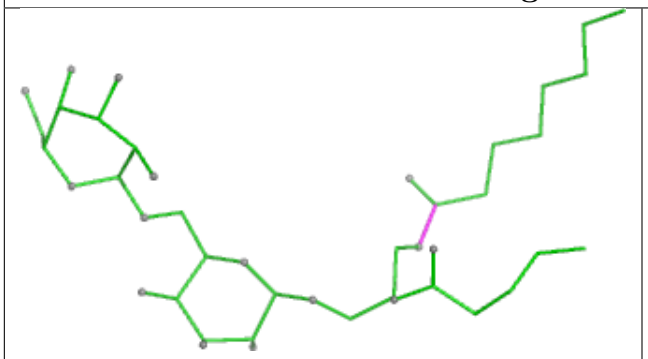
Ligand LHG d 410



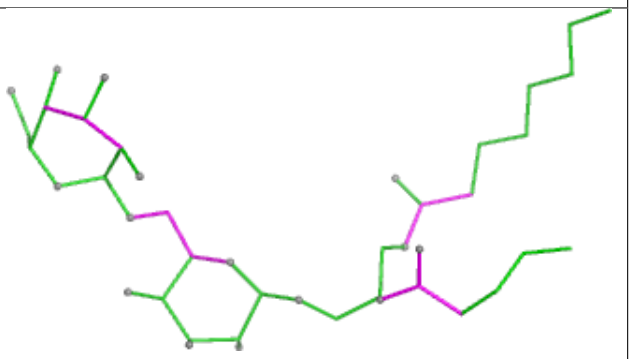
Ligand CLA C 513



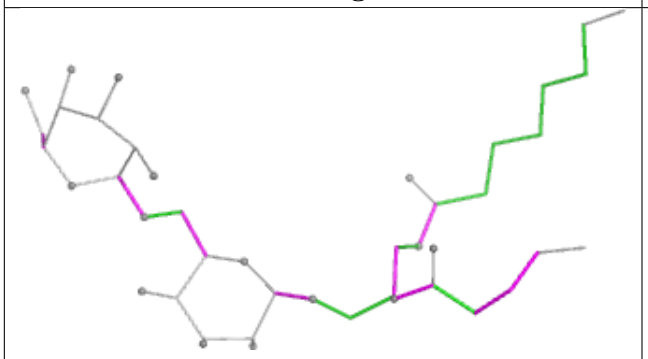
Ligand DGD B 623



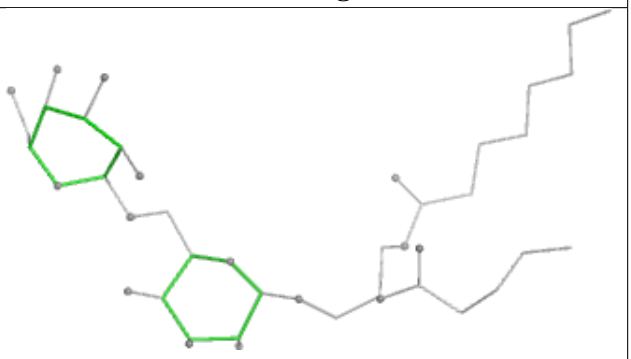
Bond lengths



Bond angles

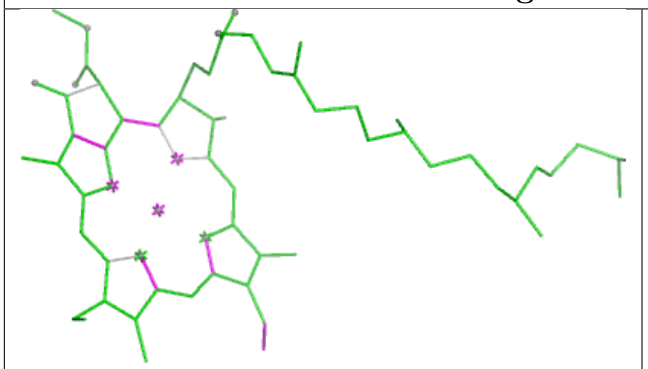


Torsions

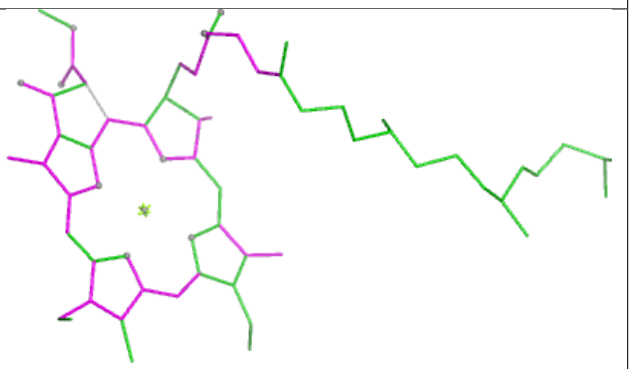


Rings

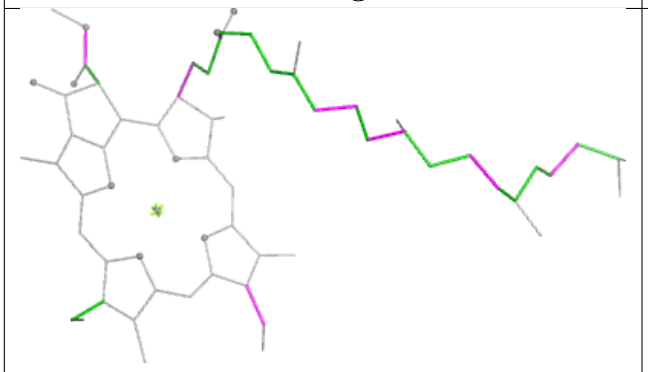
Ligand CLA C1 511



Bond lengths



Bond angles



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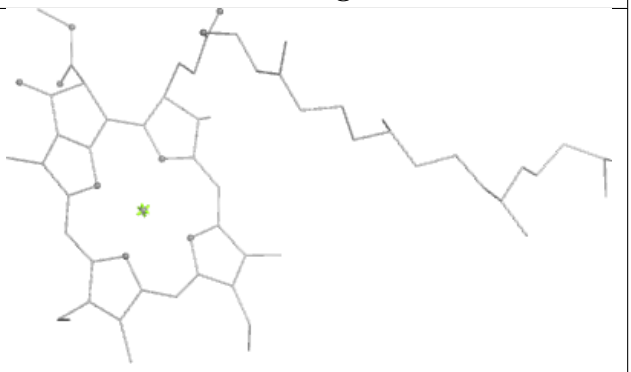
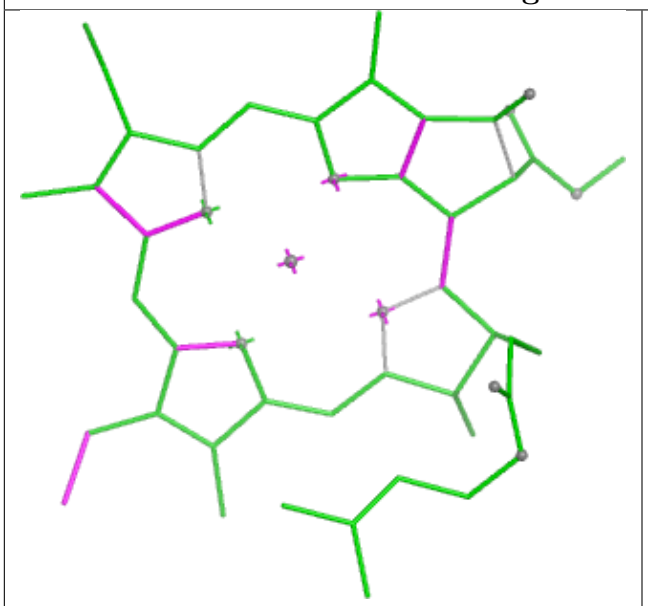
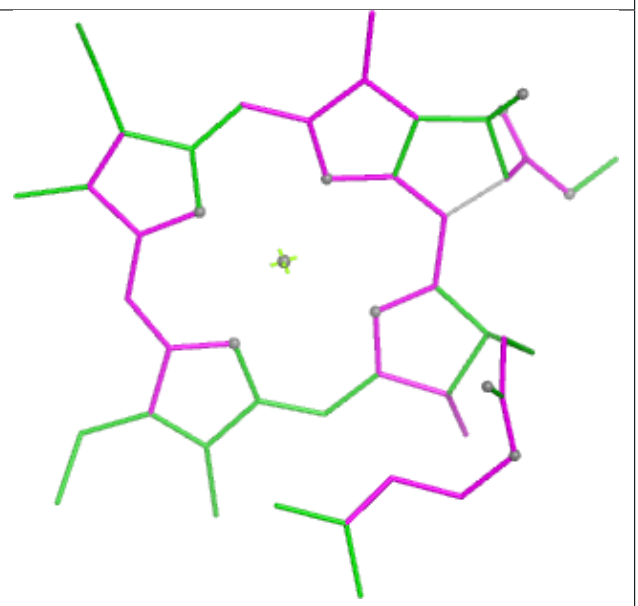


Rings

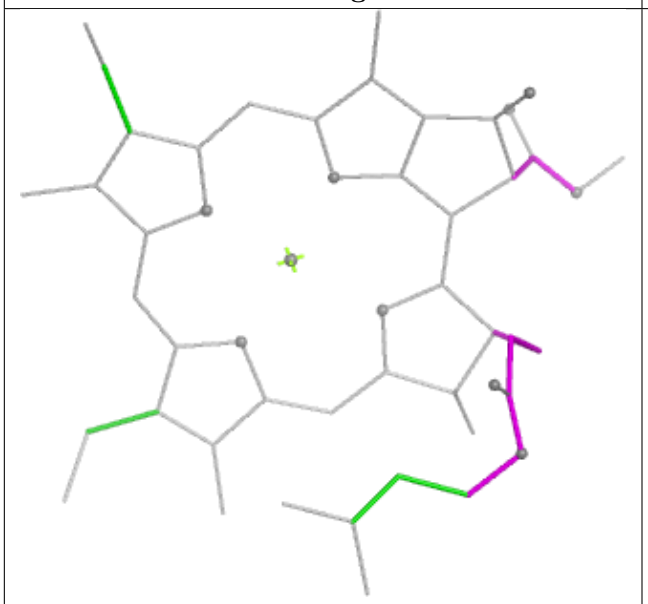
Ligand CLA s1 617



Bond lengths



Bond angles



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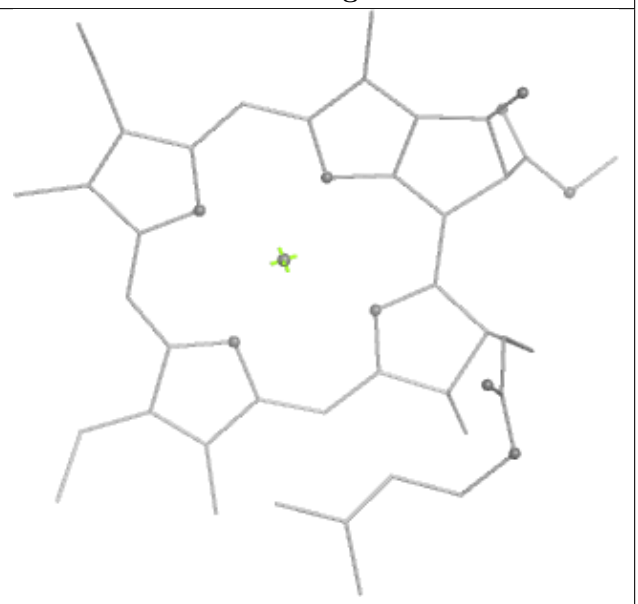
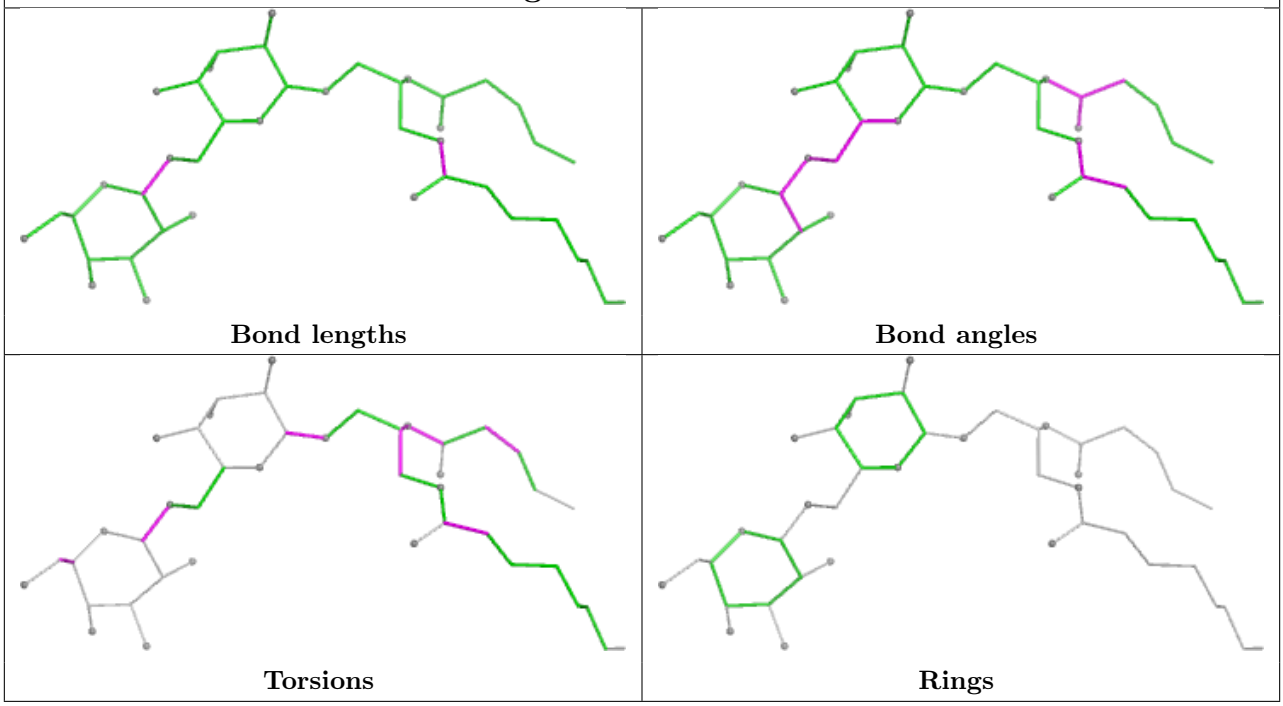
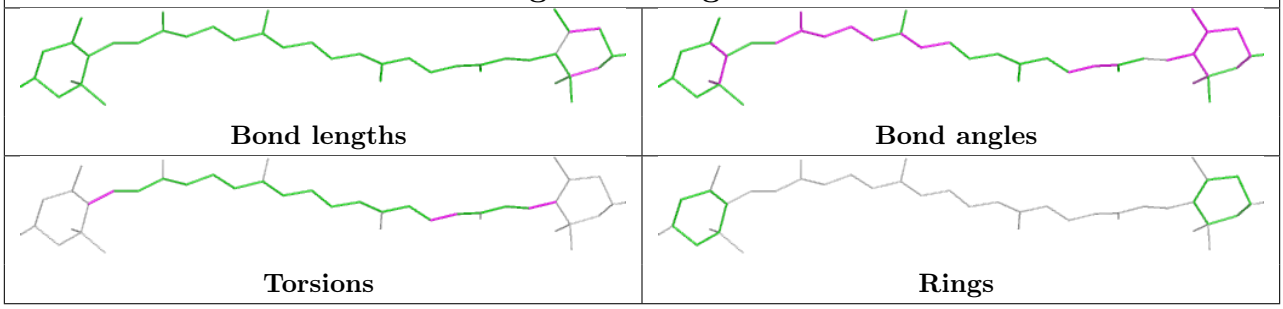


Rings

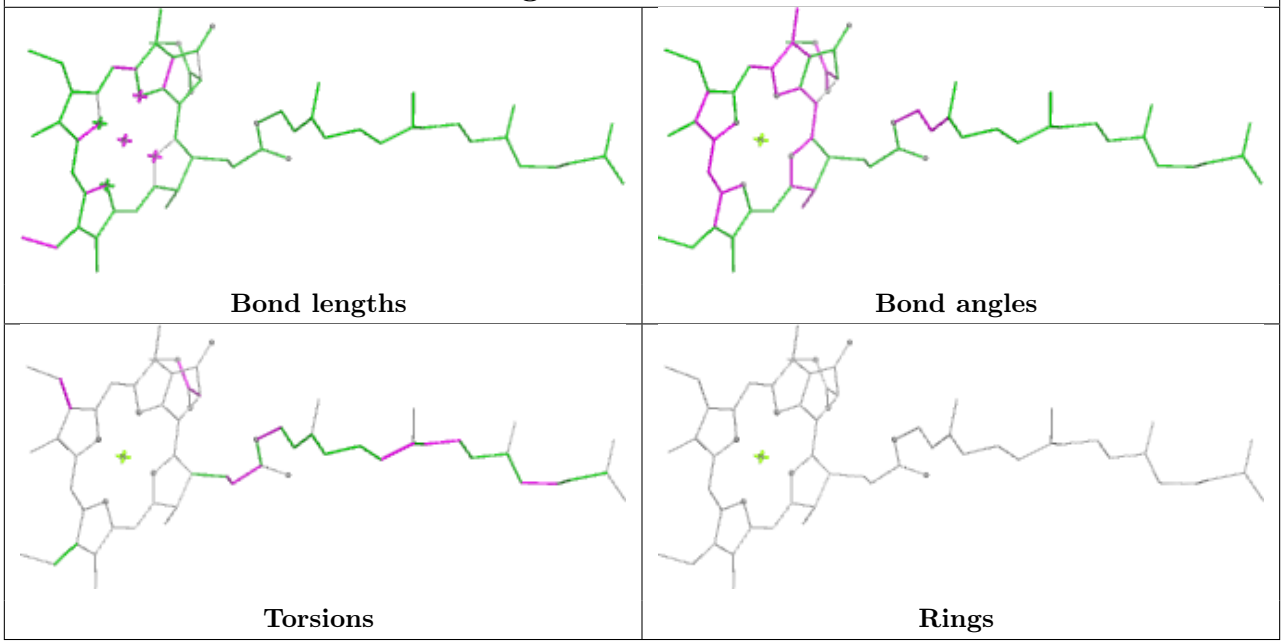
Ligand DGD b 623

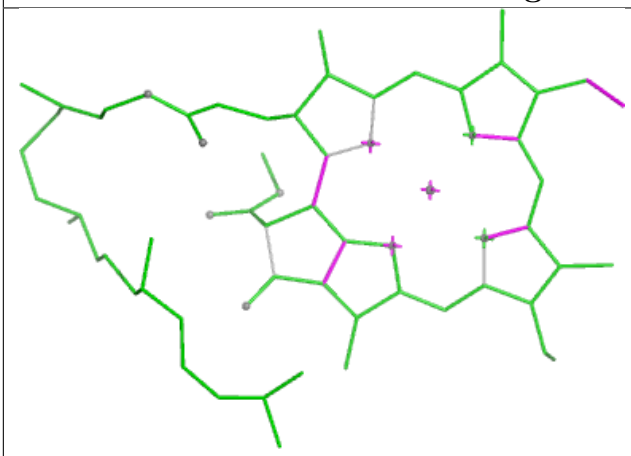
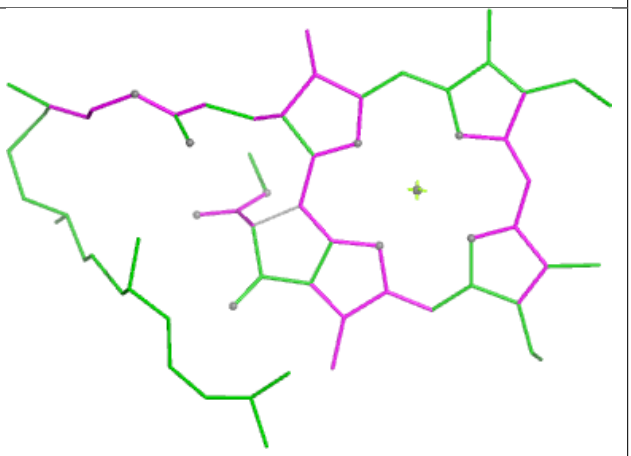
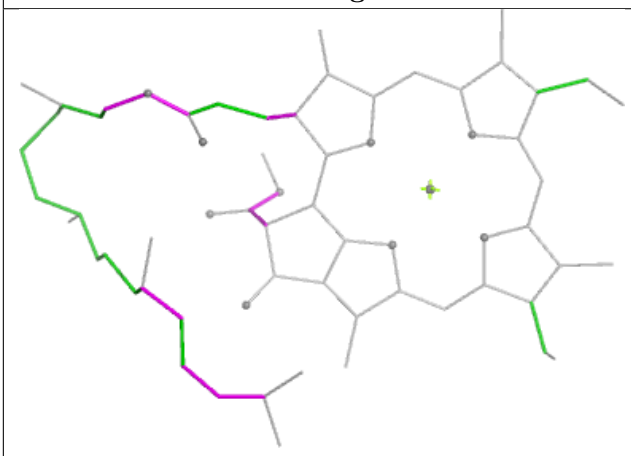
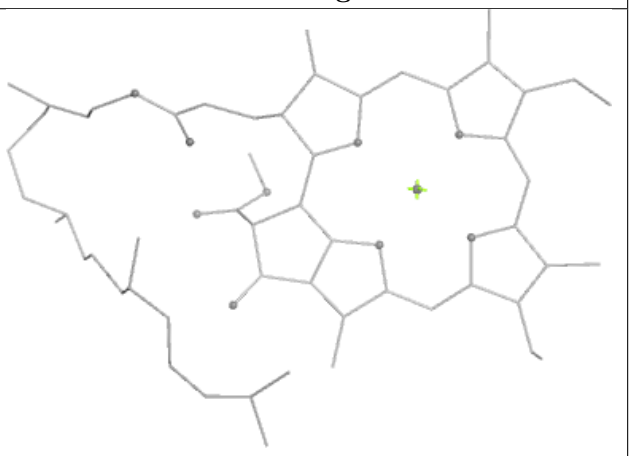


Ligand LUT g 621

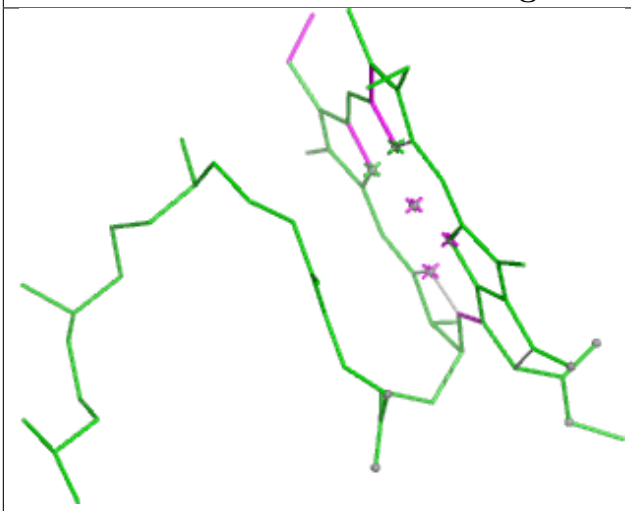


Ligand CLA c1 502

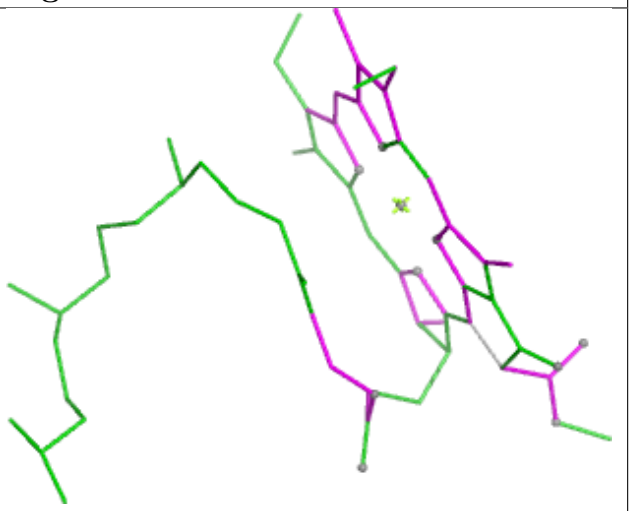


Ligand CLA B 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

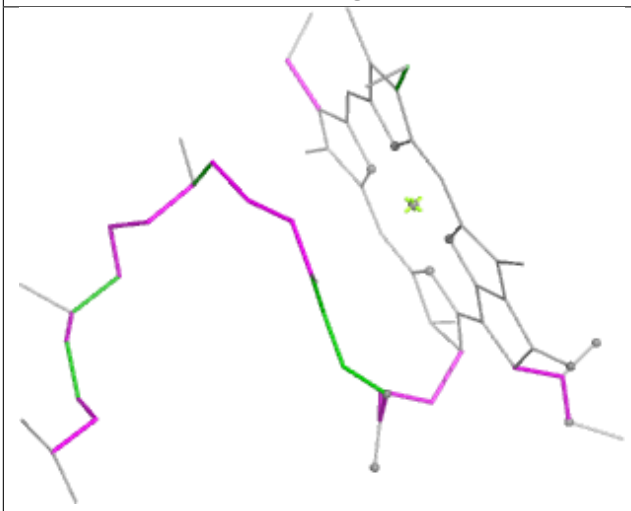
Ligand CLA g1 613



Bond lengths



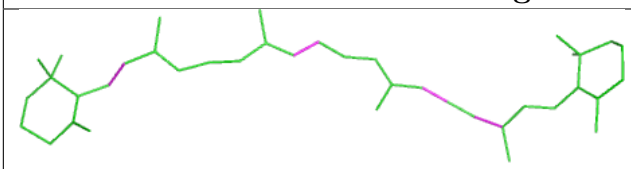
Bond angles



Torsions

Rings

Ligand BCR C1 516



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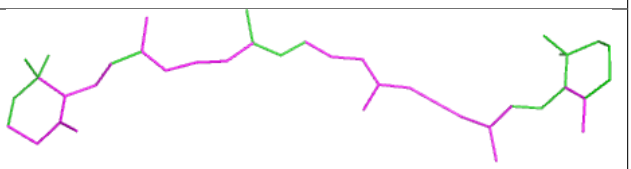
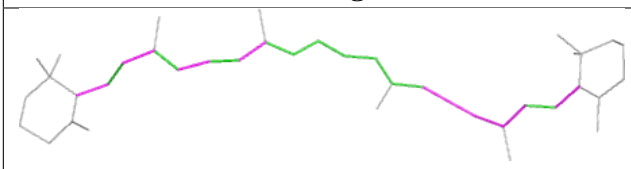


Bond angles



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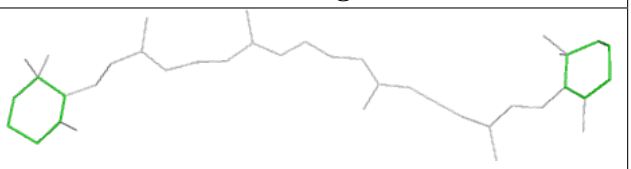
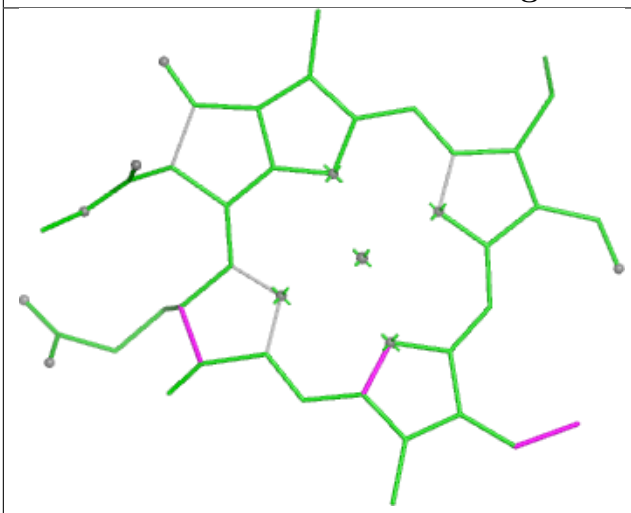
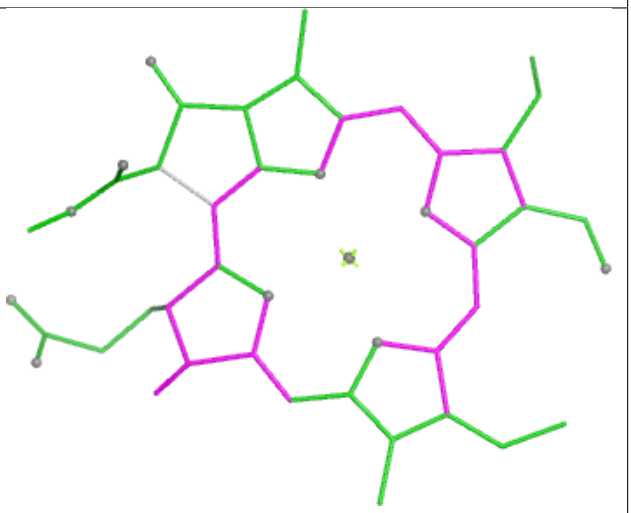
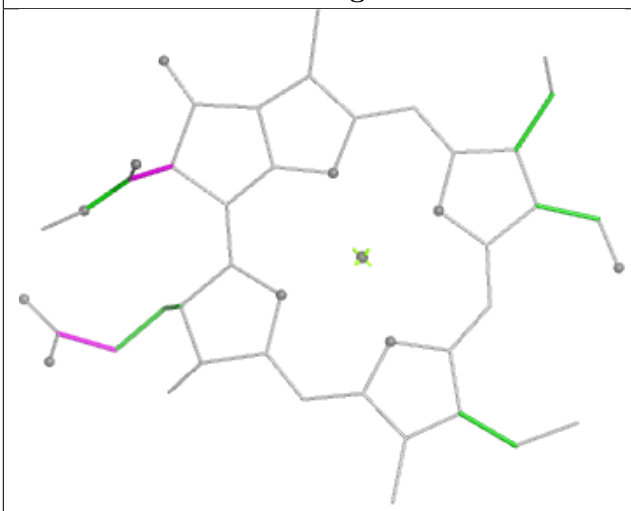
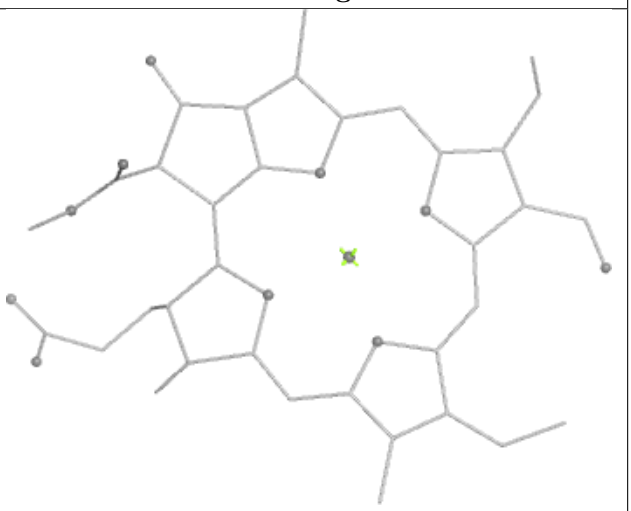
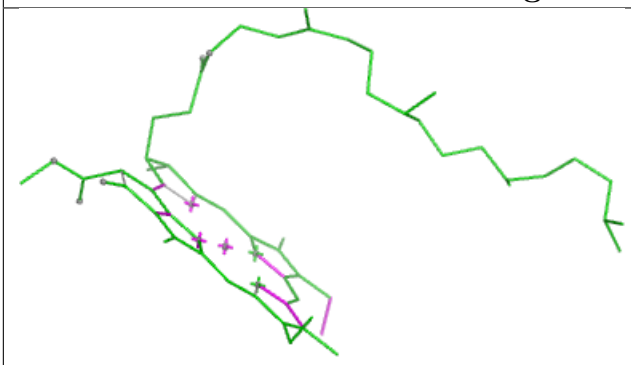
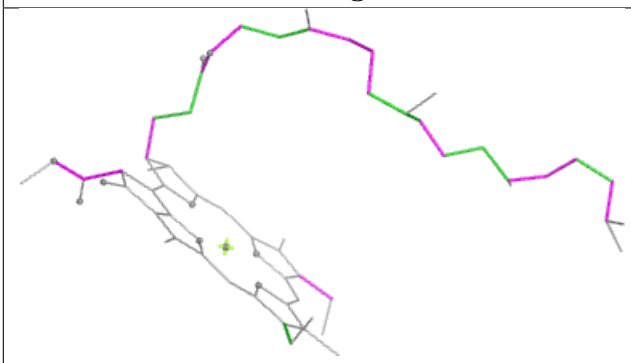
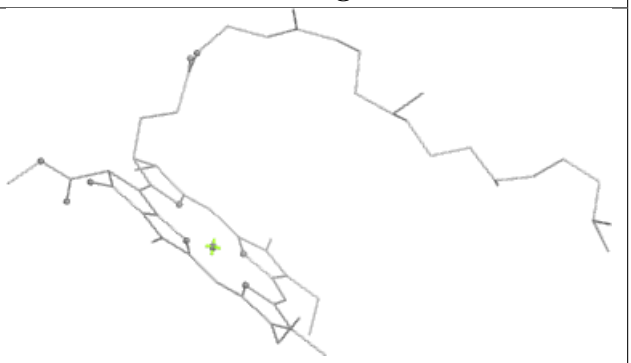
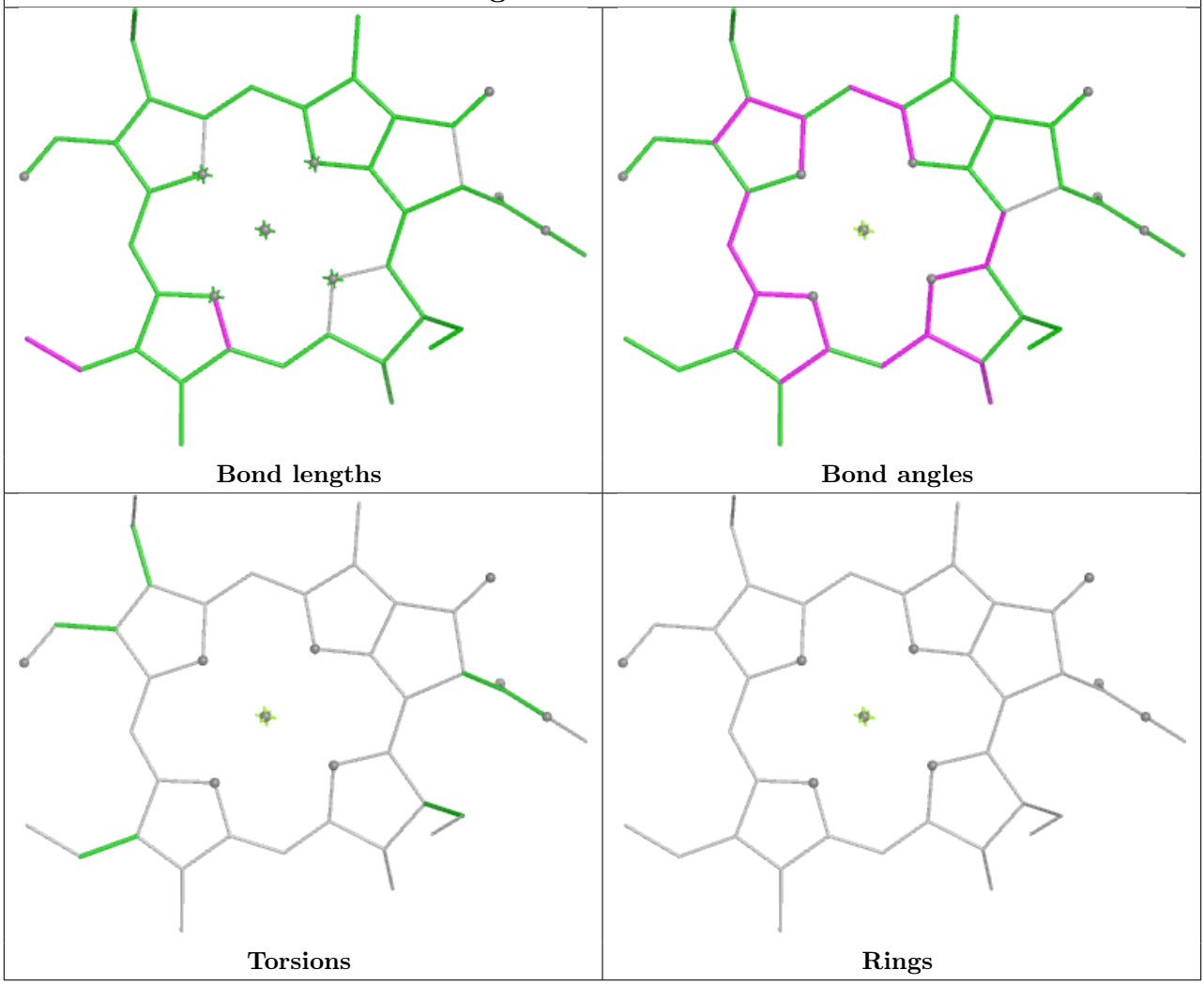


Rings

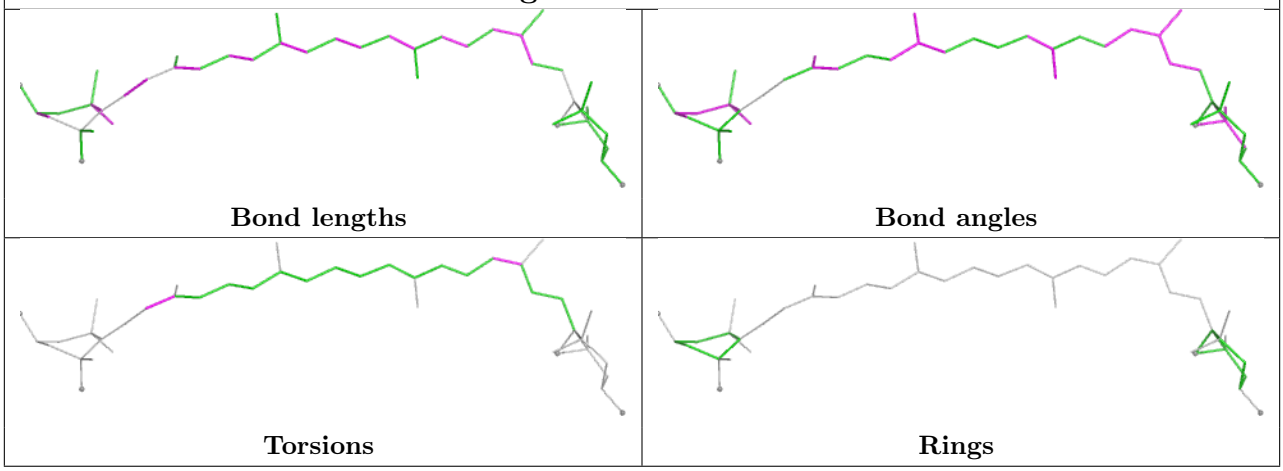
Ligand CHL s1 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Y 614	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand CHL s1 607



Ligand NEX s1 623



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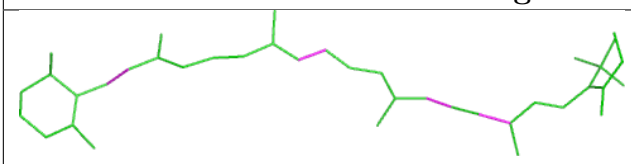
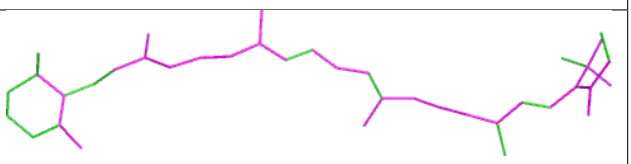
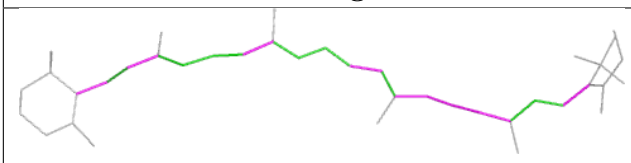
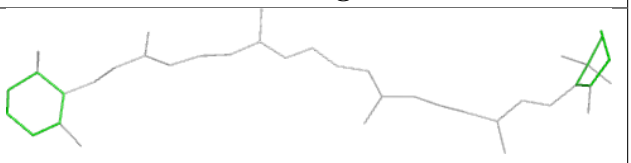
 Bond lengths	 Bond angles
 Torsions	 Rings

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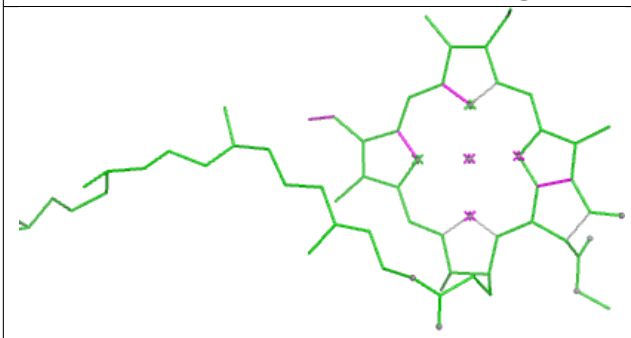
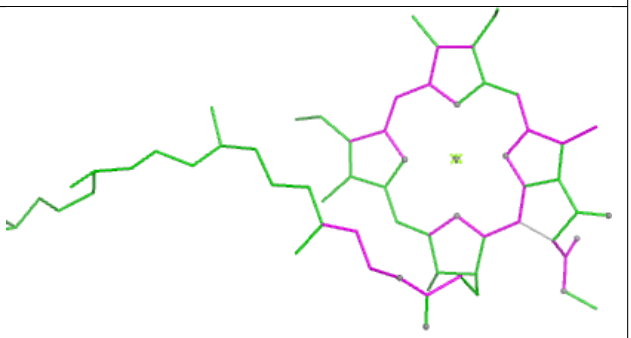
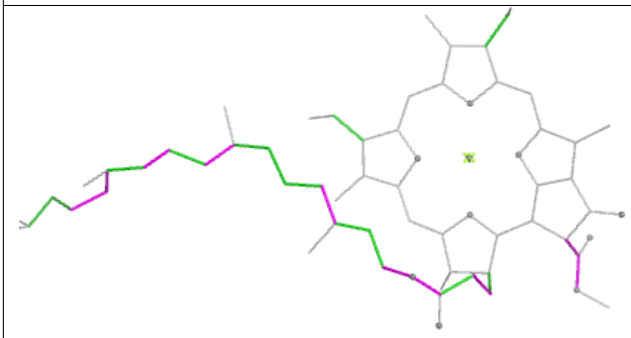
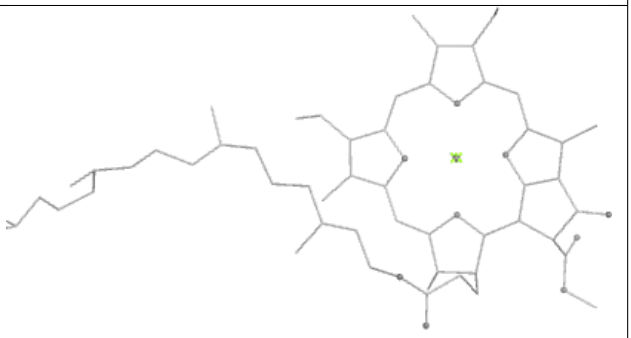
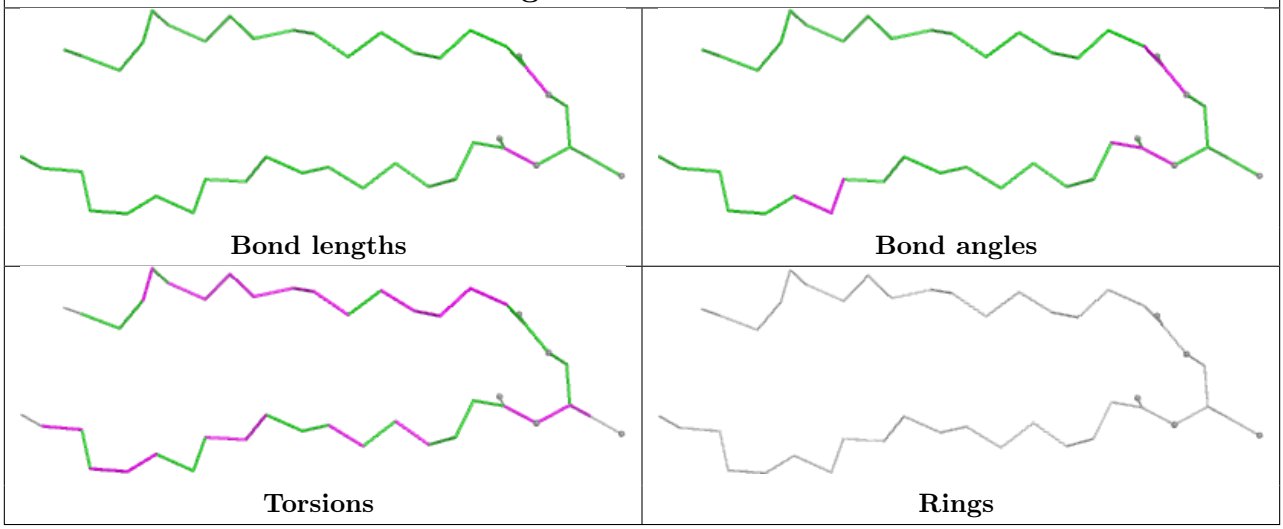
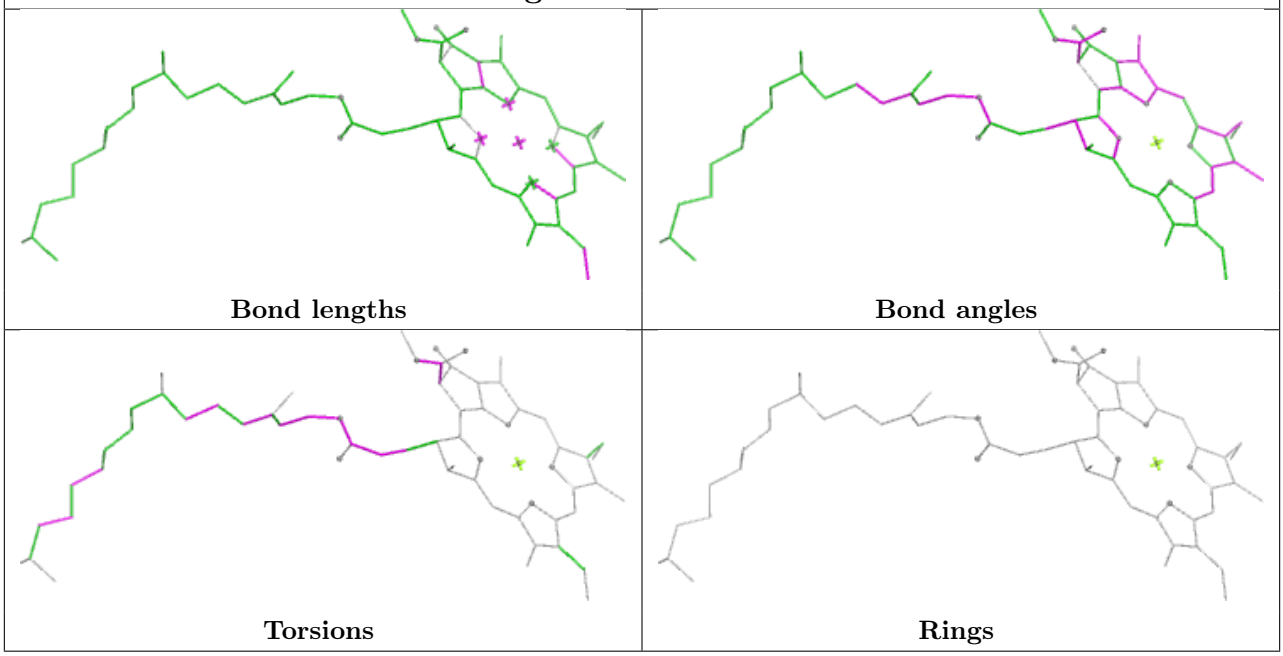
 Bond lengths	 Bond angles
 Torsions	 Rings

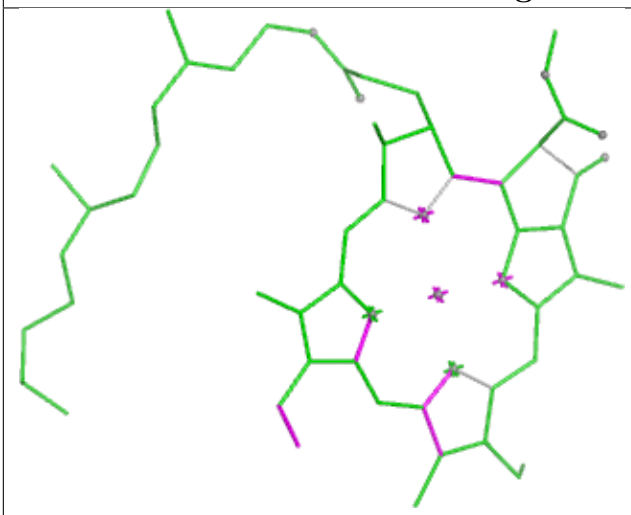
Ligand DGA B 625



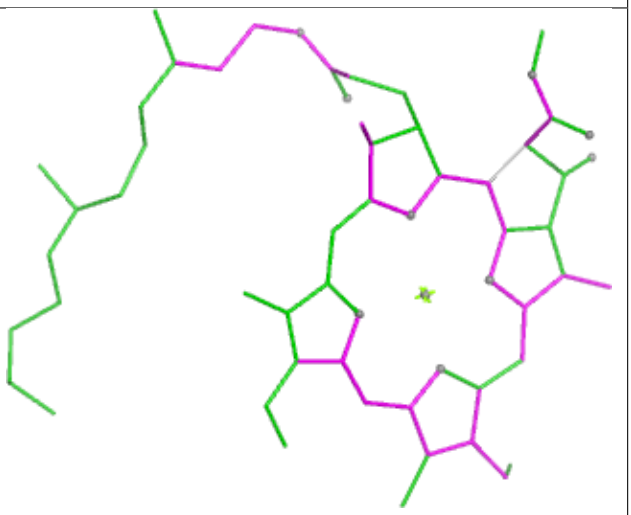
Ligand CLA A 405



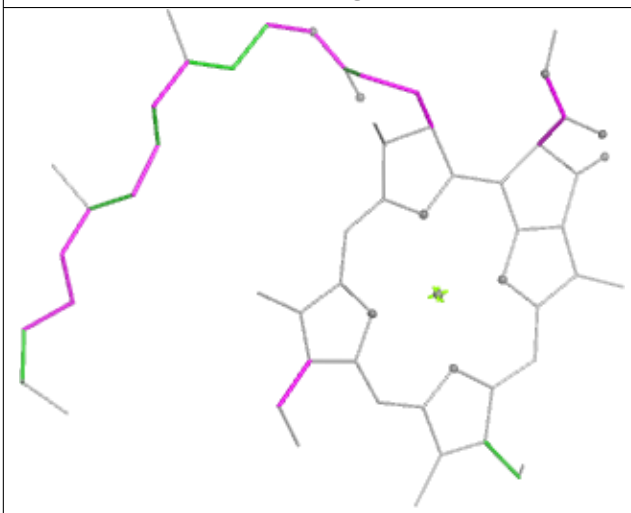
Ligand CLA R1 603



Bond lengths



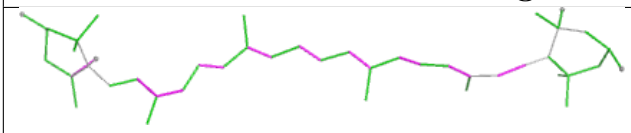
Bond angles



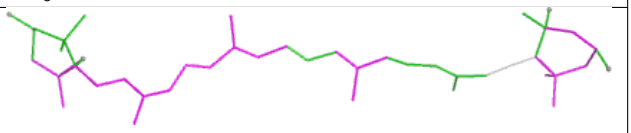
Torsions

Rings

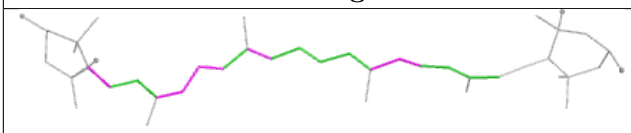
Ligand NEX y1 623



Bond lengths



Bond angles



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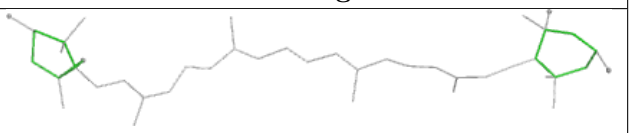
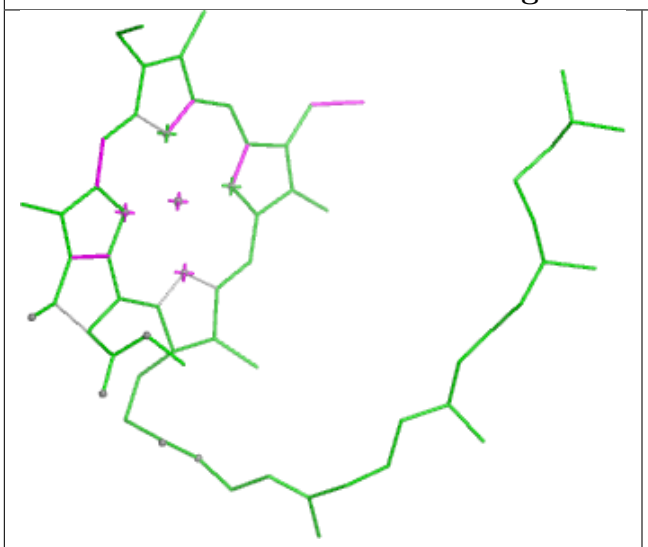
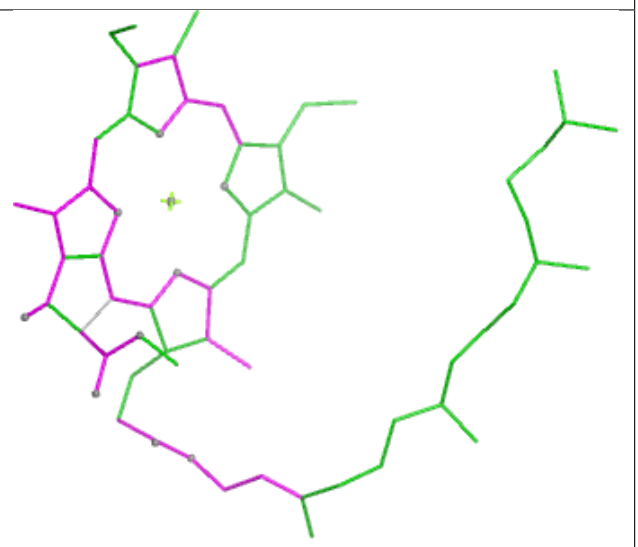


Rings

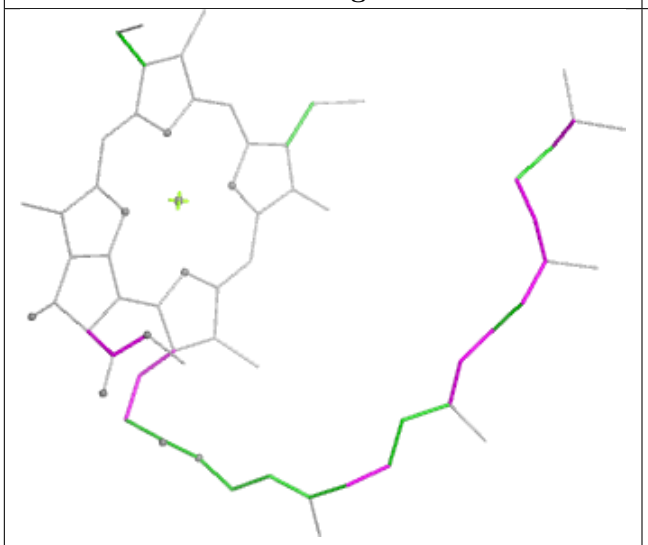
Ligand CLA c1 507



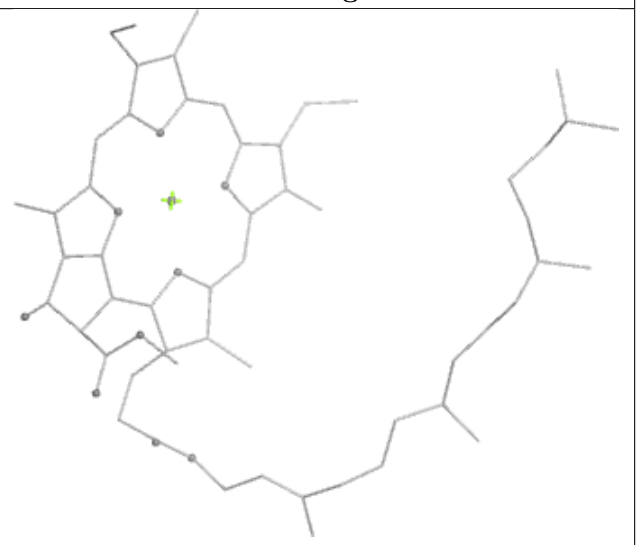
Bond lengths



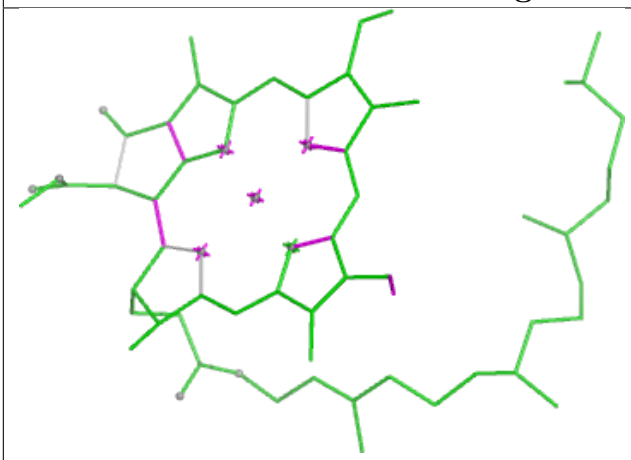
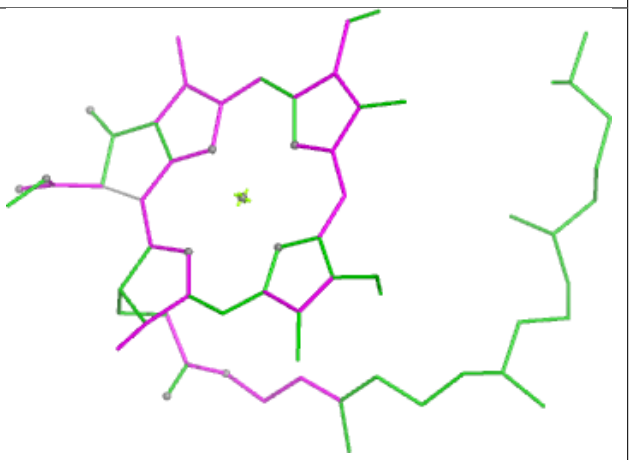
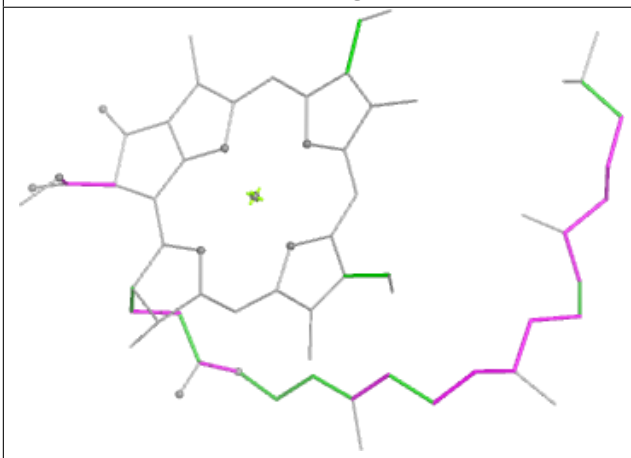
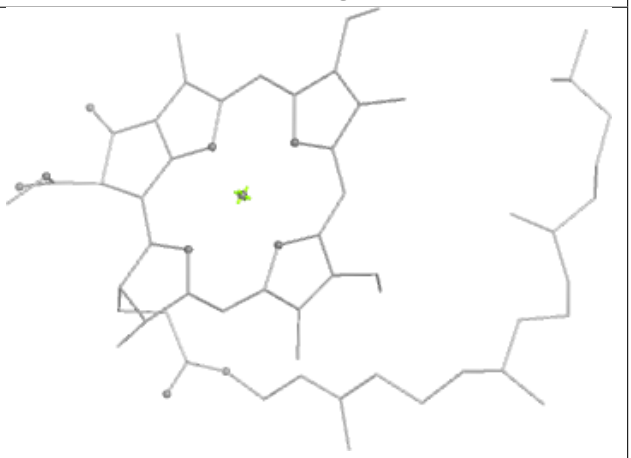
Bond angles



Torsions



Rings

Ligand CLA Y1 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

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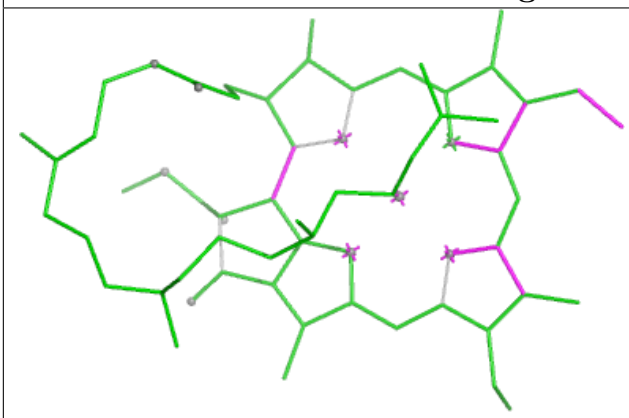
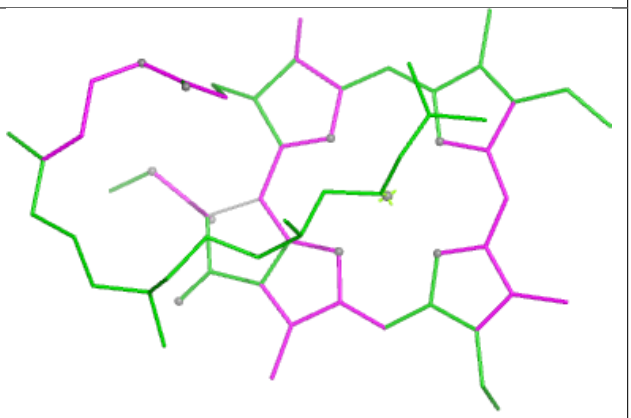
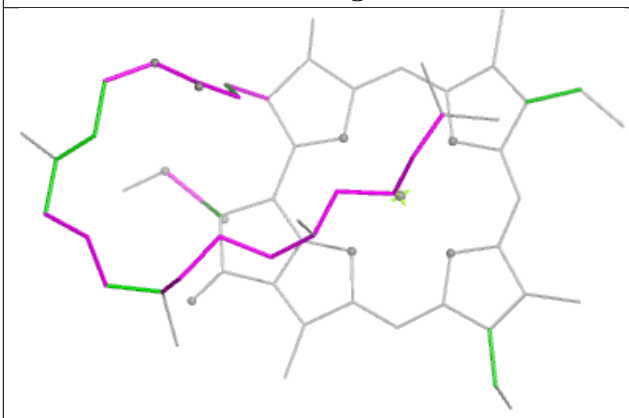
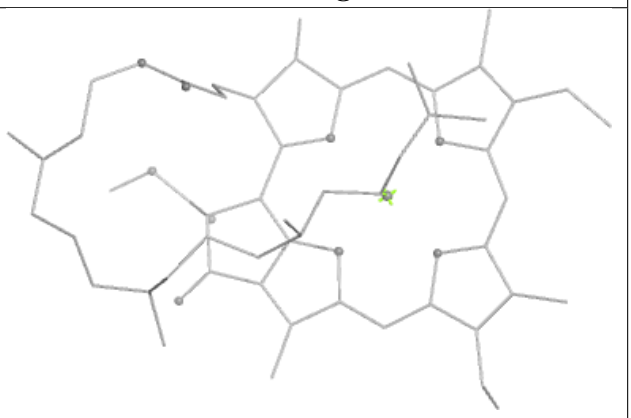
 Bond lengths	 Bond angles
 Torsions	 Rings

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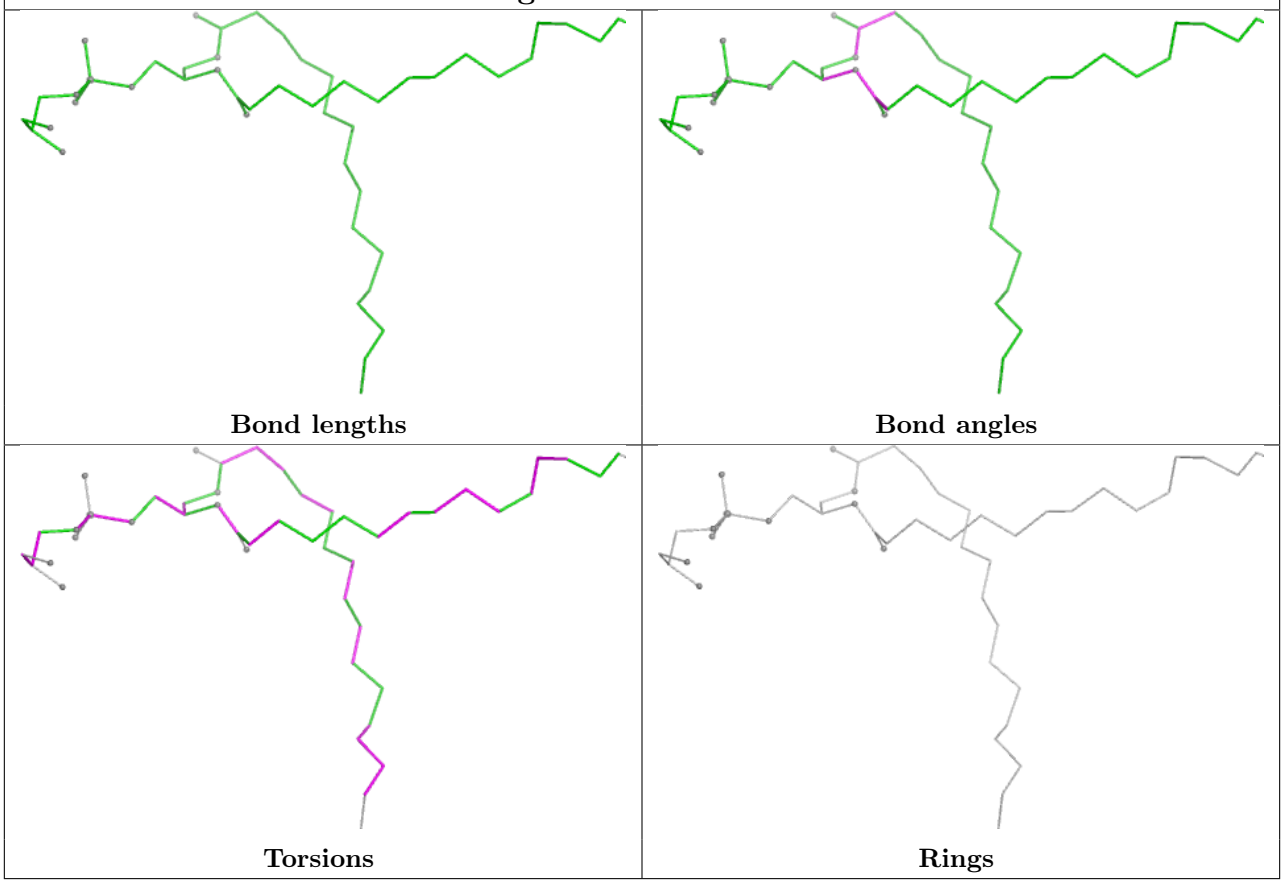

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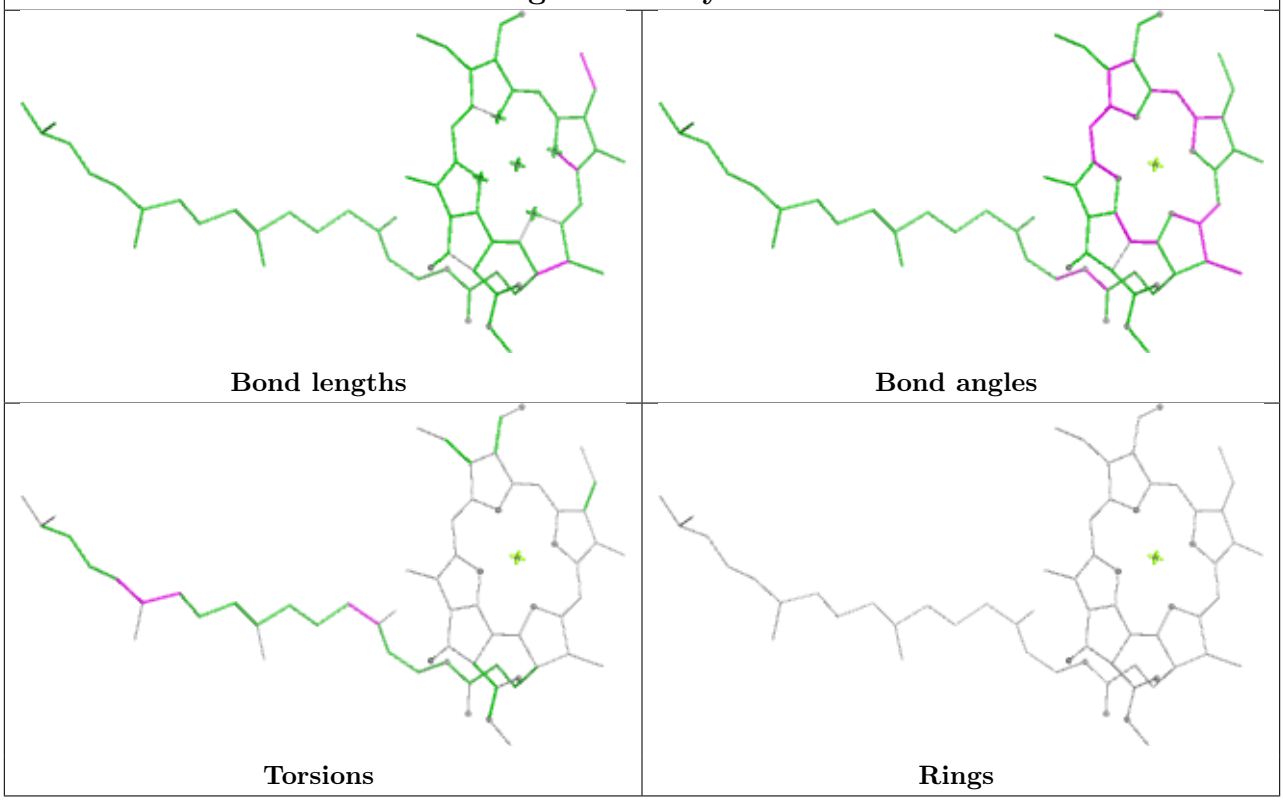

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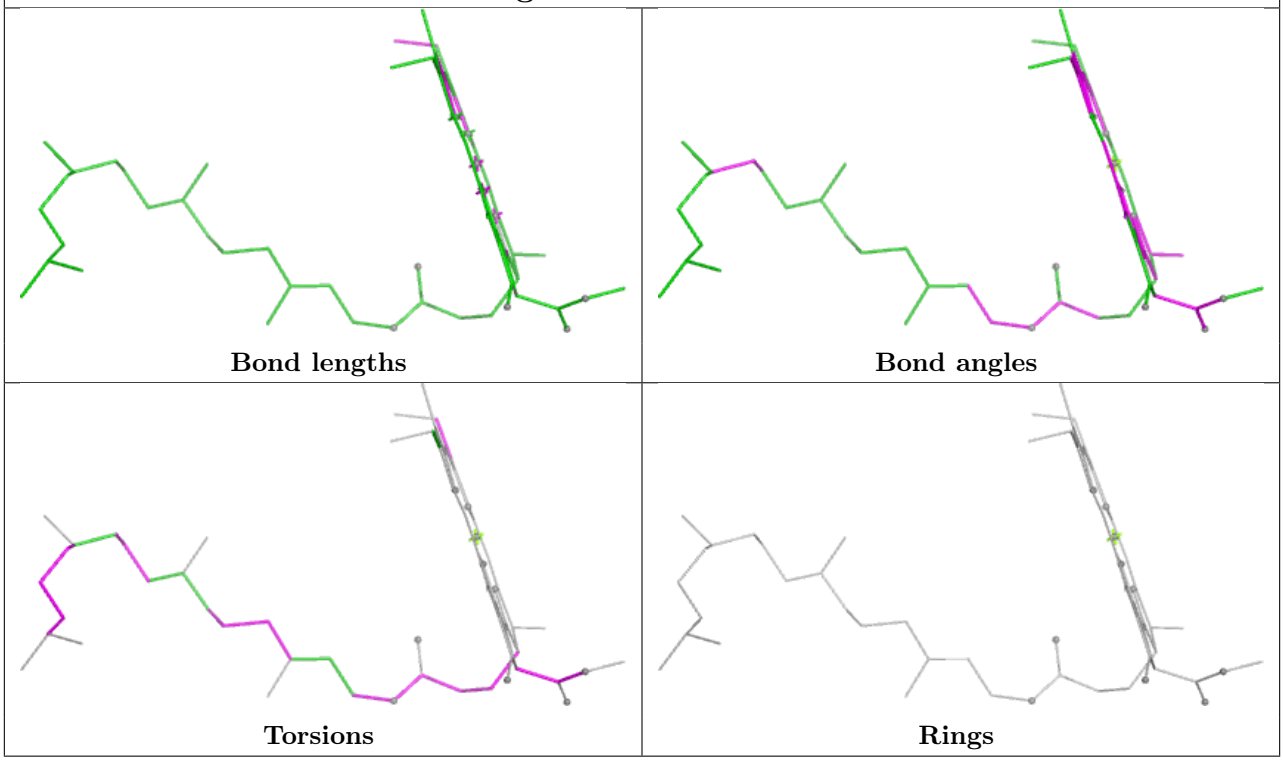
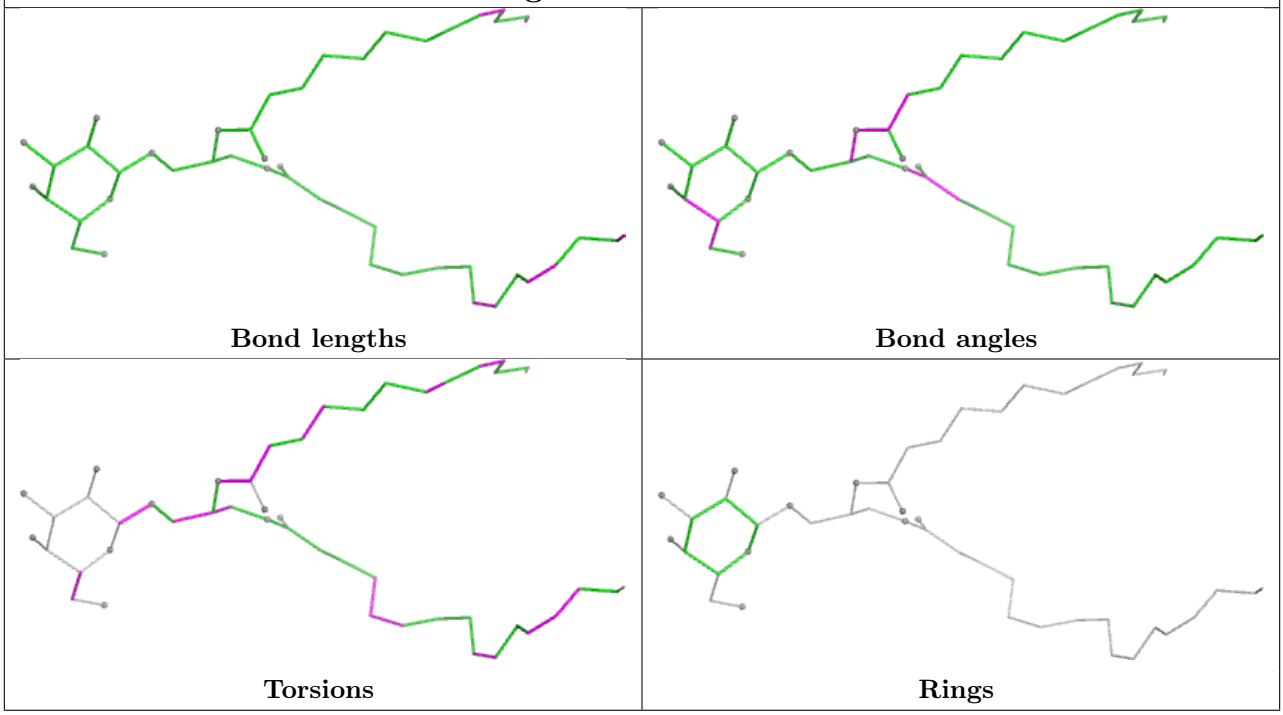
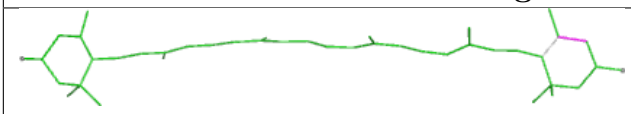


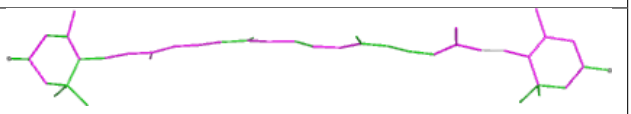
Ligand LMG a 413



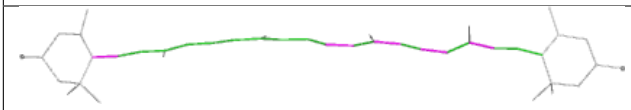
Ligand LUT N1 620



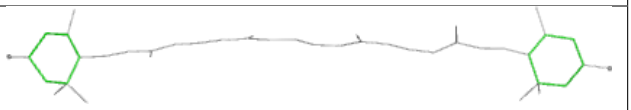
Bond lengths



Bond angles

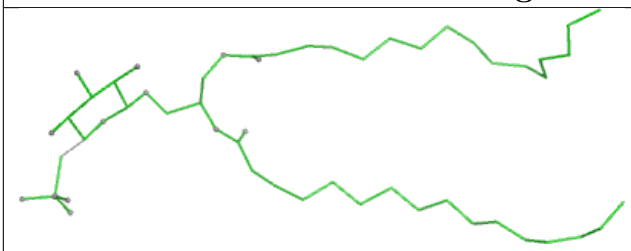


Torsions



Rings

Ligand SQD C1 526



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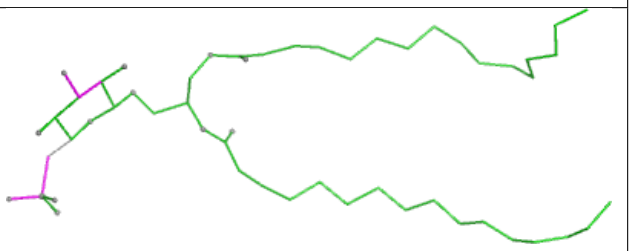
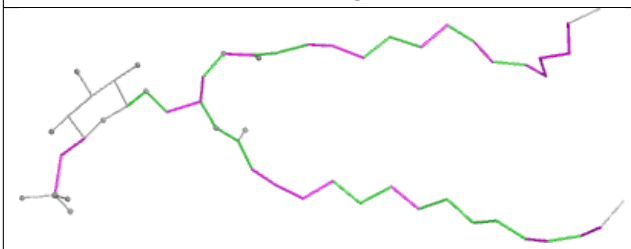


Bond angles



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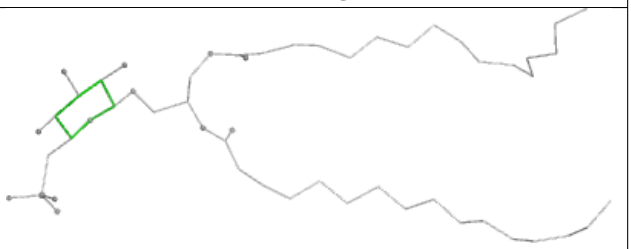
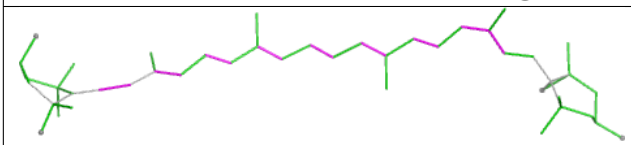


Rings

Ligand NEX n1 623



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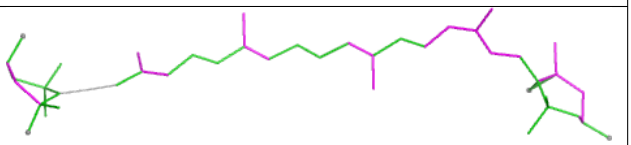
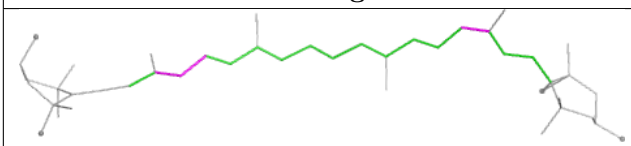


Bond angles



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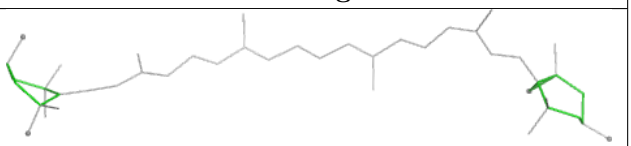
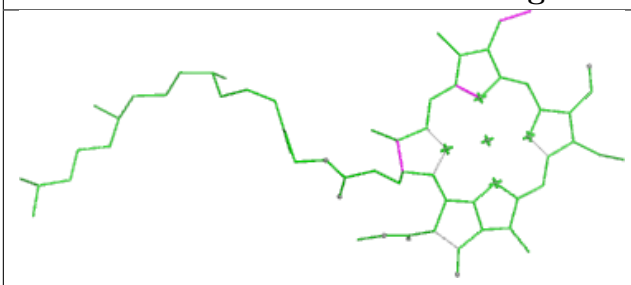
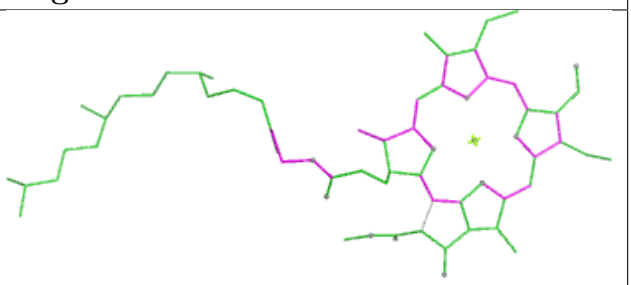
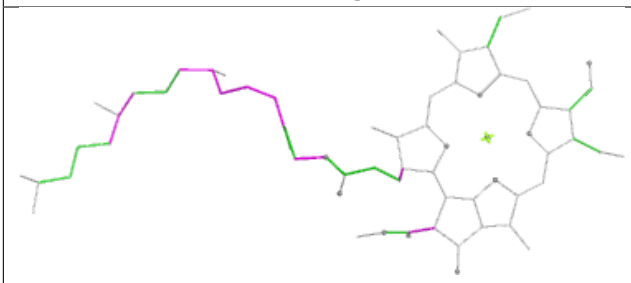
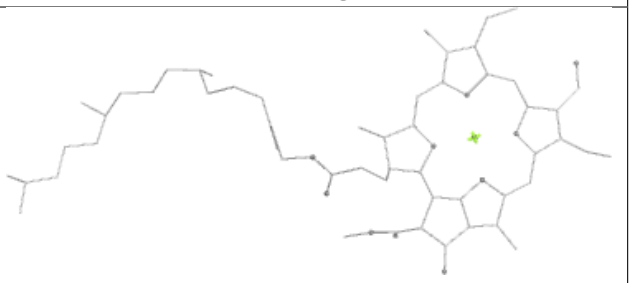


Rings

Ligand CHL g 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

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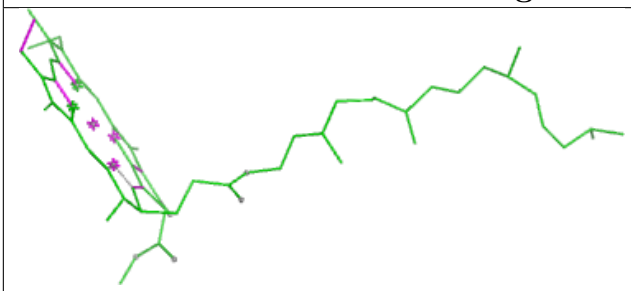
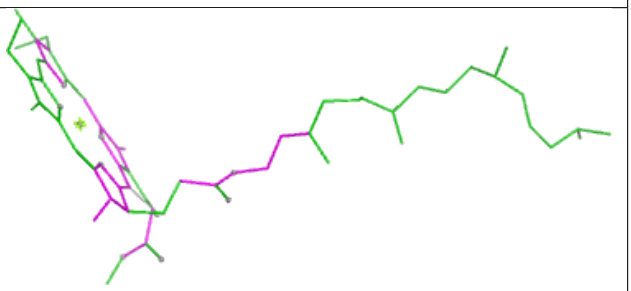
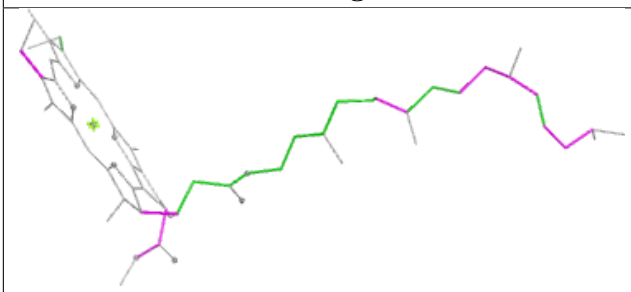
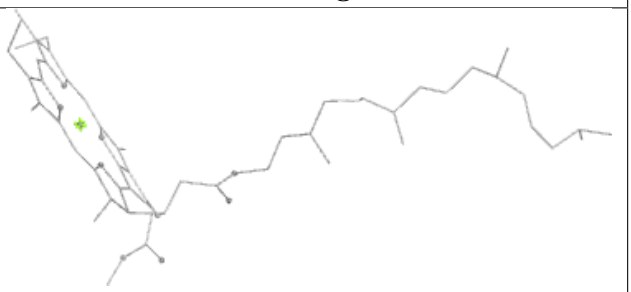
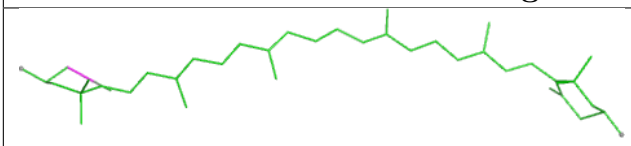
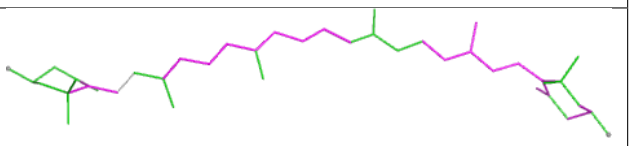
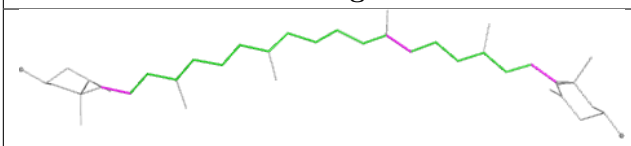
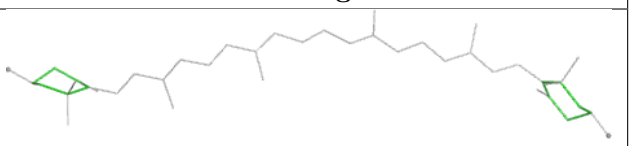
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT s1 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

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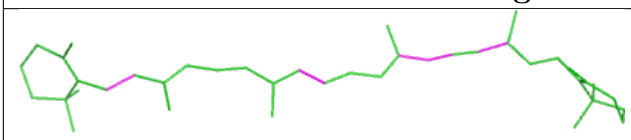
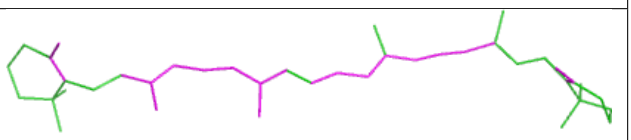
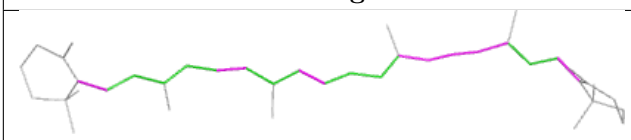
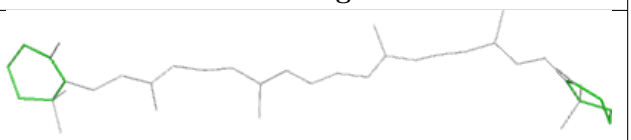
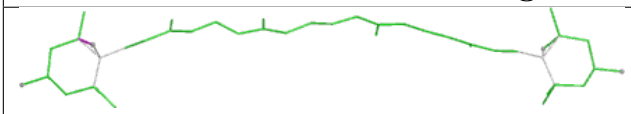
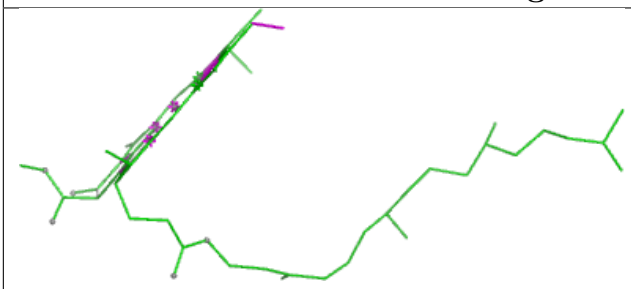
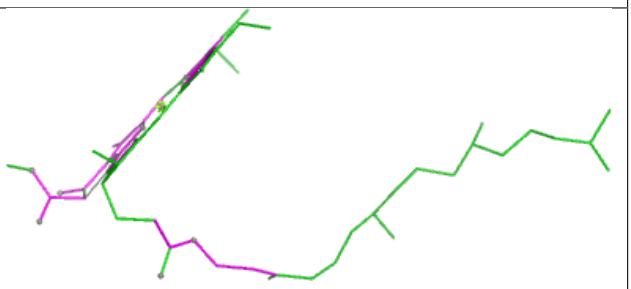
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT y1 622	
 Bond lengths	Bond angles
Torsions	Rings

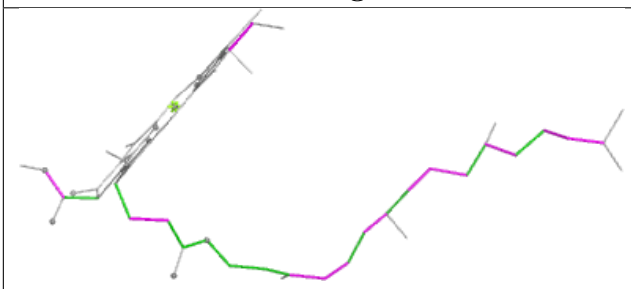
Ligand CLA n 604



Bond lengths



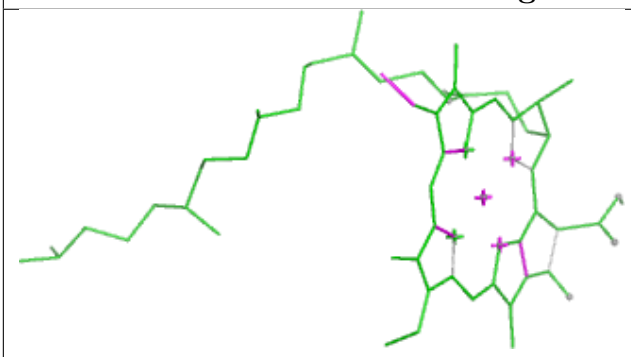
Bond angles



Torsions

Rings

Ligand CLA S1 610



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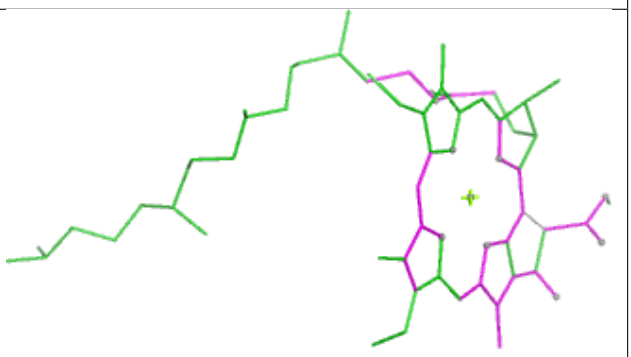
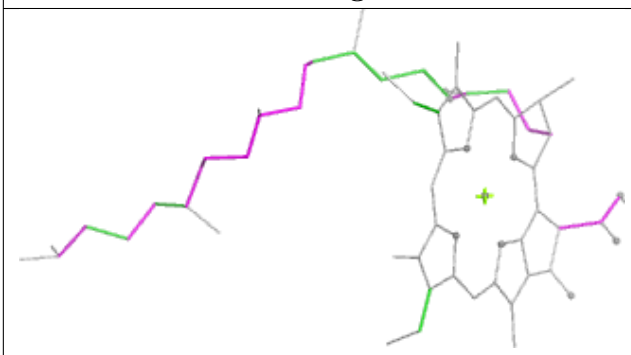
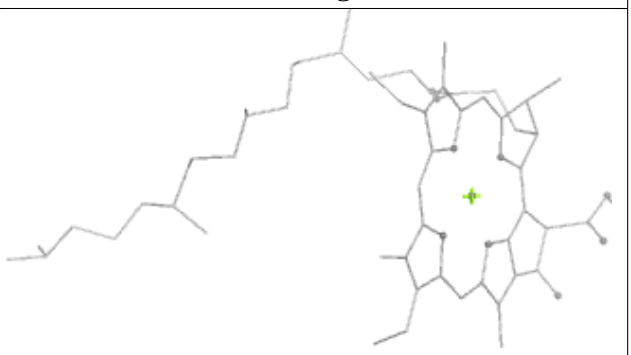


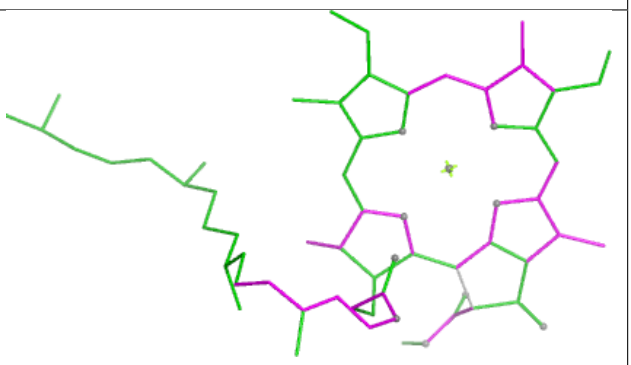
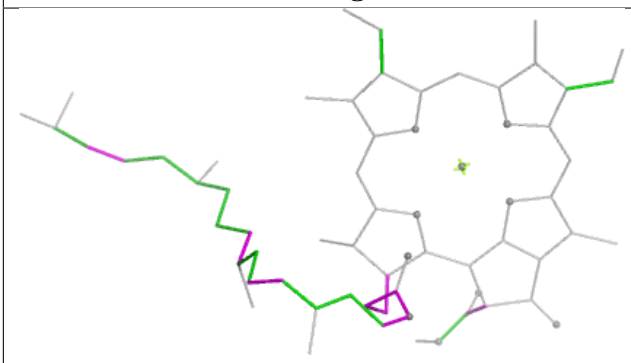
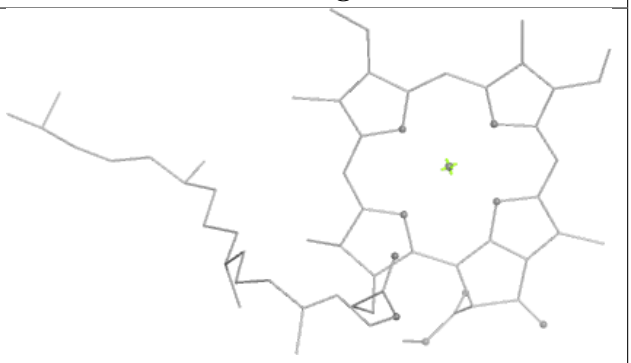
Bond angles



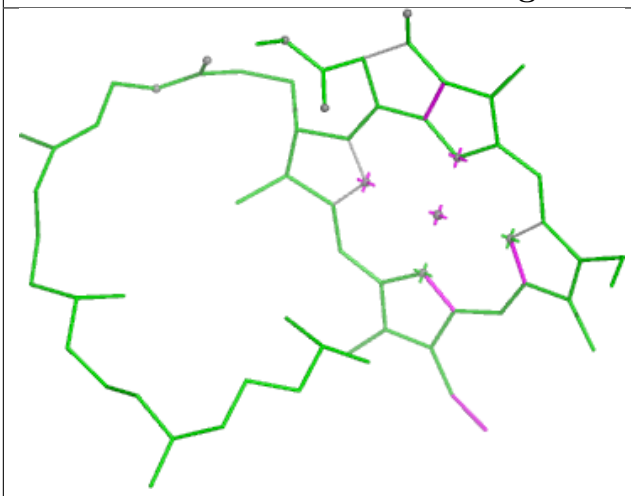
Torsions



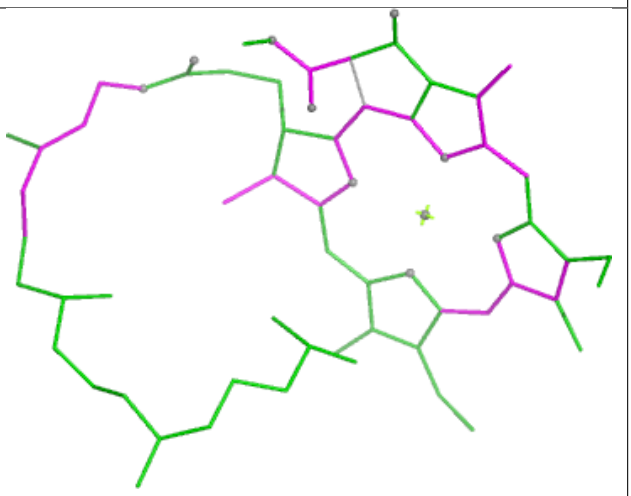
Rings

Ligand CLA A 406	
Bond lengths	 Bond angles
 Torsions	 Rings

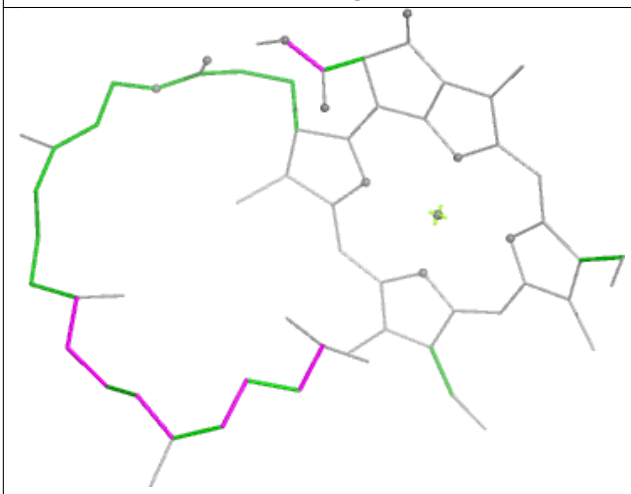
Ligand CLA b1 616



Bond lengths



Bond angles



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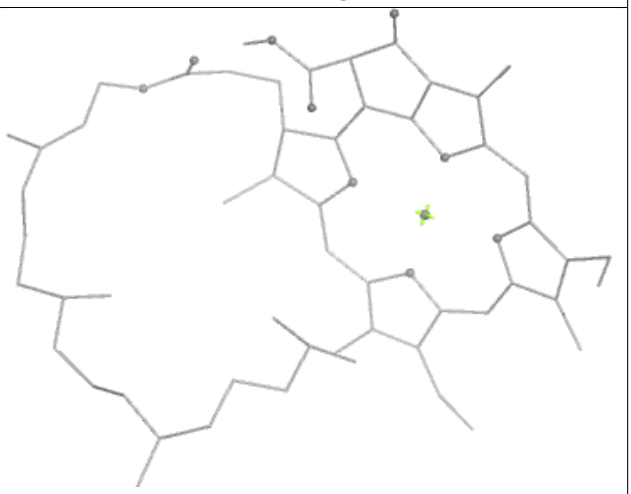
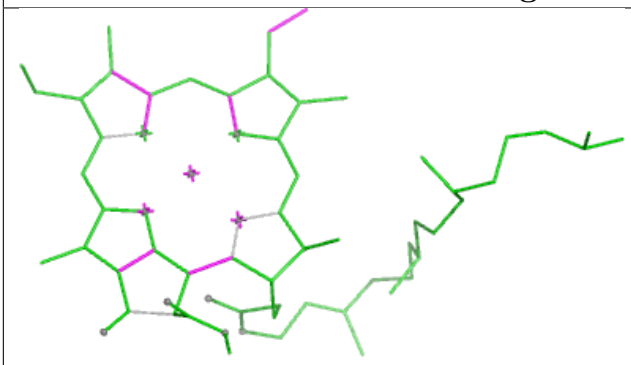
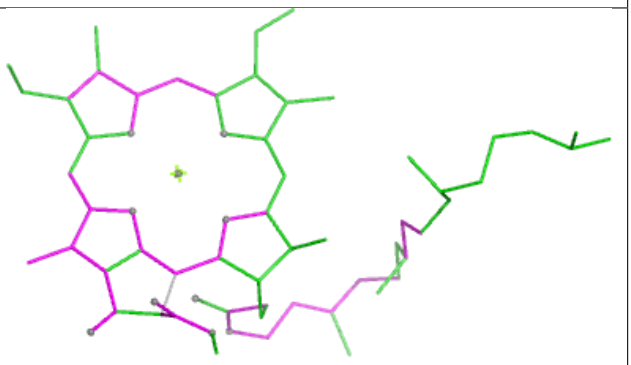
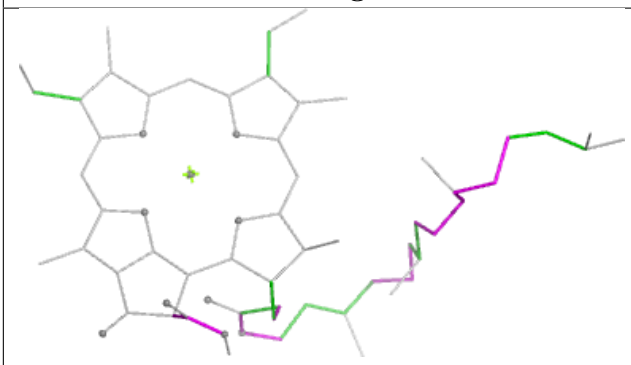
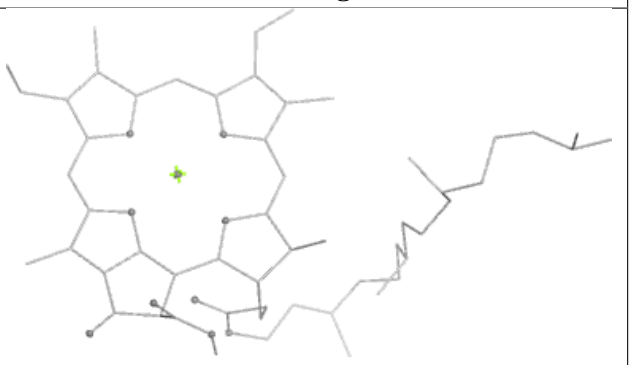
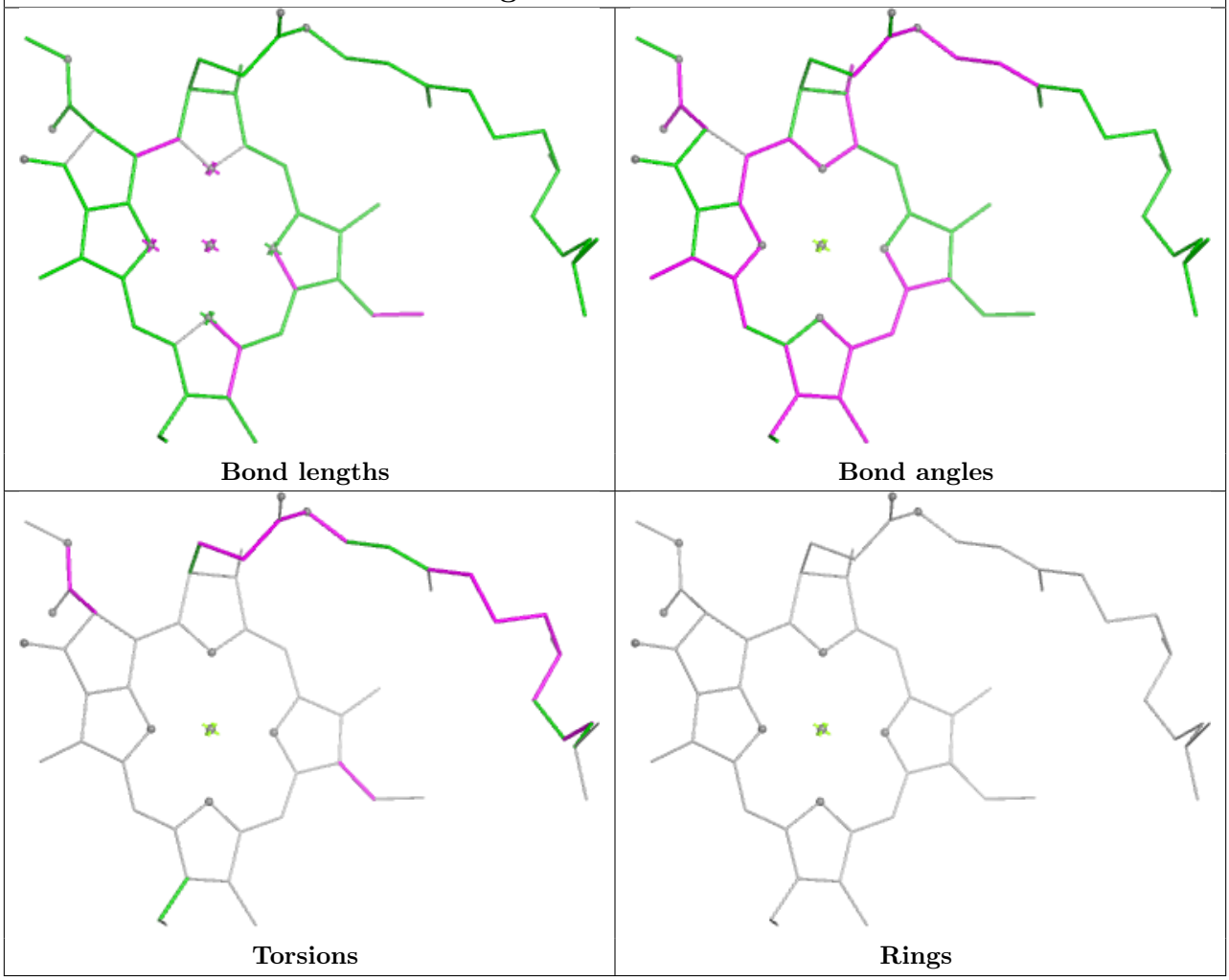


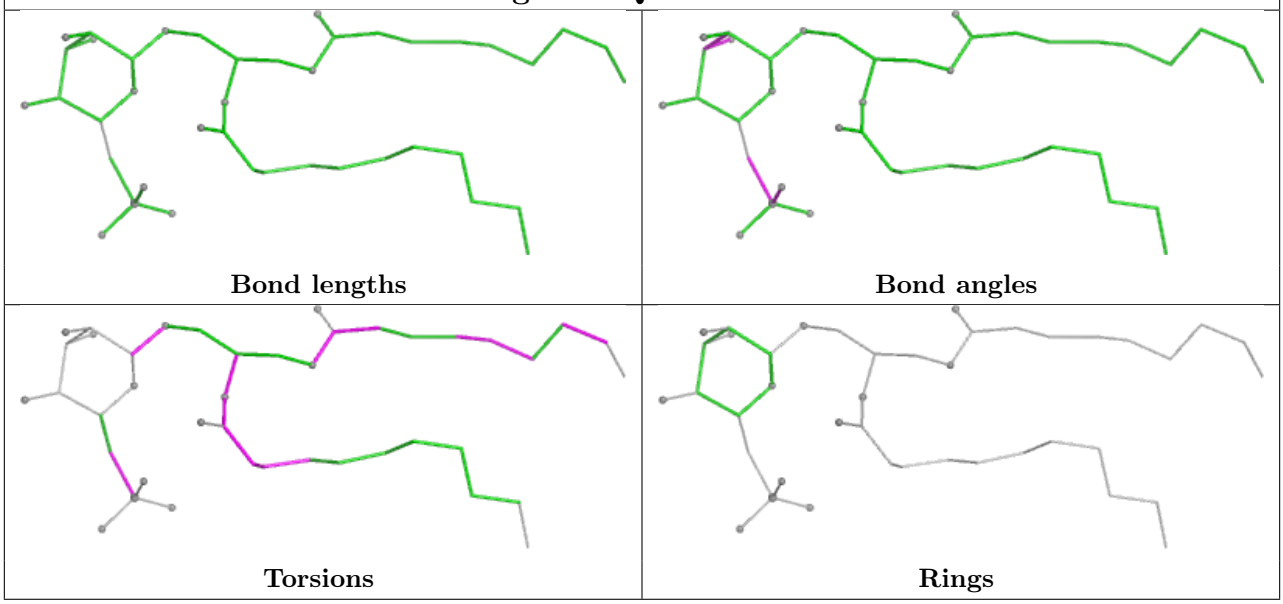
Rings

Ligand CLA a1 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

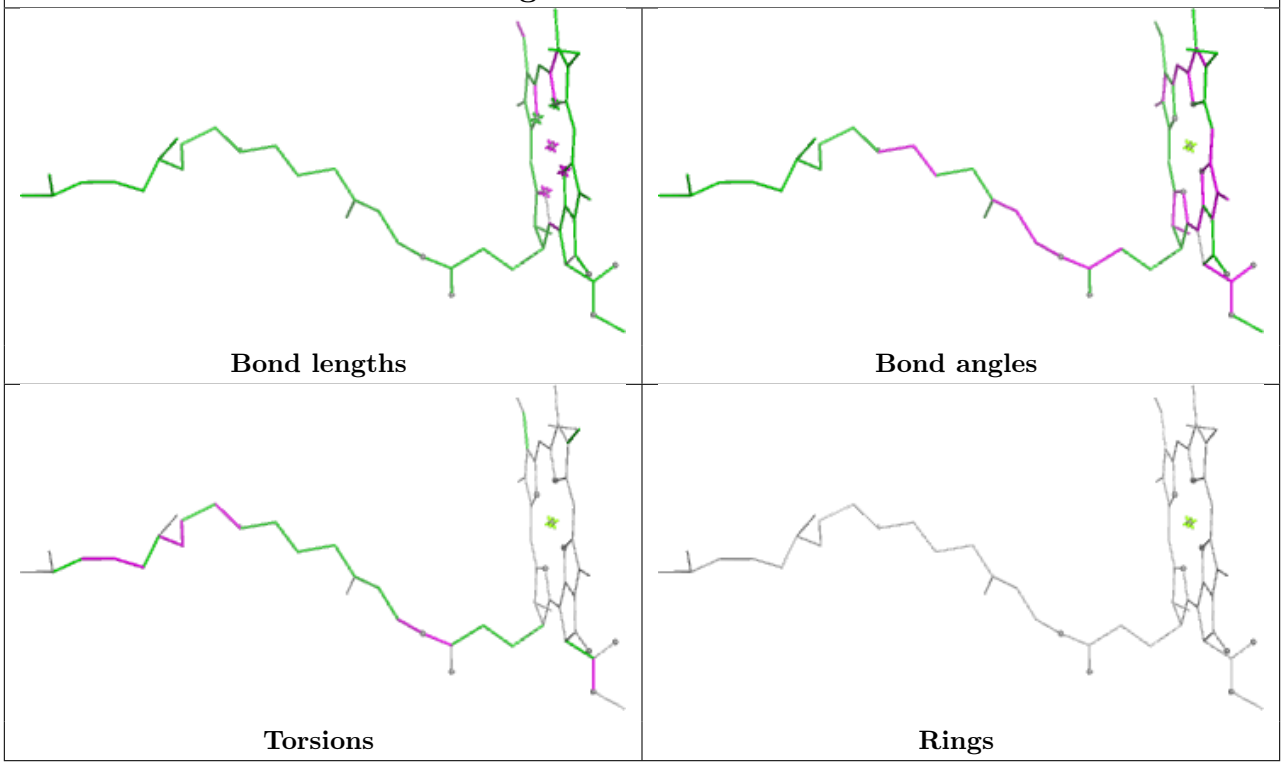
Ligand CLA r1 609



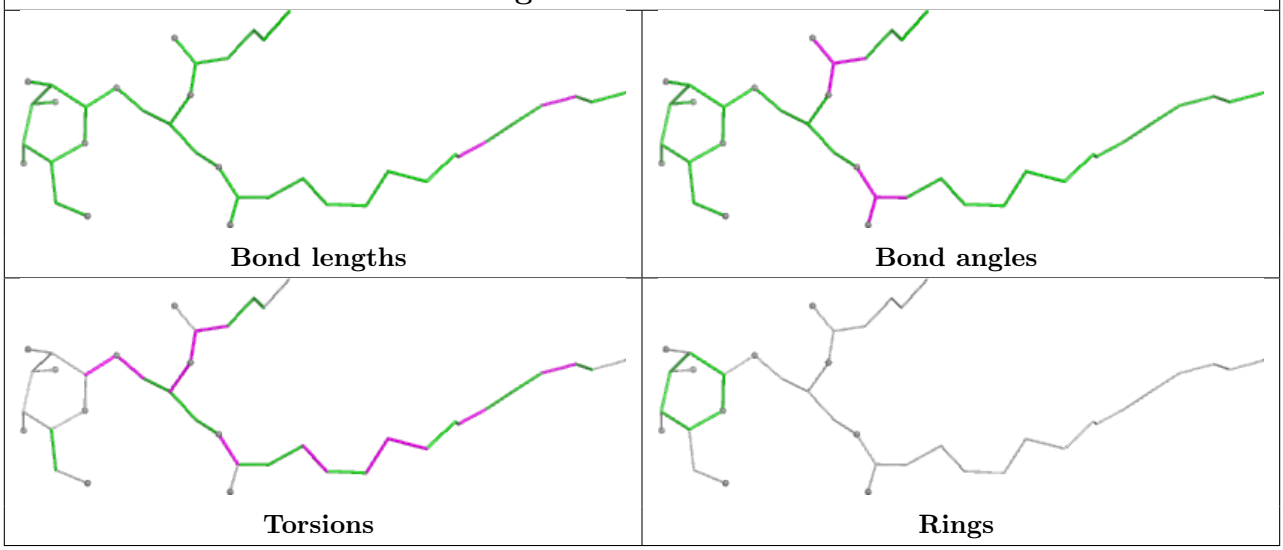
Ligand SQD M1 101

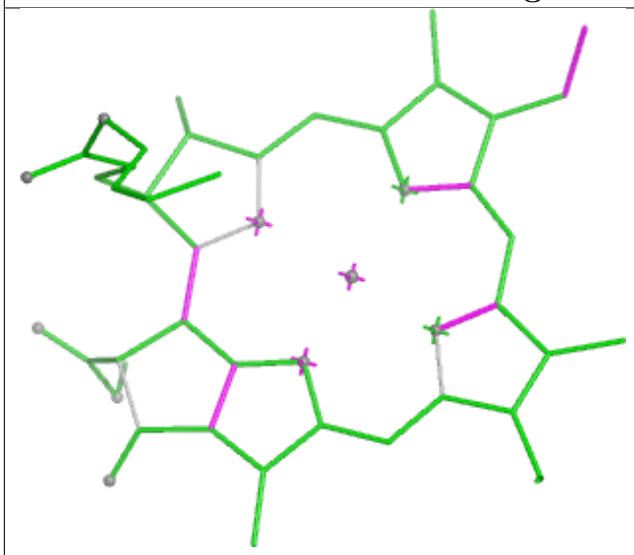
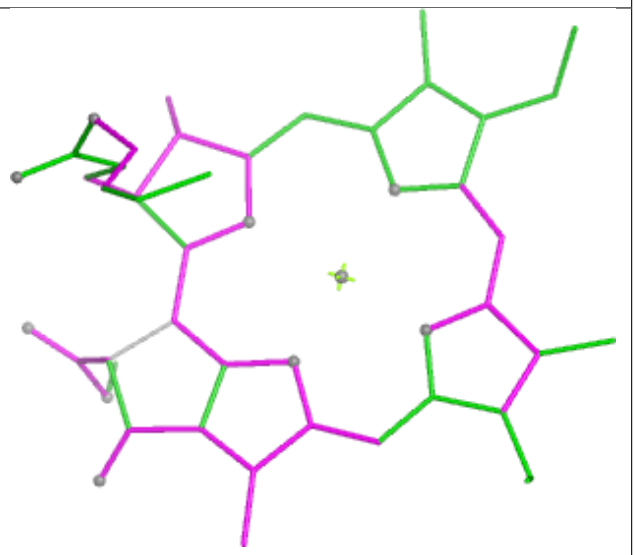
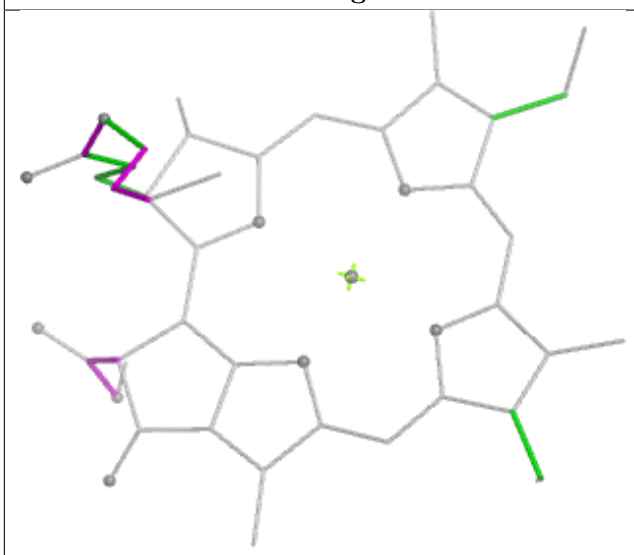
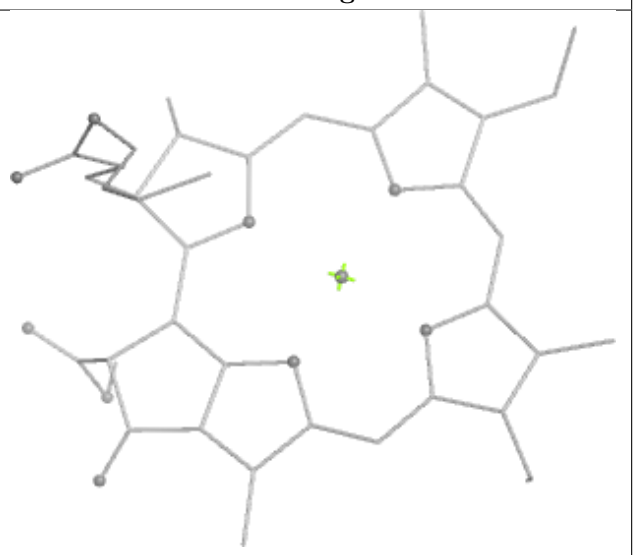


Ligand CLA d1 403

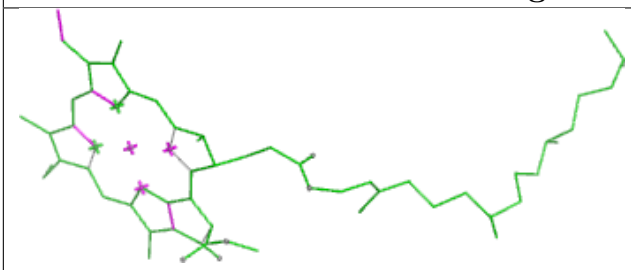


Ligand LMG W 201



Ligand CLA G 604	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA a 405



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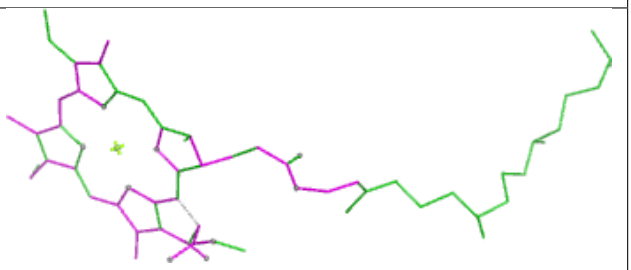
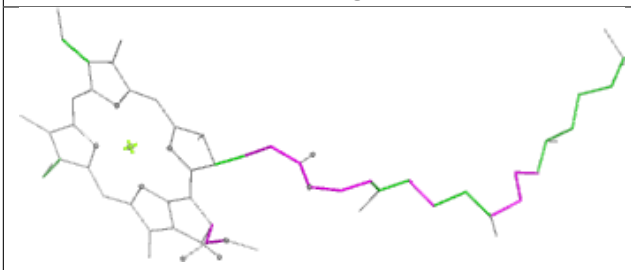


Bond angles



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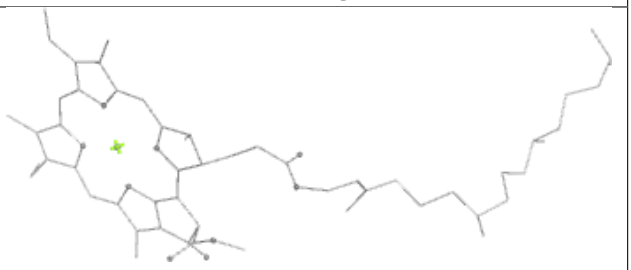
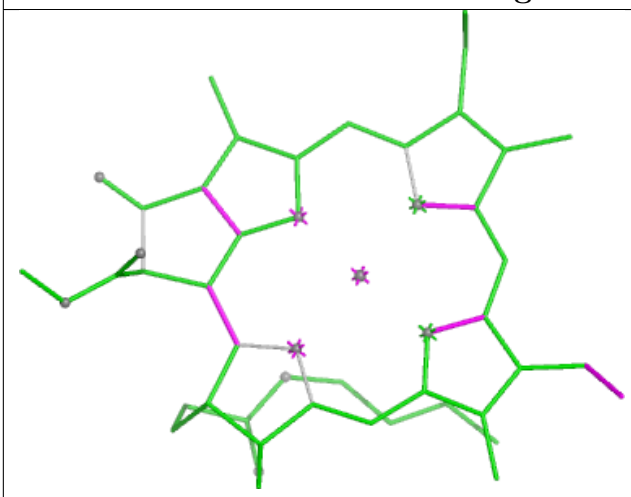


Rings

Ligand CLA N1 614



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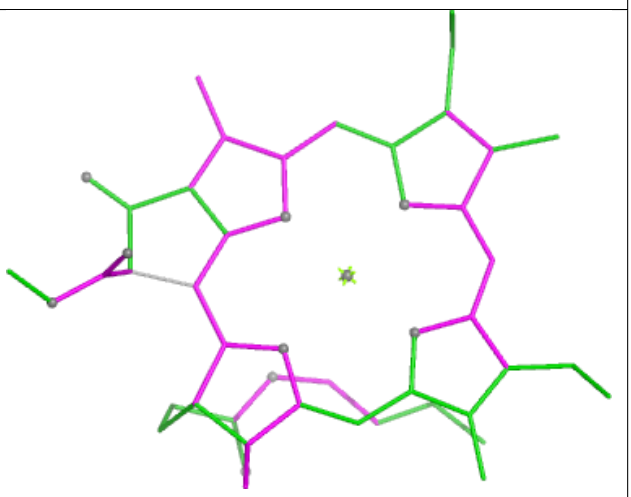
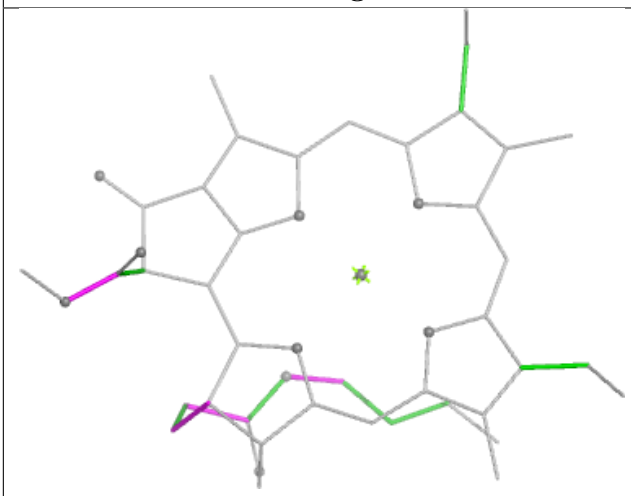


Bond angles



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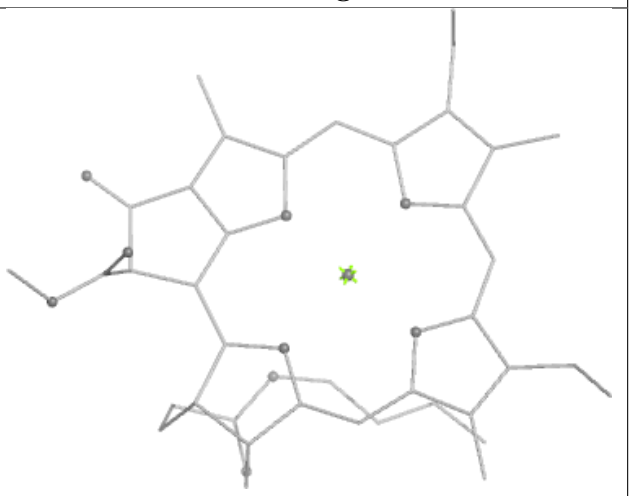
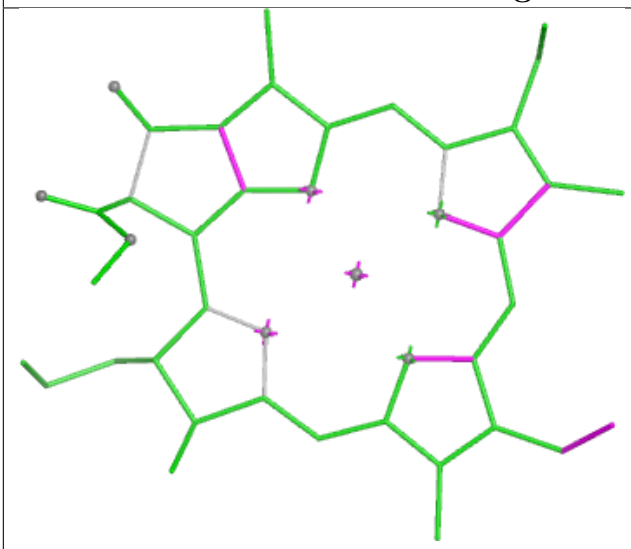


Rings

Ligand CLA G1 612



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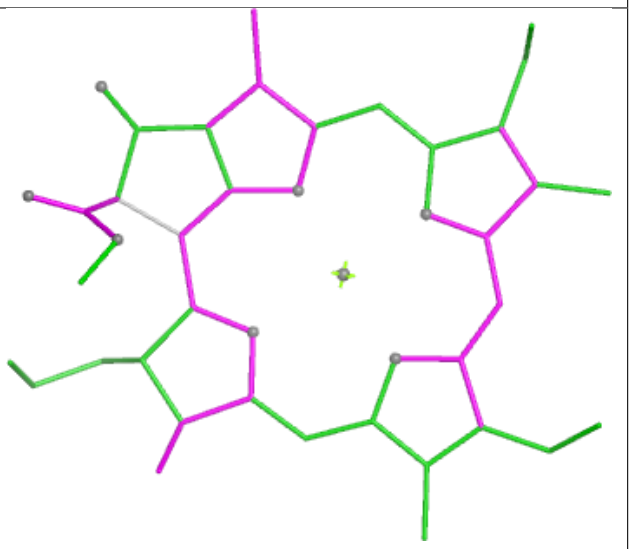

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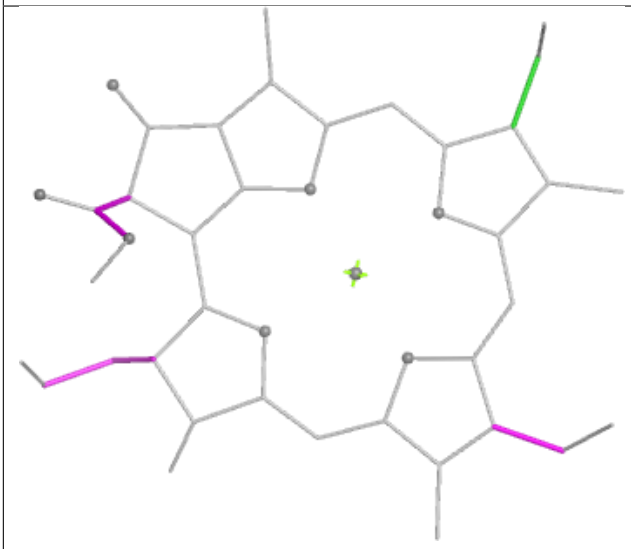

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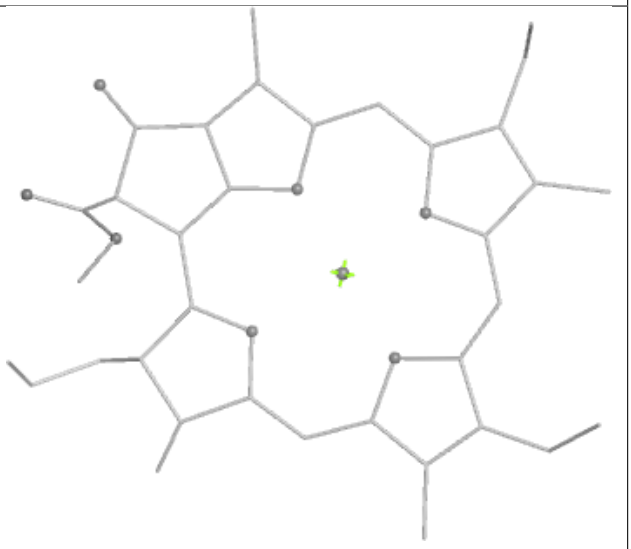
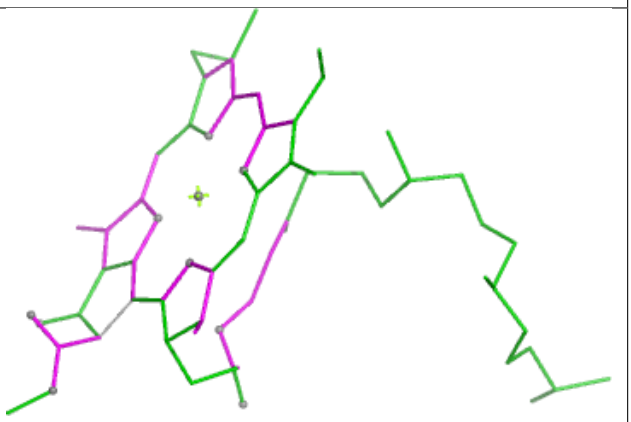


Rings

Ligand CLA Y1 613

Bond lengths



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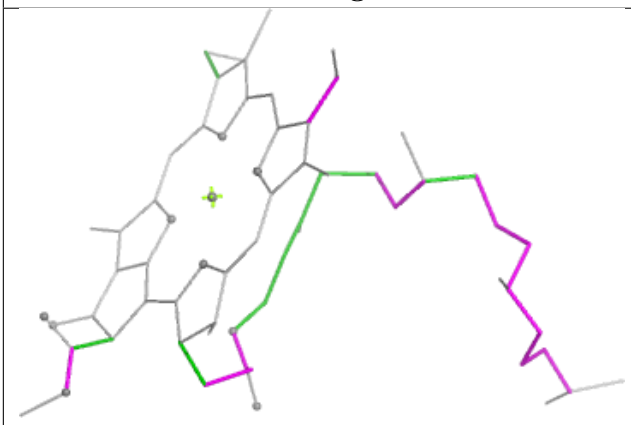

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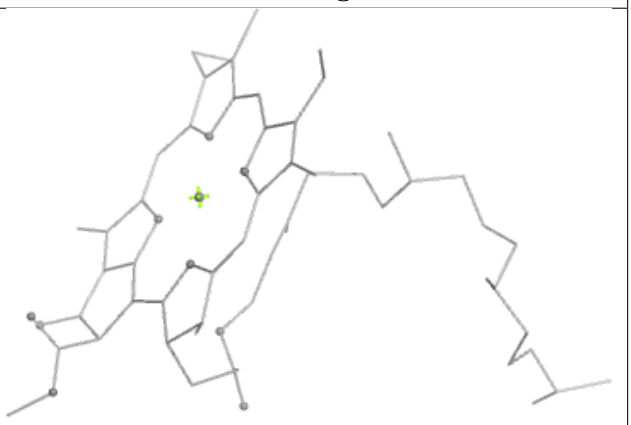
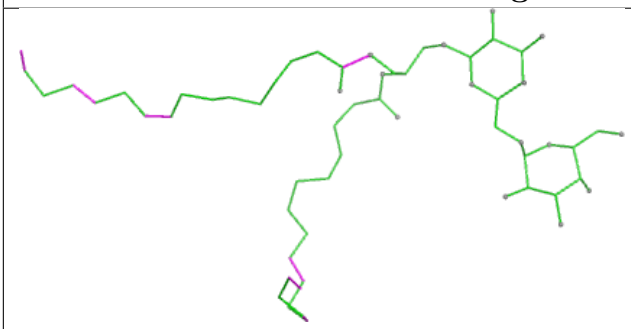


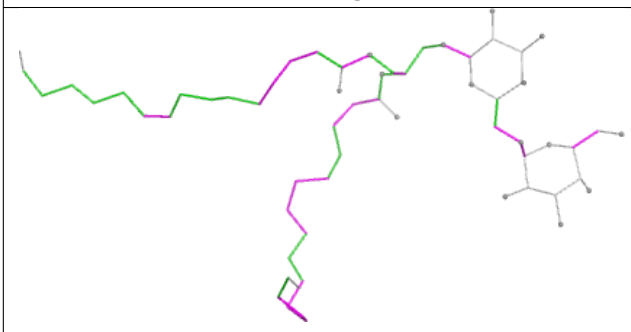
Rings

Ligand DGD C1 519



Bond lengths

Bond angles



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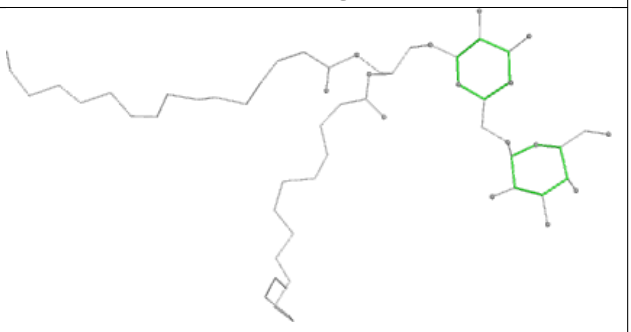
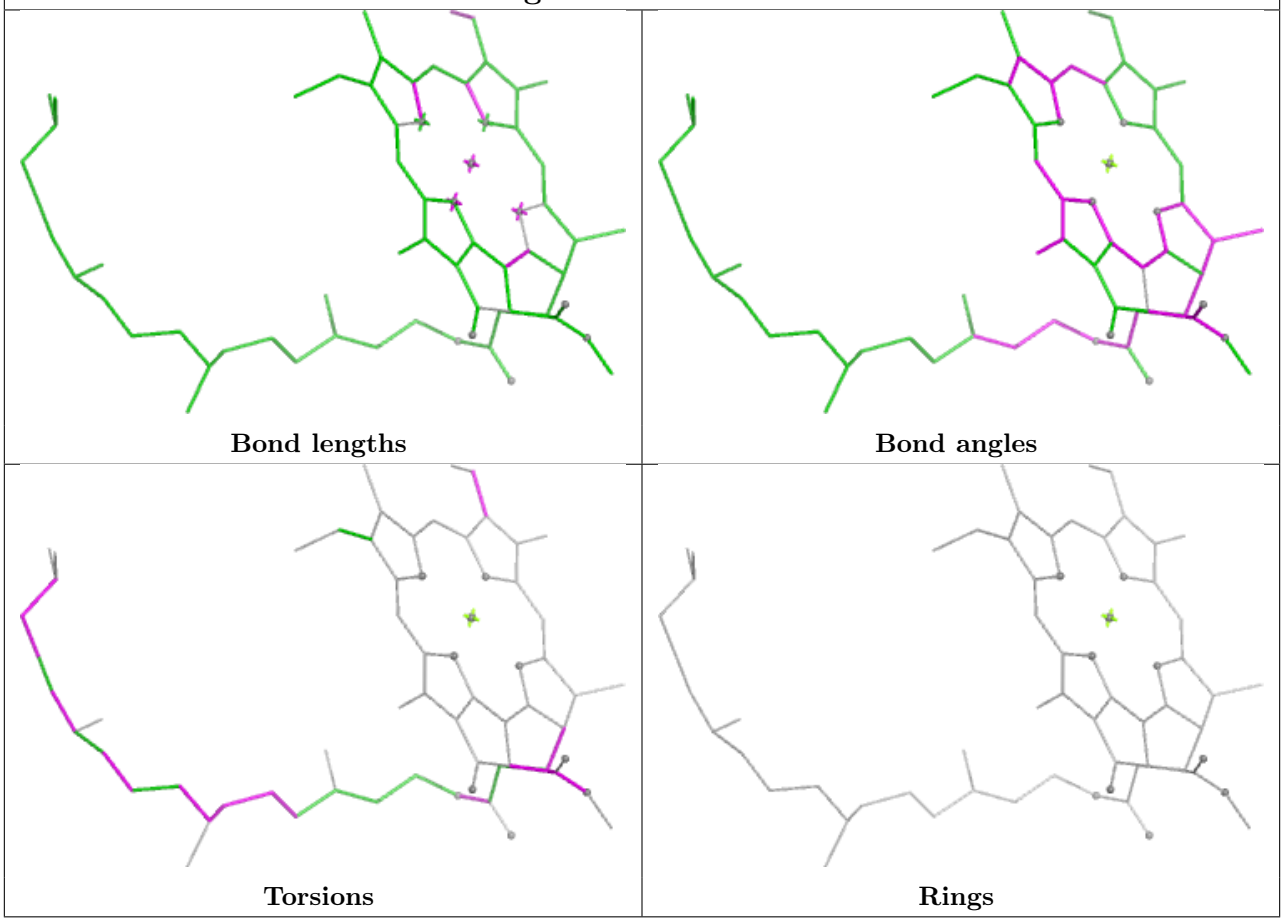
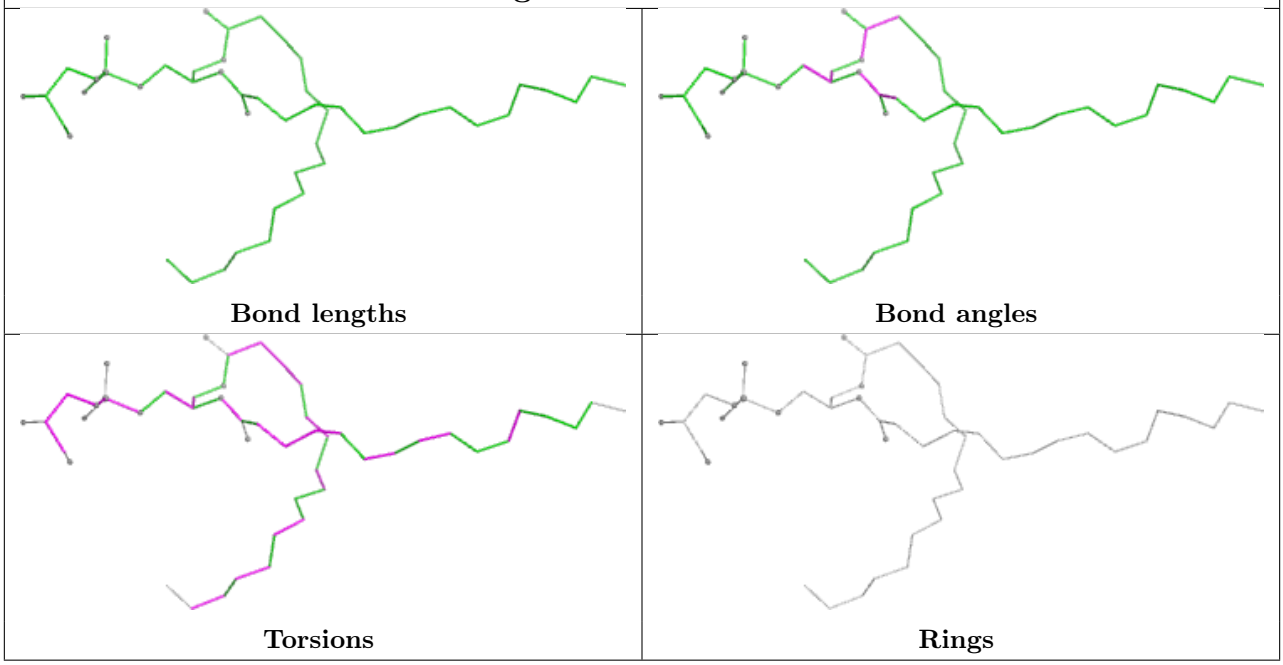


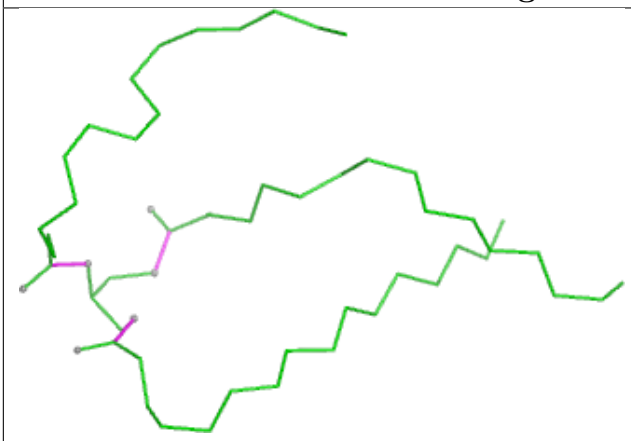
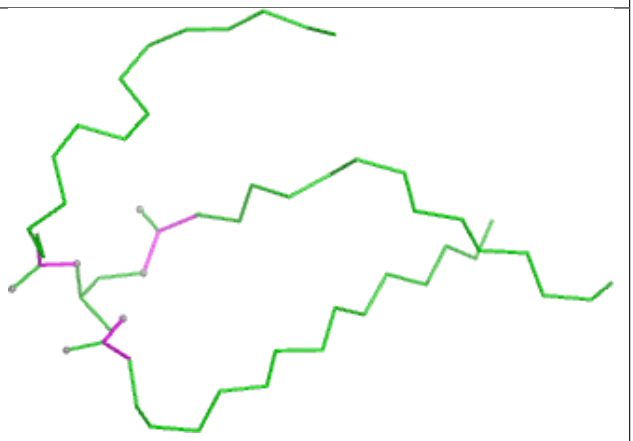
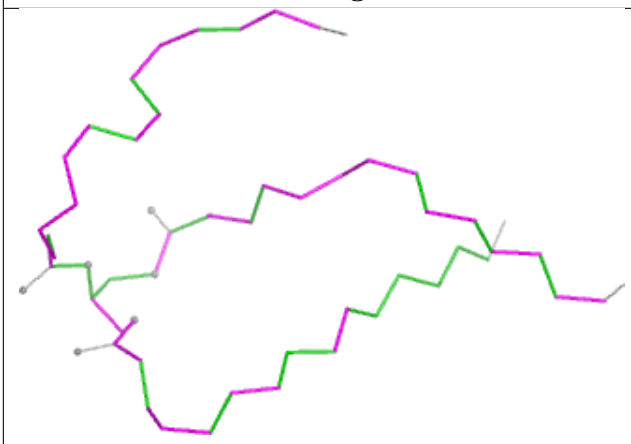
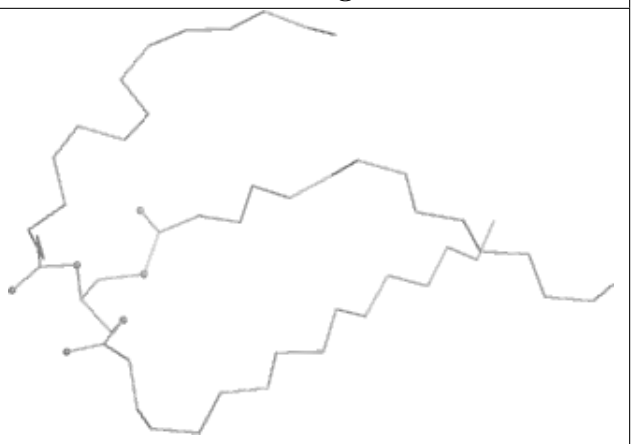
Rings

Ligand CLA G 611

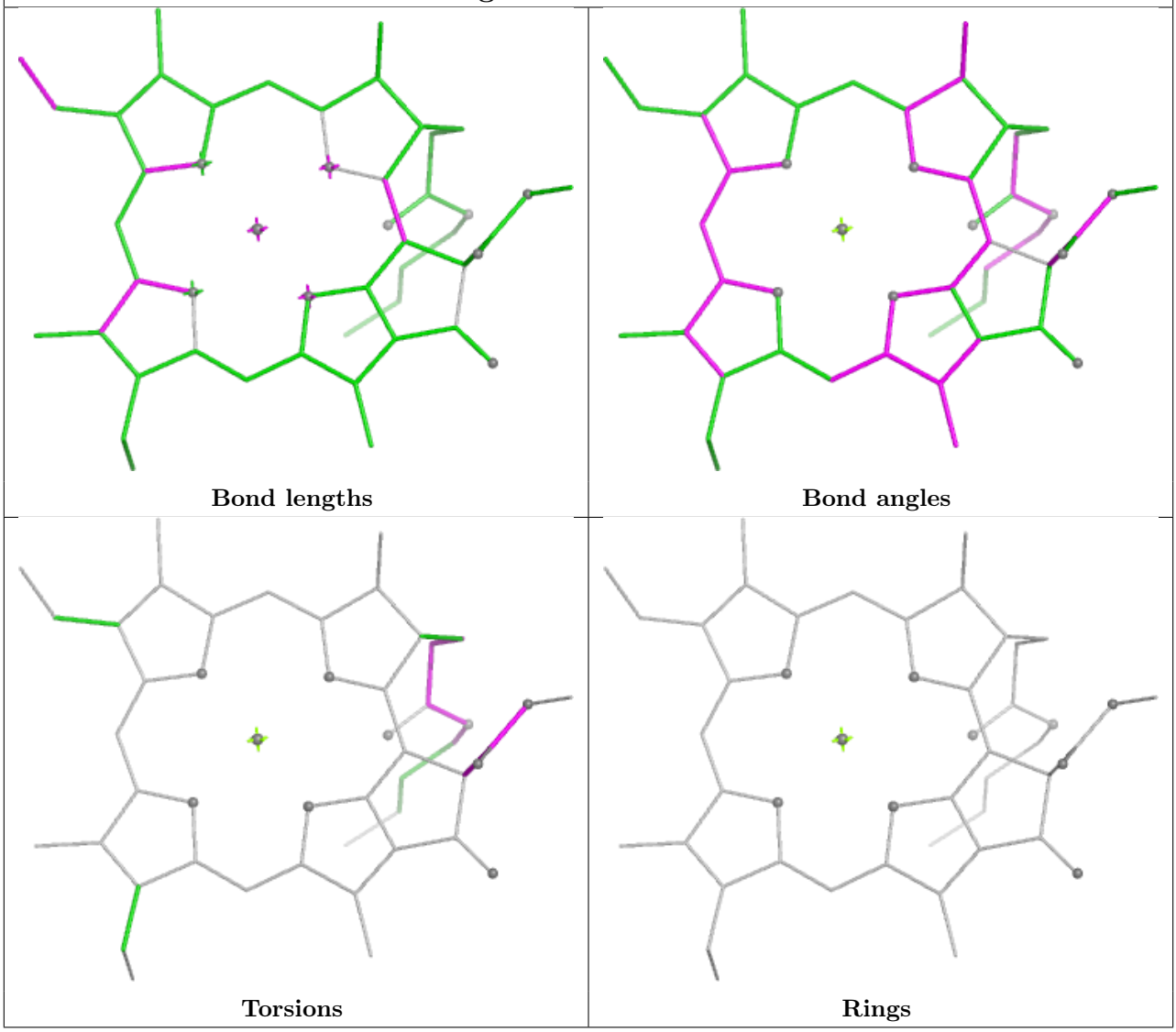


Ligand LHG G1 624



Ligand 4RF K1 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r1 604



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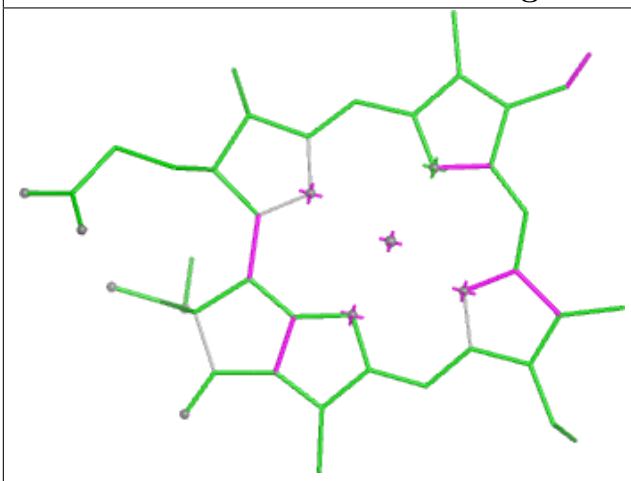
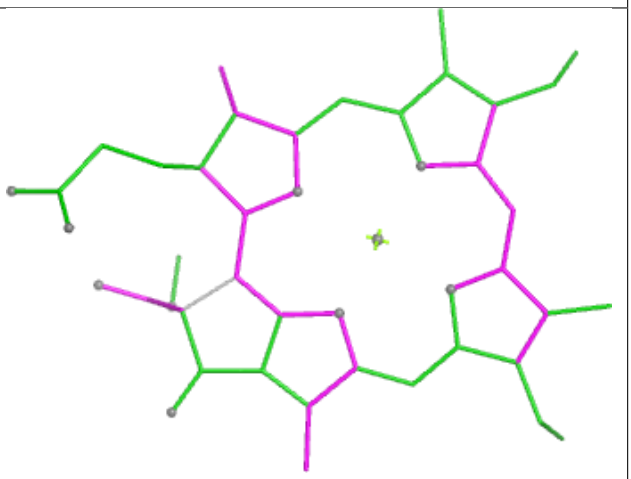
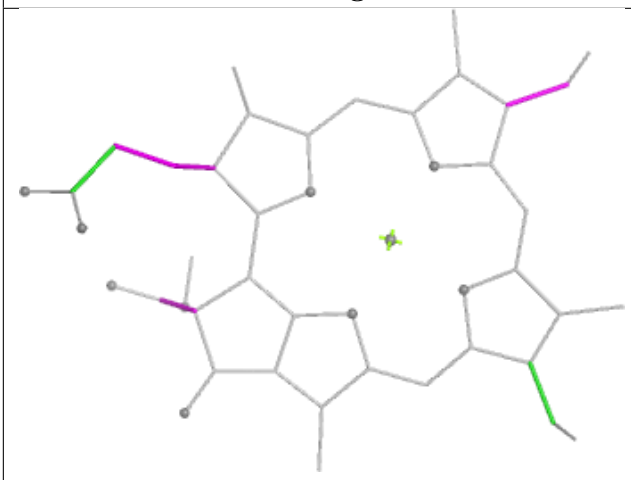


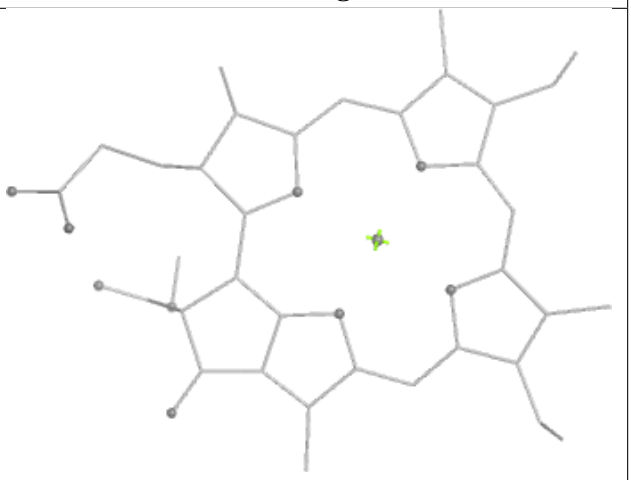
Bond lengths



Bond angles

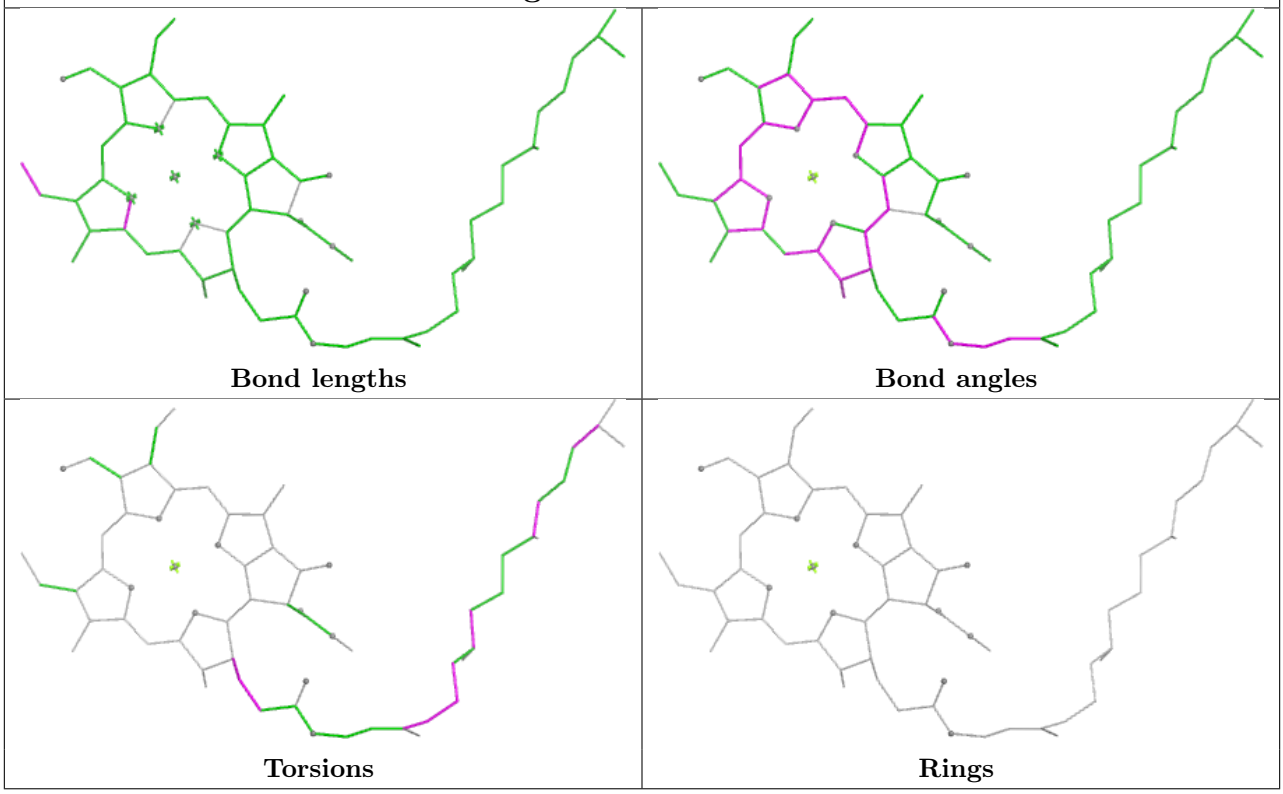


Torsions

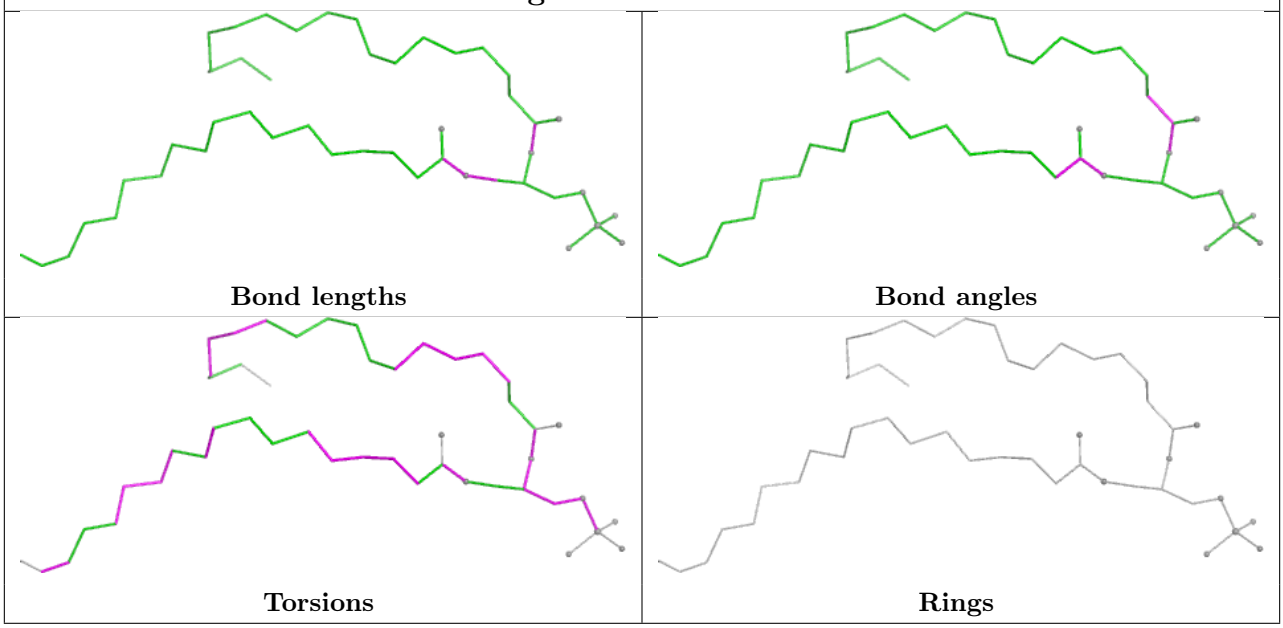


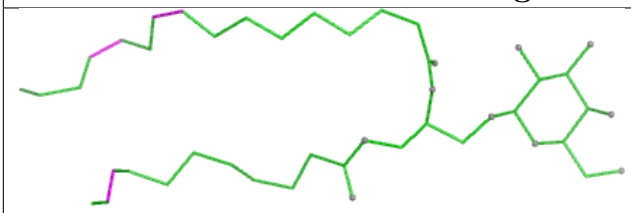
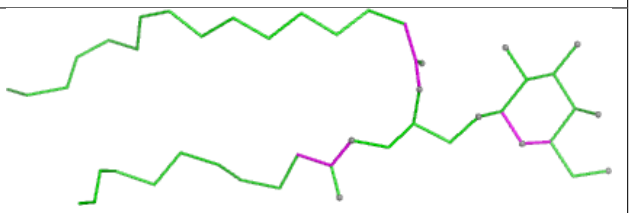
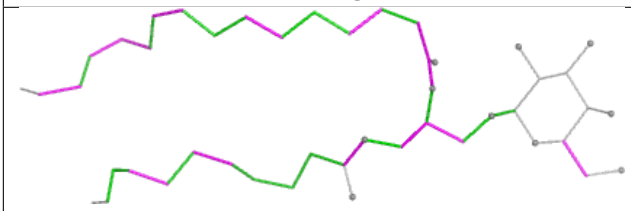
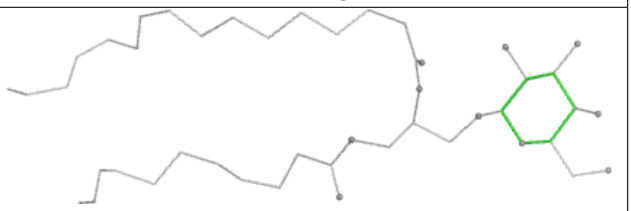
Rings

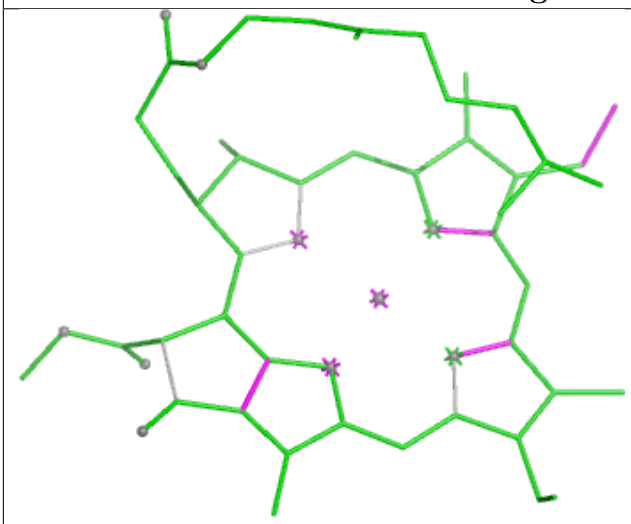
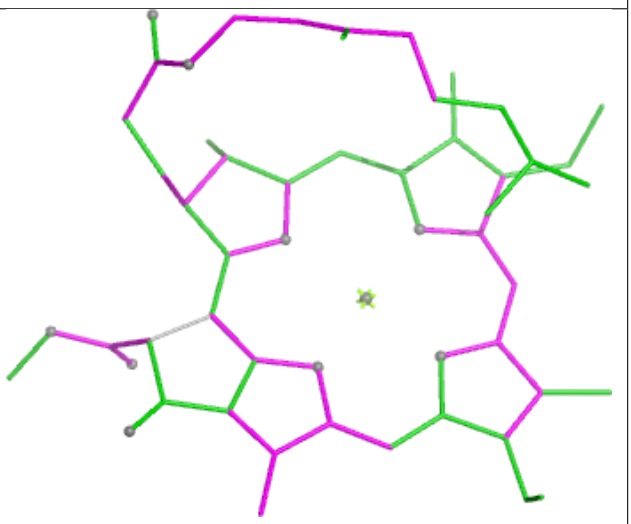
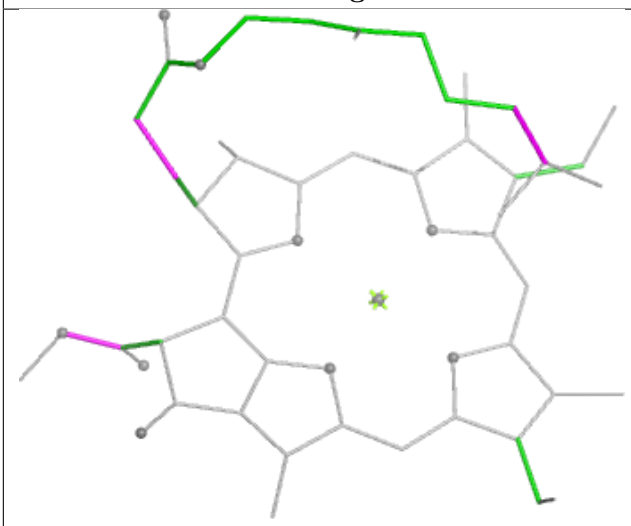
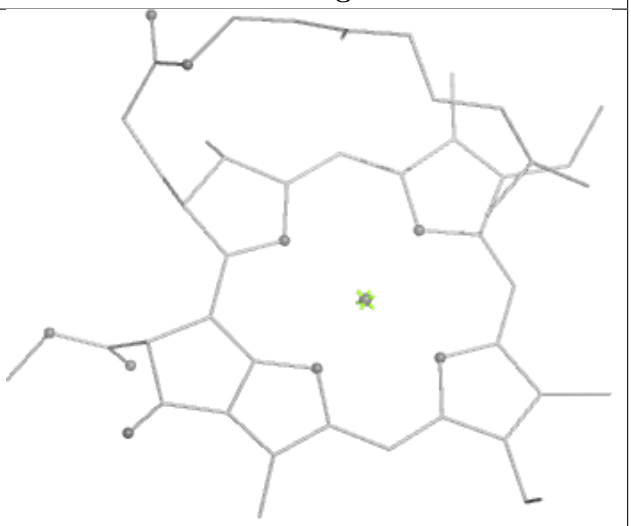
Ligand CHL N 606



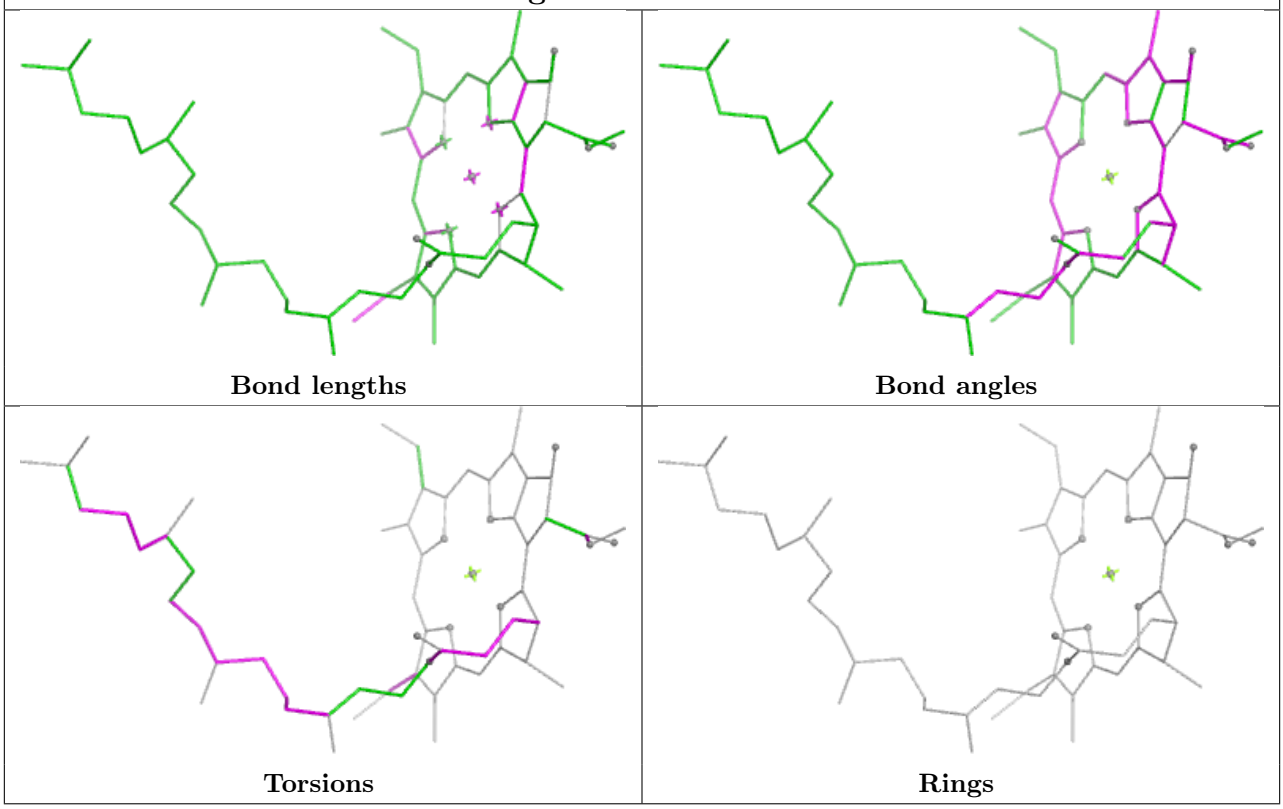
Ligand 3PH T 101



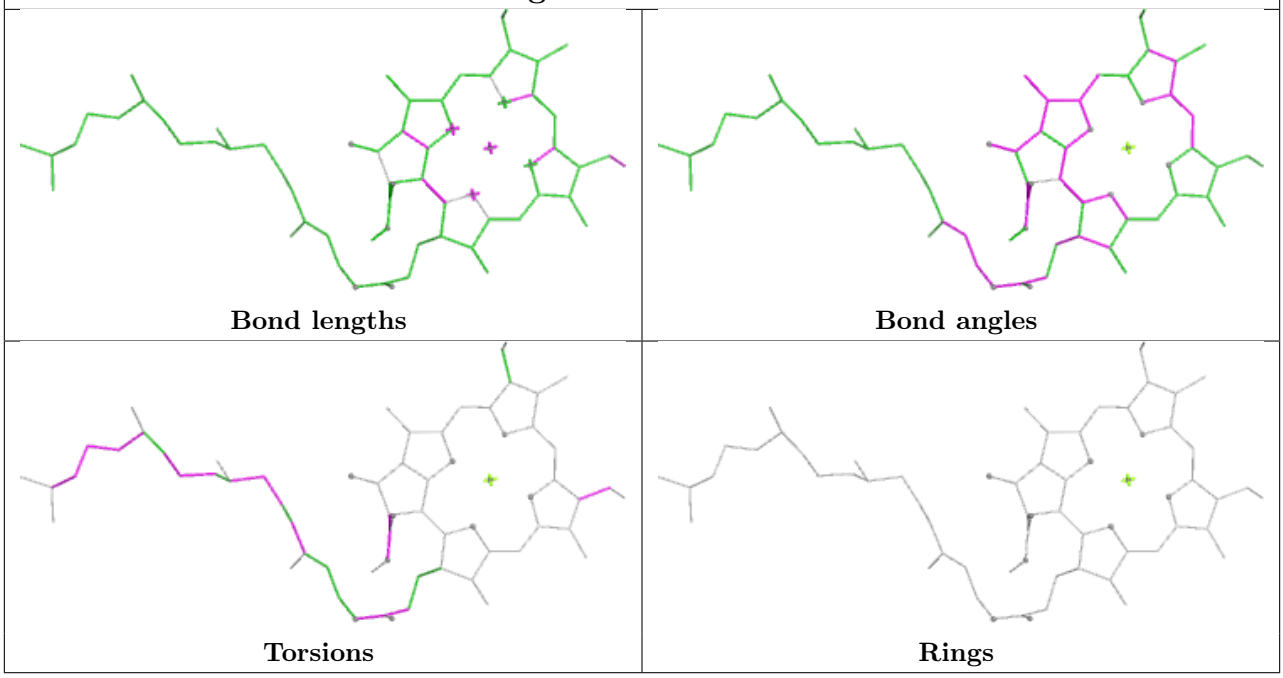
Ligand LMG d1 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 610

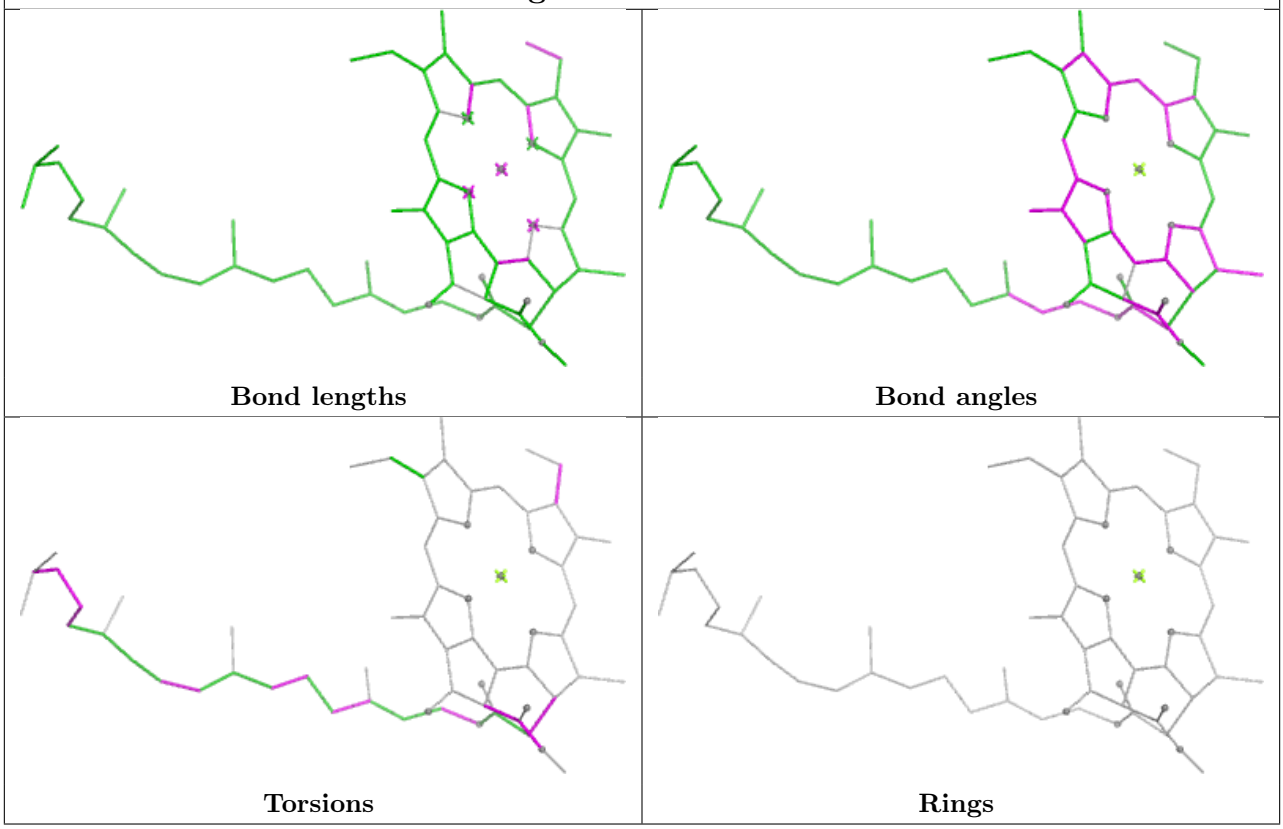


Ligand CLA b 603

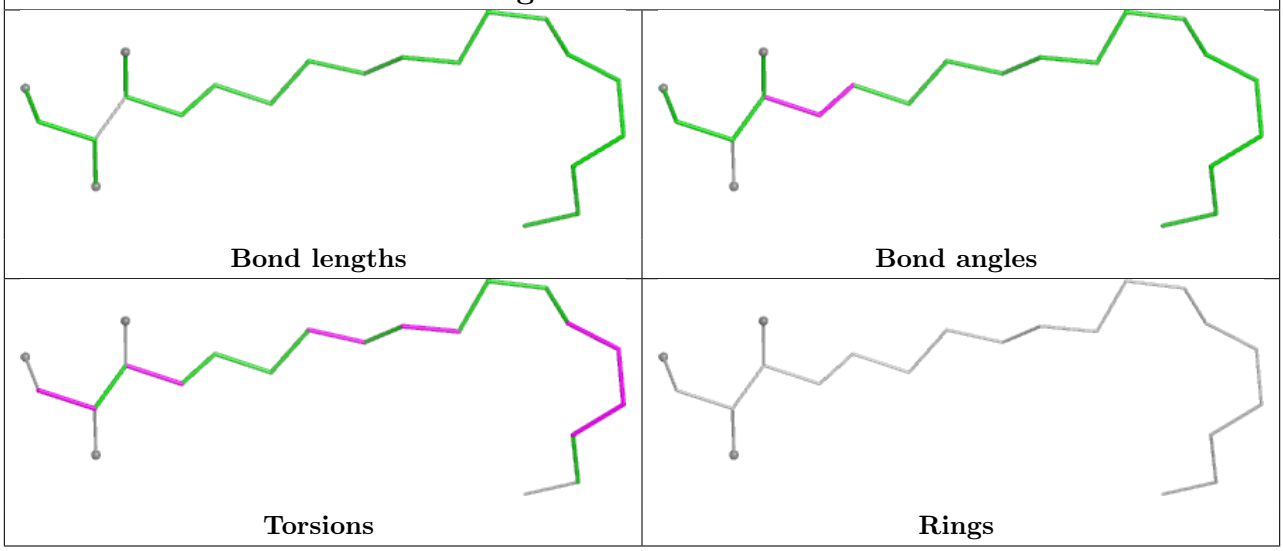


Ligand BCR a 411

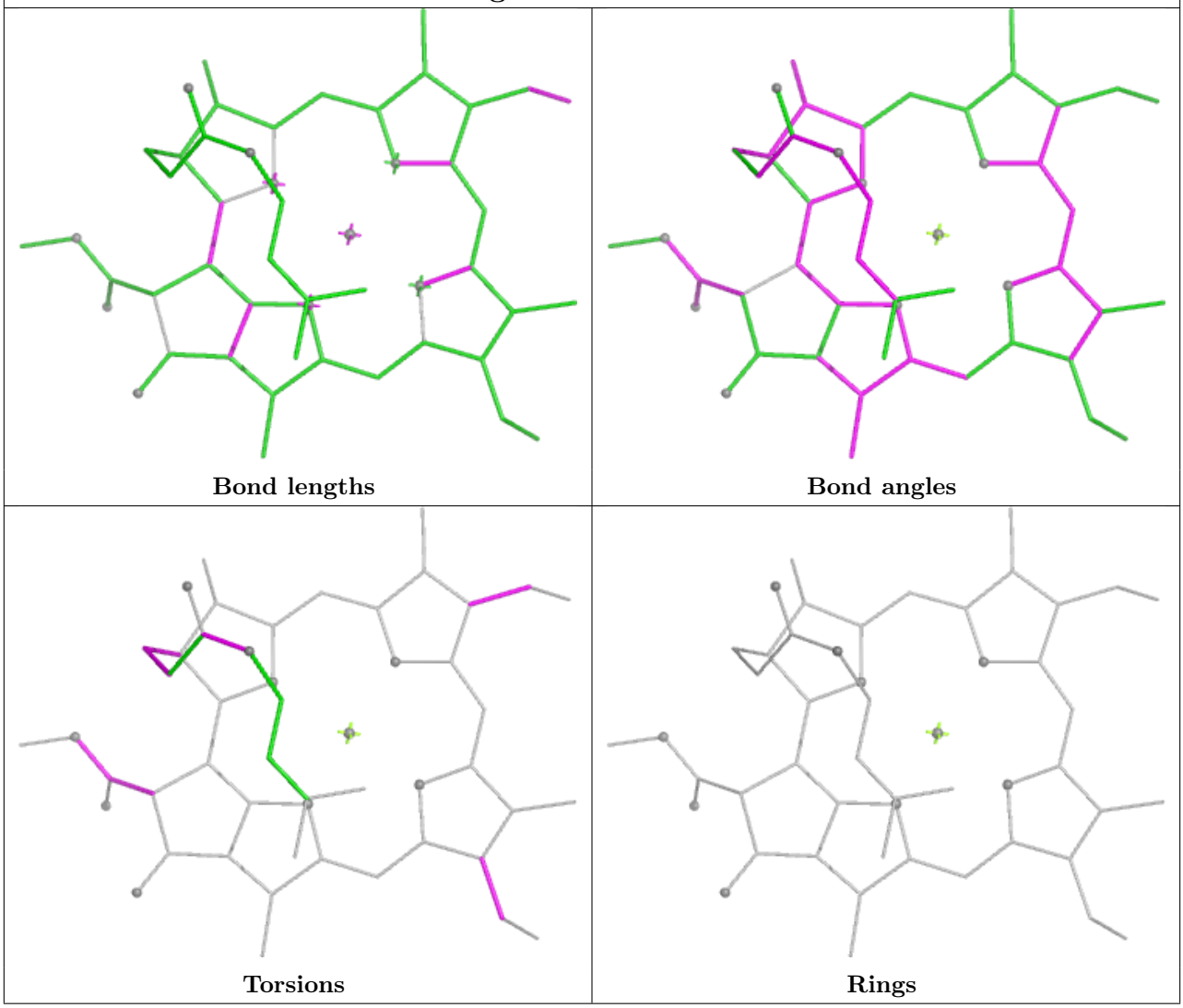
Ligand CLA S 611



Ligand SPH Y1 625



Ligand CLA s 605



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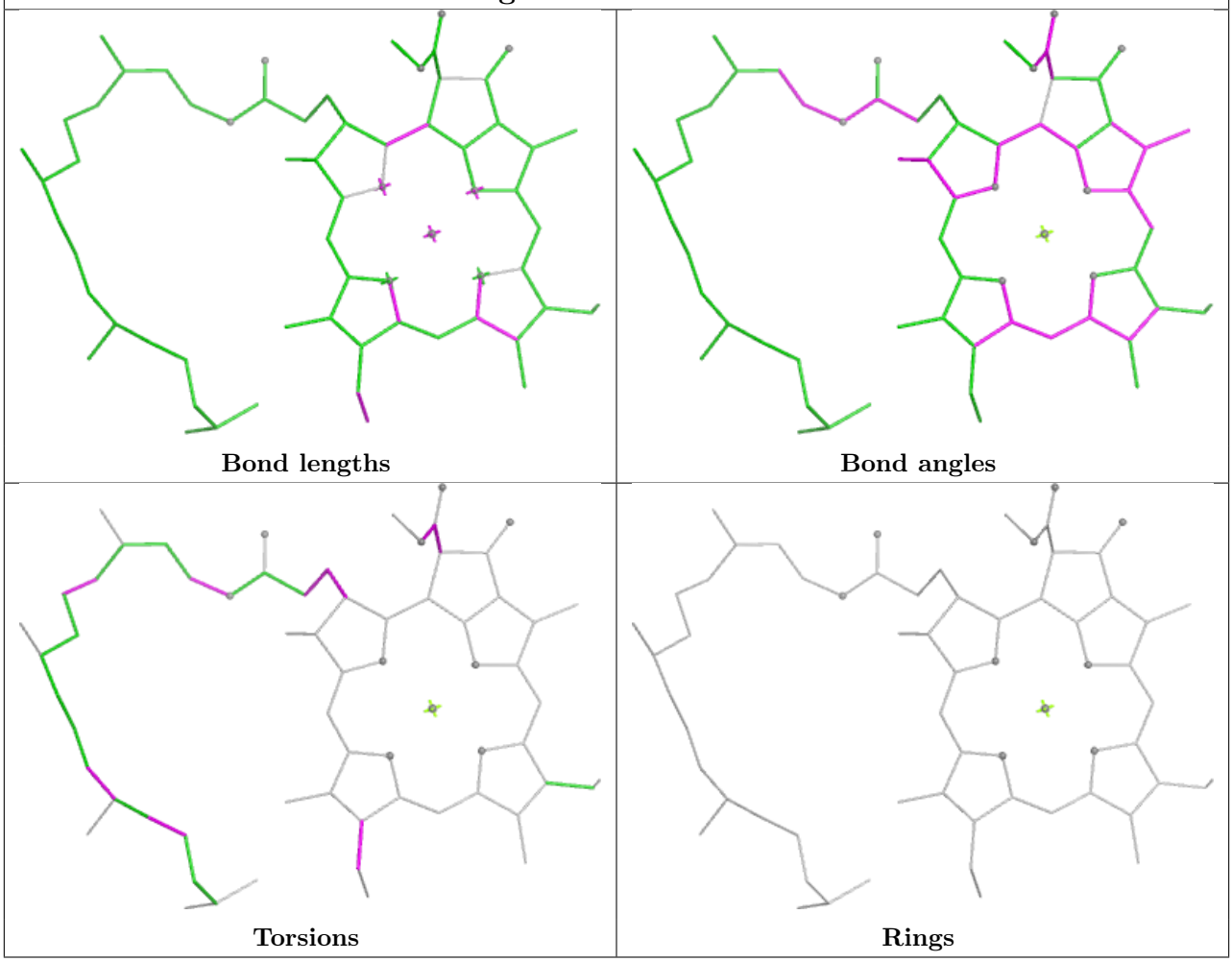
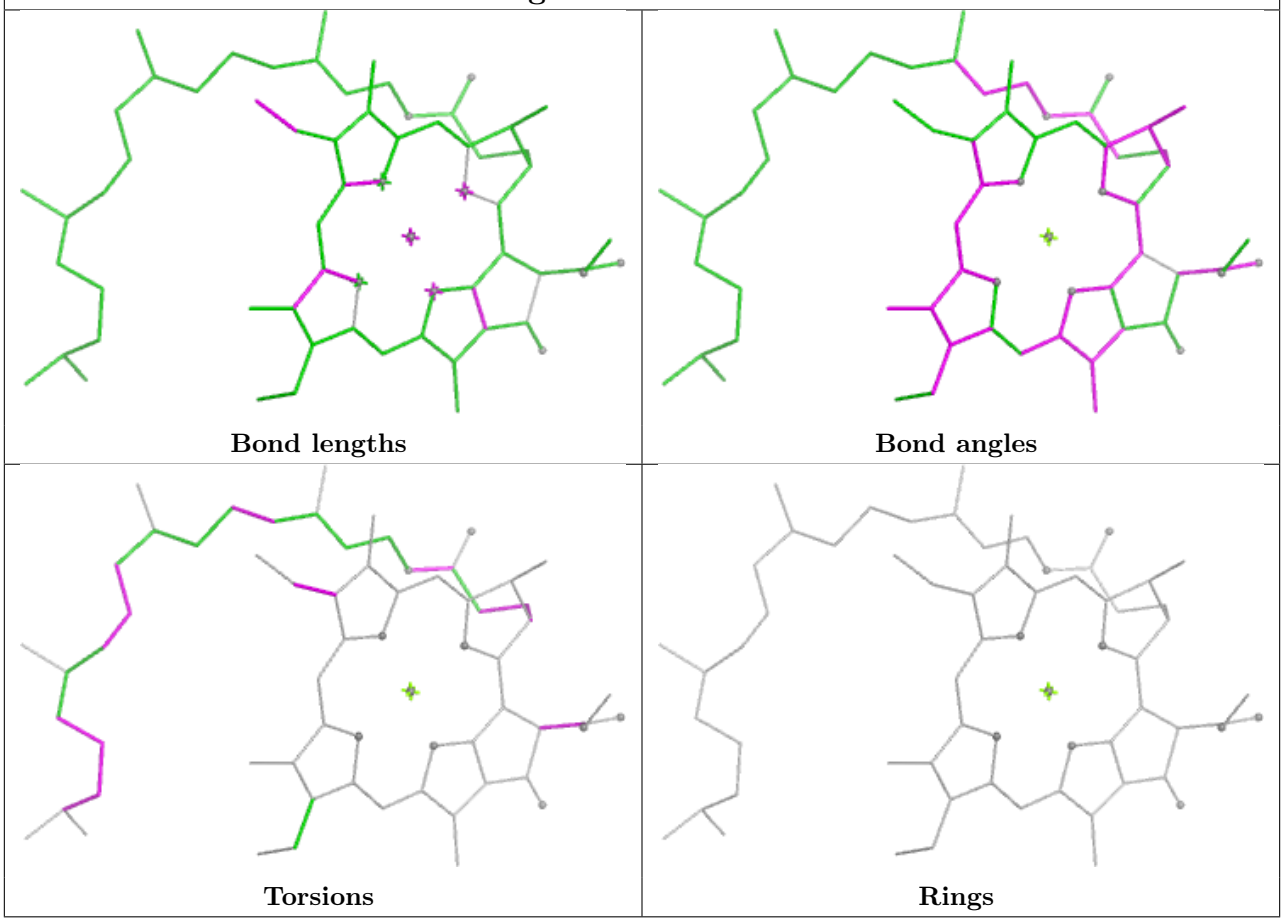
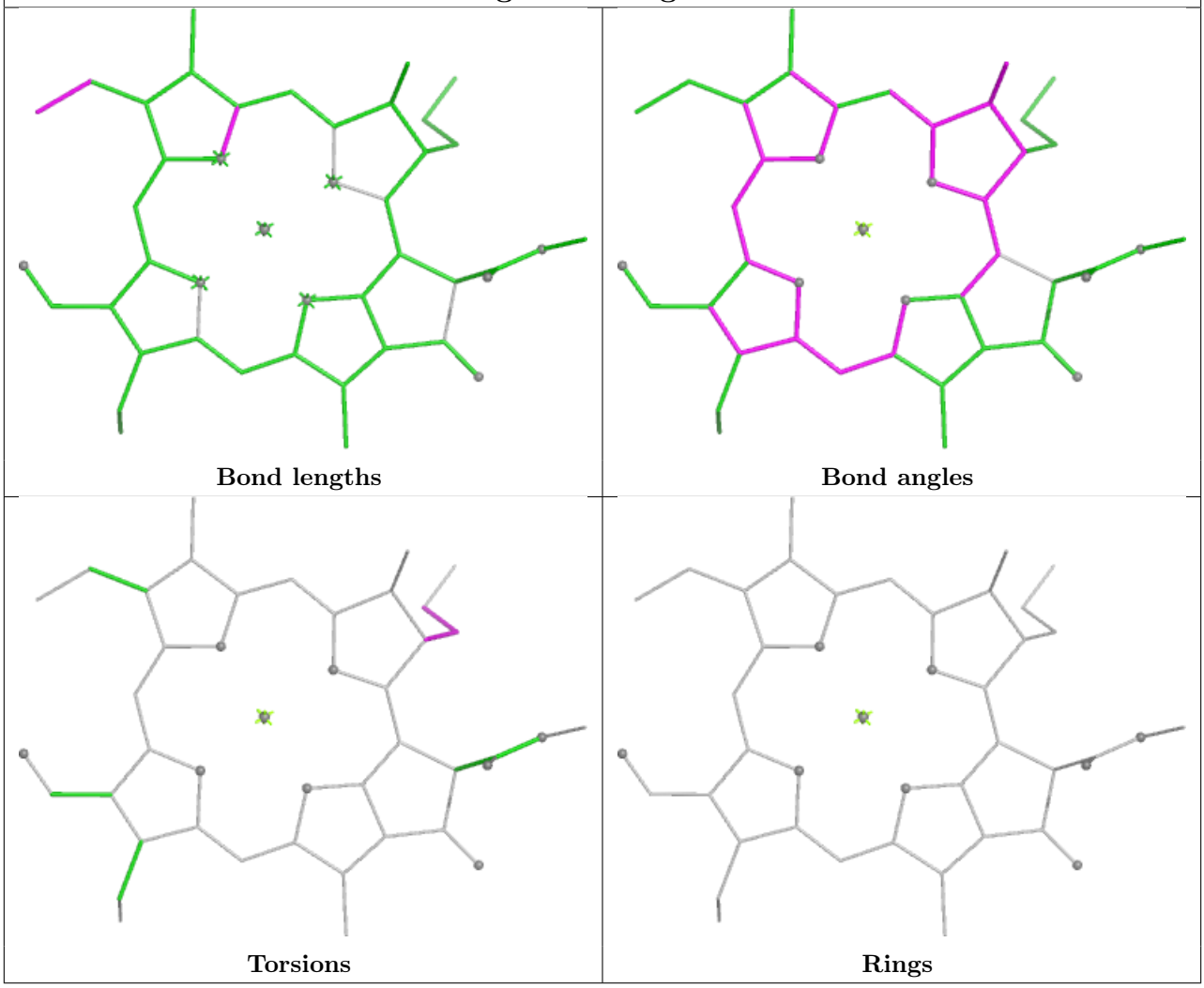


Ligand CLA n 602



Ligand CHL g 608



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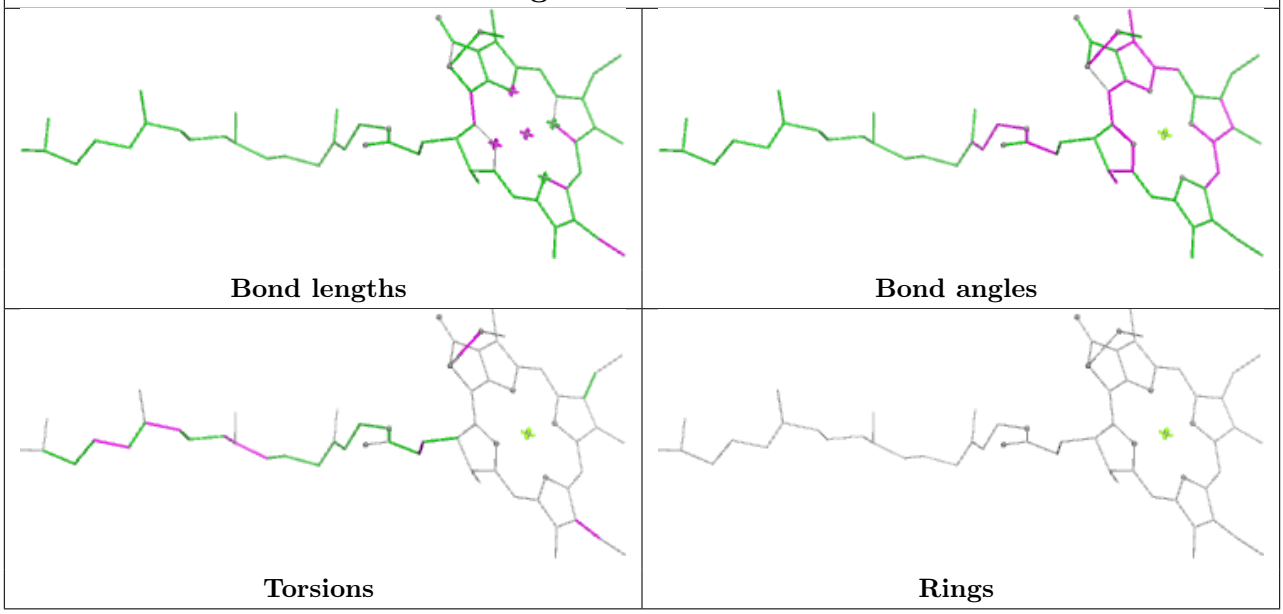
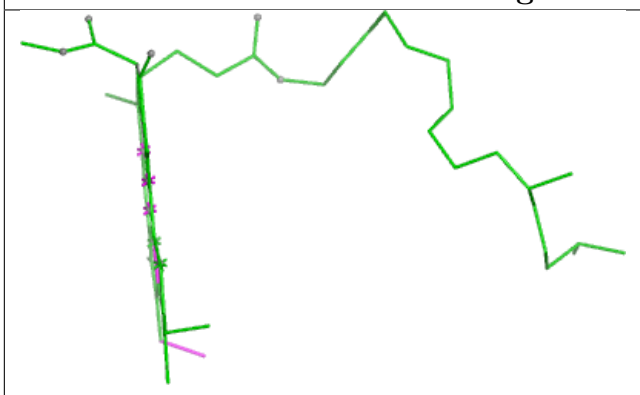
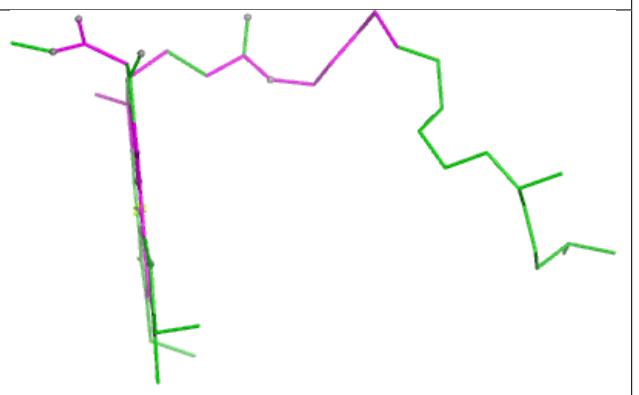
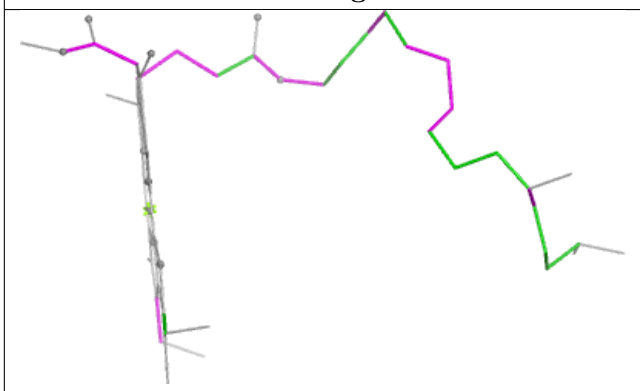
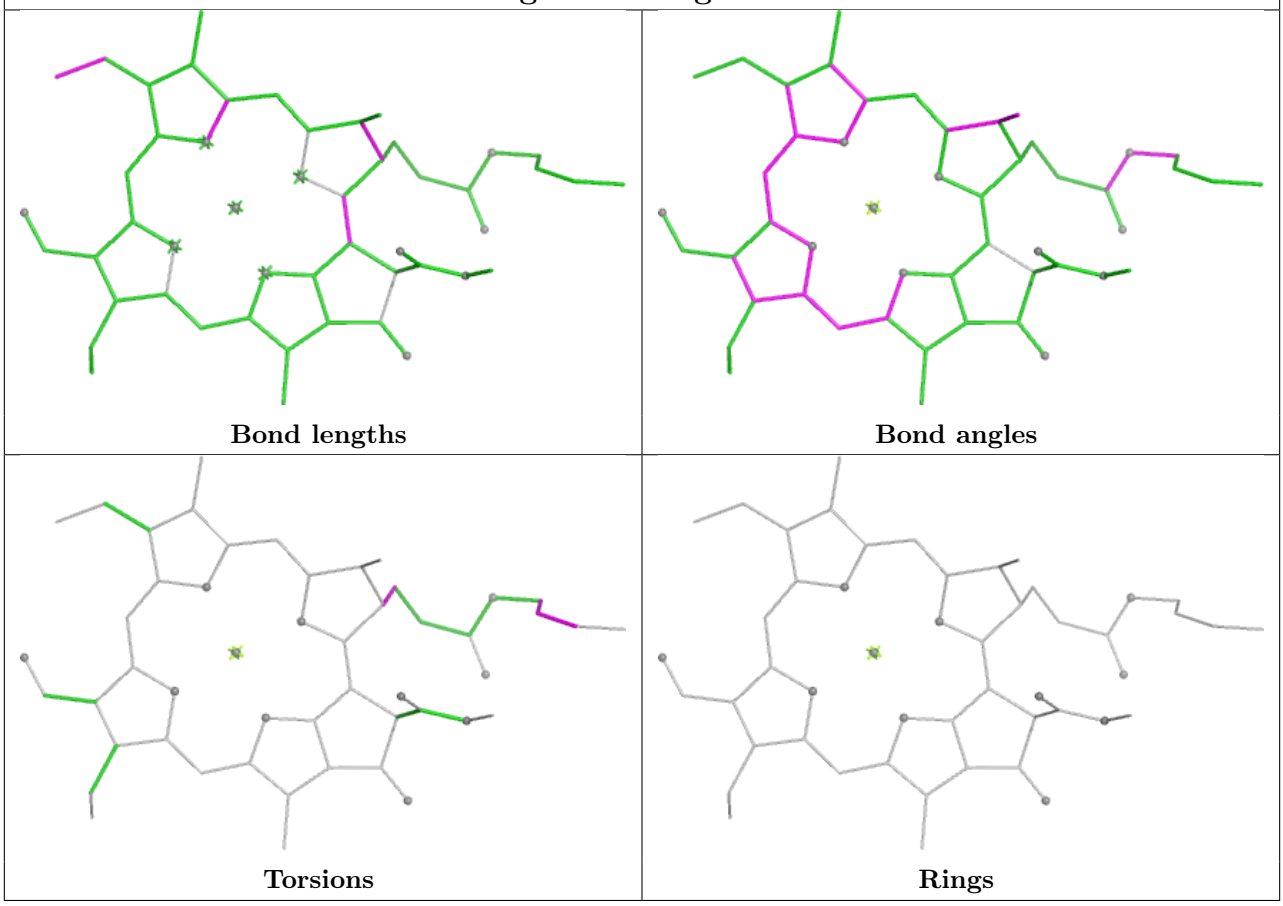


Ligand CLA C1 506	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CHL g1 606



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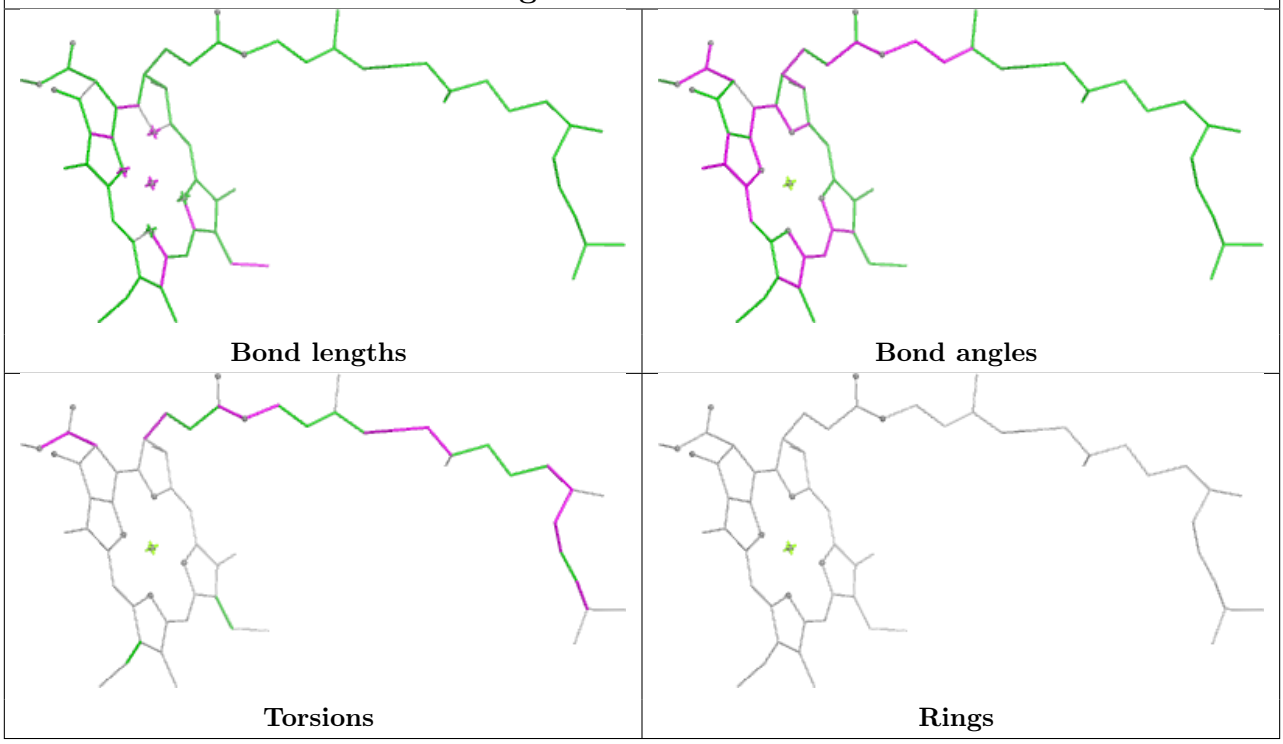

Ligand CLA S1 604

Bond lengths

Bond angles

Torsions

Rings

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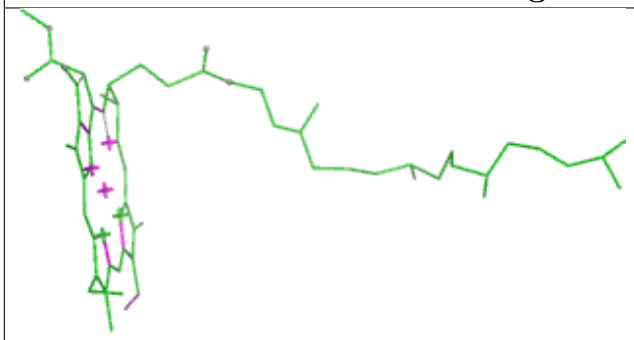
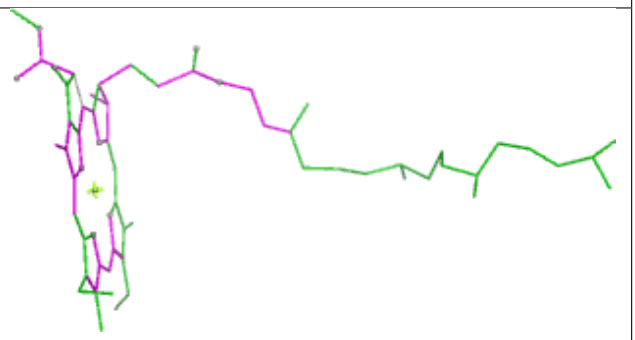
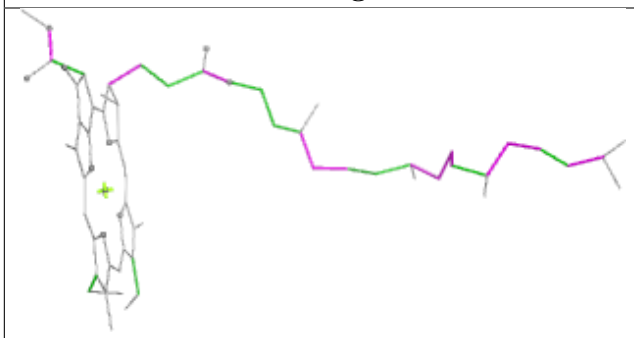
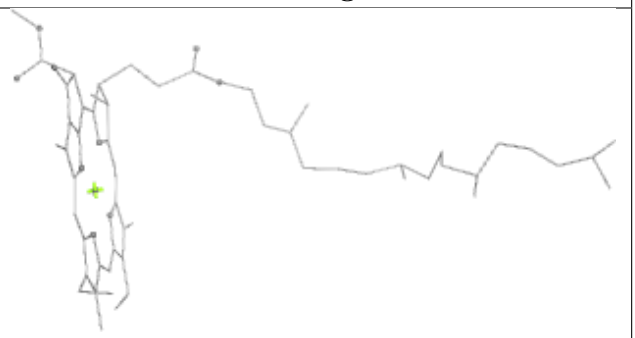
 Bond lengths	 Bond angles
 Torsions	 Rings

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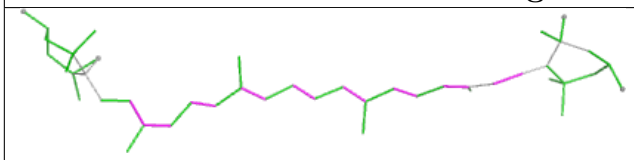
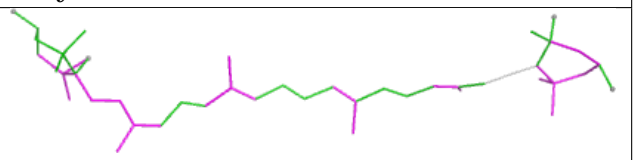
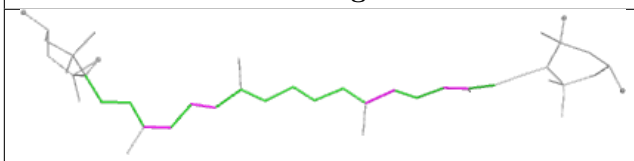
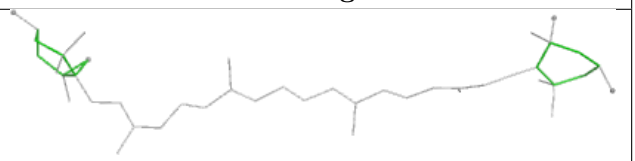
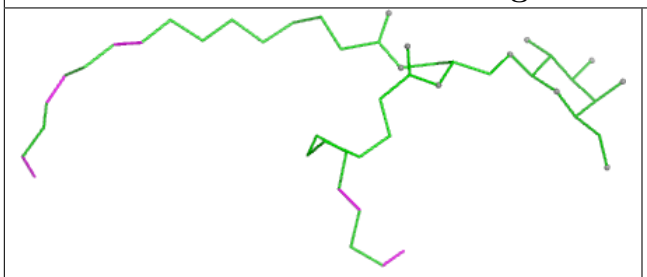
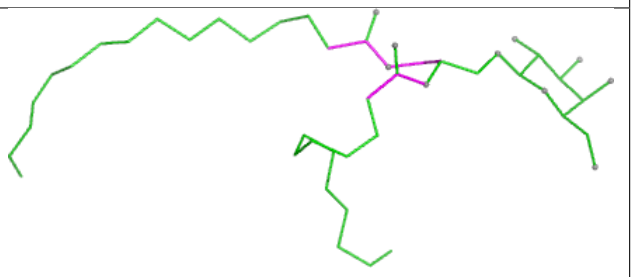
 Bond lengths	 Bond angles
 Torsions	 Rings

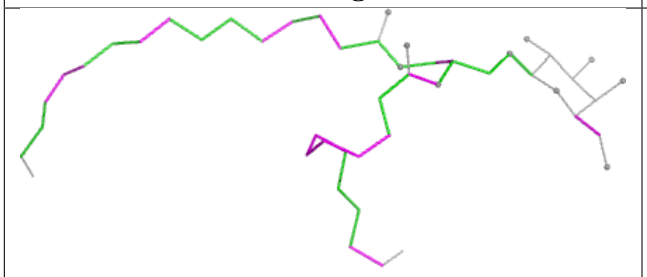
Ligand LMG H1 102



Bond lengths



Bond angles



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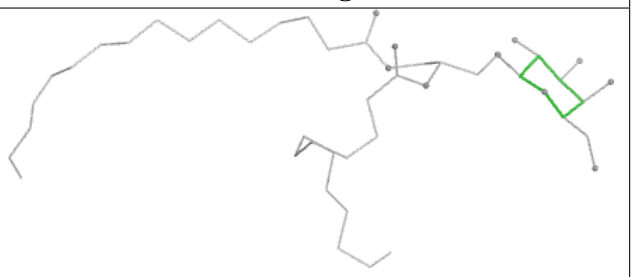
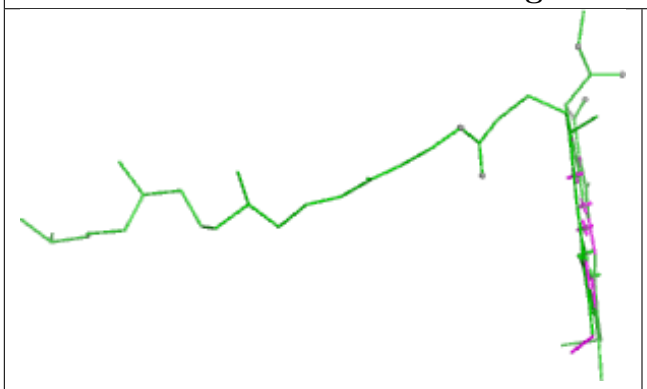


Rings

Ligand CLA B 607



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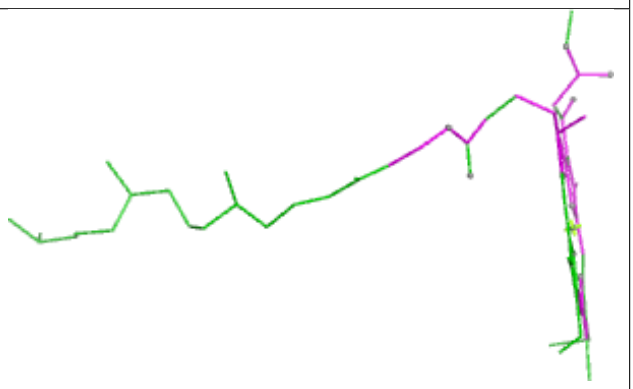

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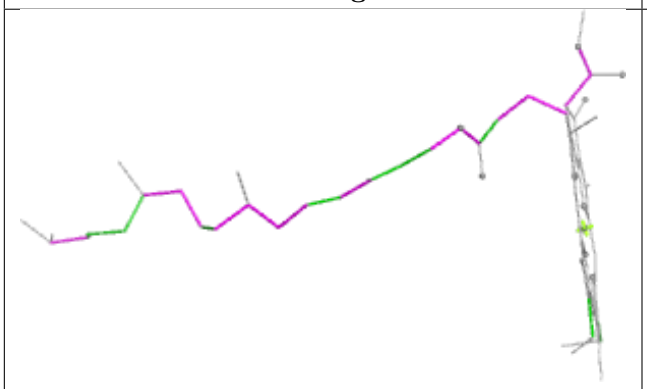

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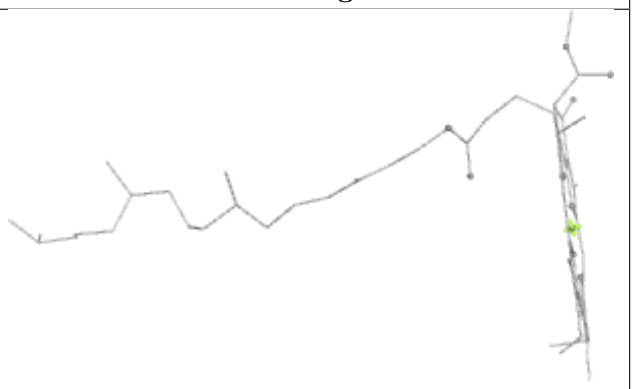
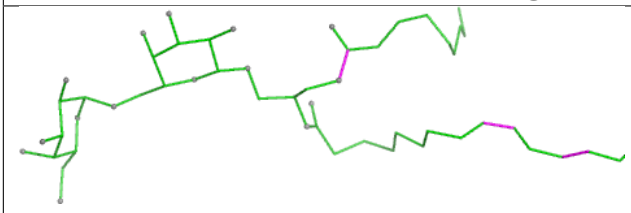
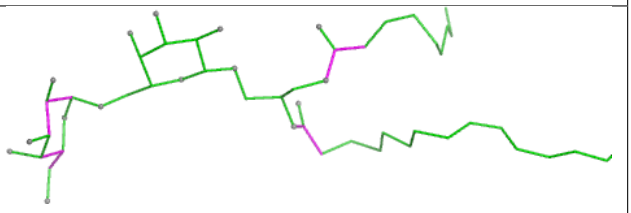
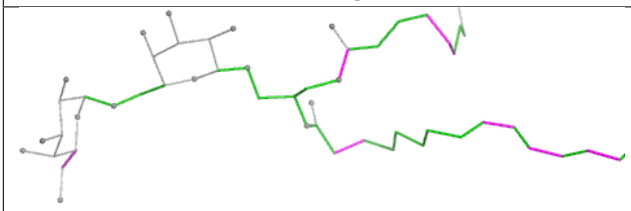
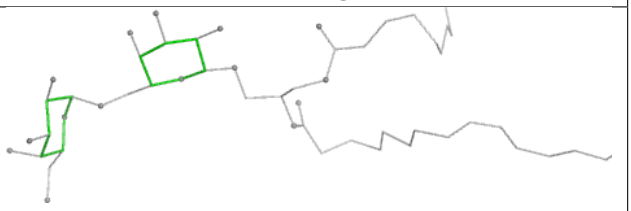


Rings

Ligand DGD c 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

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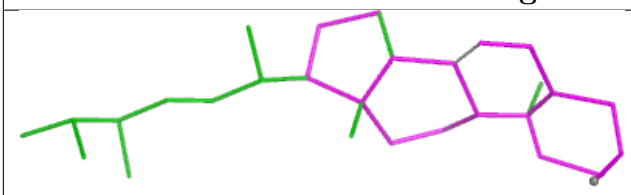
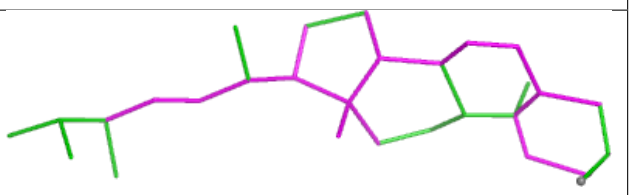
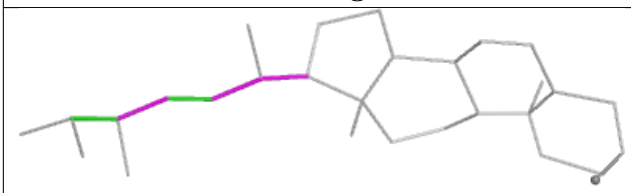
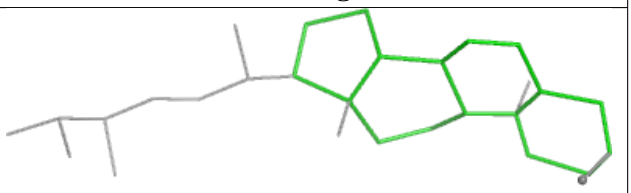
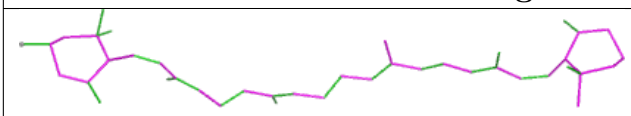
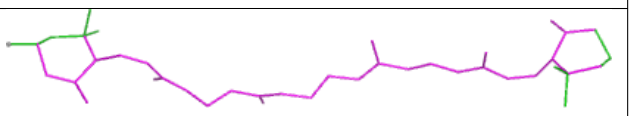
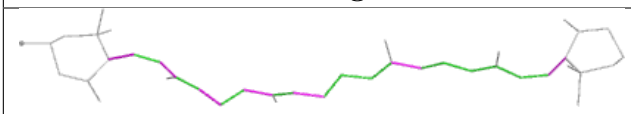
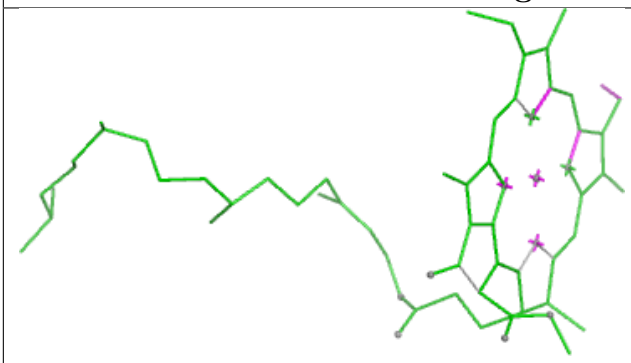
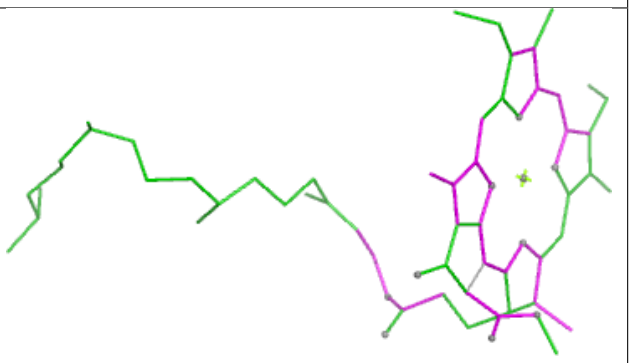
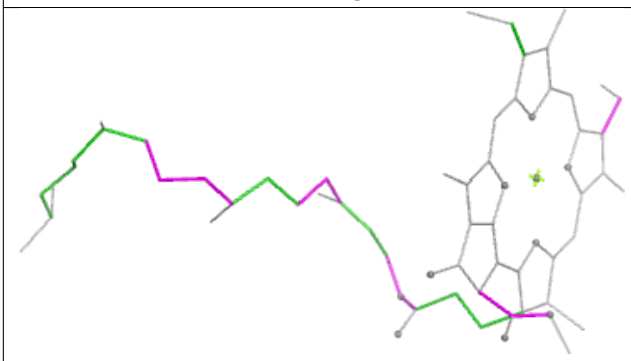
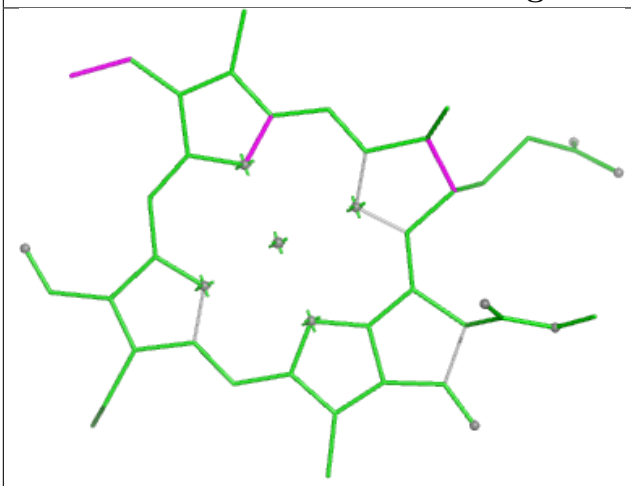
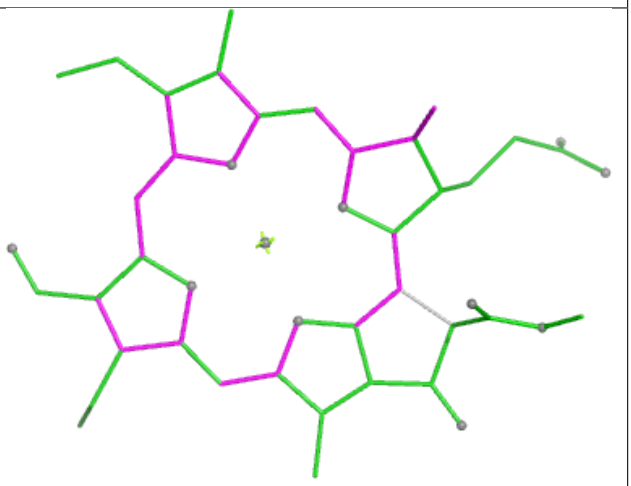
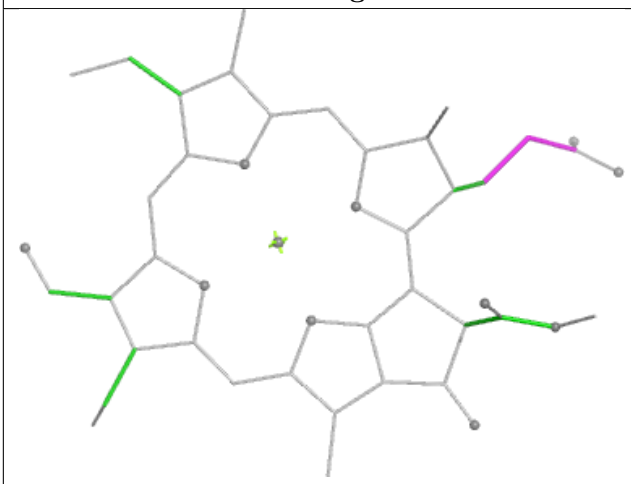
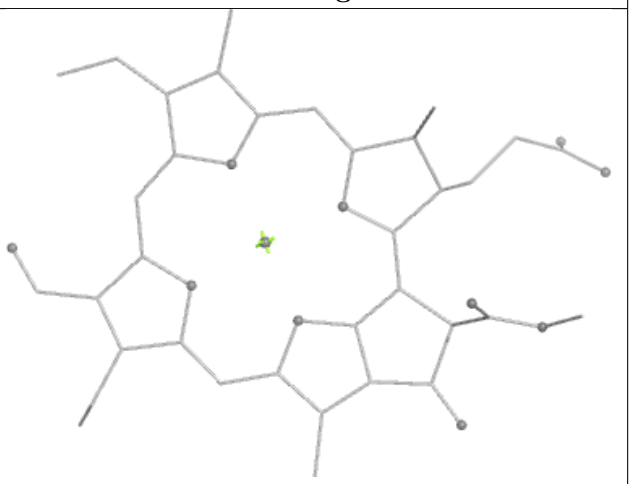
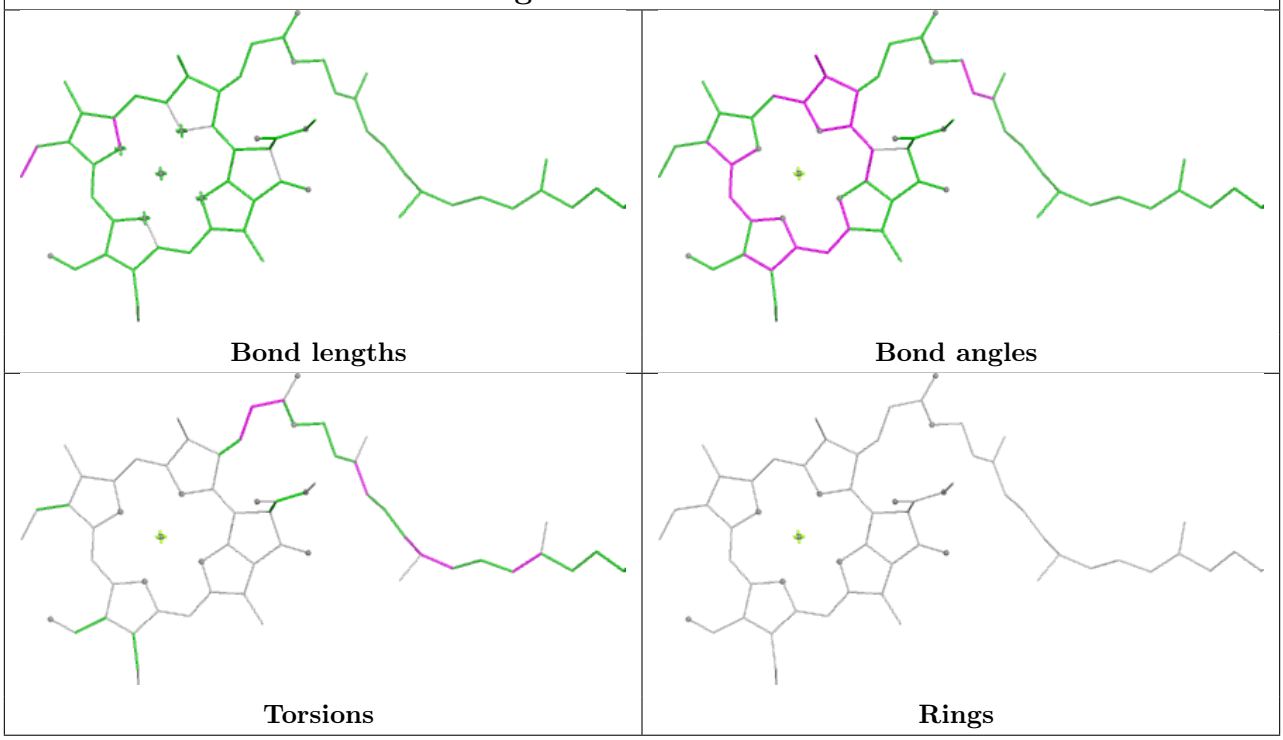
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand RRX h1 101	
 Bond lengths	 Bond angles
 Torsions	Rings

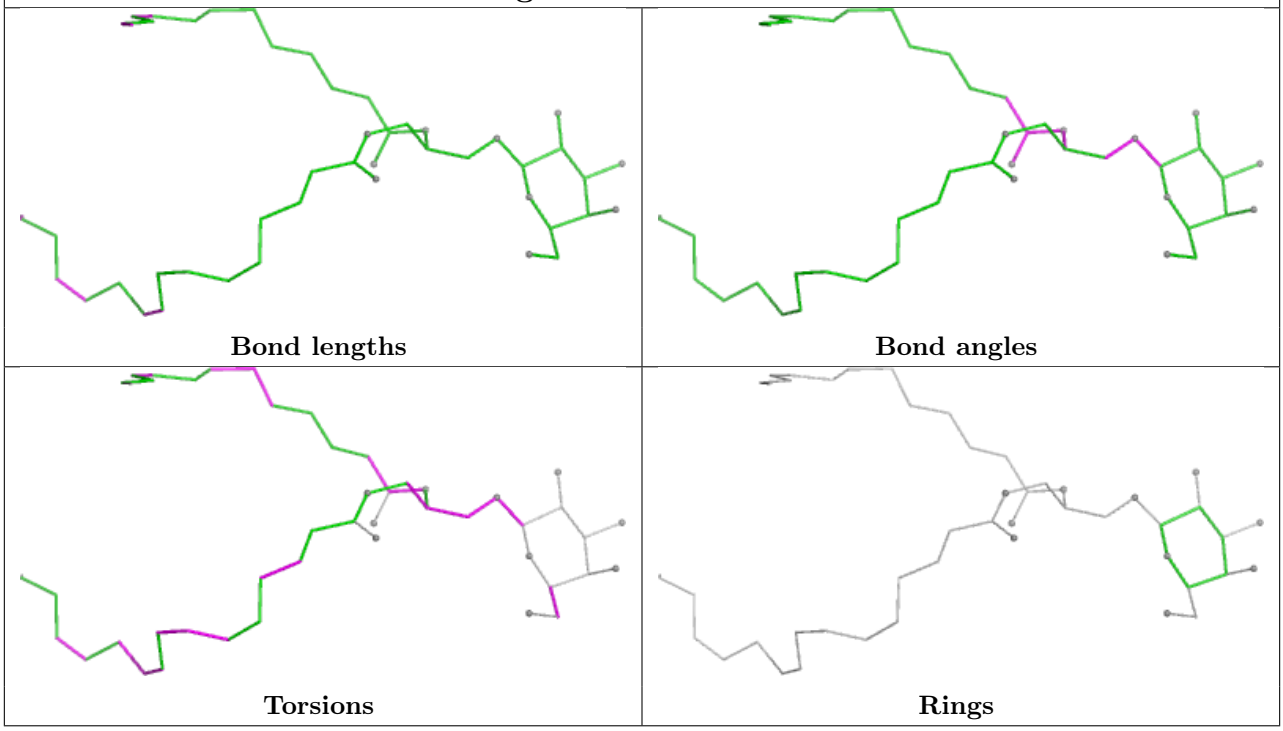
Ligand CLA Y1 604	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CHL S 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

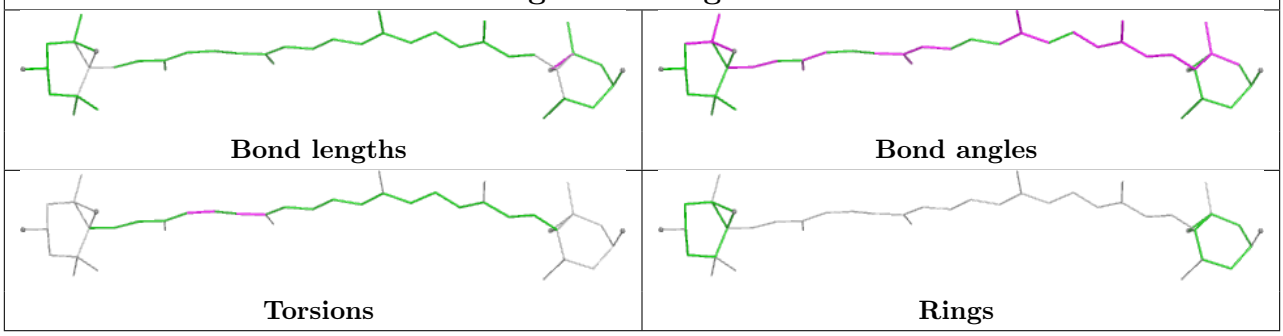
Ligand CHL N1 605



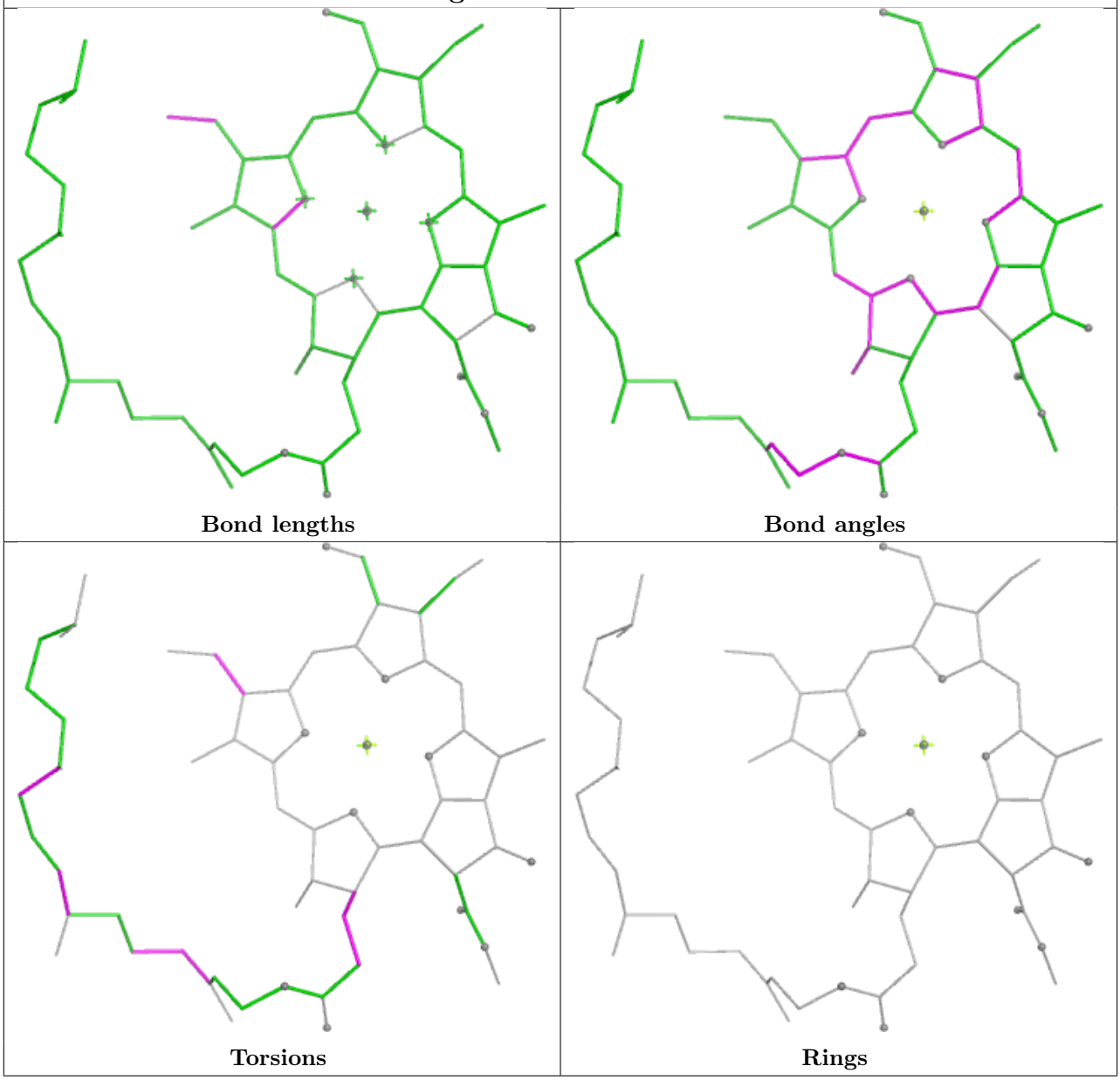
Ligand LMG a1 413



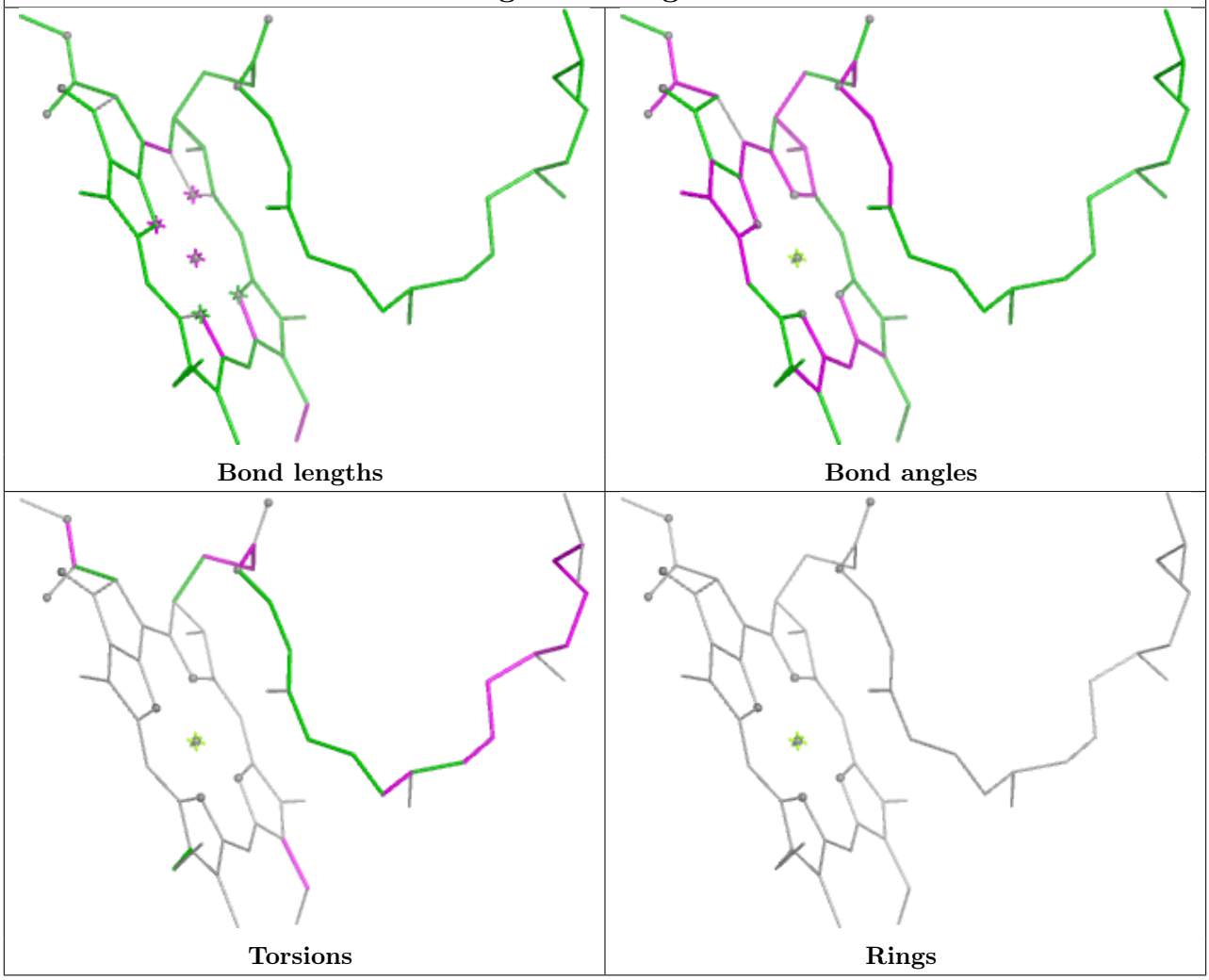
Ligand XAT g 622



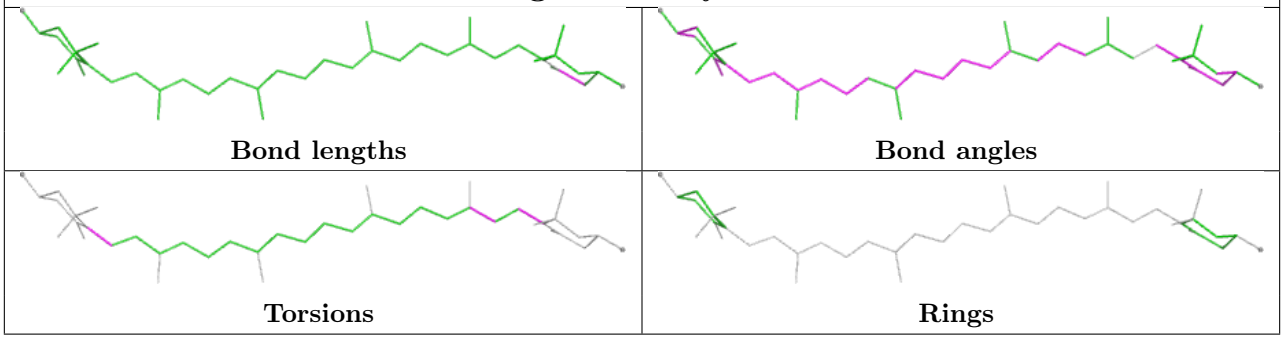
Ligand CHL N1 607

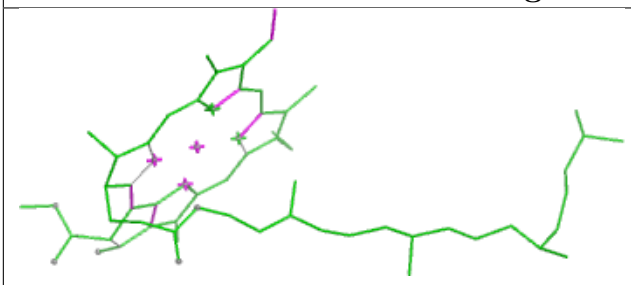
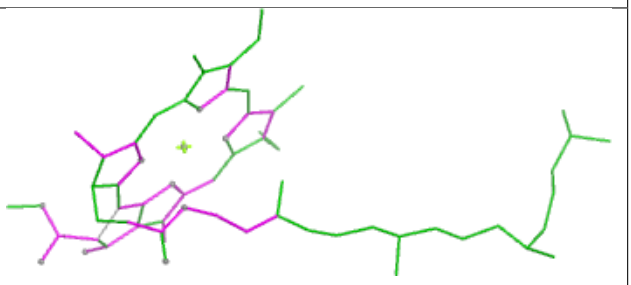
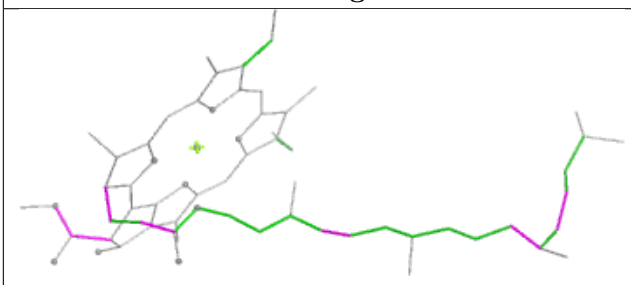
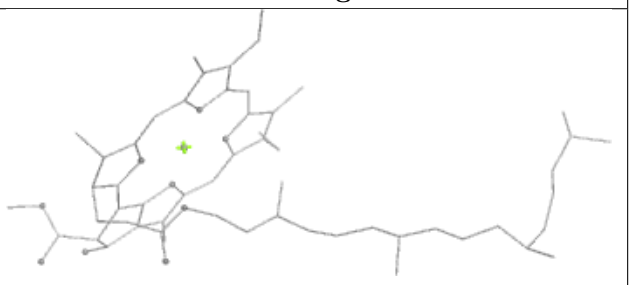


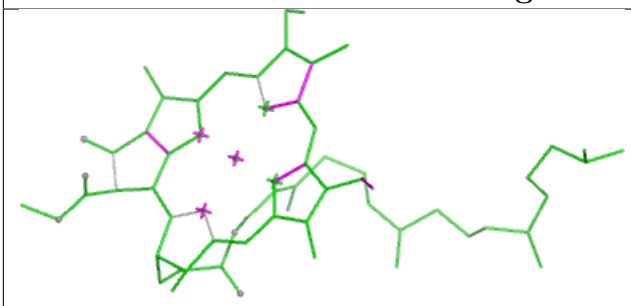
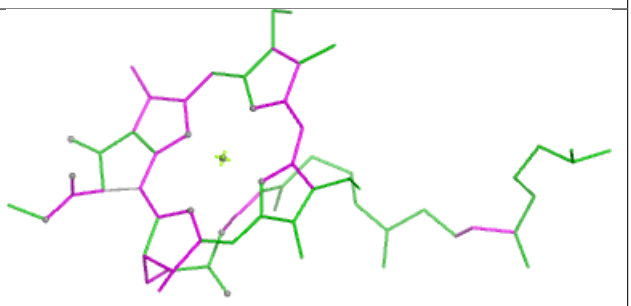
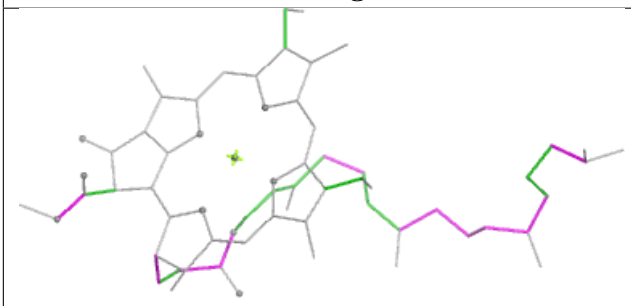
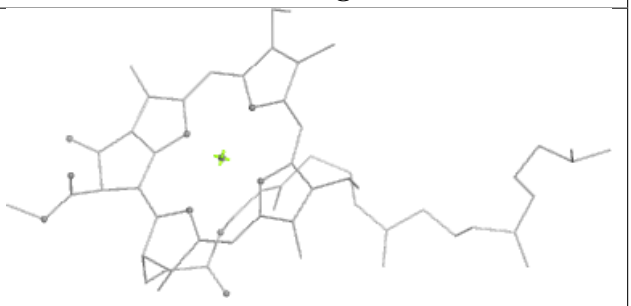
Ligand CLA g 613

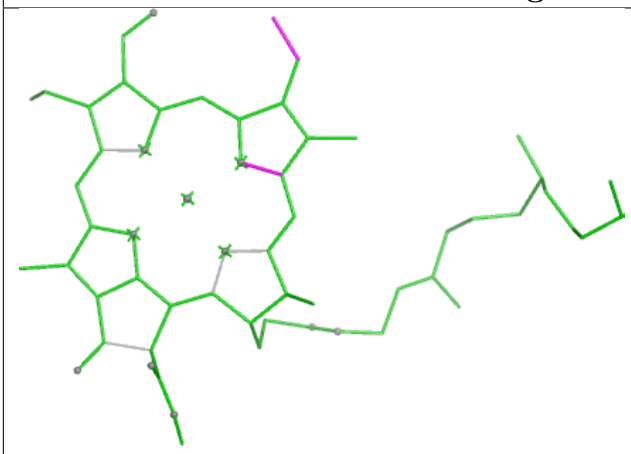
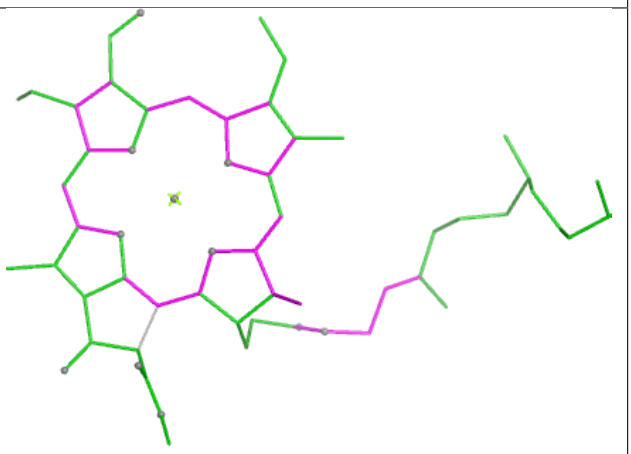
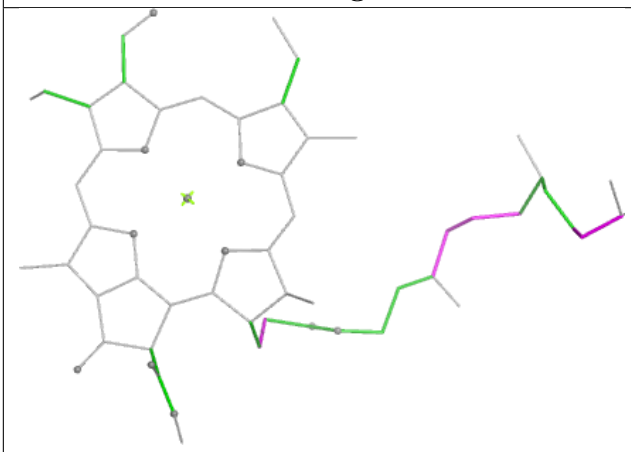
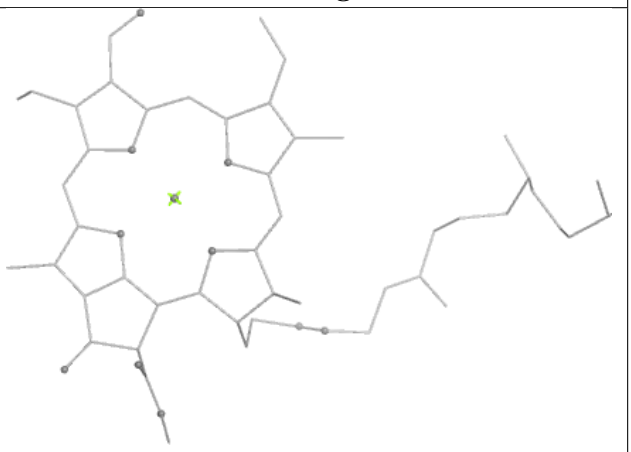


Ligand LUT y 620

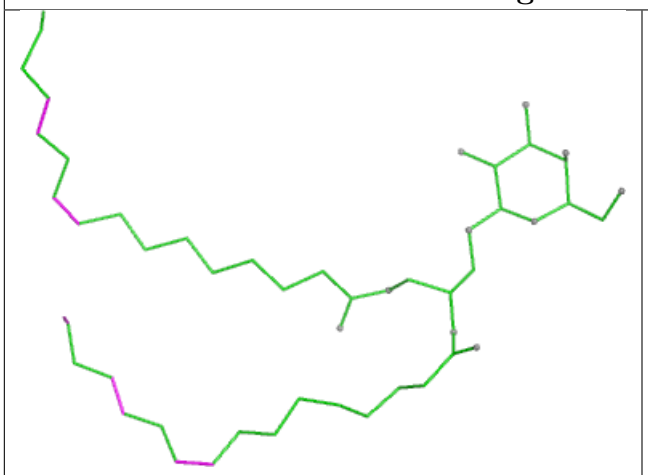


Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C1 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL S 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG c1 521



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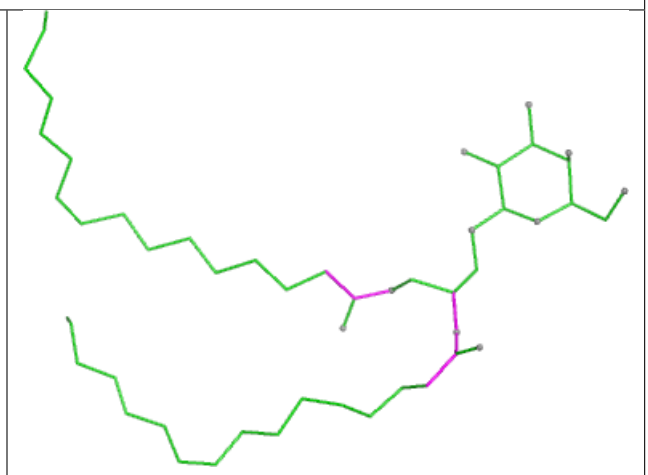

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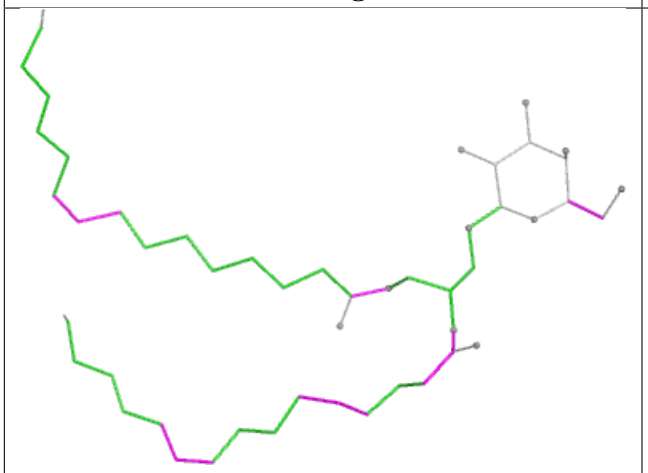
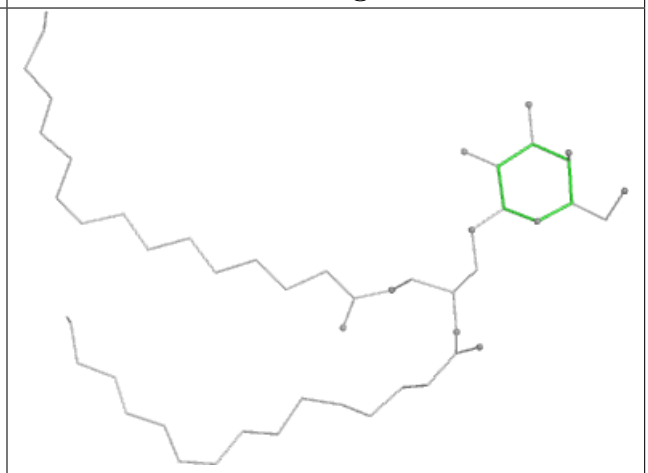
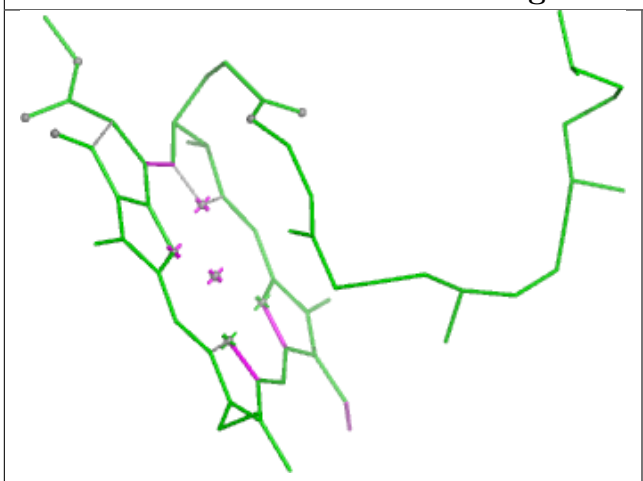
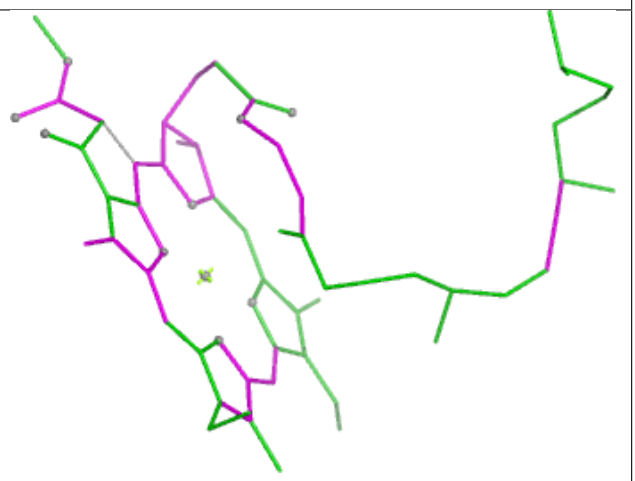


Torsions



Rings

Ligand CLA n 613	
	
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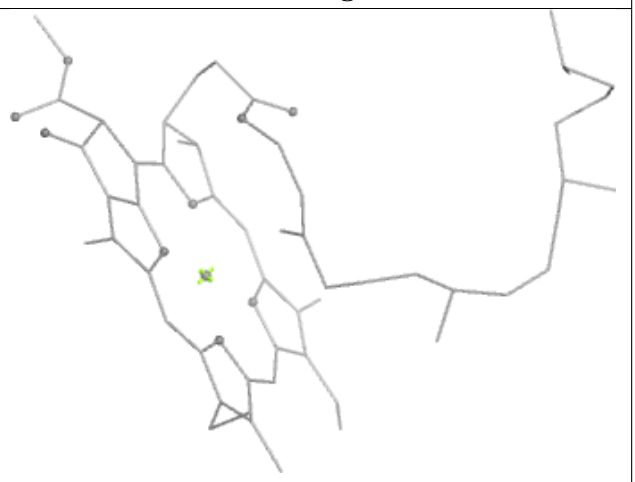
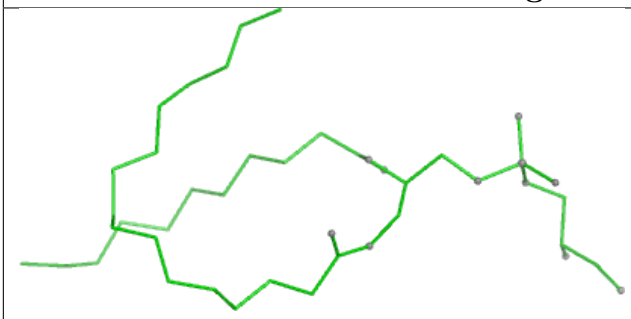
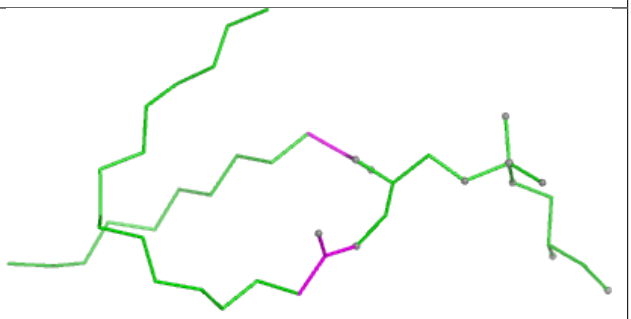
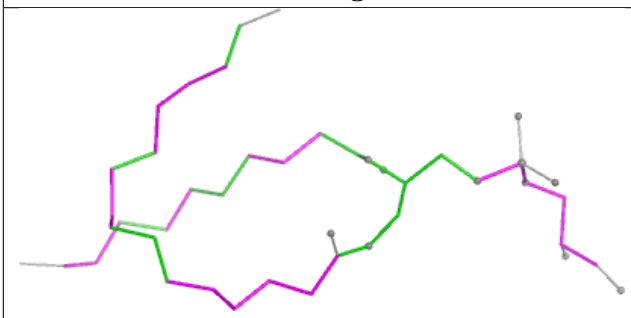
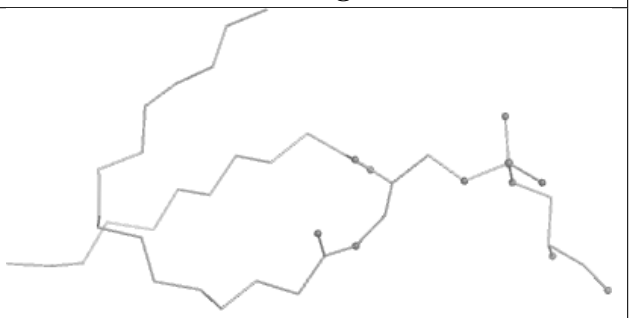
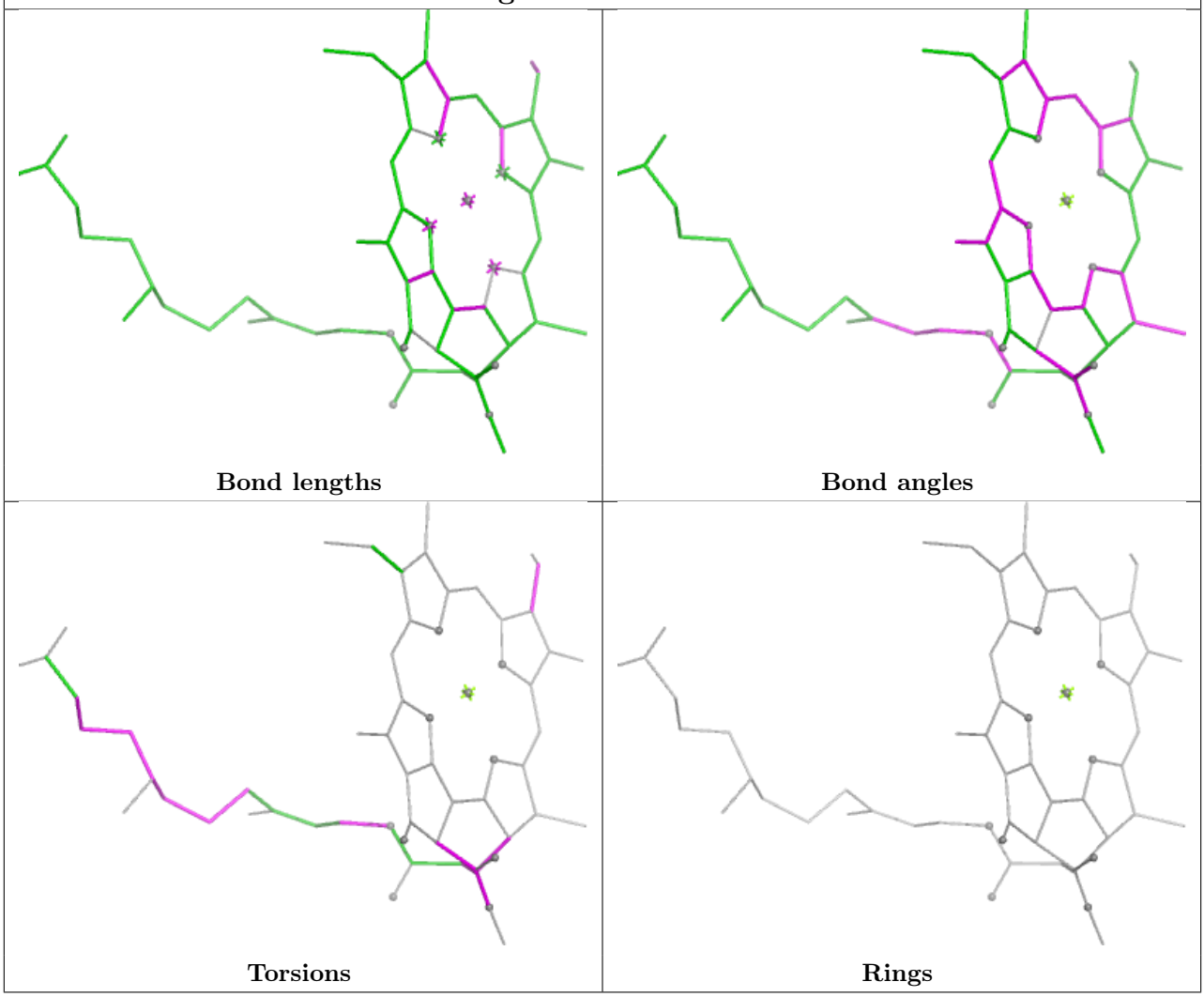
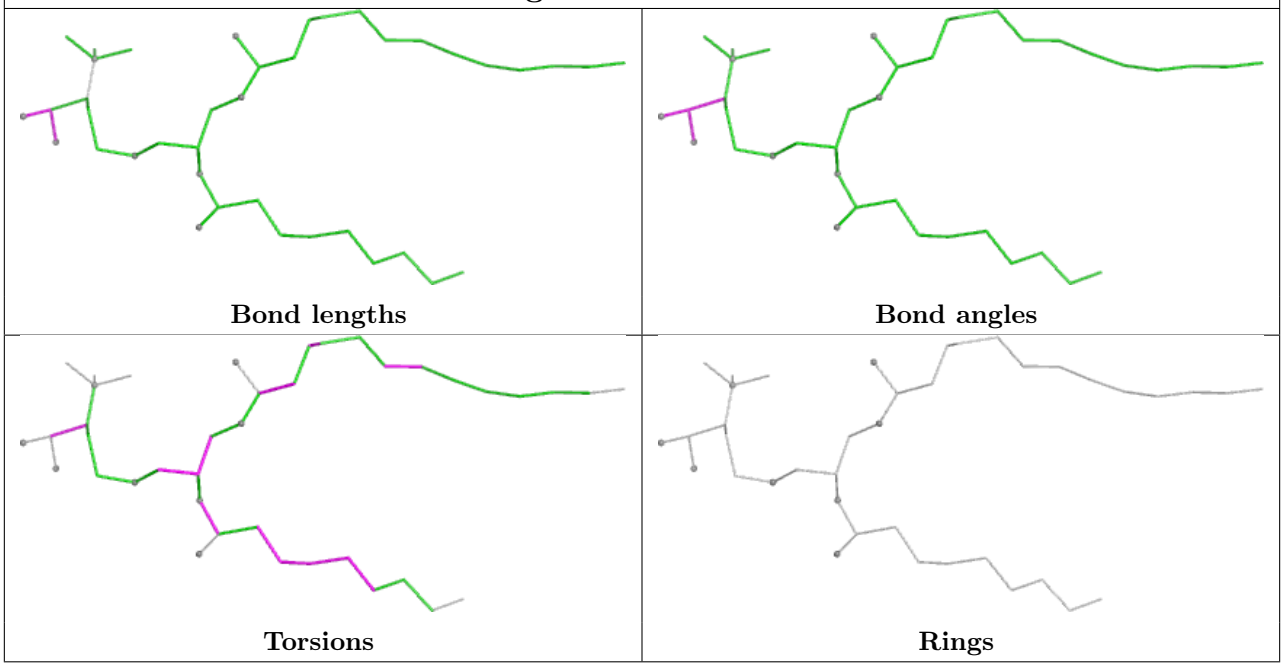
	
Torsions	**Rings**

Ligand LHG d 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 609



Ligand LMK c 527



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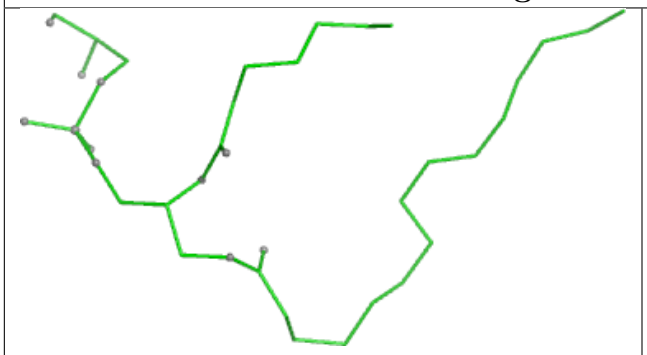
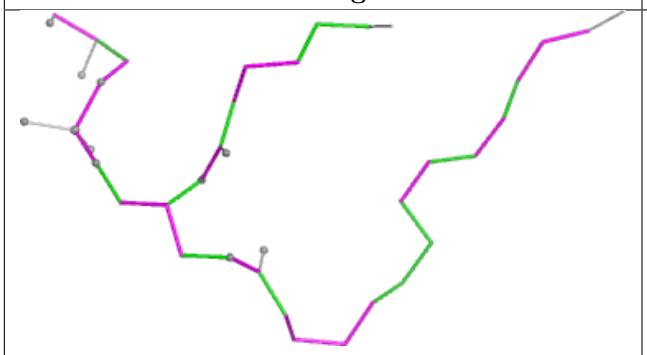
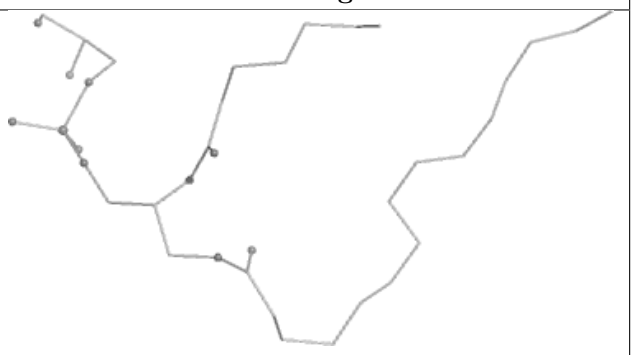
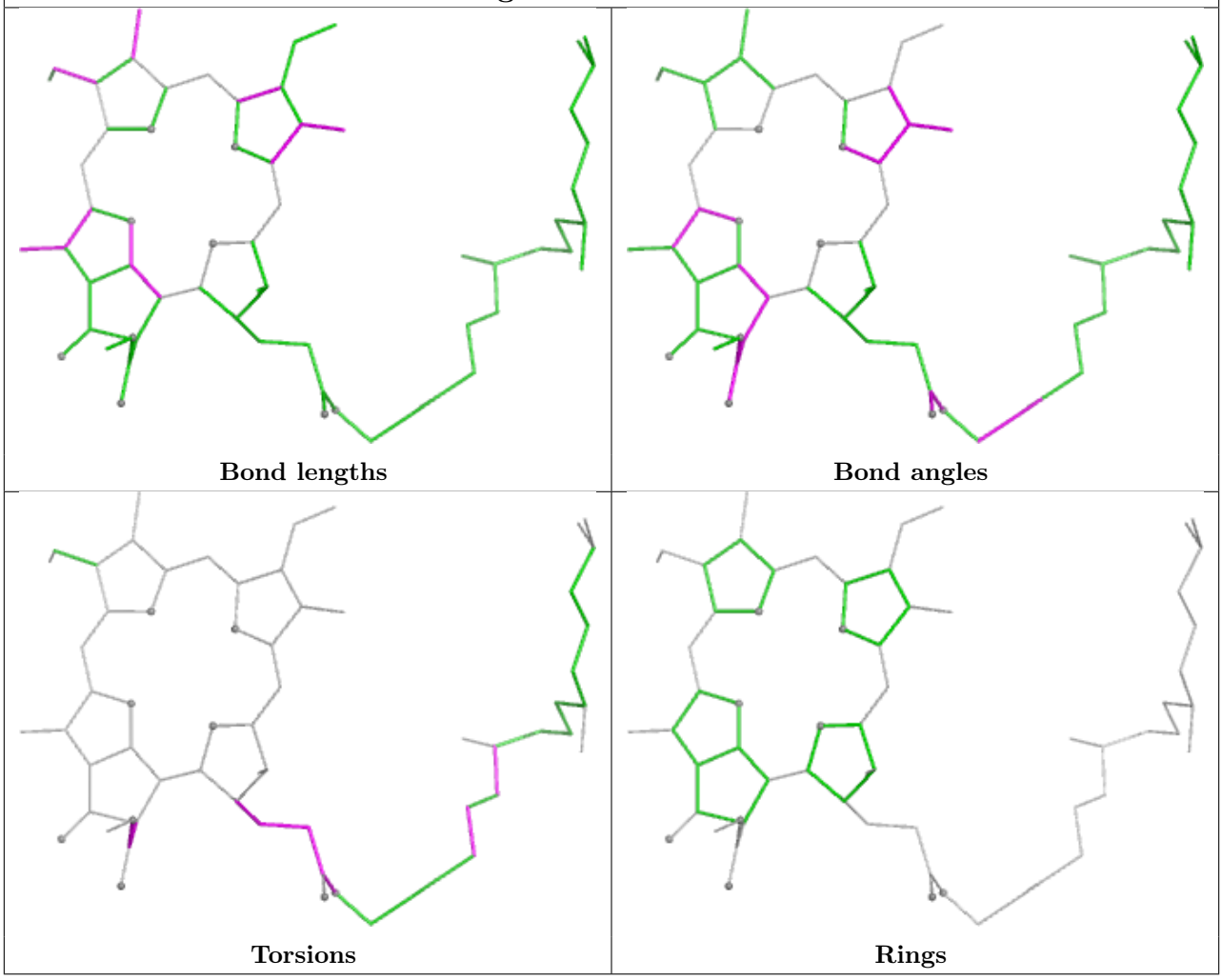
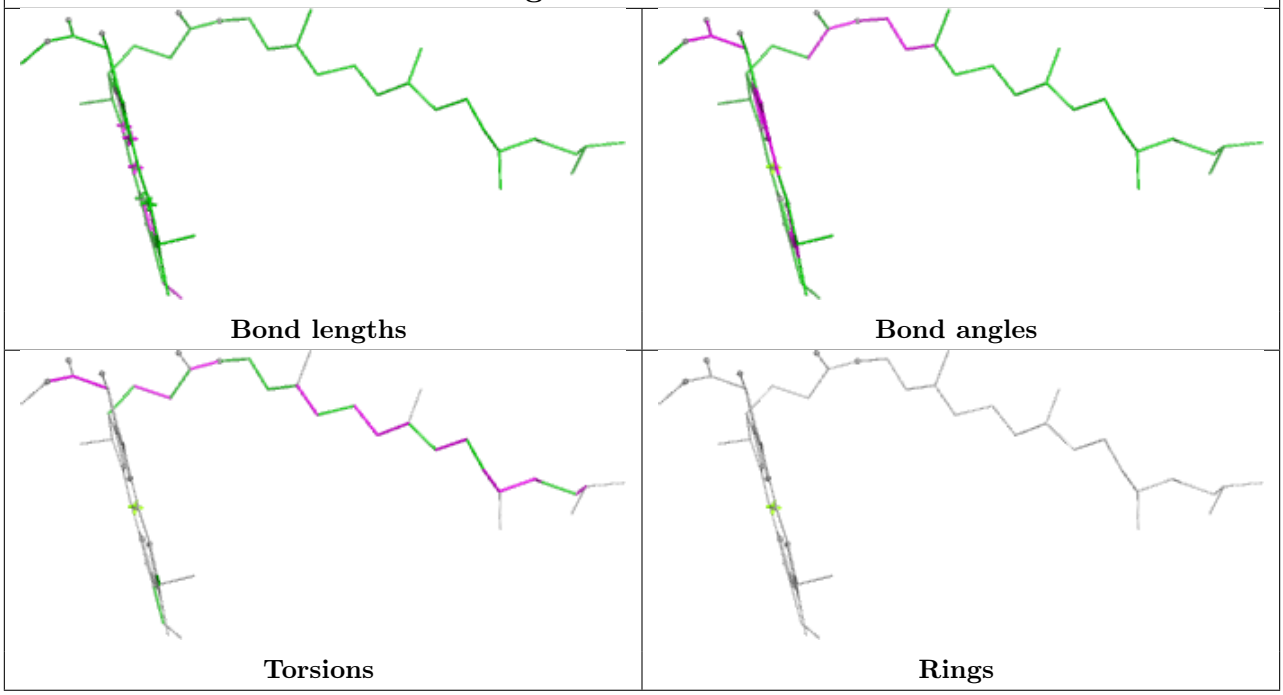
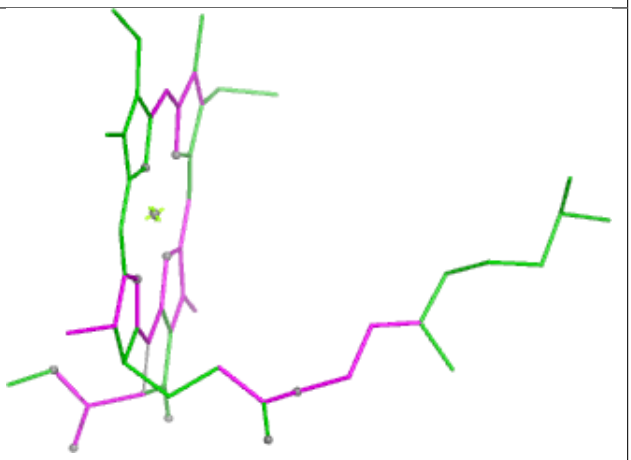
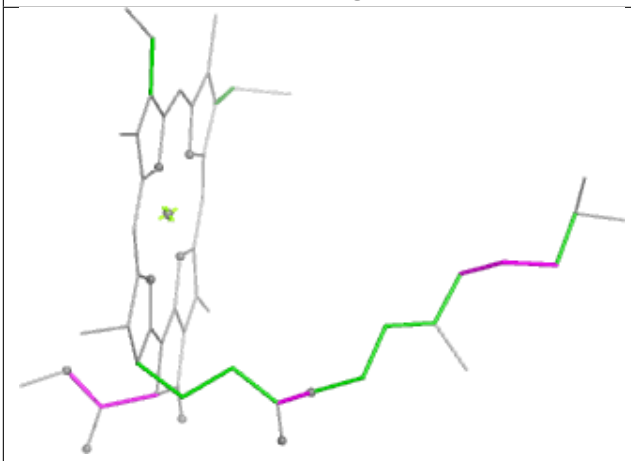
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand PHO A 409

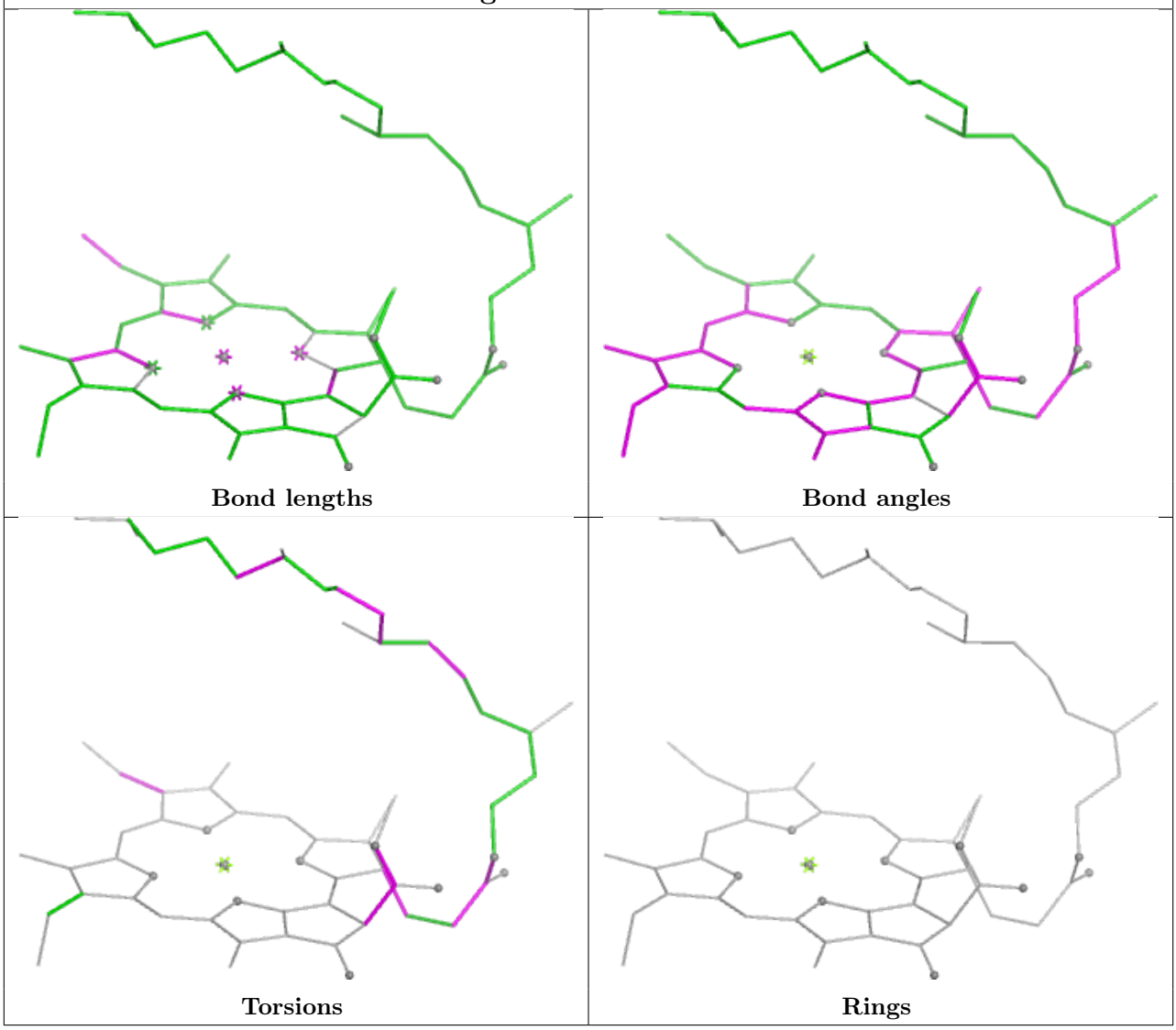


Ligand CLA B 606



Ligand CLA s1 604	
Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA G 603



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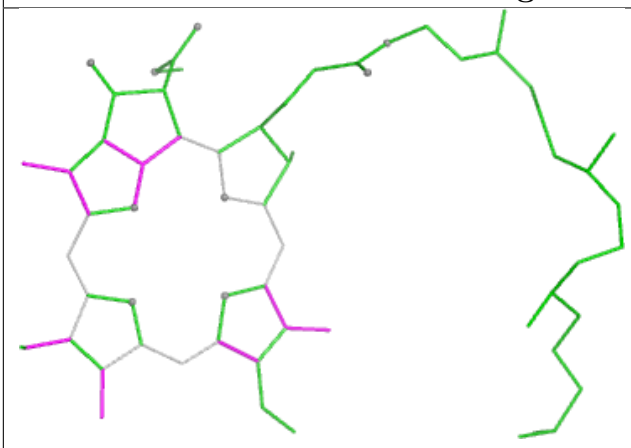
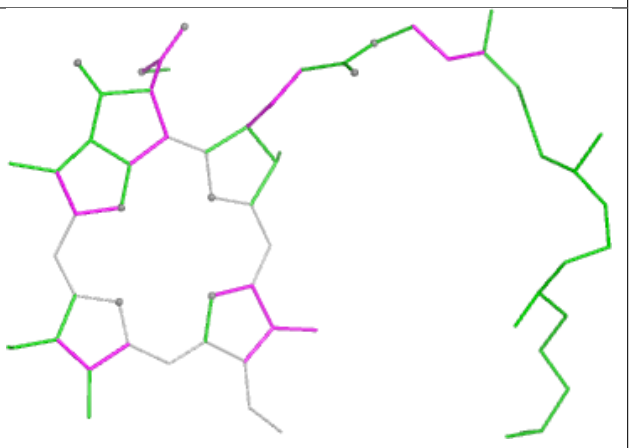
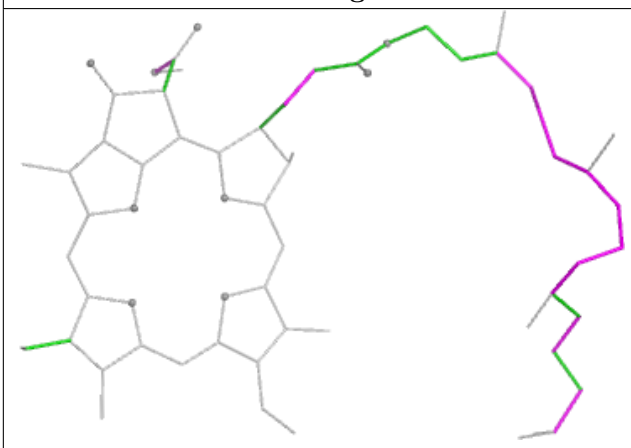
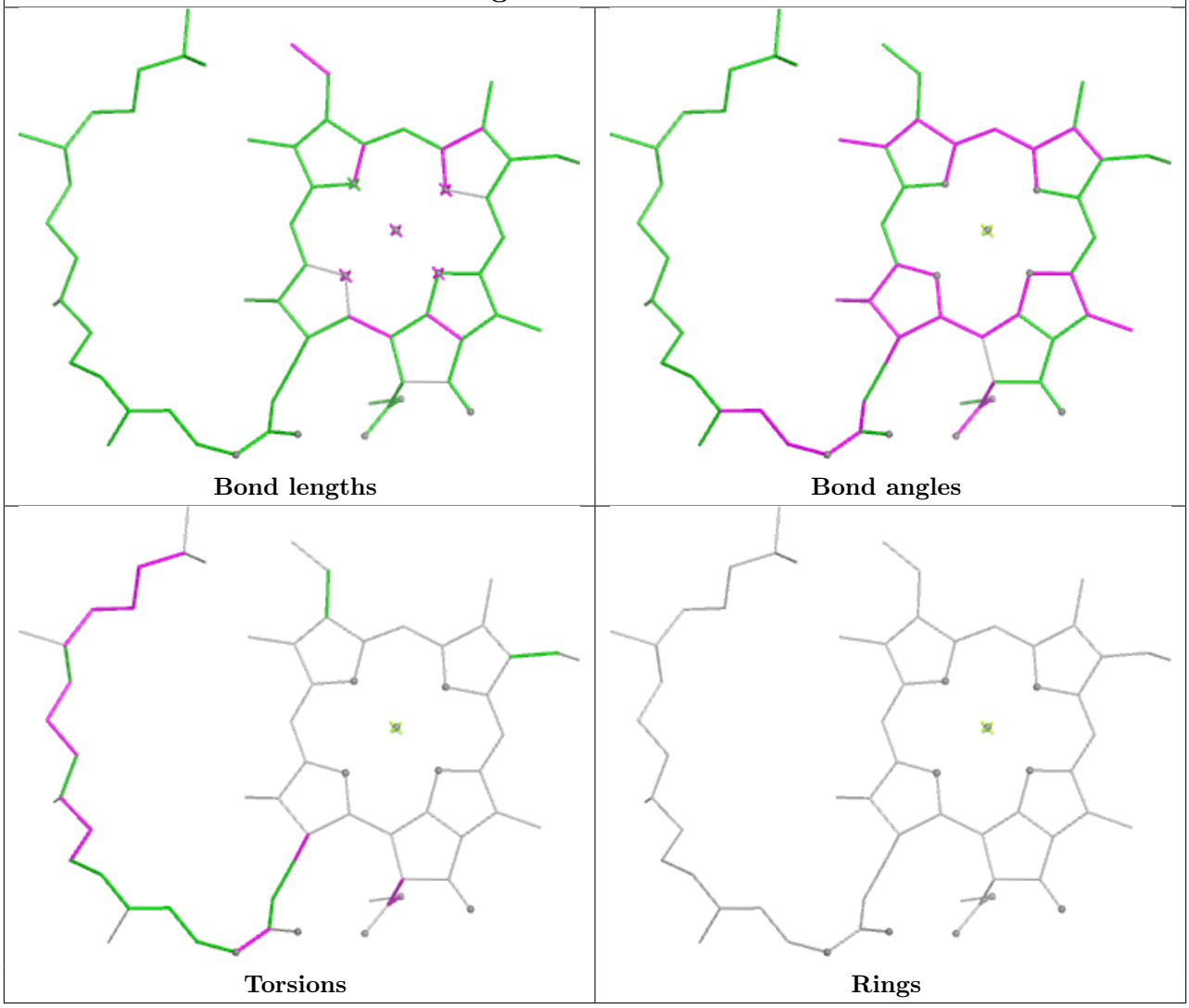
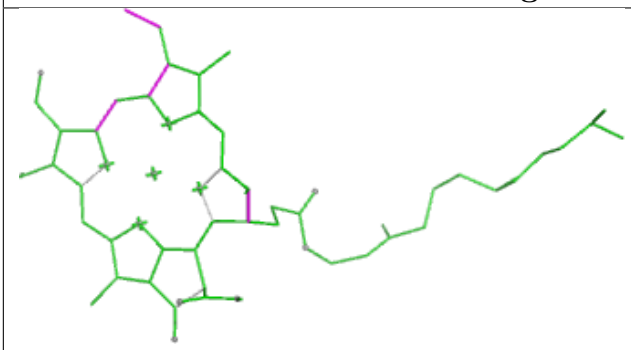
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA c 512



Ligand CHL s1 608



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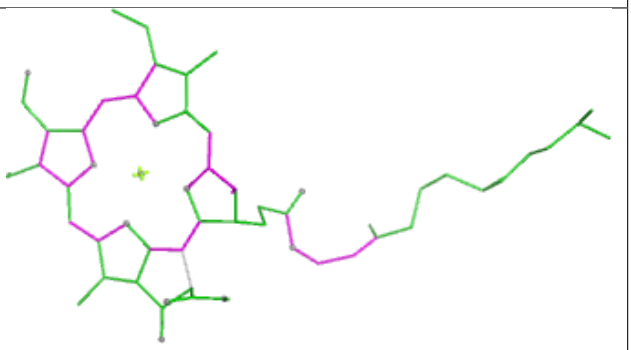
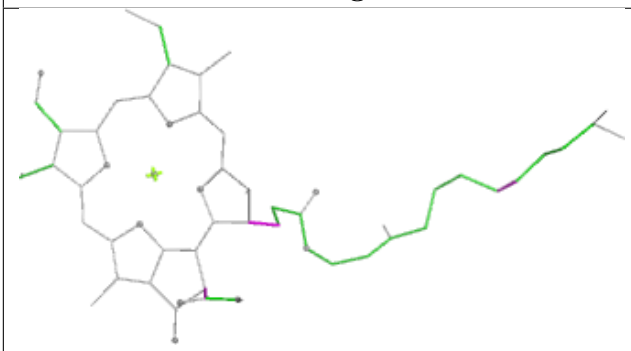


Bond angles



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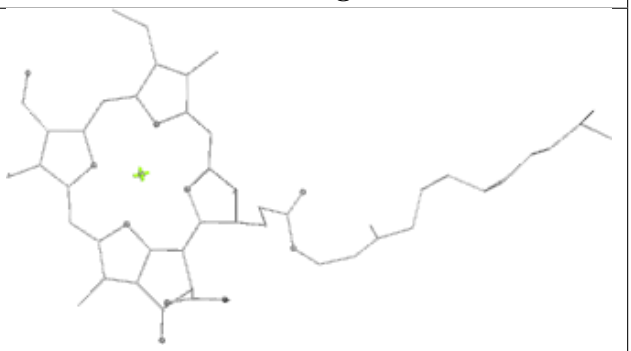
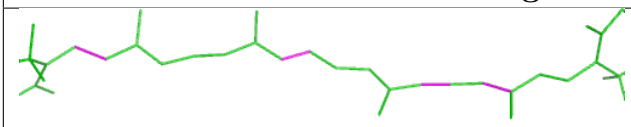


Rings

Ligand BCR A 411



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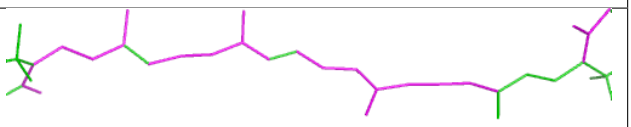
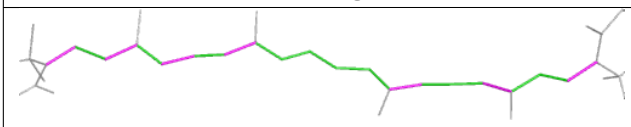
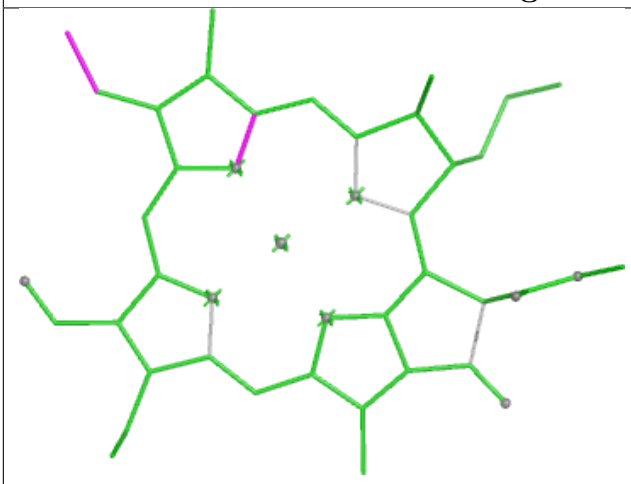
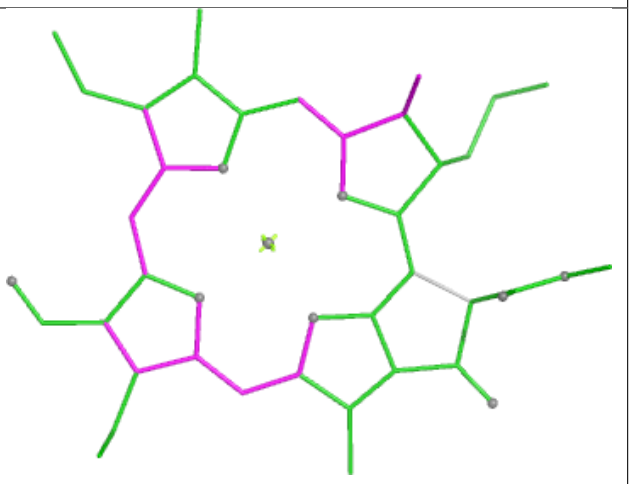


Bond angles



Torsions

Rings

Ligand CHL s1 606	
	
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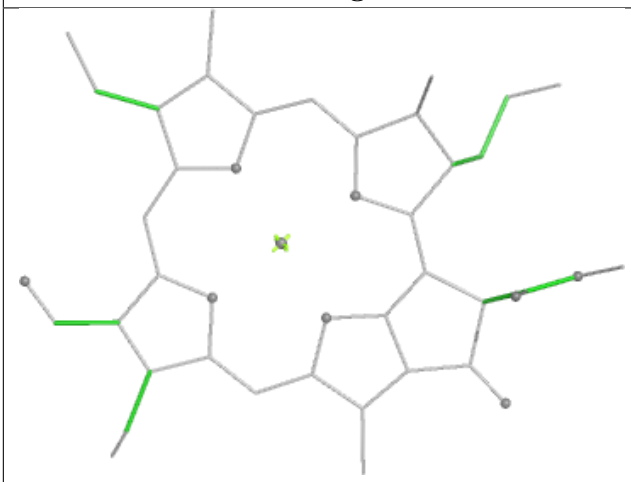
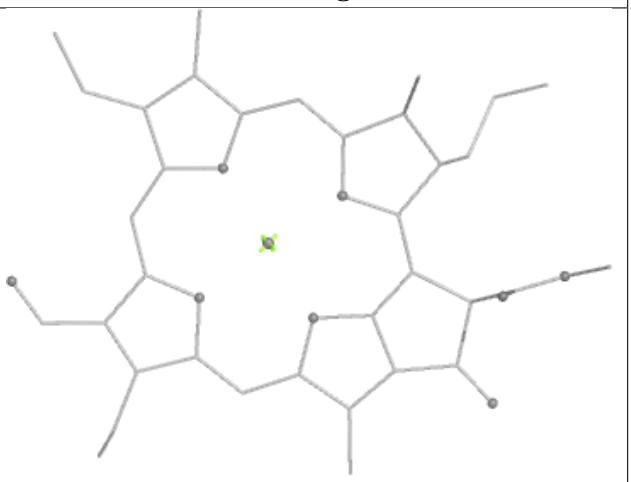
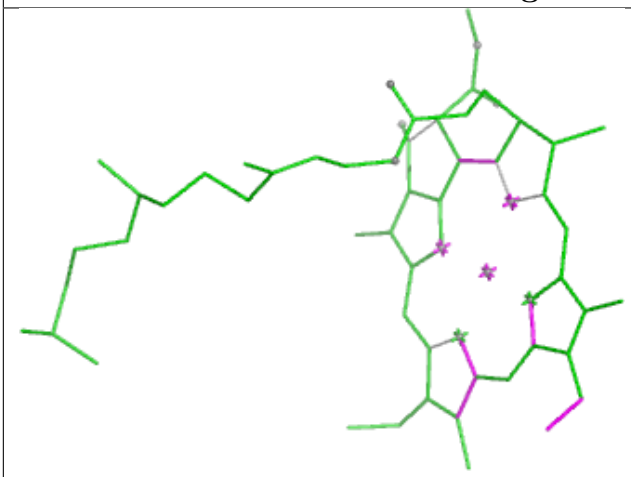
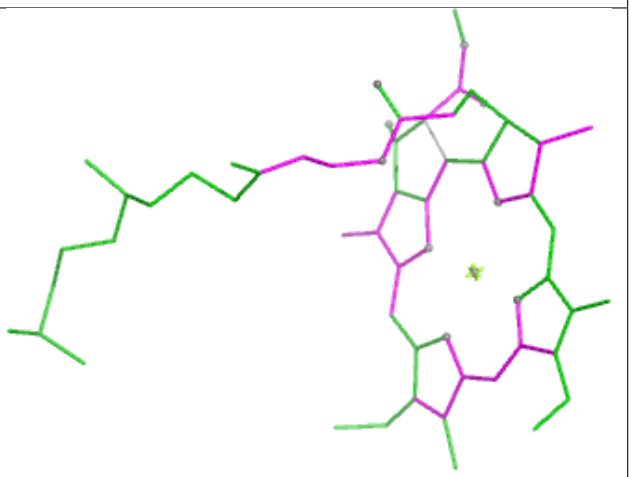
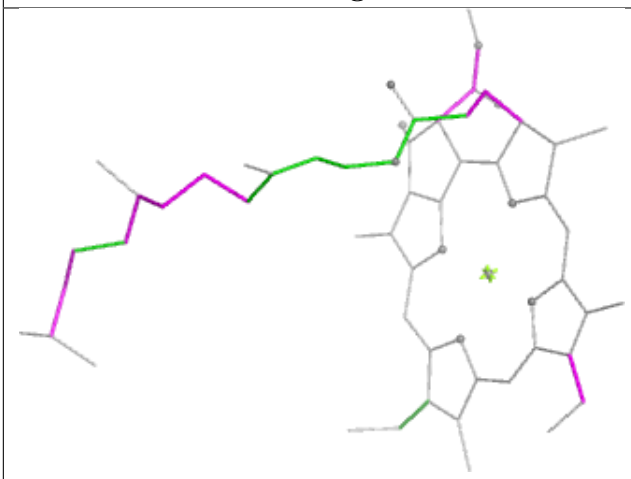
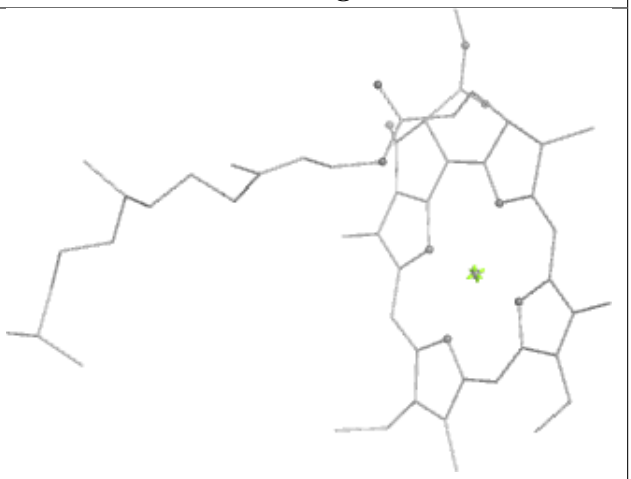
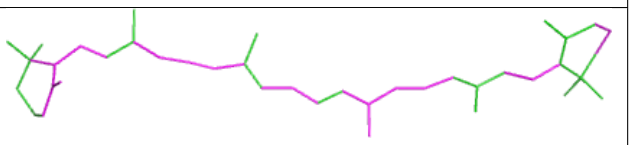
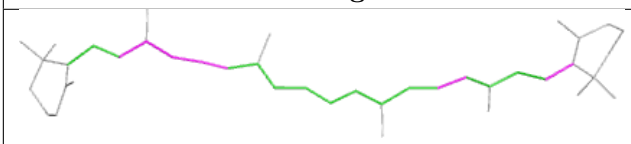
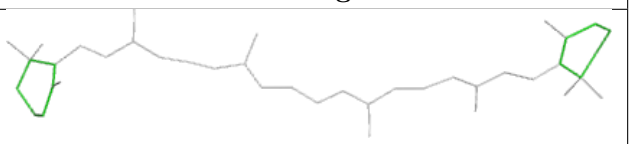
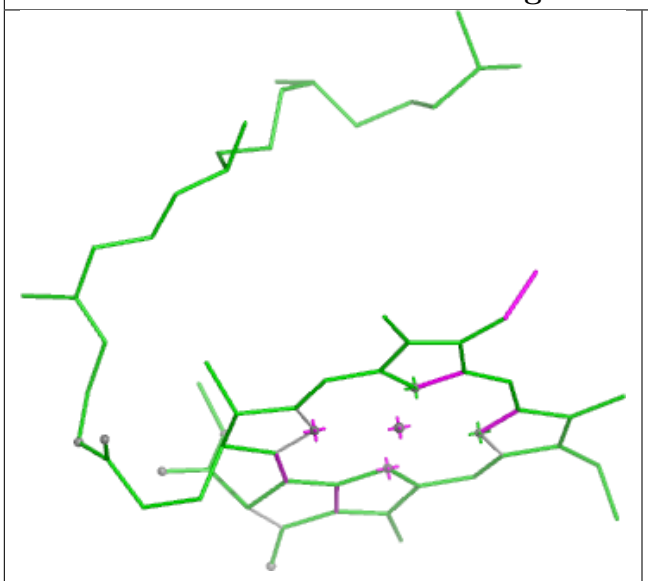
	
Torsions	**Rings**

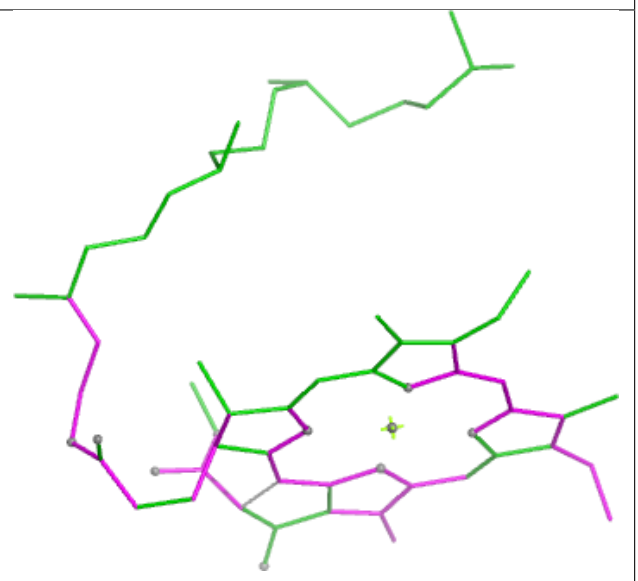
Ligand CLA s1 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b1 619	
Bond lengths	 Bond angles
 Torsions	 Rings

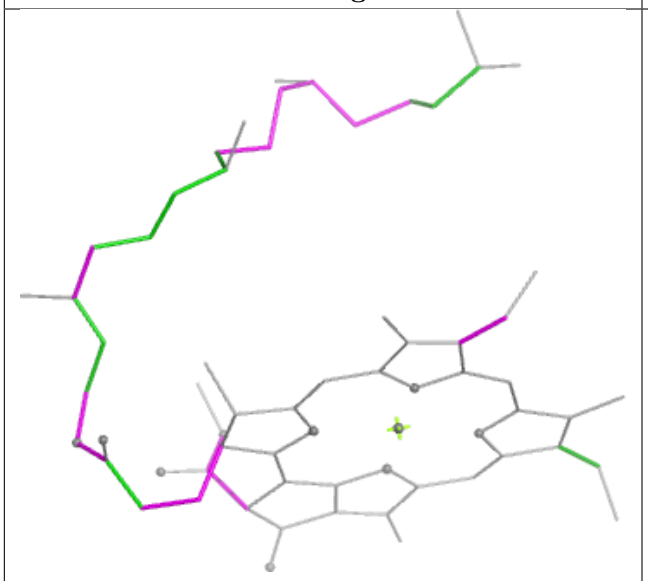
Ligand CLA N 603



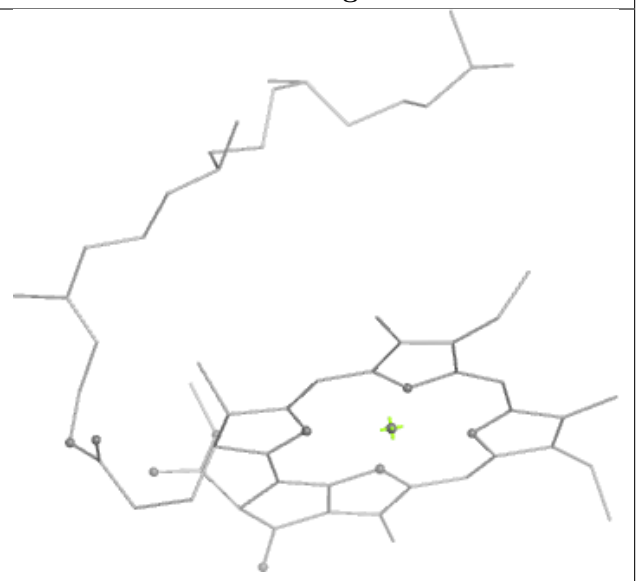
Bond lengths



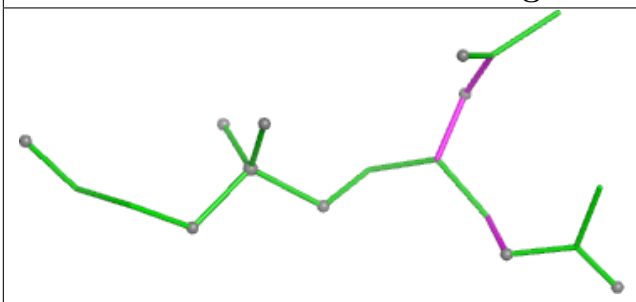
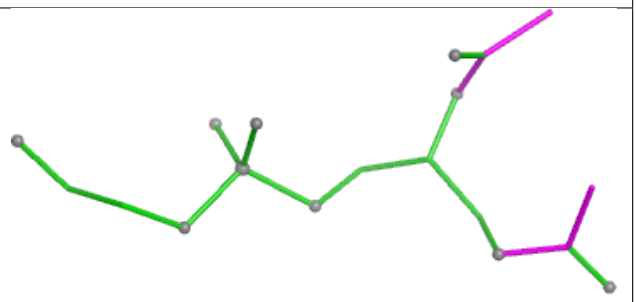
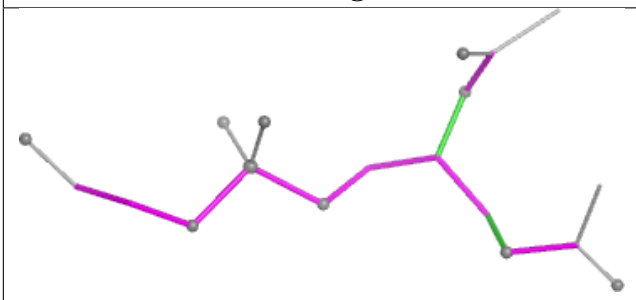
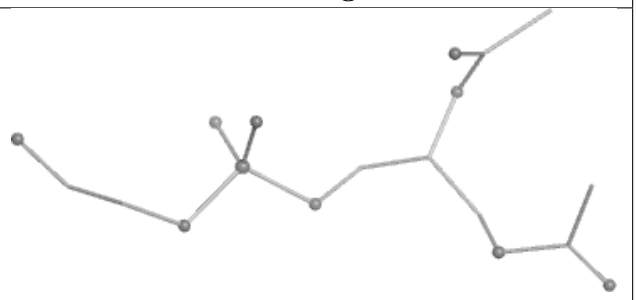
Bond angles



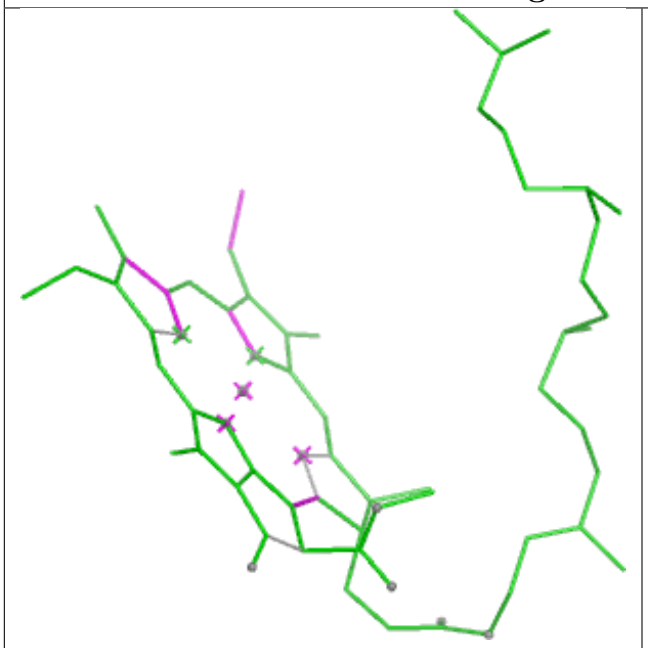
Torsions



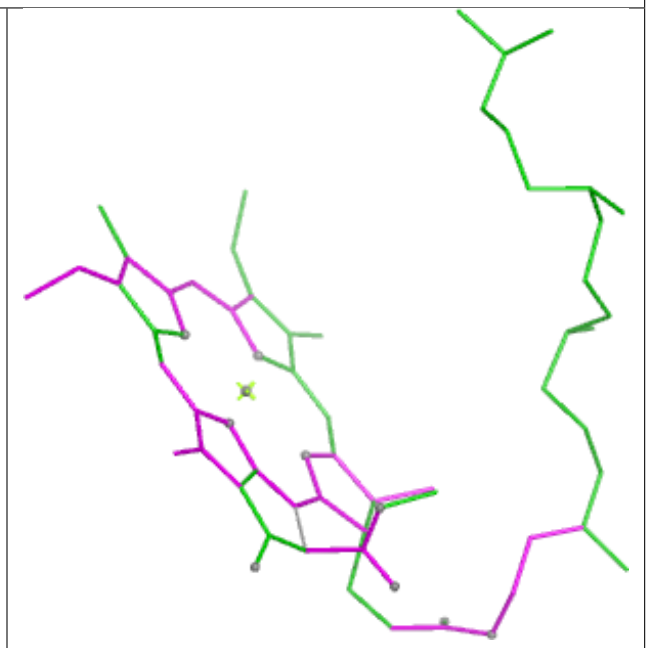
Rings

Ligand PTY Y 627	
 Bond lengths	 Bond angles
 Torsions	 Rings

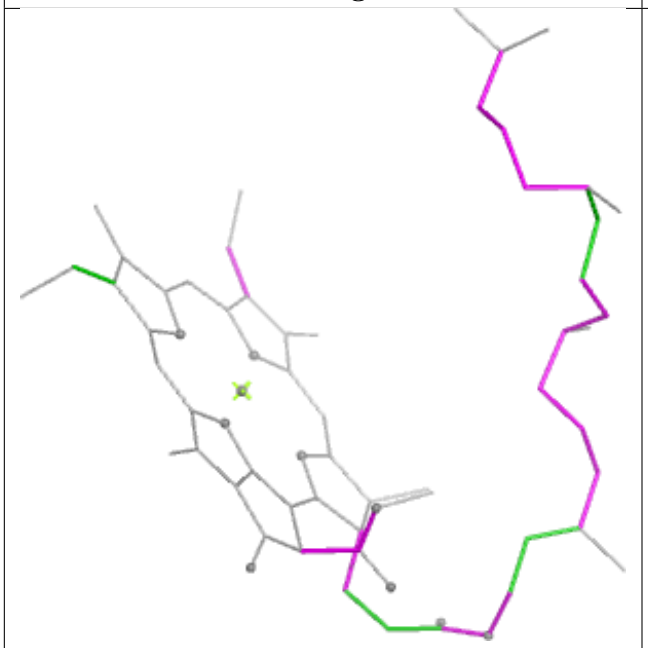
Ligand CLA n 603



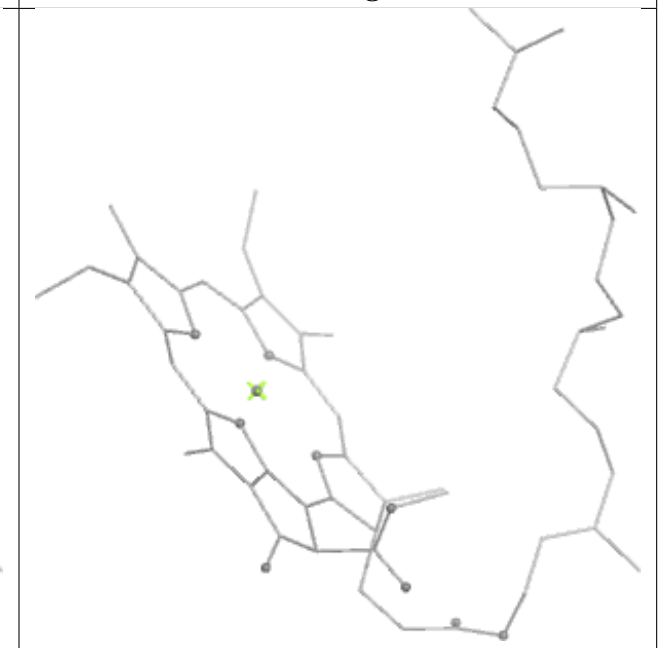
Bond lengths



Bond angles

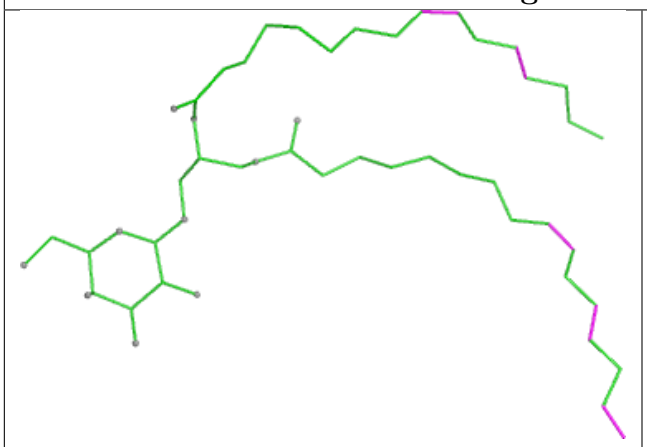


Torsions



Rings

Ligand LMG C 521



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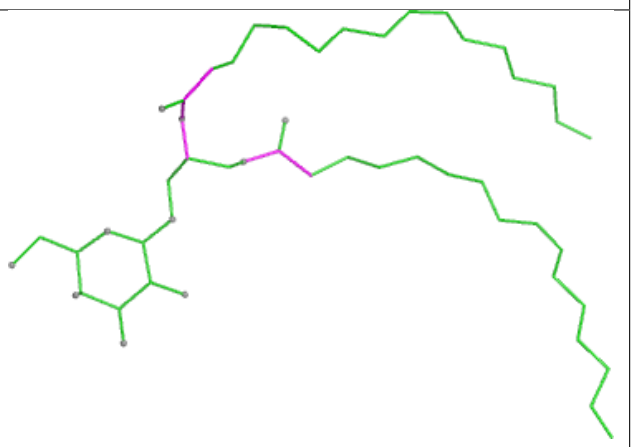
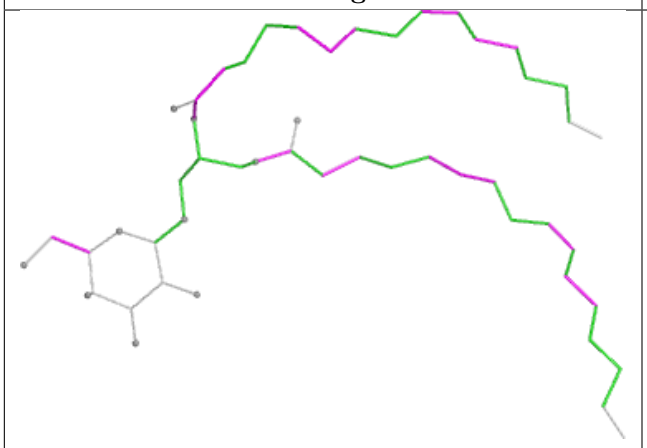


Bond angles



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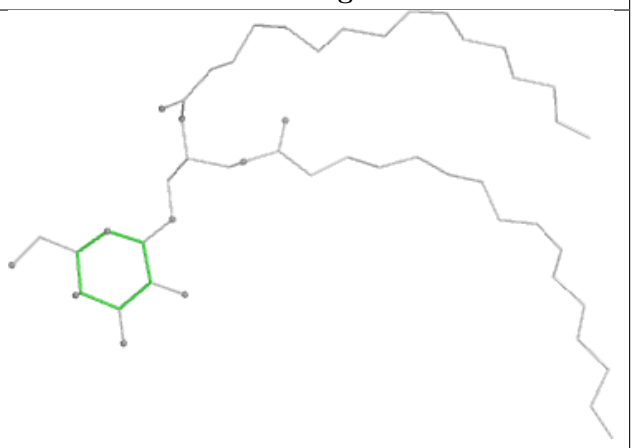
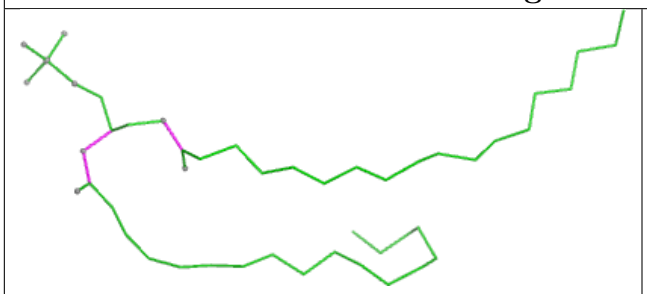


Rings

Ligand 3PH t1 101



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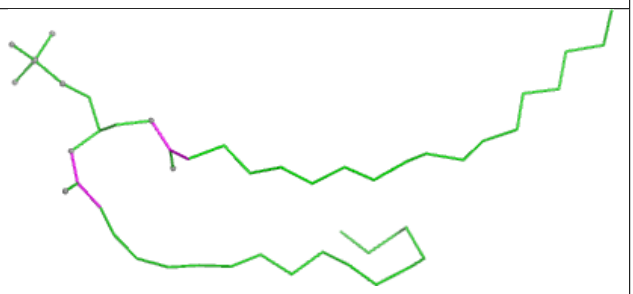
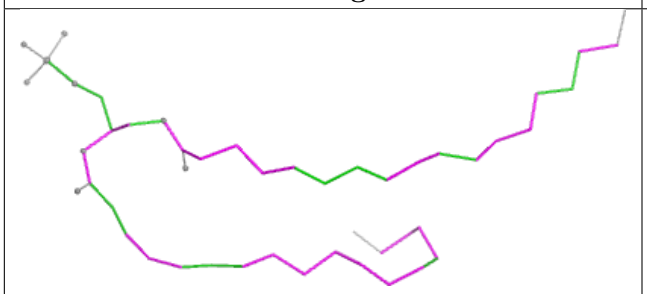


Bond angles



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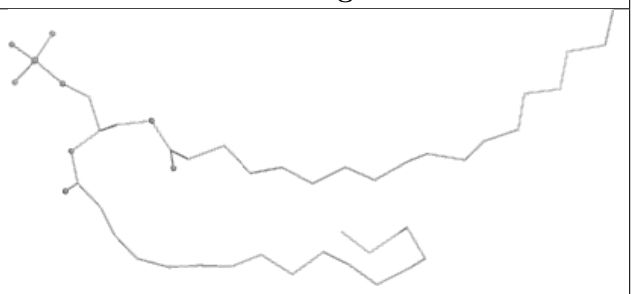
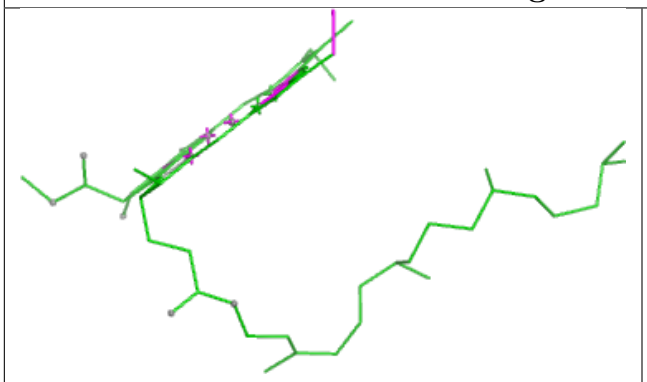


Rings

Ligand CLA y 614



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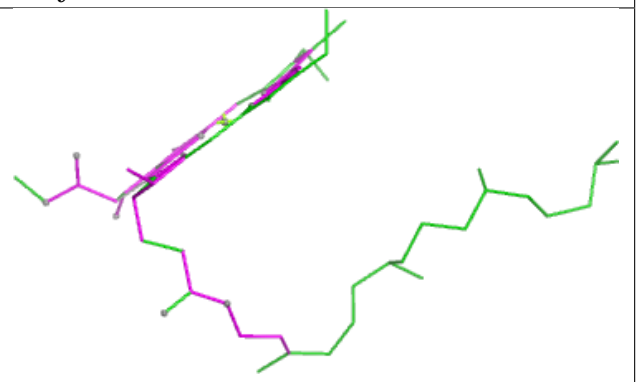
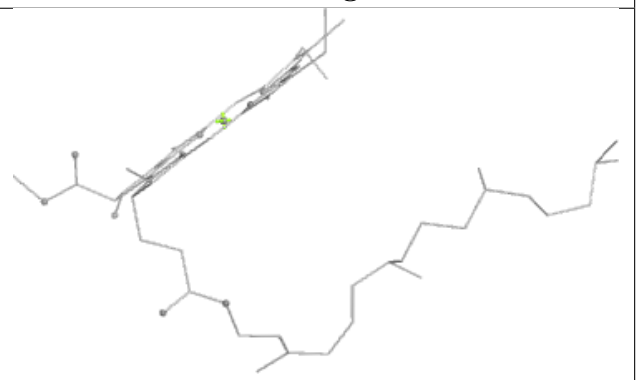


Bond angles

Torsions

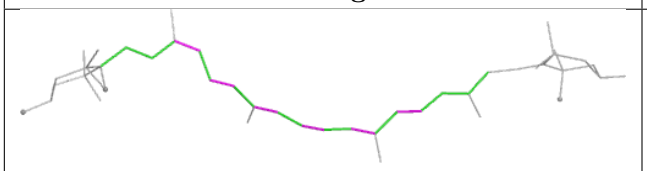


Rings

Ligand NEX R 622

Bond lengths

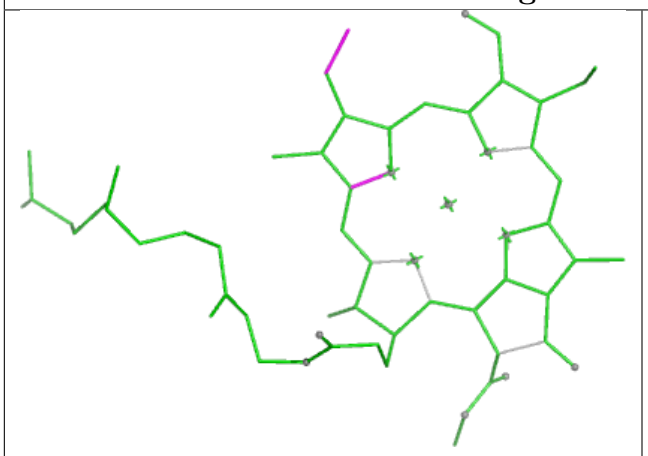
Bond angles



Torsions

Rings

Ligand CHL S1 608



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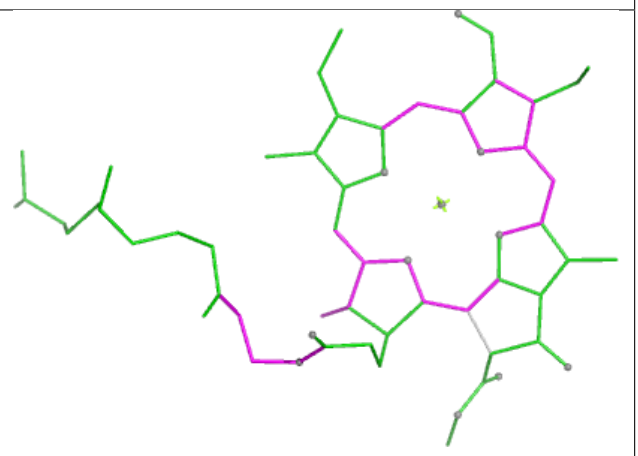

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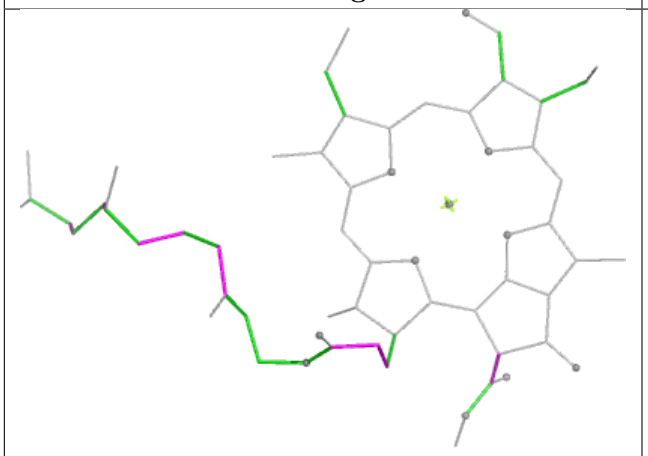

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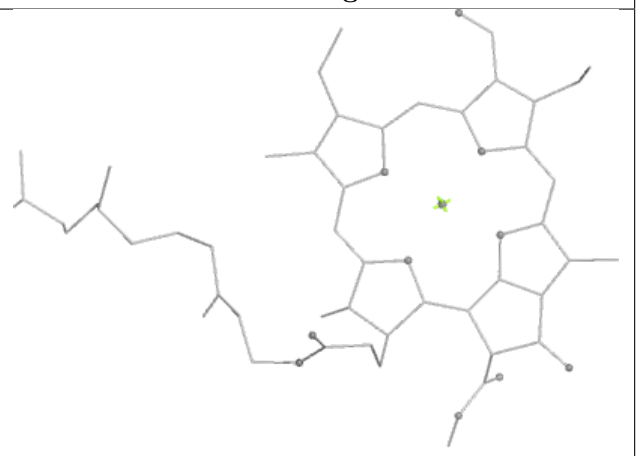
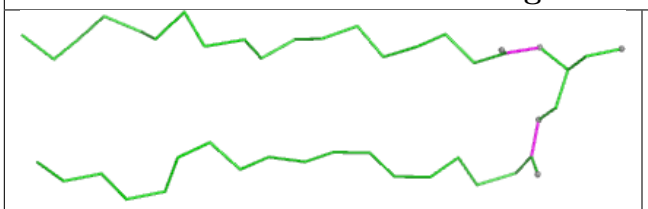


Rings

Ligand DGA b 625



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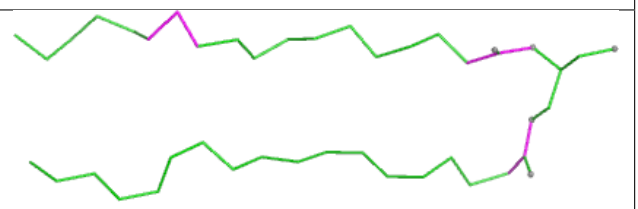
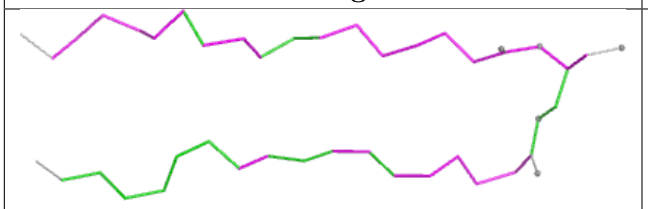


Bond angles



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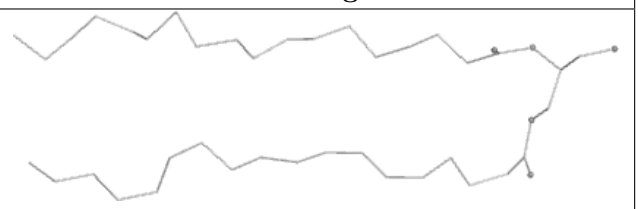
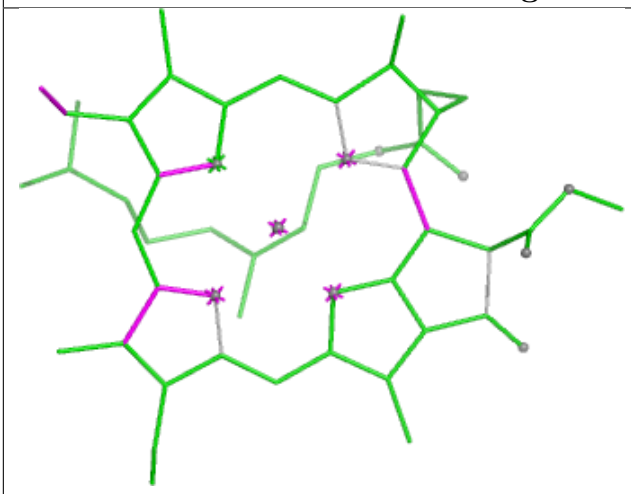


Rings

Ligand CLA s1 613



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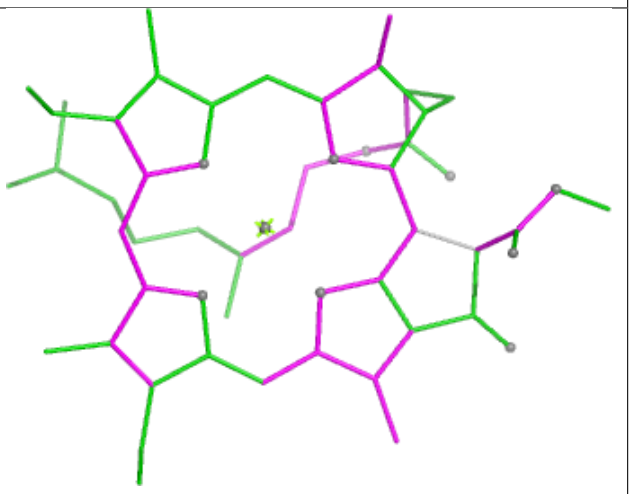
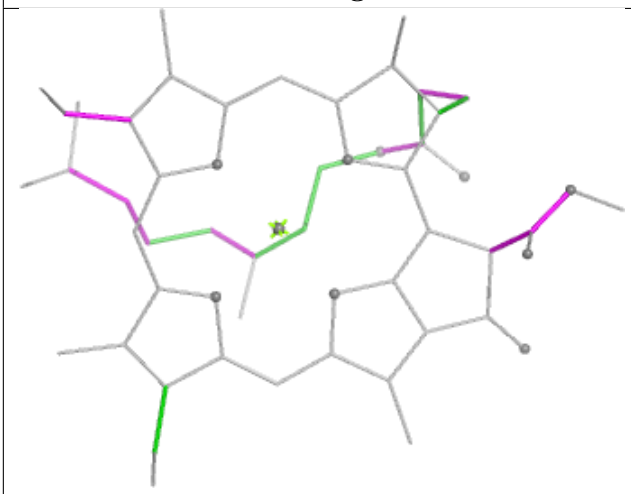


Bond angles



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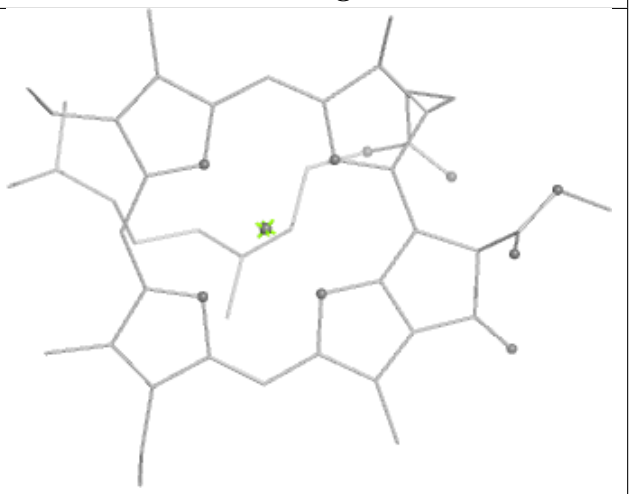
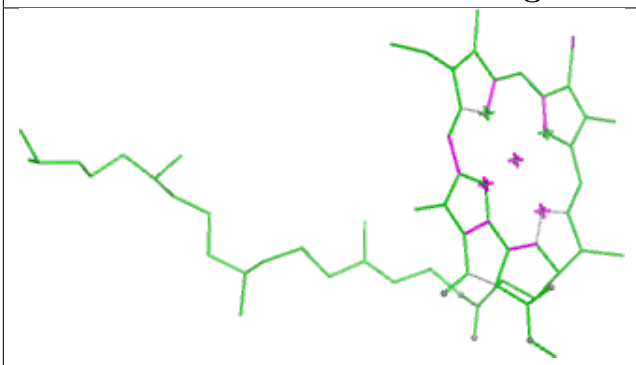
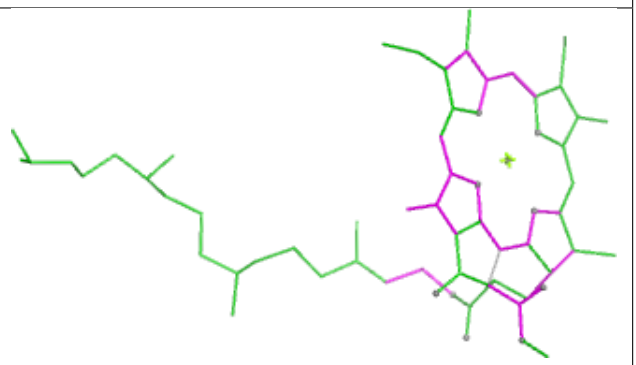
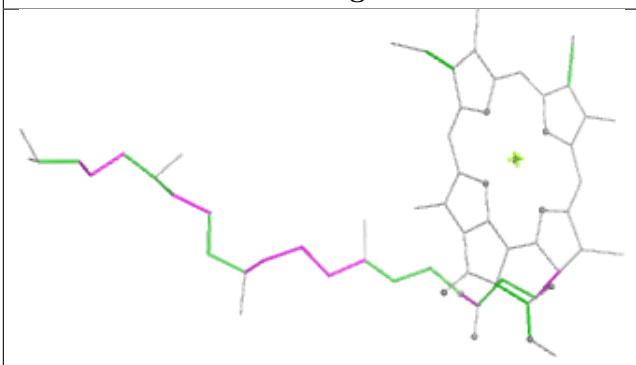
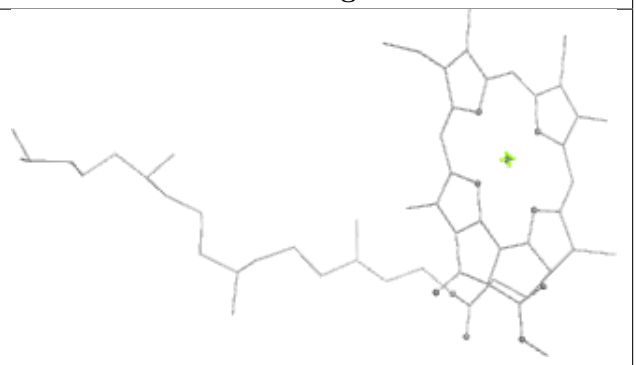
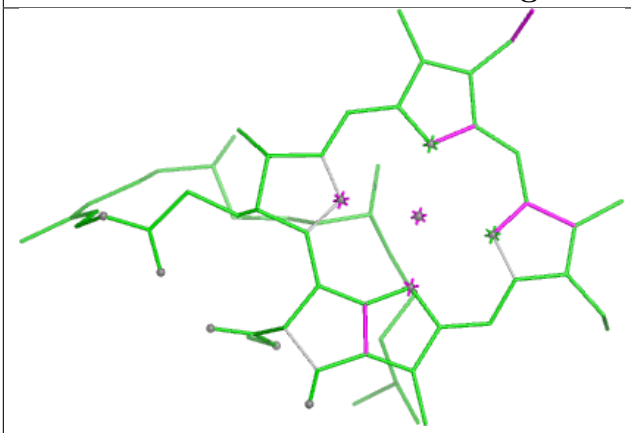
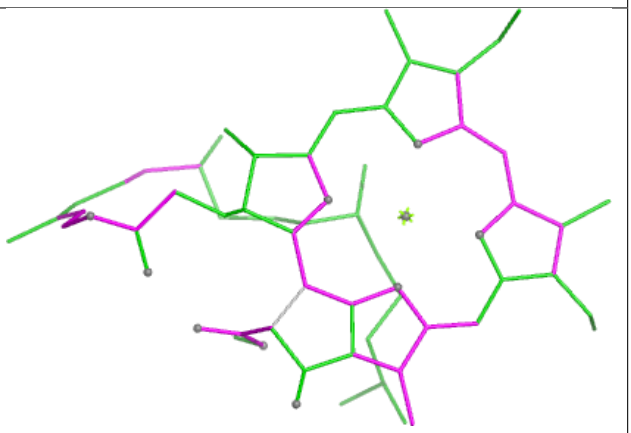
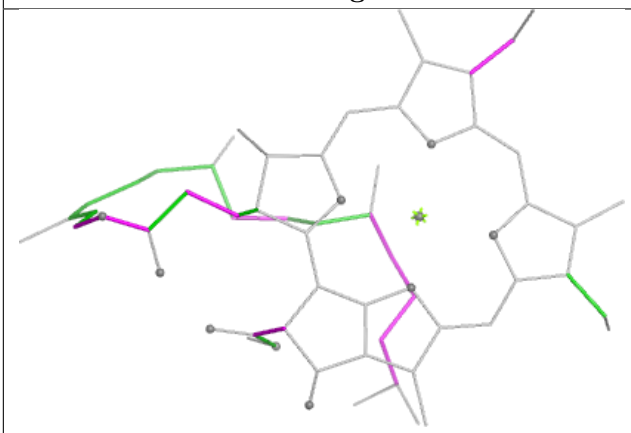
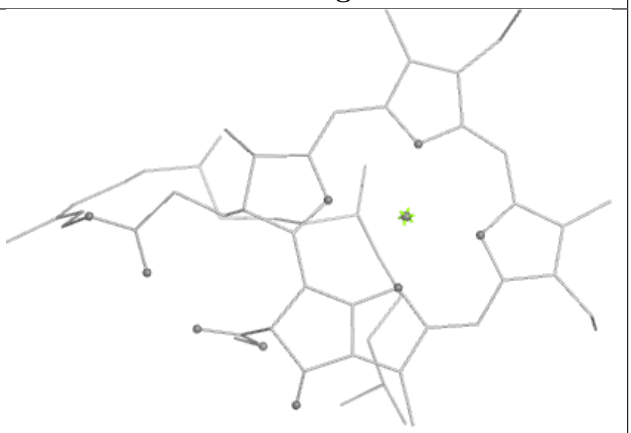
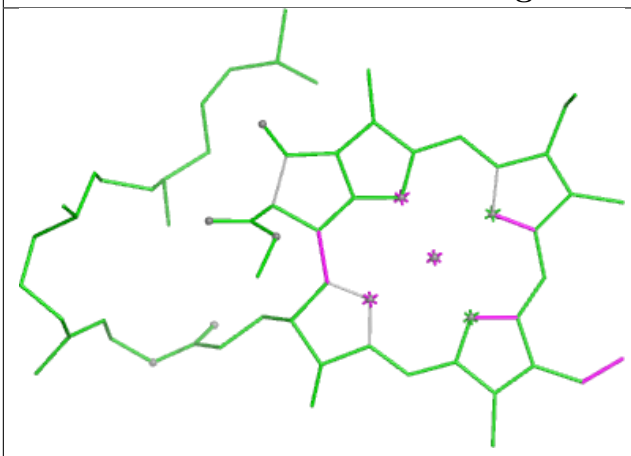
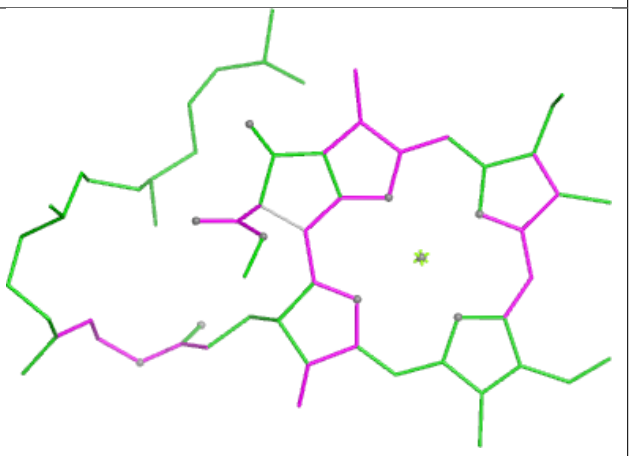
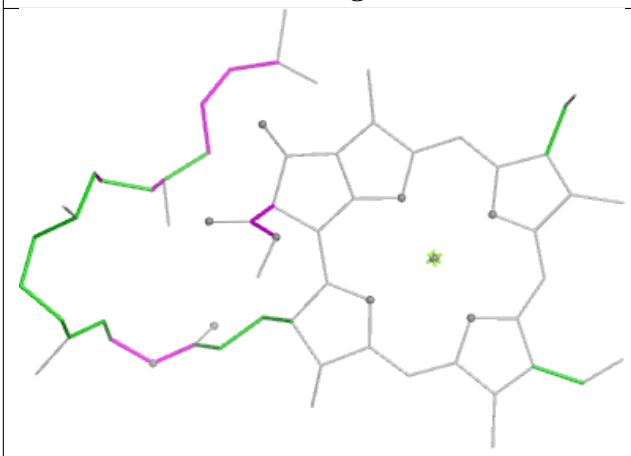
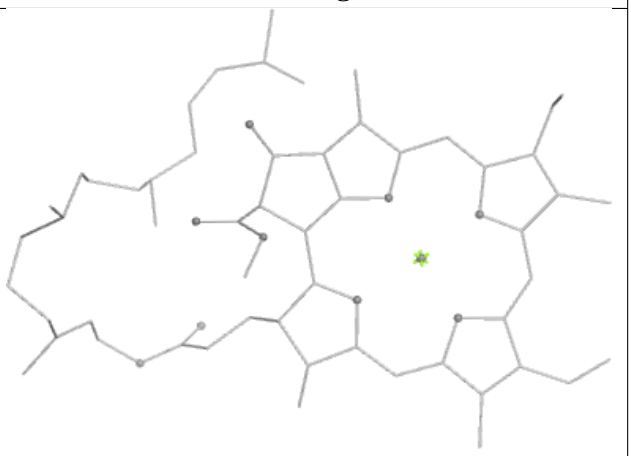
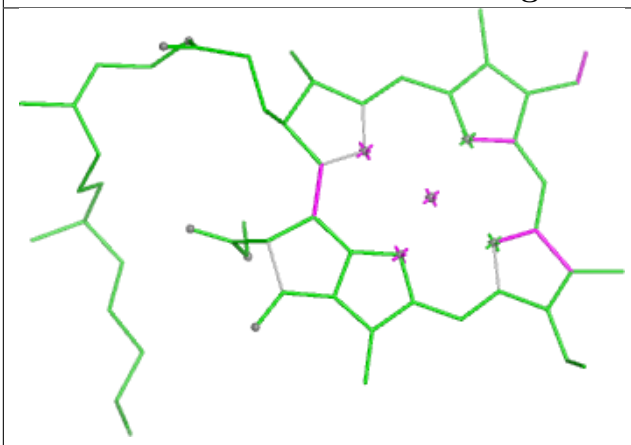
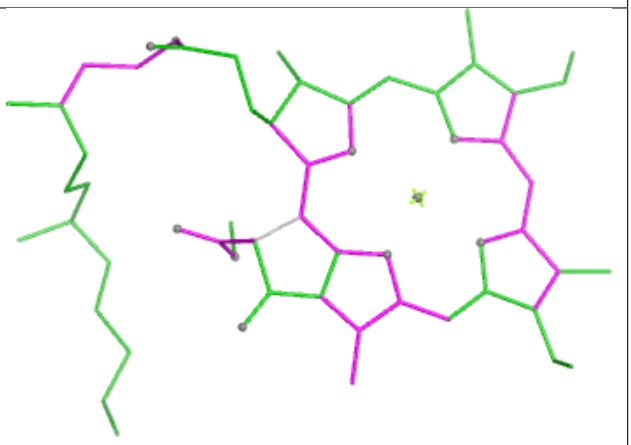
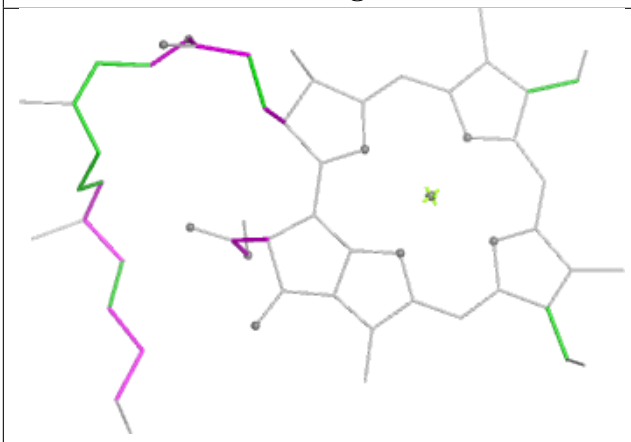
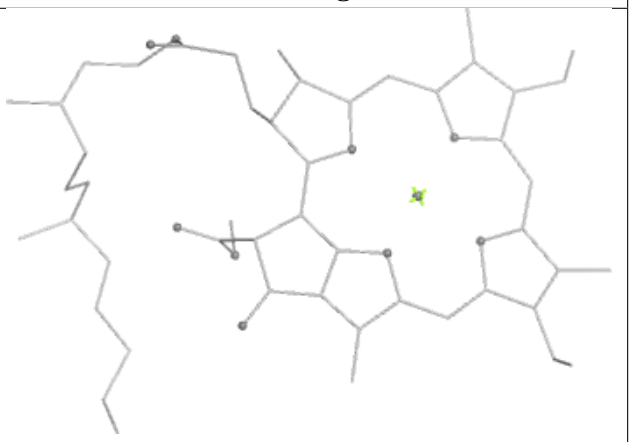


Rings

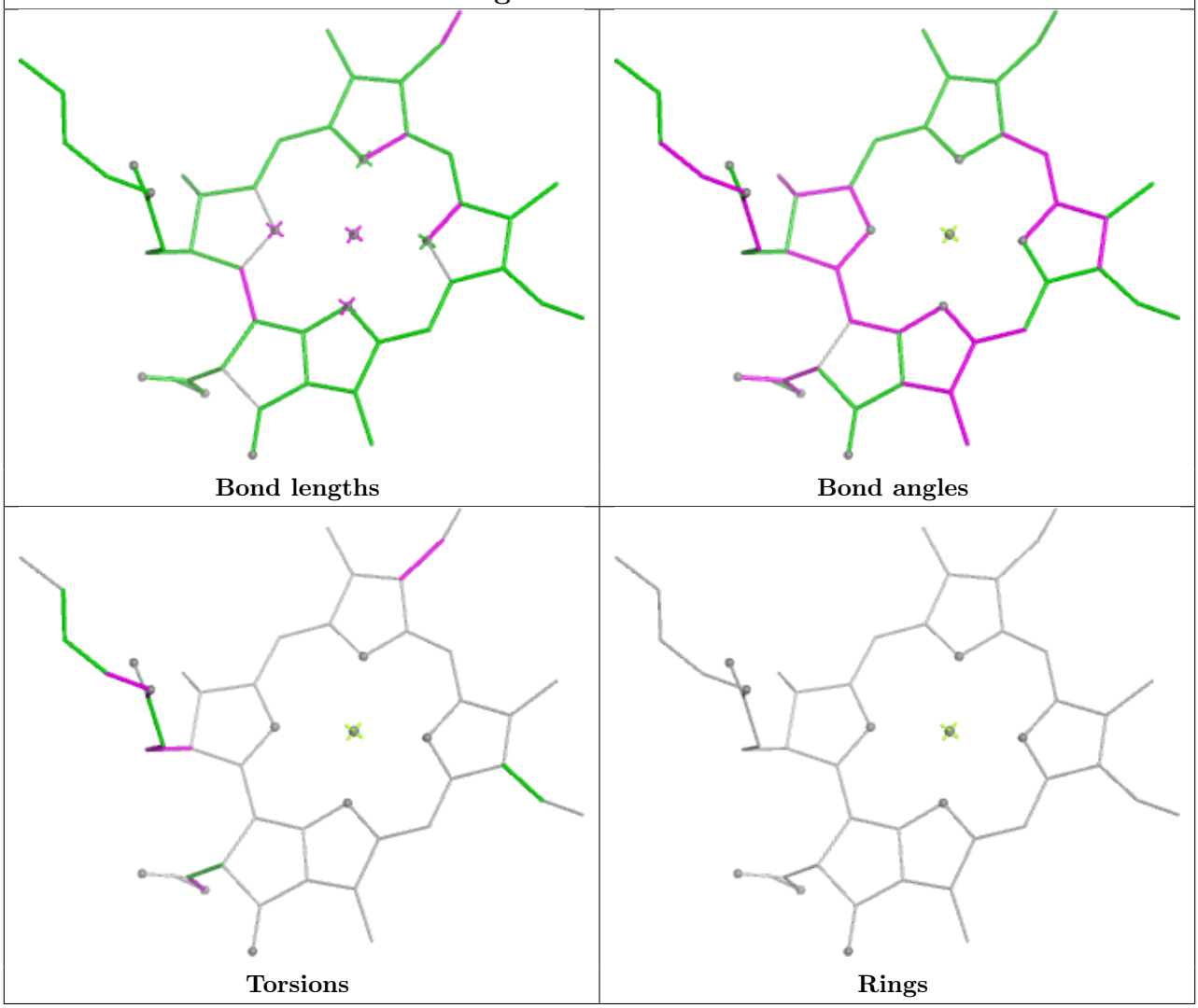
Ligand CLA Y 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c1 510	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

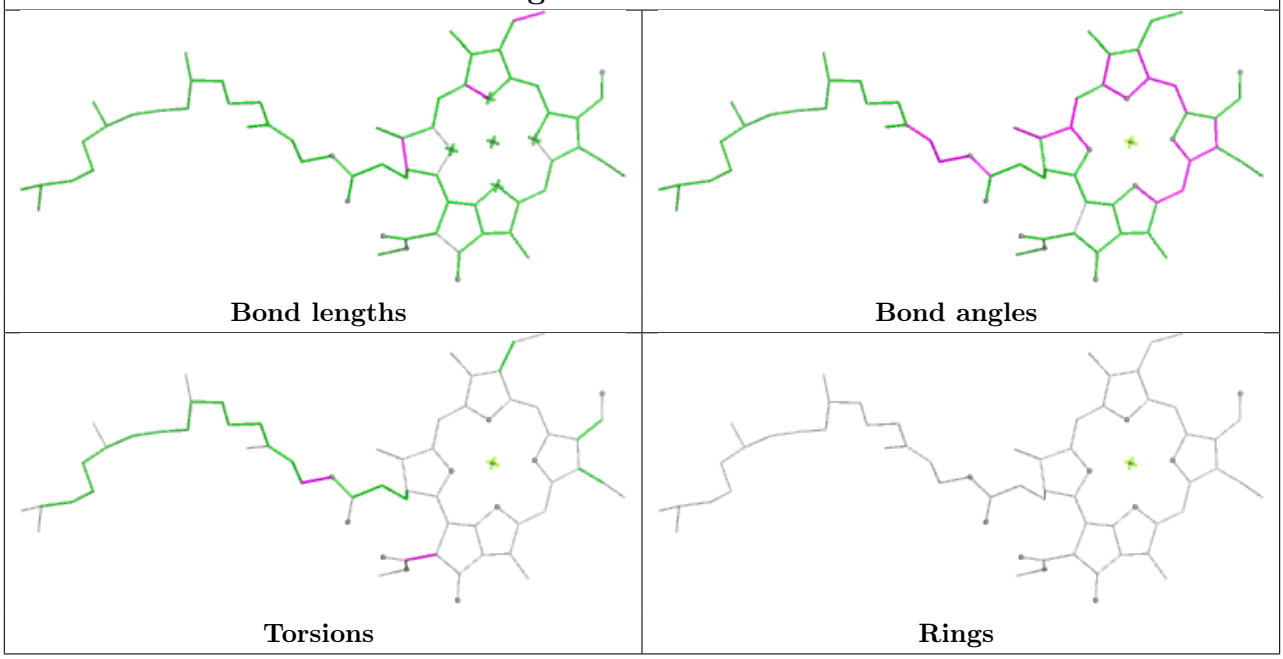
Ligand CLA B1 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r1 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 407



Ligand CHL n 601



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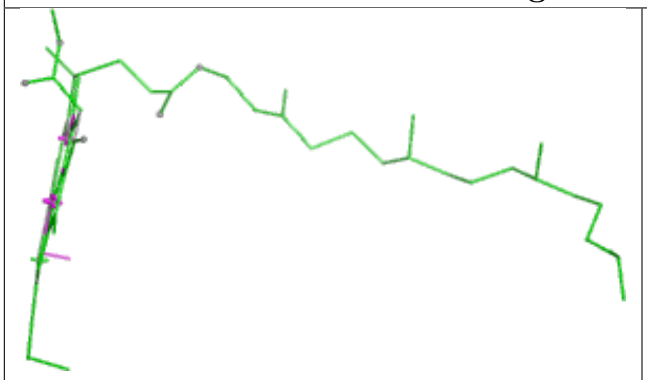
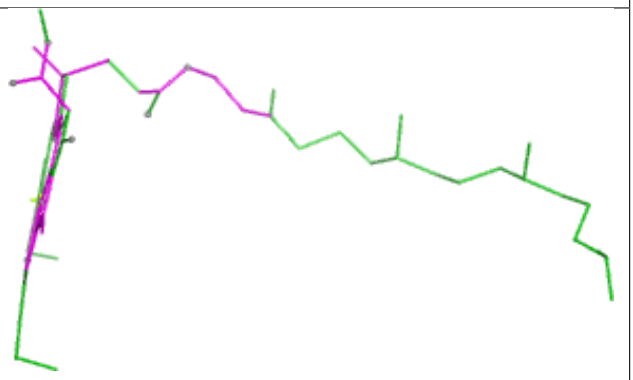
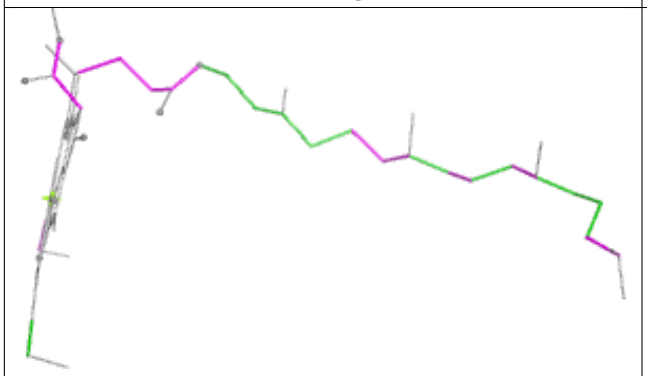


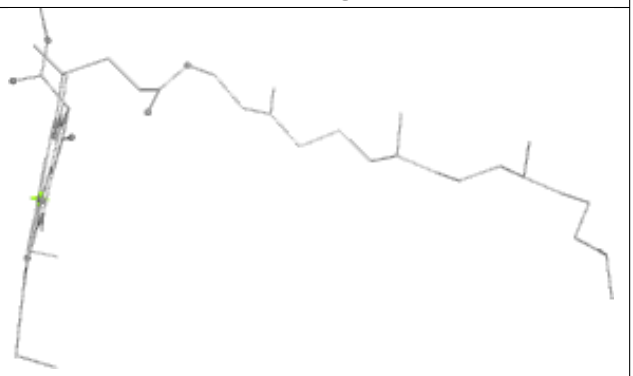
Bond lengths



Bond angles

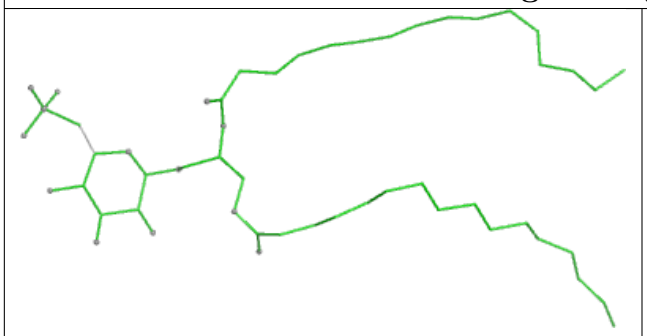


Torsions

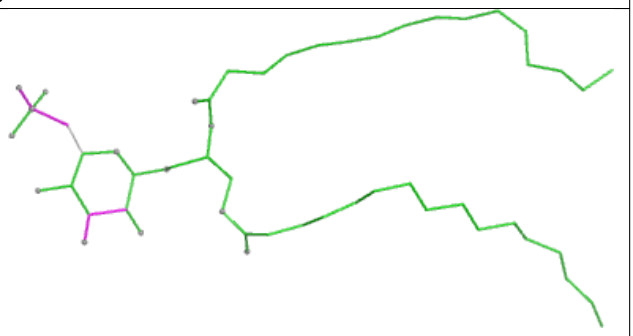


Rings

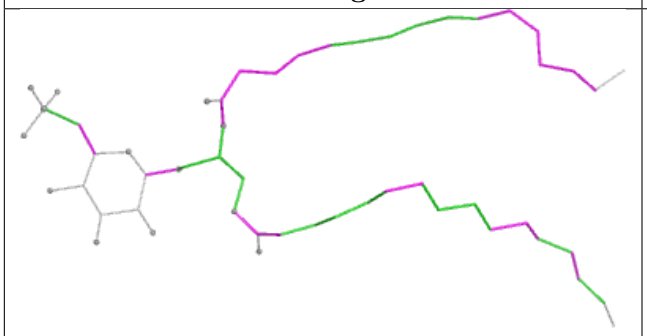
Ligand SQD c1 526



Bond lengths



Bond angles



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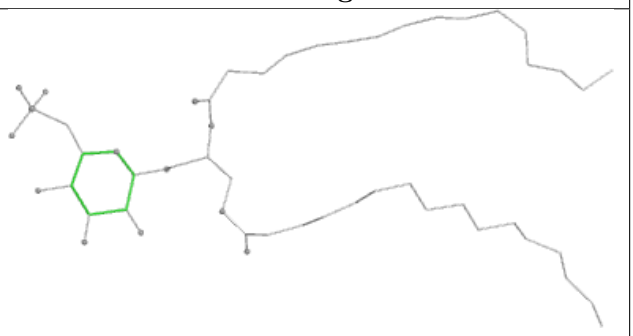
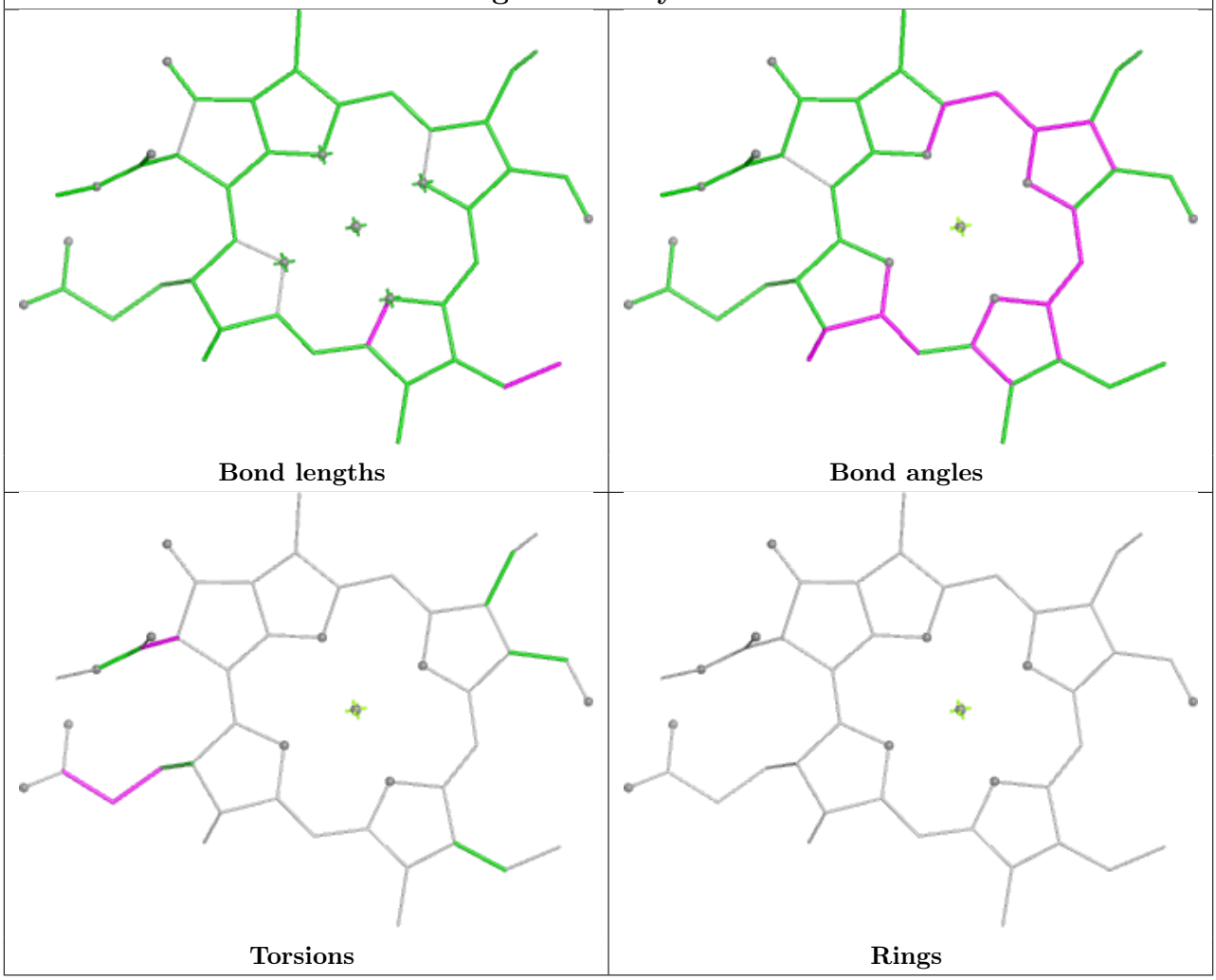
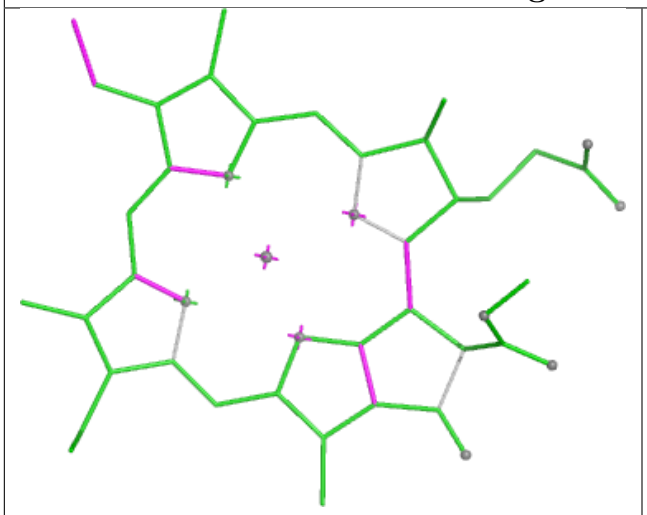


Rings

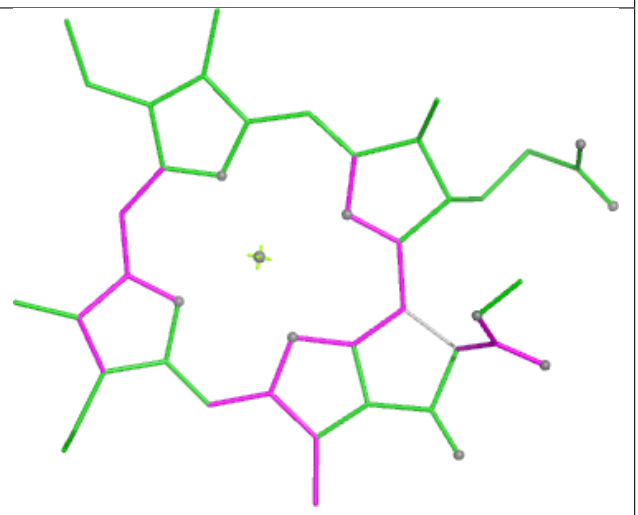
Ligand CHL y1 605



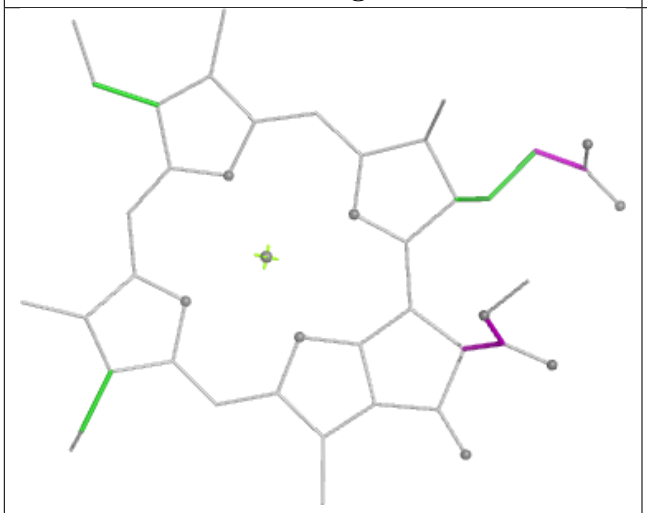
Ligand CLA S 612



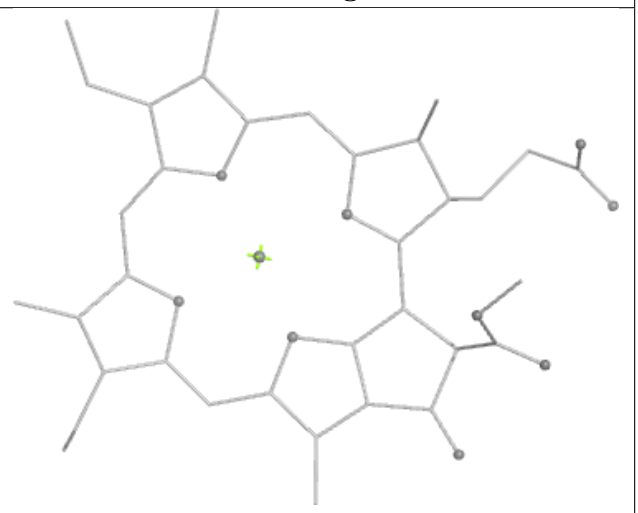
Bond lengths



Bond angles



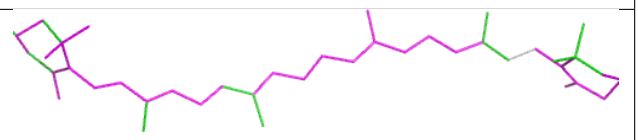
Torsions



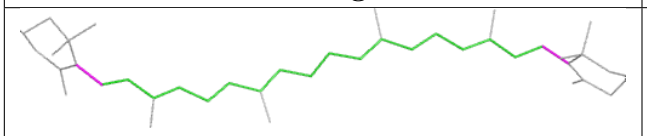
Rings

Ligand LUT S 620

Bond lengths



Bond angles



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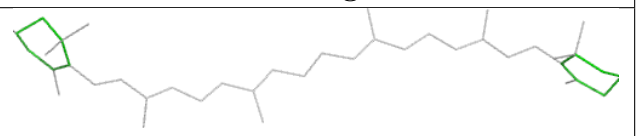
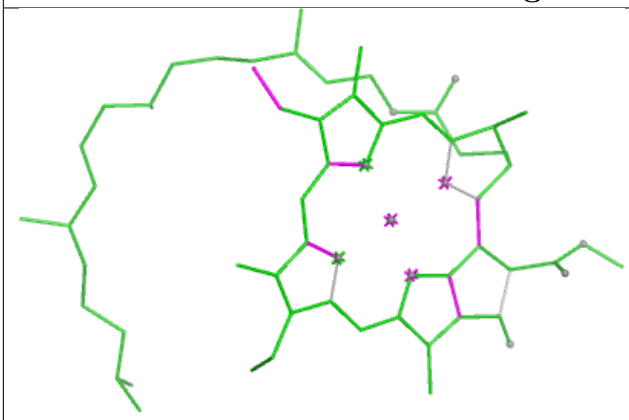
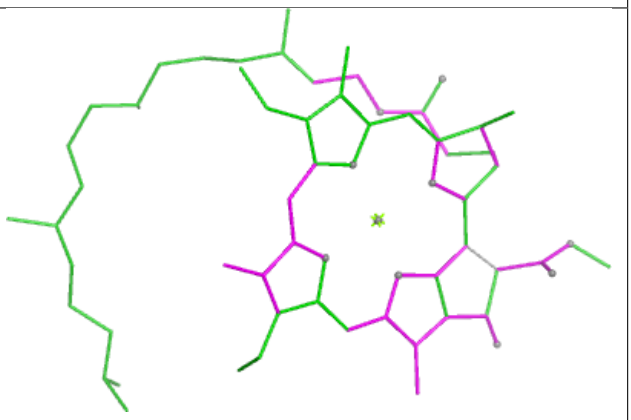
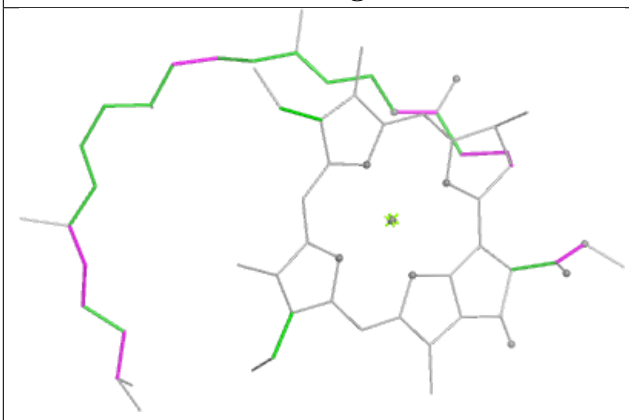
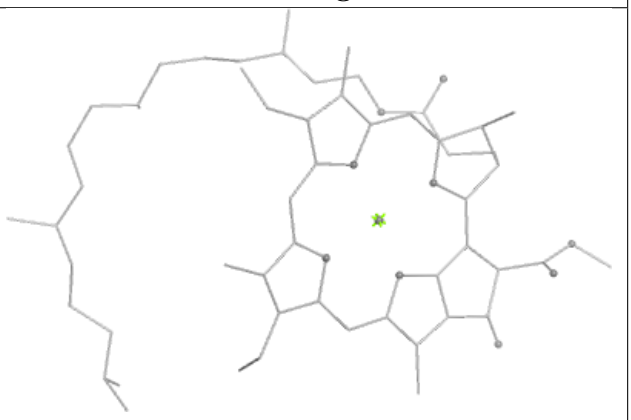
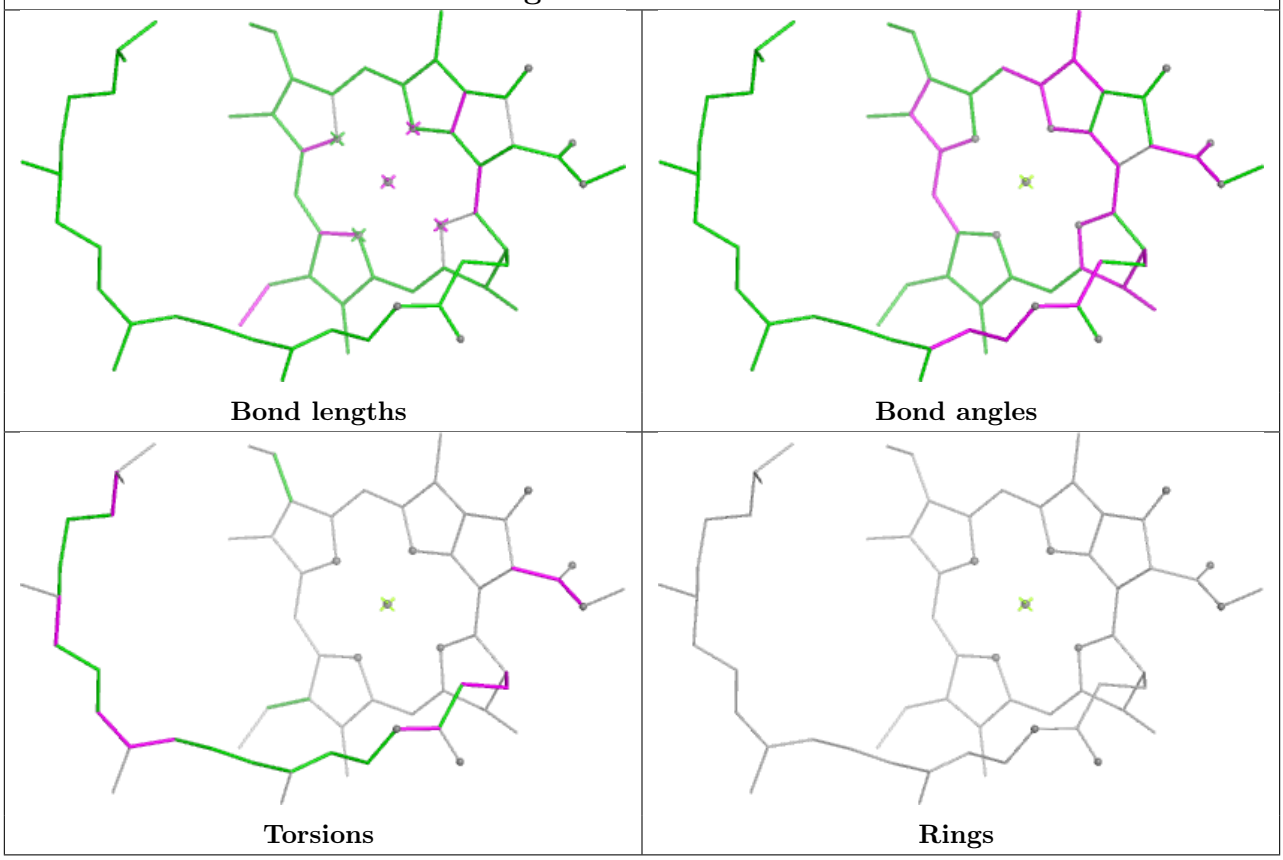


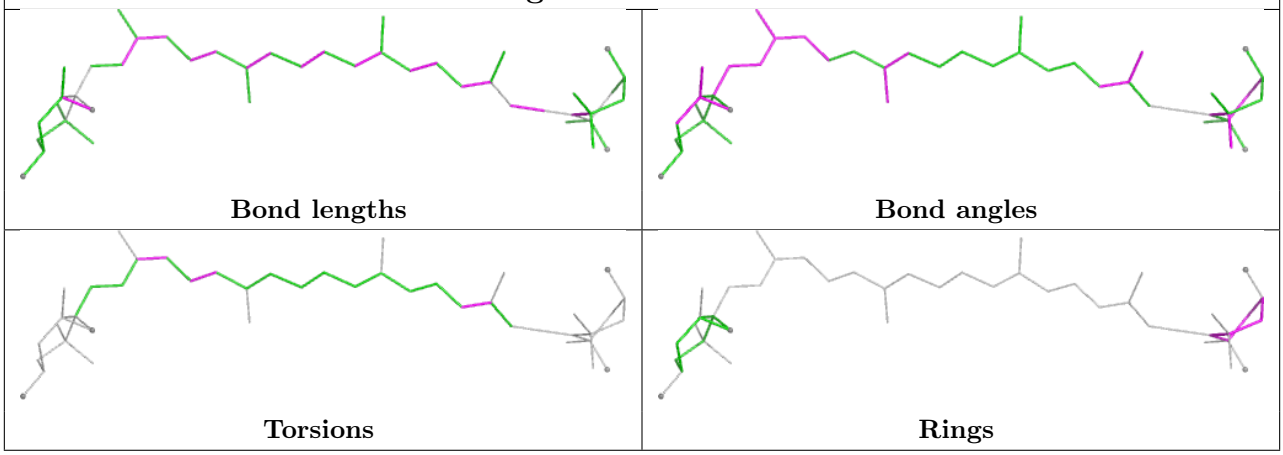
Rings

Ligand CLA Y 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 610



Ligand NEX n 623



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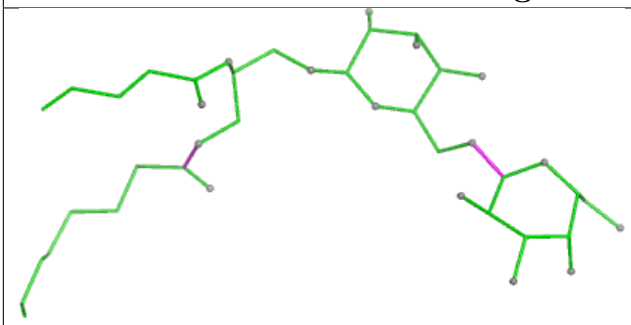
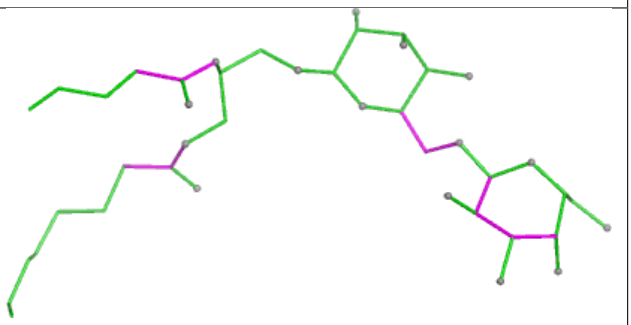
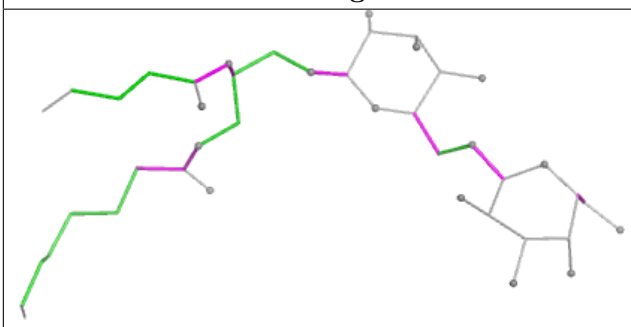
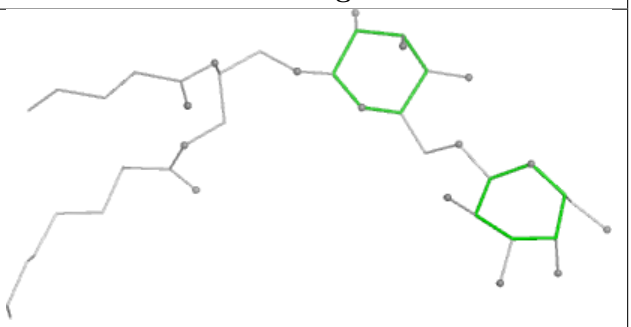
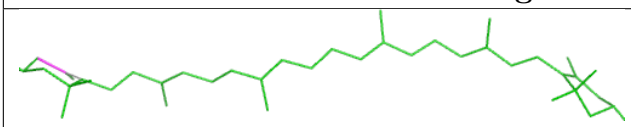
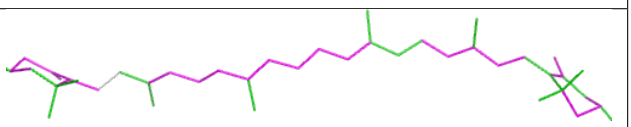
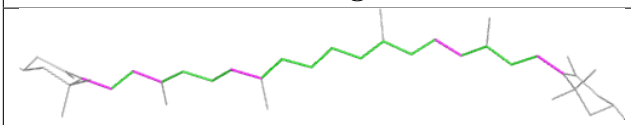
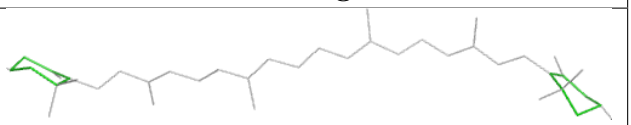
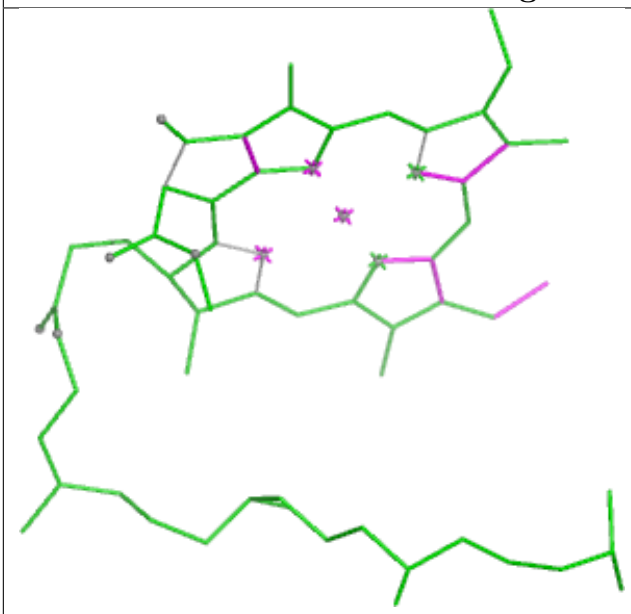
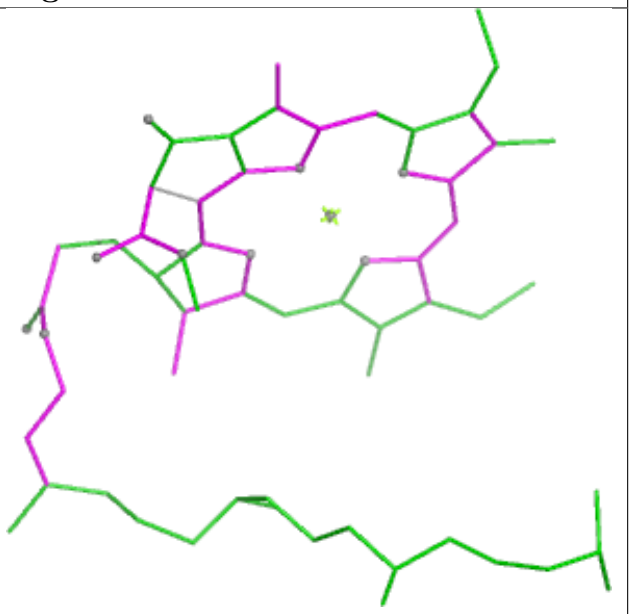
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT Y1 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

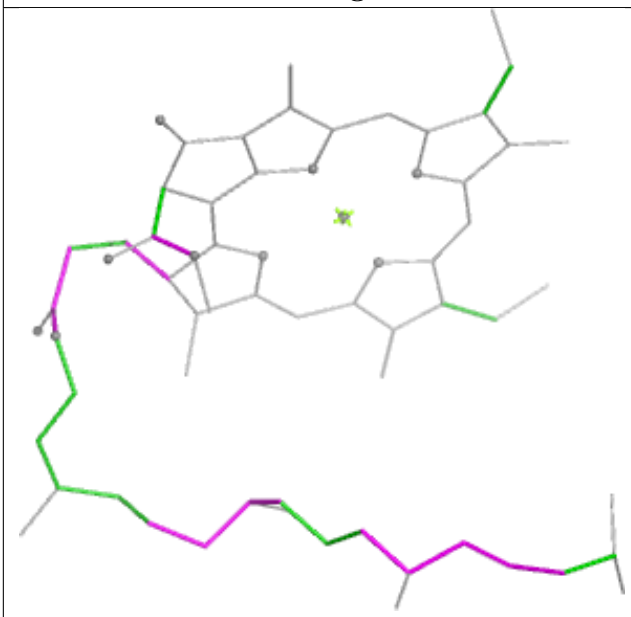
Ligand CLA g1 603



Bond lengths



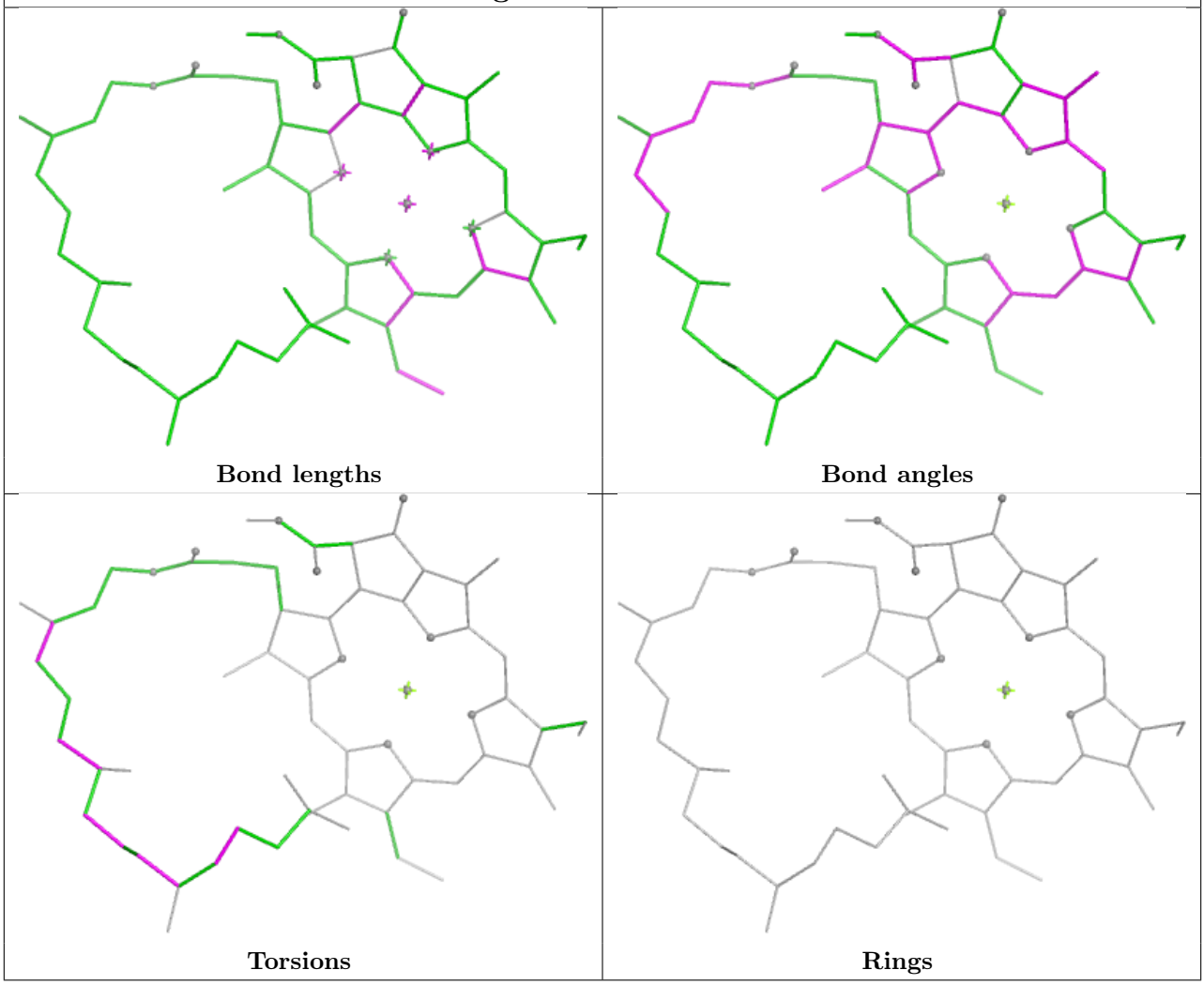
Bond angles



Torsions

Rings

Ligand CLA B 616



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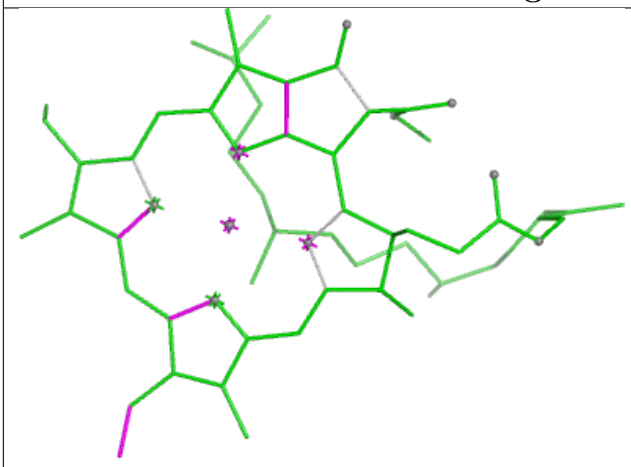

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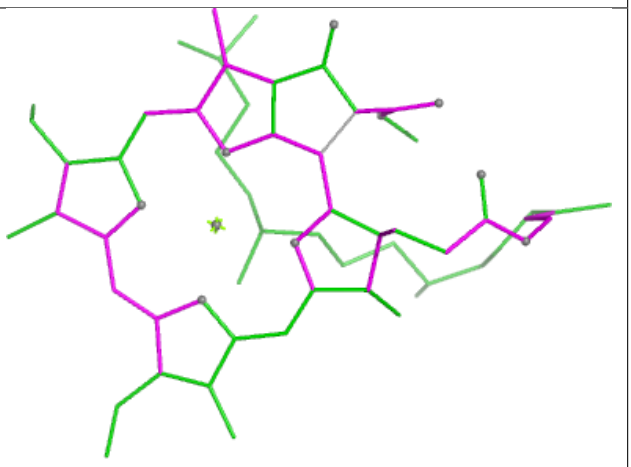

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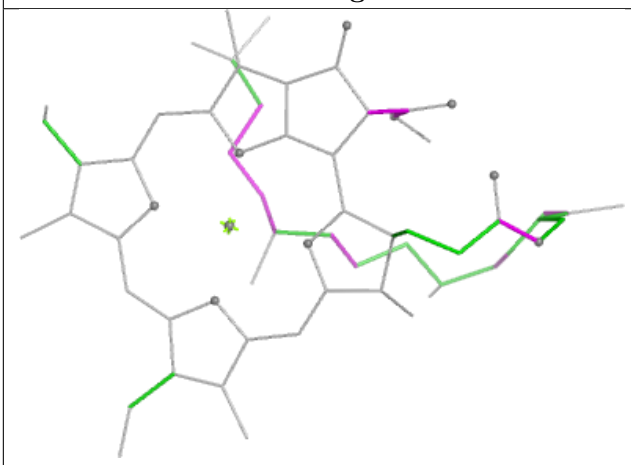

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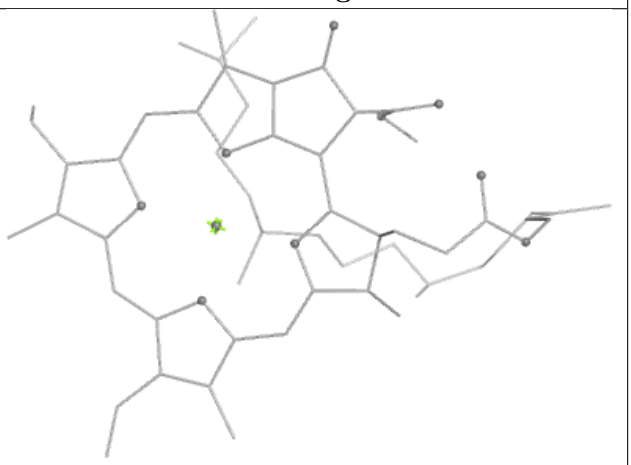
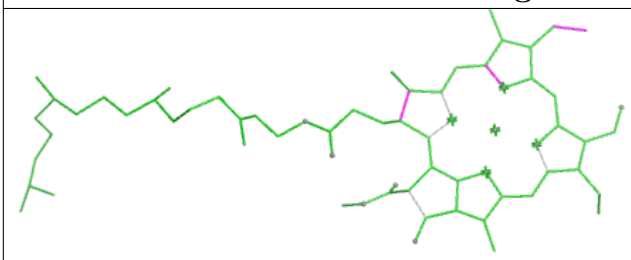


Rings

Ligand CHL Y1 606



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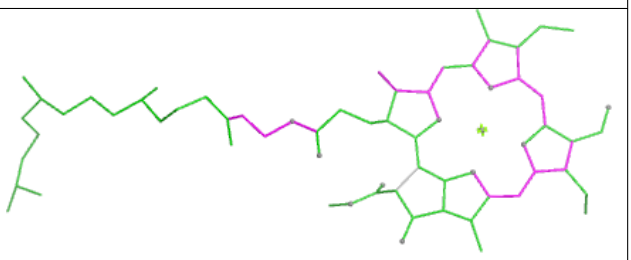

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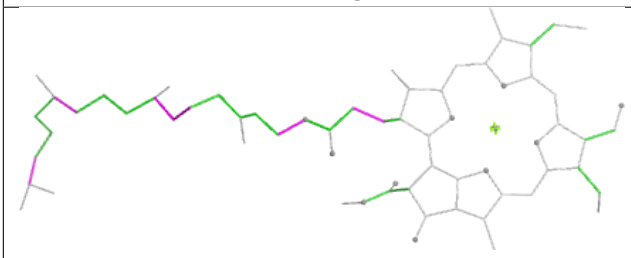

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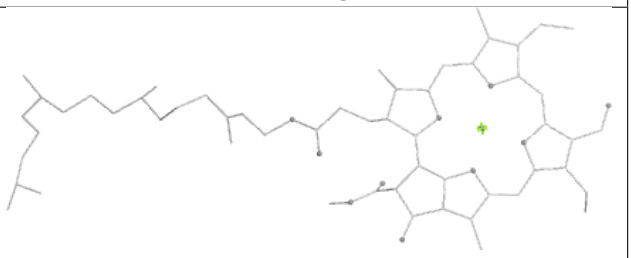
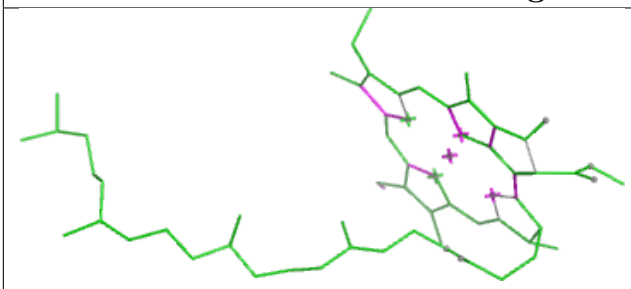


Rings

Ligand CLA b 609



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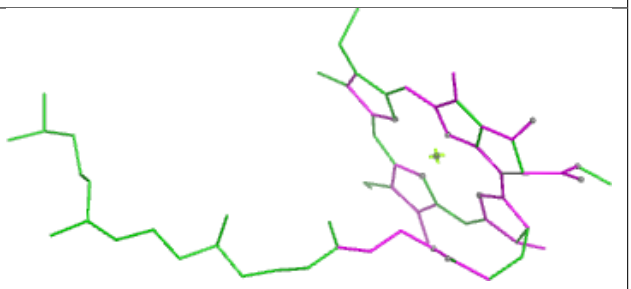
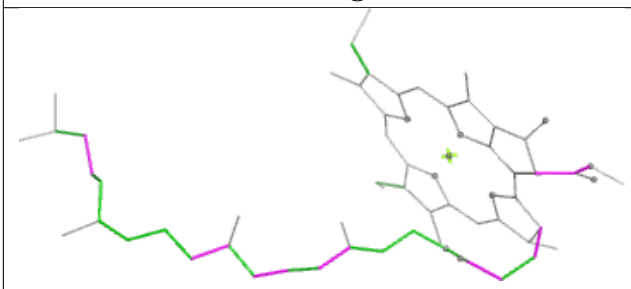


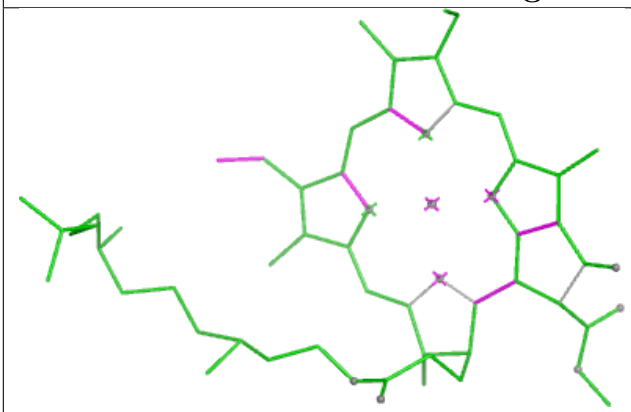
Bond angles



Torsions

Rings

Ligand CLA R 609



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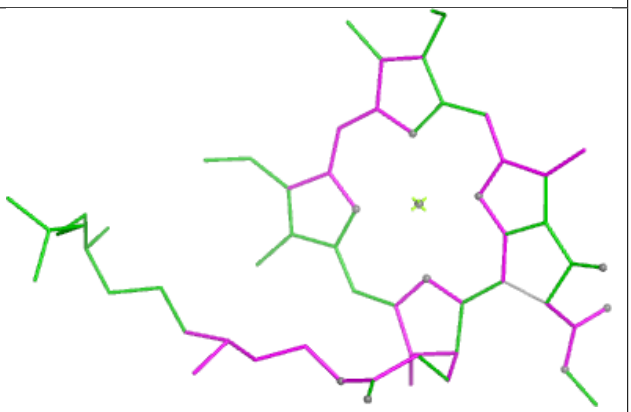

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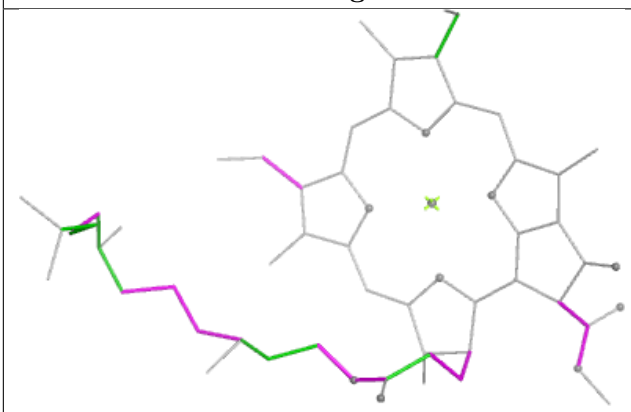

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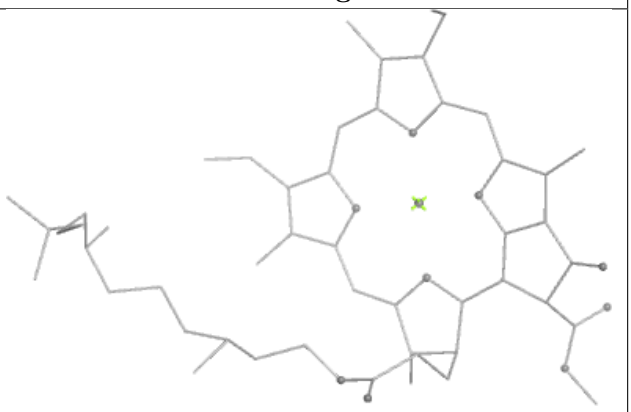
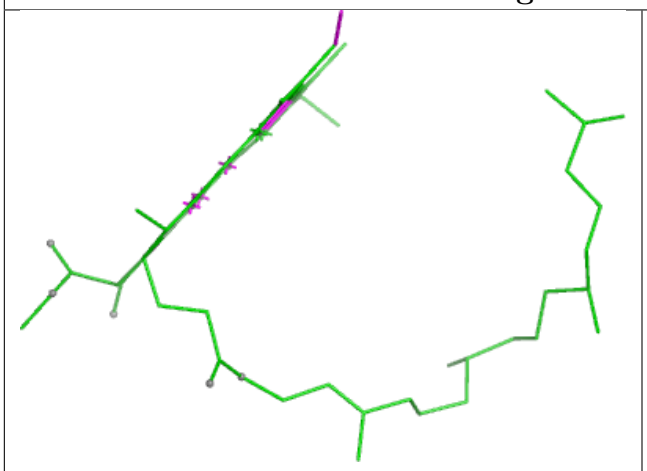


Rings

Ligand CLA B1 612



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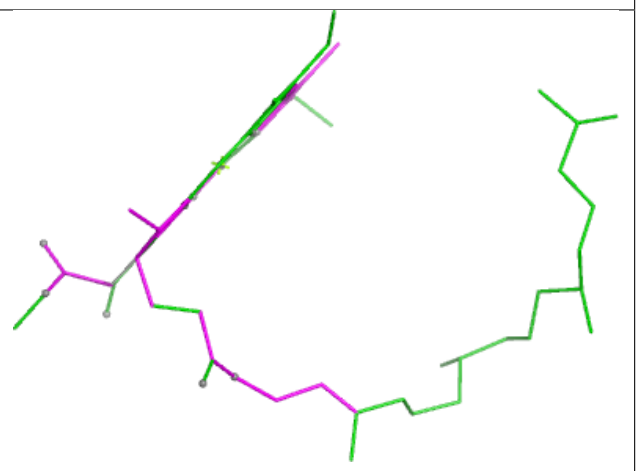
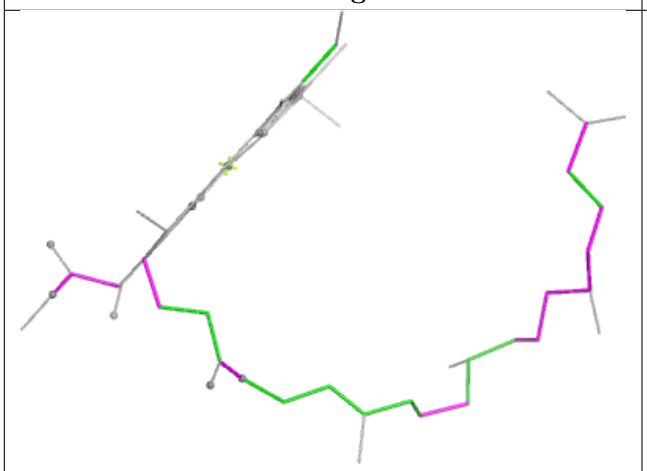


Bond angles



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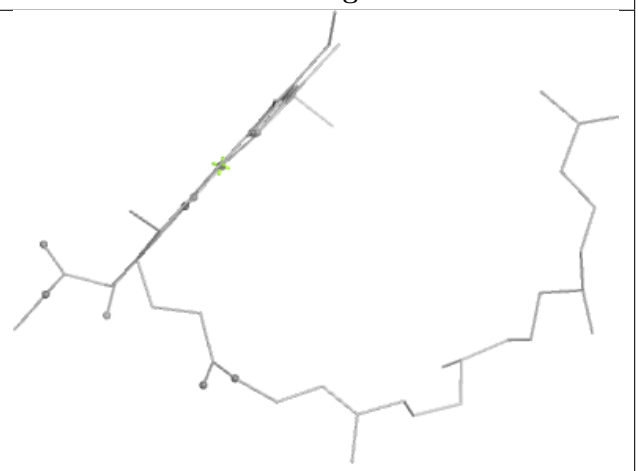
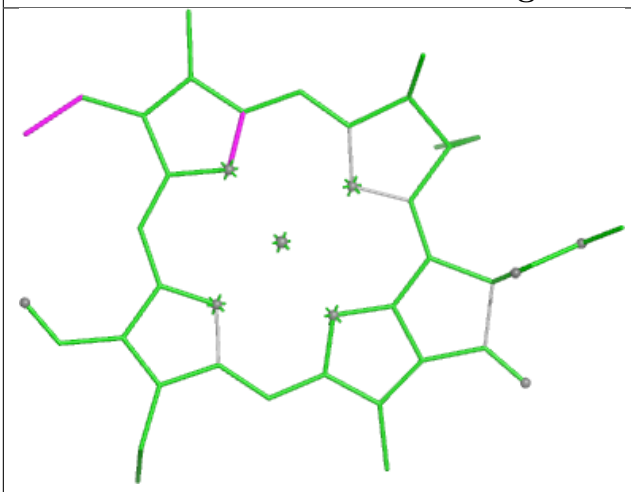


Rings

Ligand CHL S1 607



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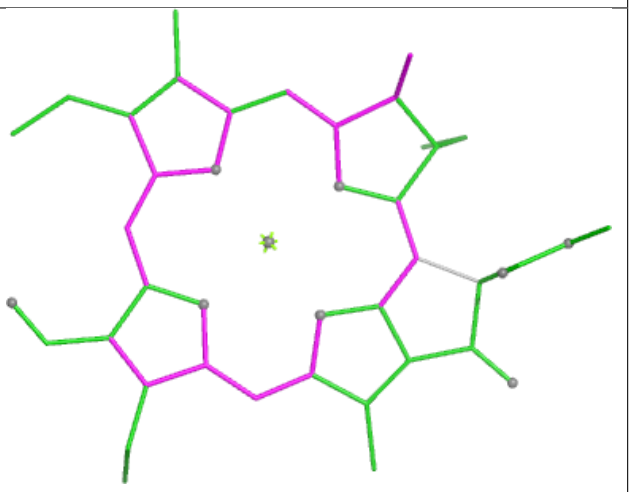

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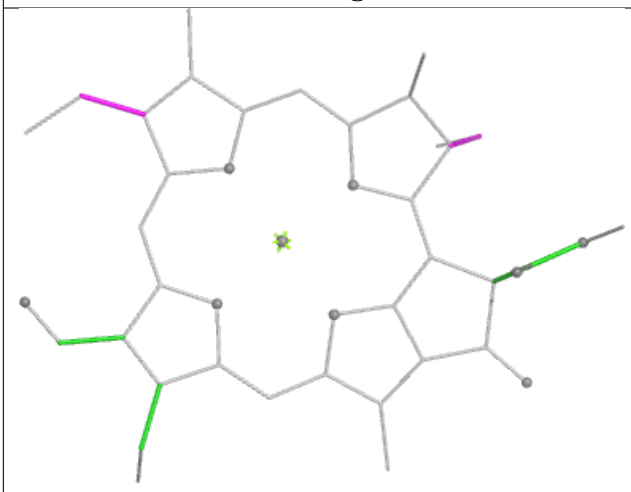

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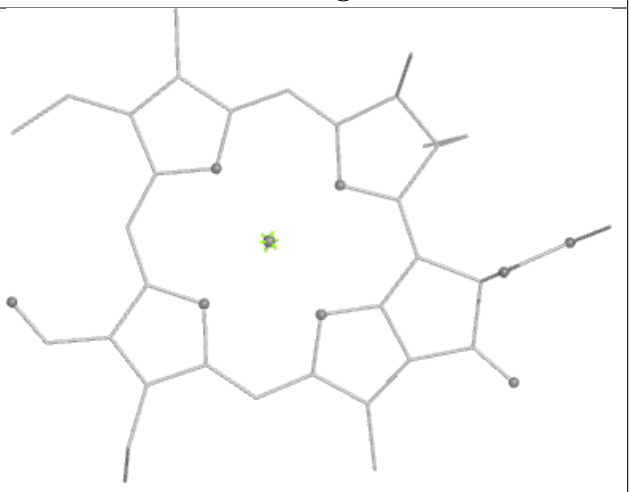
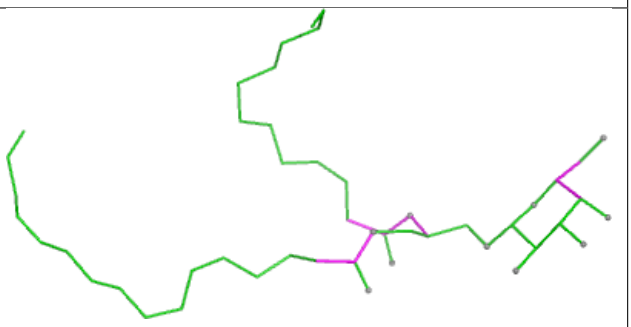
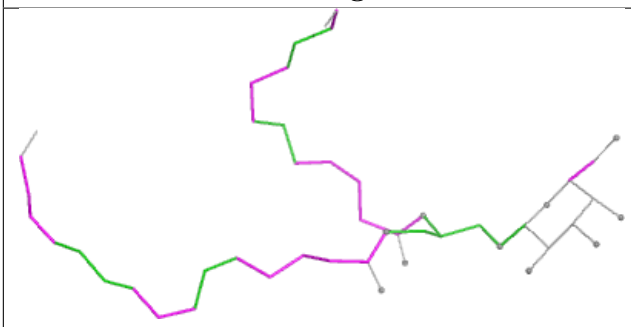
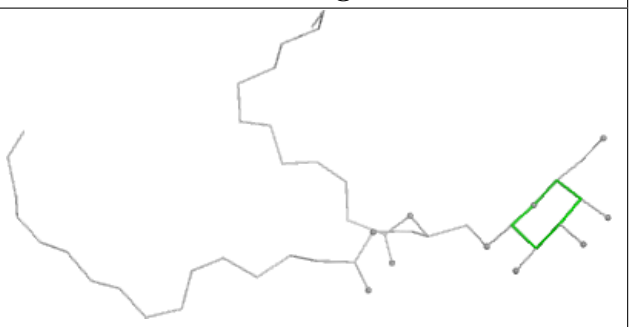
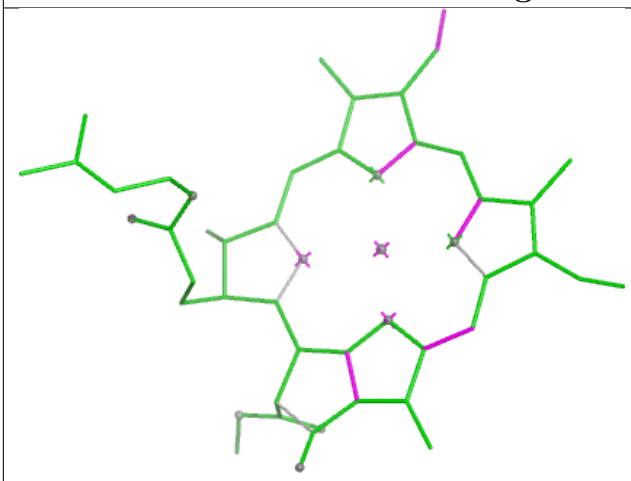


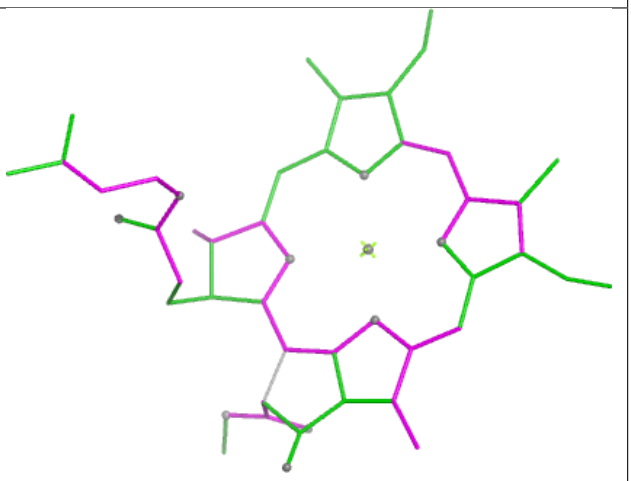
Rings

Ligand LMG h1 102	
Bond lengths	 Bond angles
 Torsions	 Rings

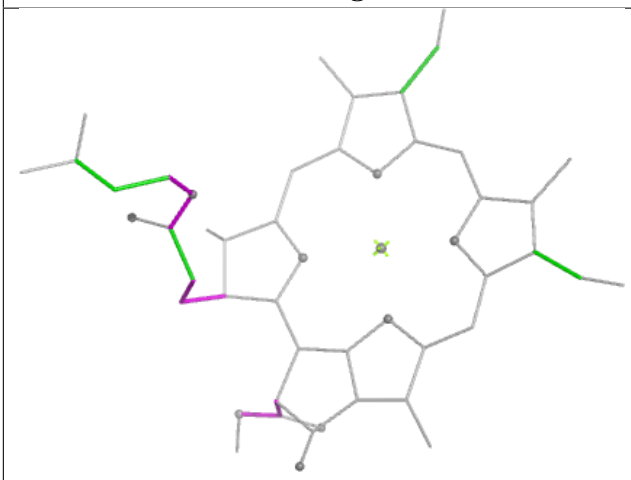
Ligand CLA A1 407



Bond lengths



Bond angles



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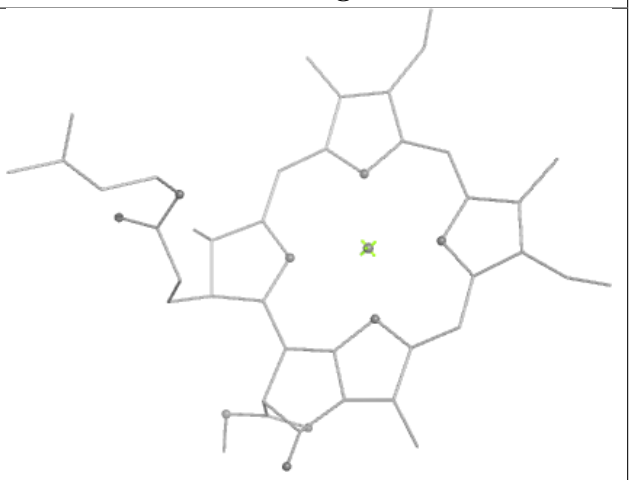
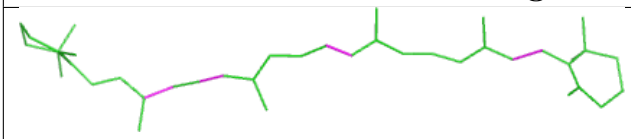
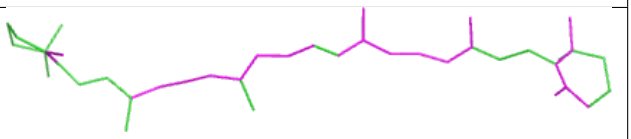


Rings

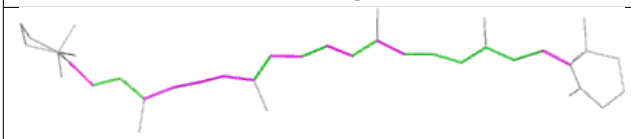
Ligand BCR c 514



Bond lengths



Bond angles



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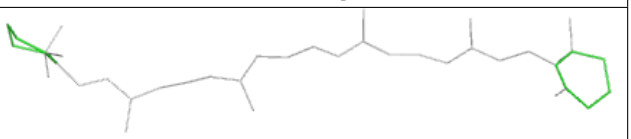
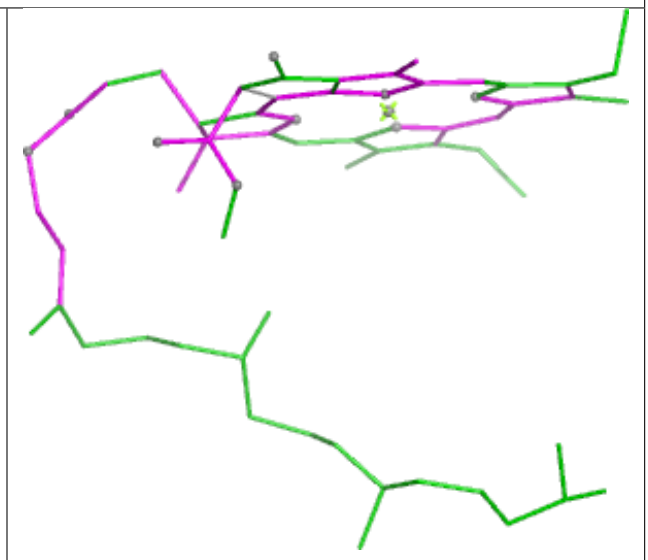


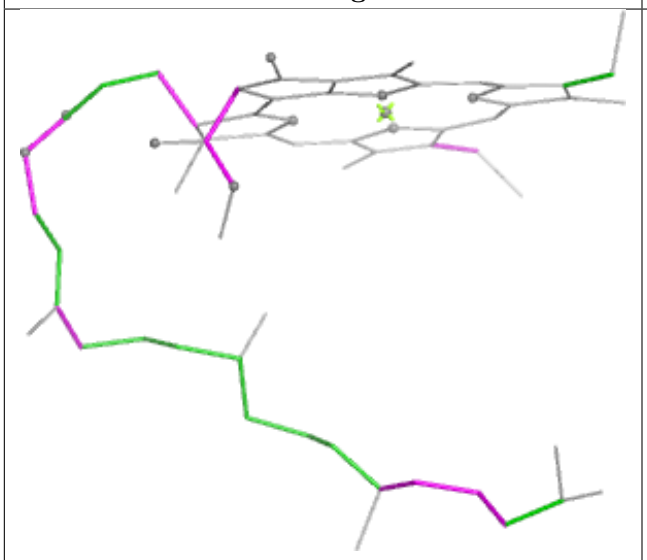
Rings

Ligand CLA Y1 603

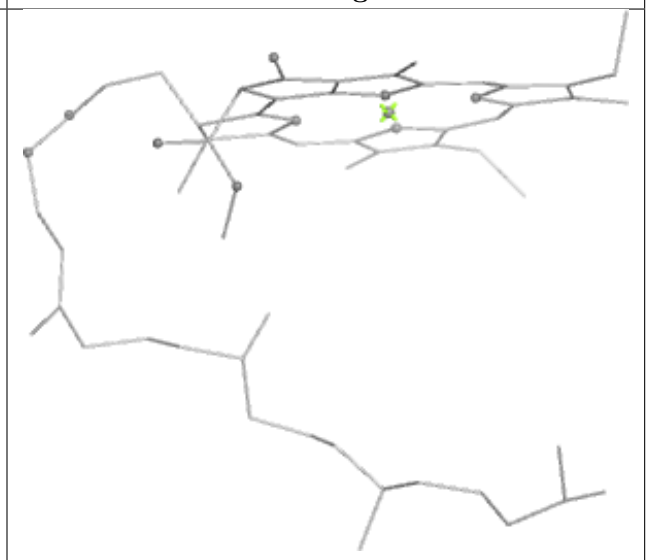
Bond lengths



Bond angles

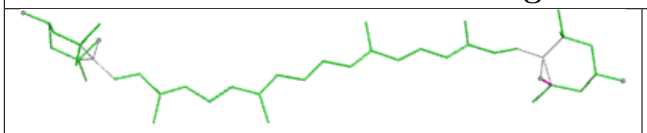


Torsions

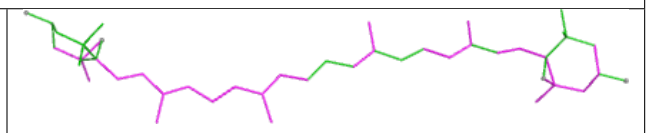


Rings

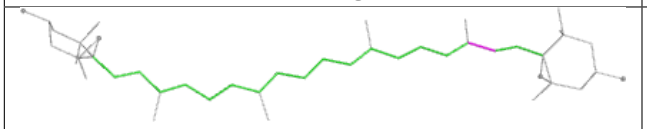
Ligand XAT R 621



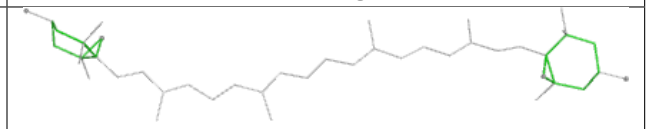
Bond lengths



Bond angles

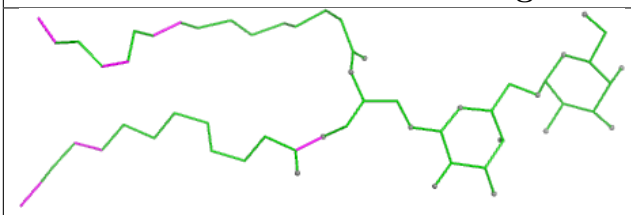


Torsions

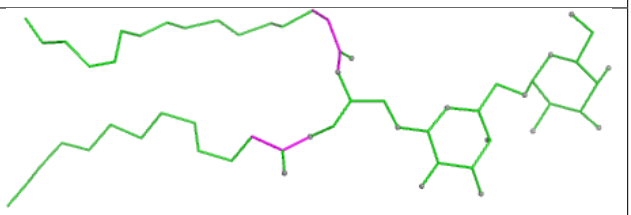


Rings

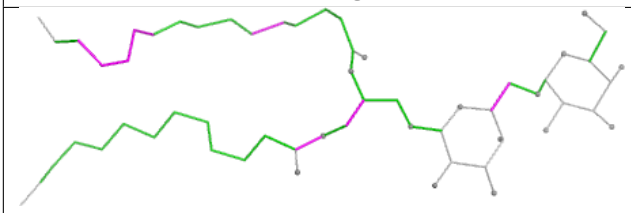
Ligand DGD c1 520



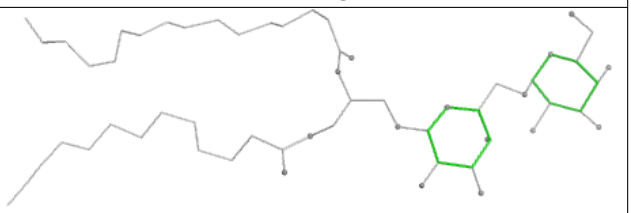
Bond lengths



Bond angles

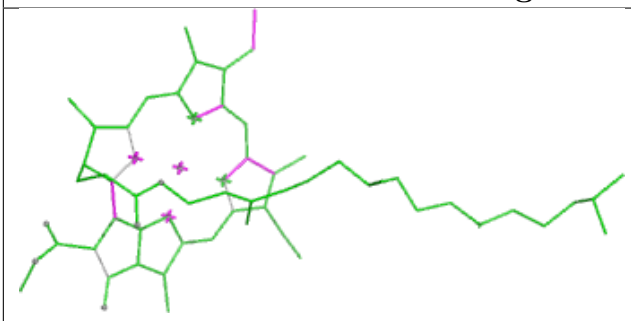


Torsions

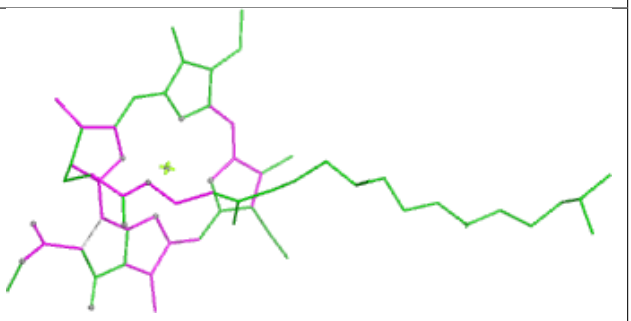


Rings

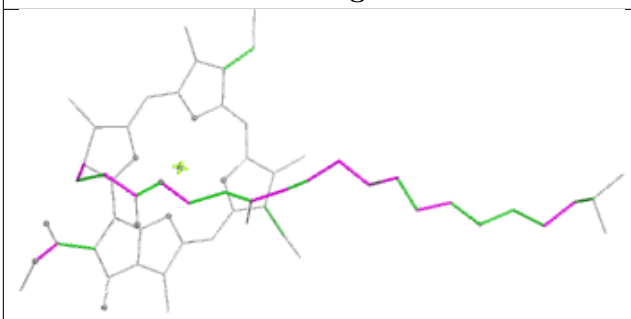
Ligand CLA B1 615



Bond lengths



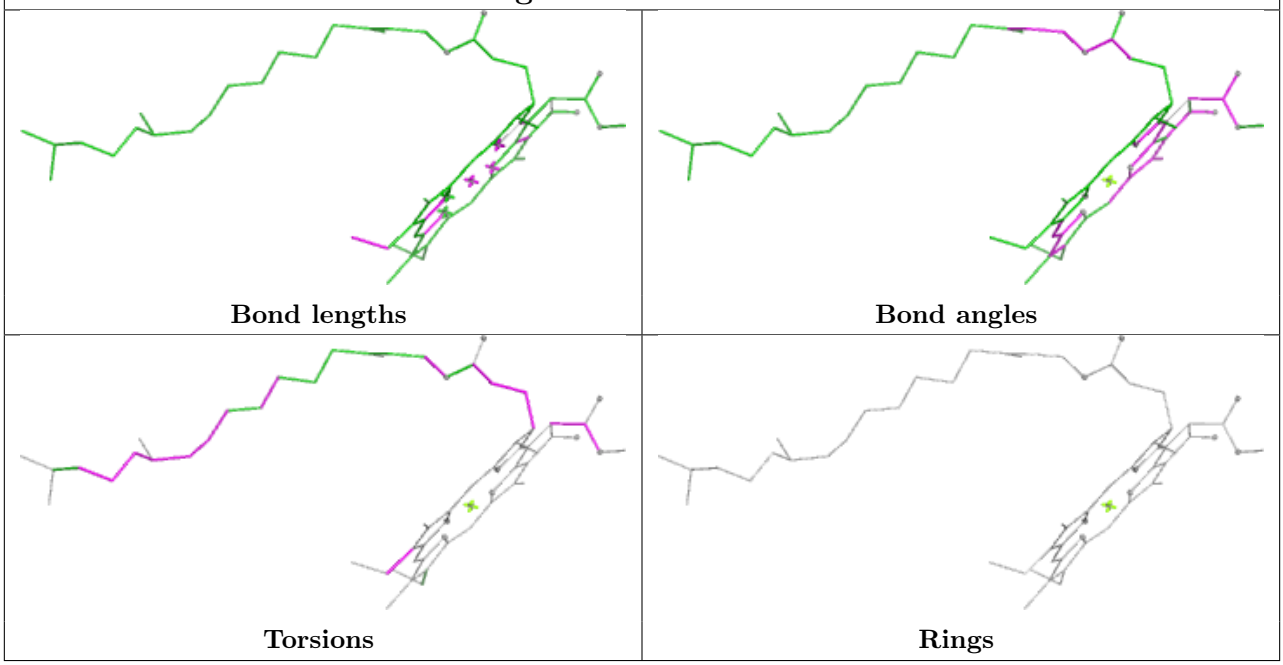
Bond angles



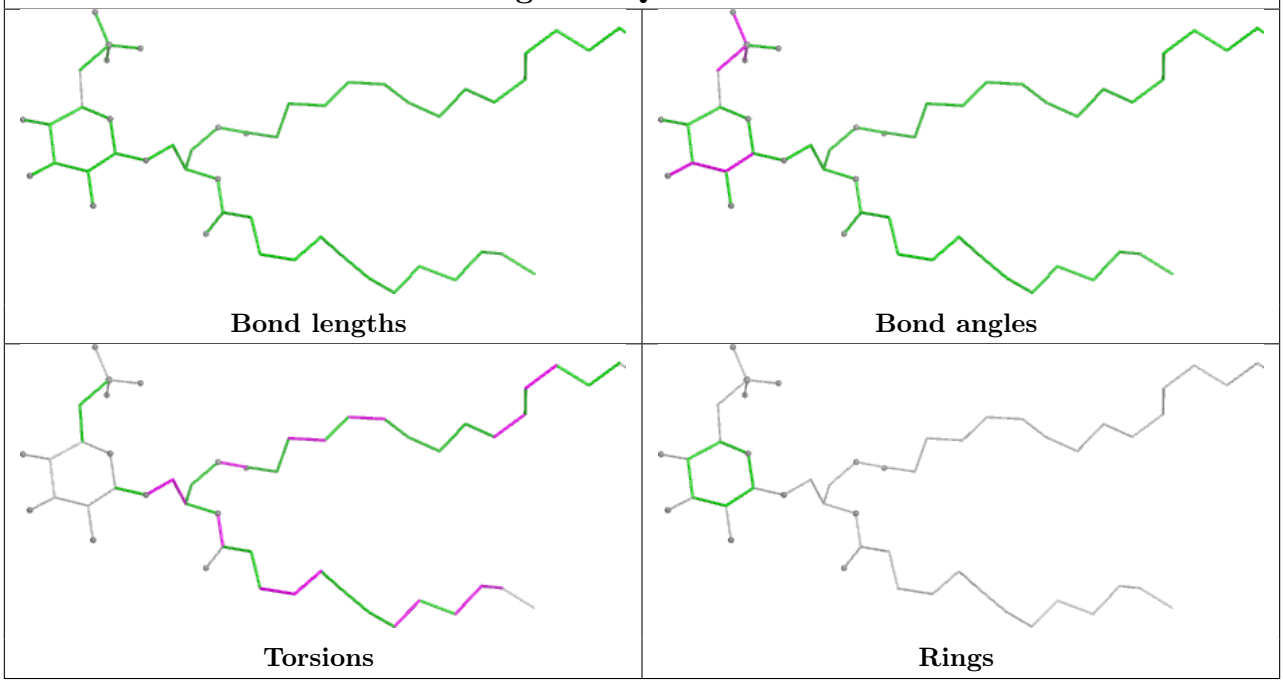
Torsions

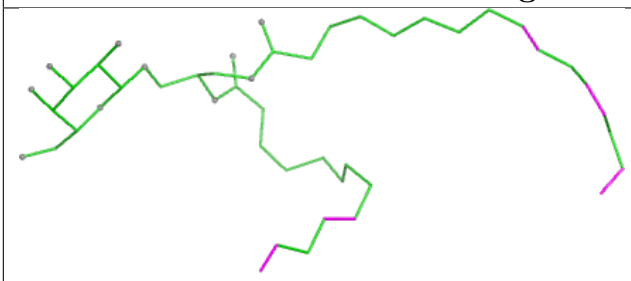
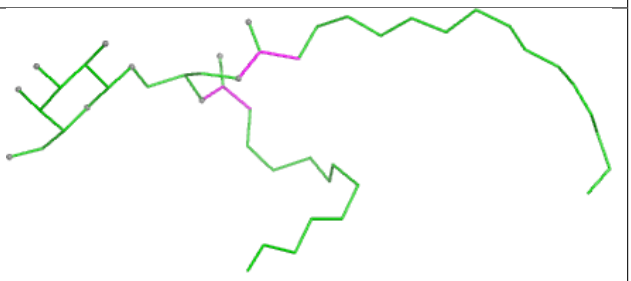
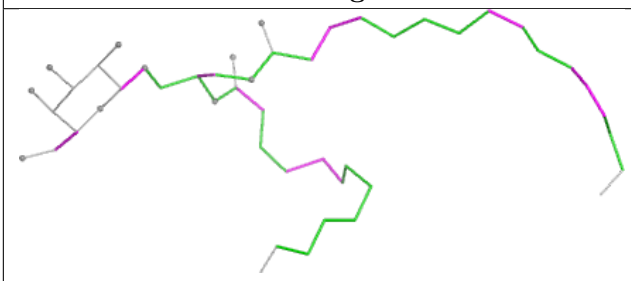
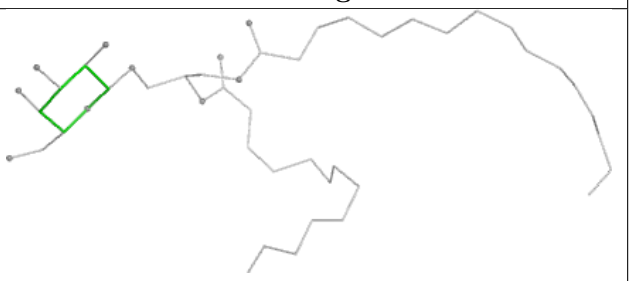
Rings

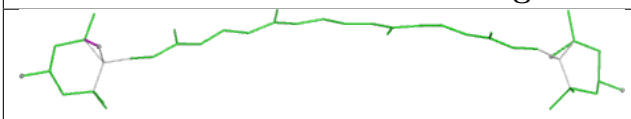
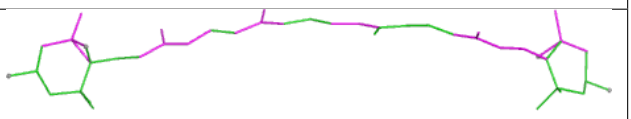
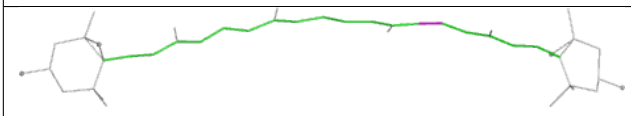
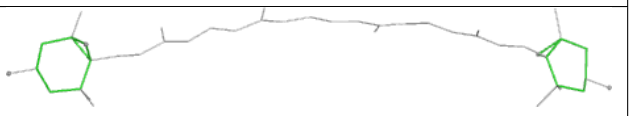
Ligand CLA N1 604



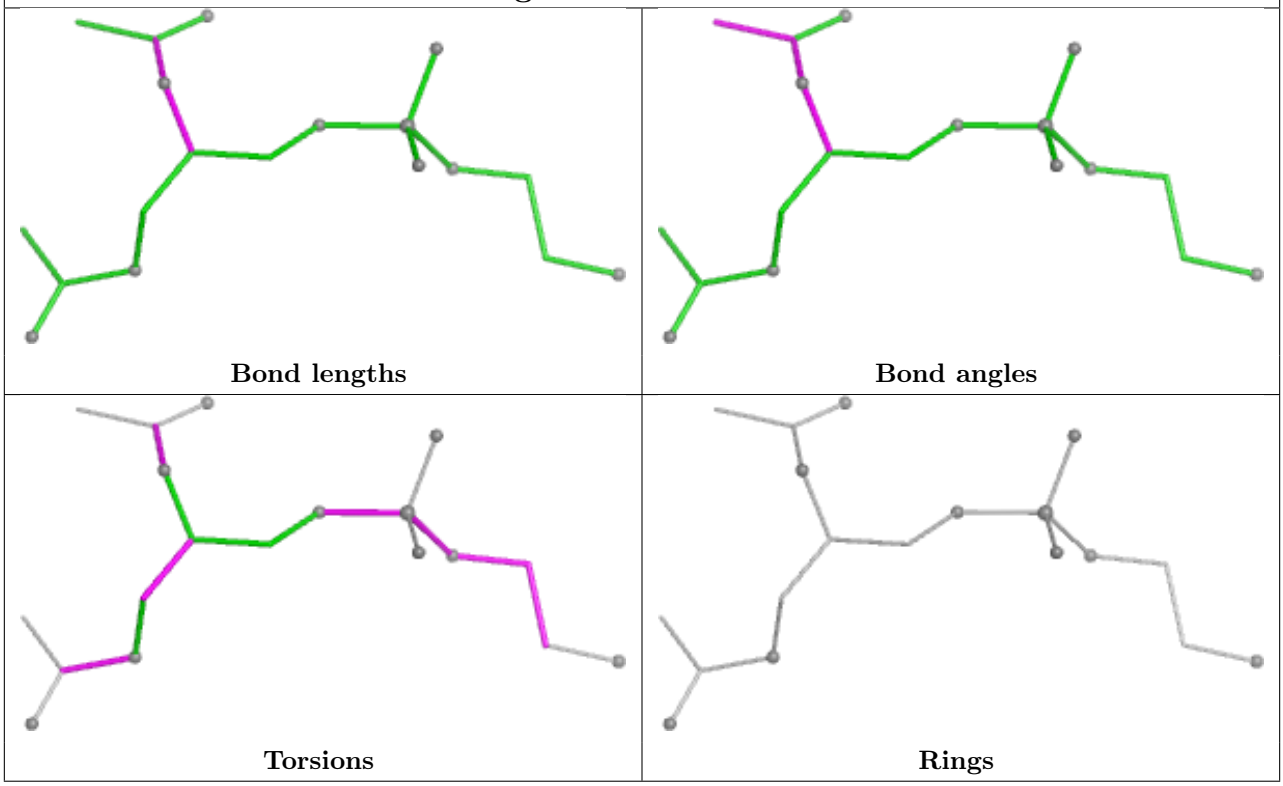
Ligand SQD A1 412



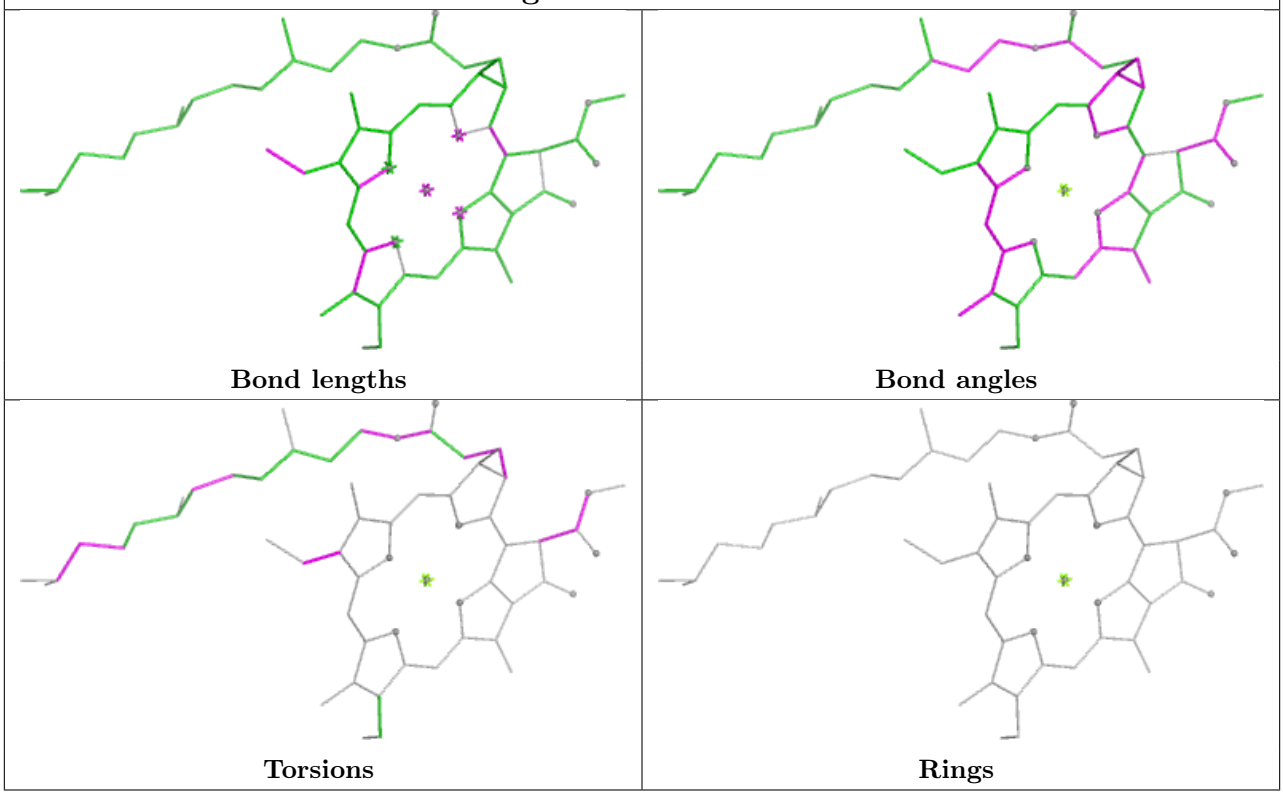
Ligand LMG H 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT N1 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

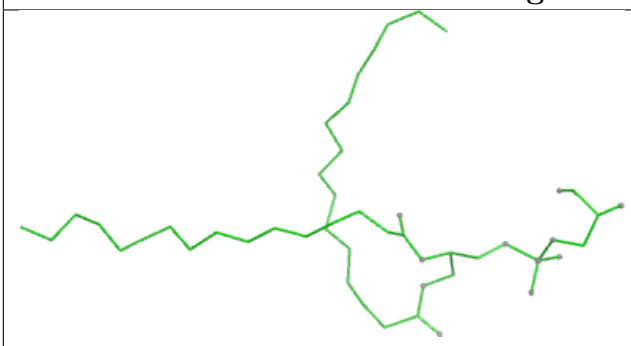
Ligand PTY Y1 627



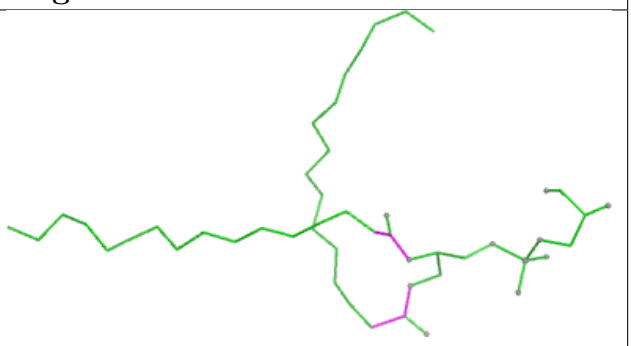
Ligand CLA r1 610



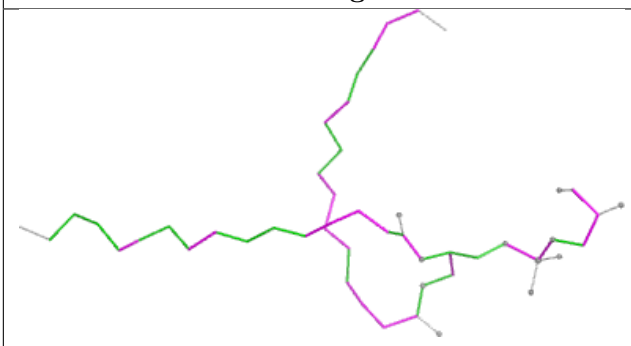
Ligand LHG g 624



Bond lengths



Bond angles



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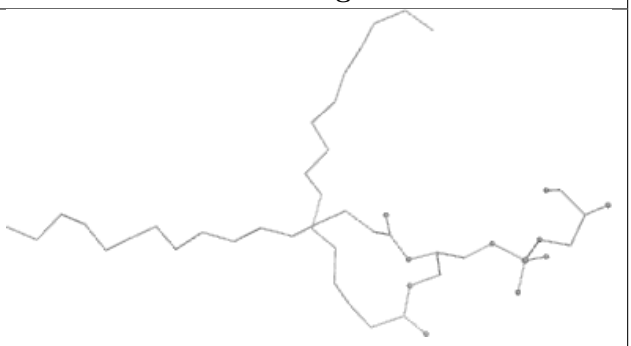
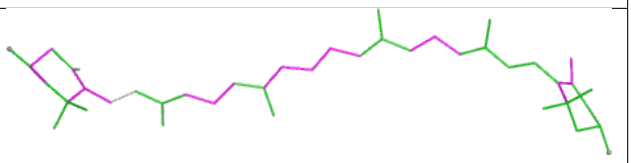


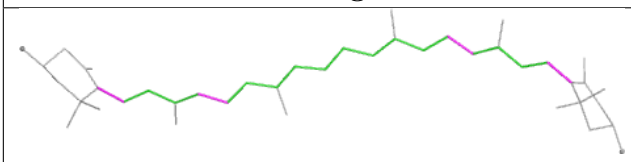
Rings

Ligand LUT S1 620

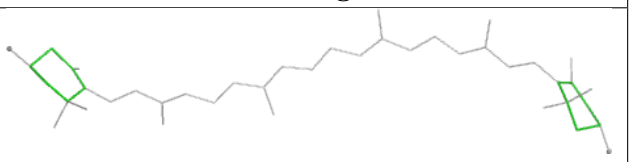
Bond lengths



Bond angles



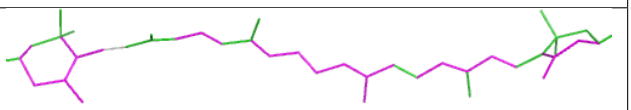
Torsions



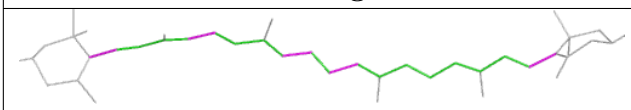
Rings

Ligand LUT Y1 621

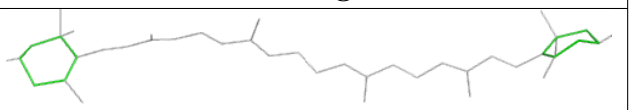
Bond lengths



Bond angles

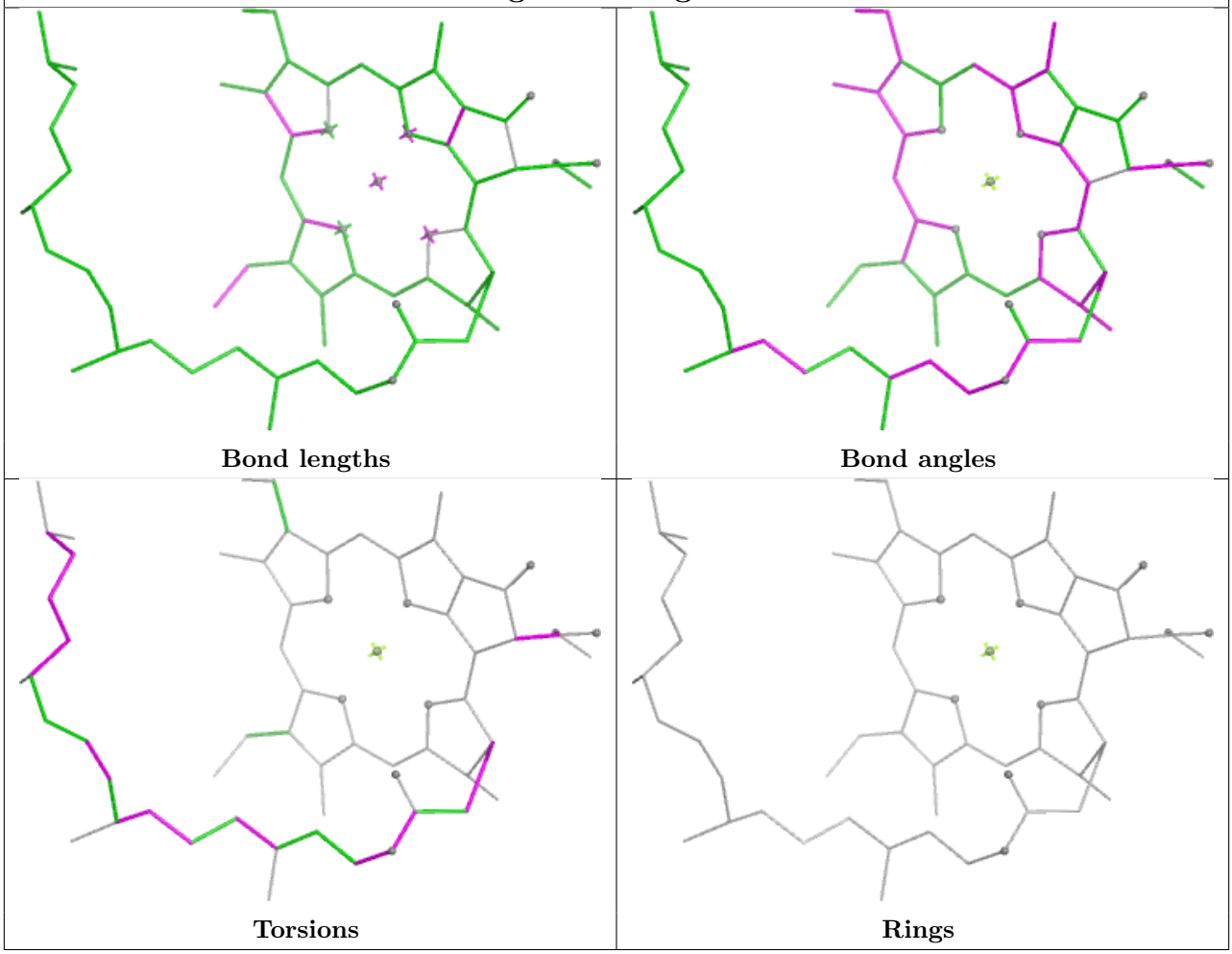


Torsions

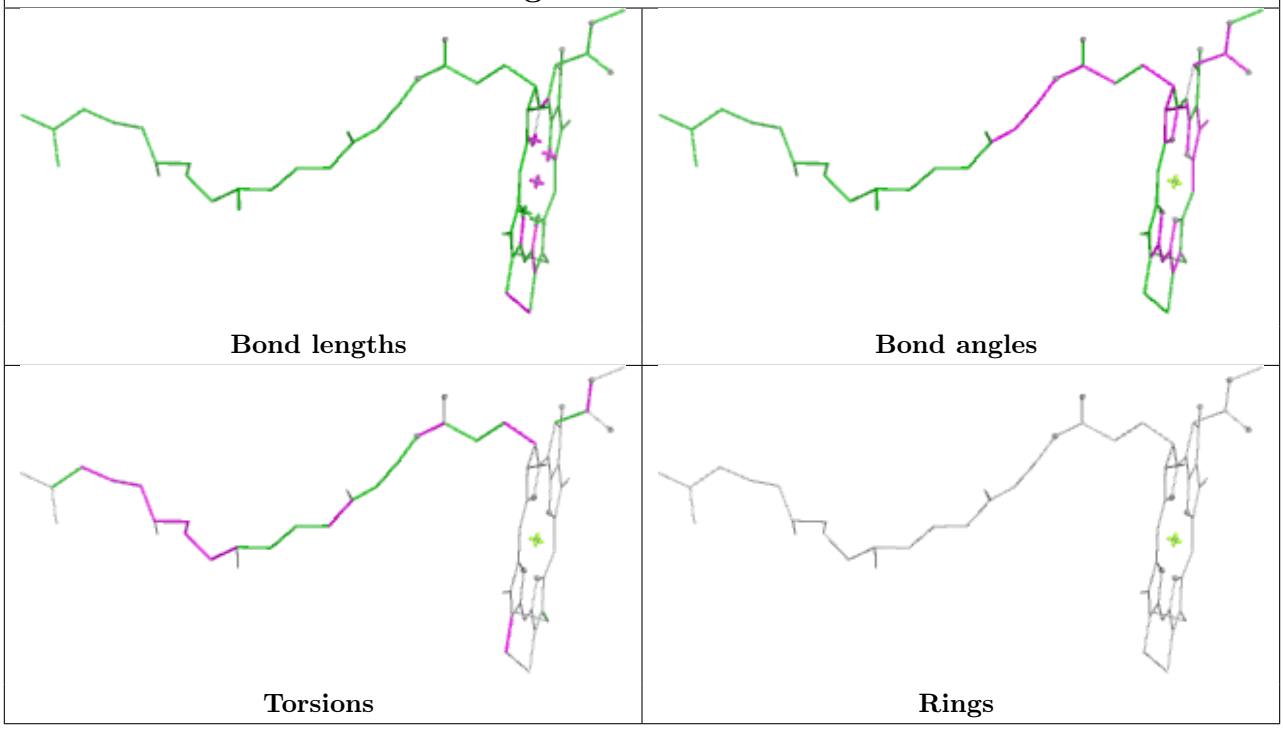


Rings

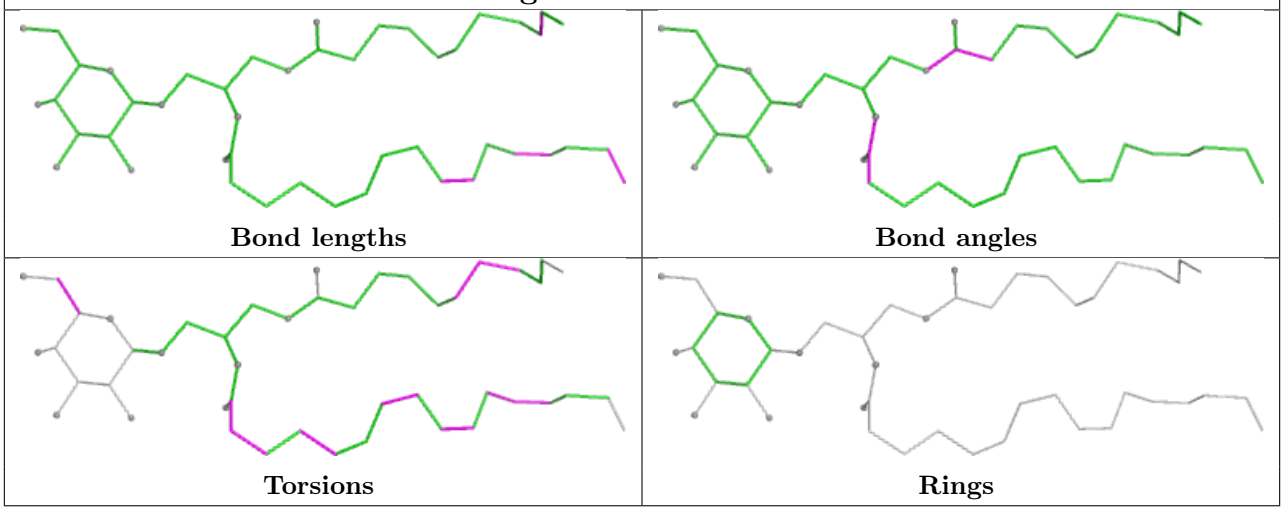
Ligand CLA g 602



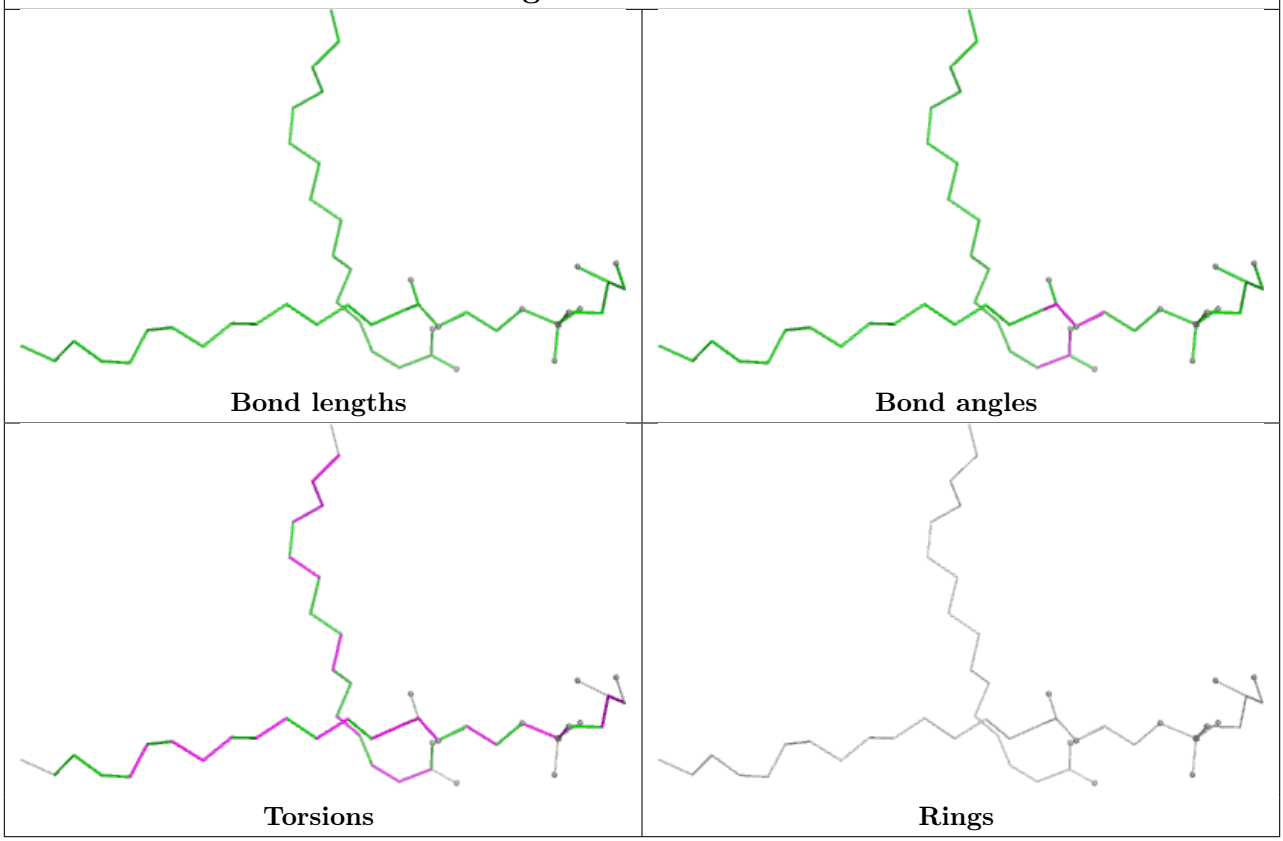
Ligand CLA D 403



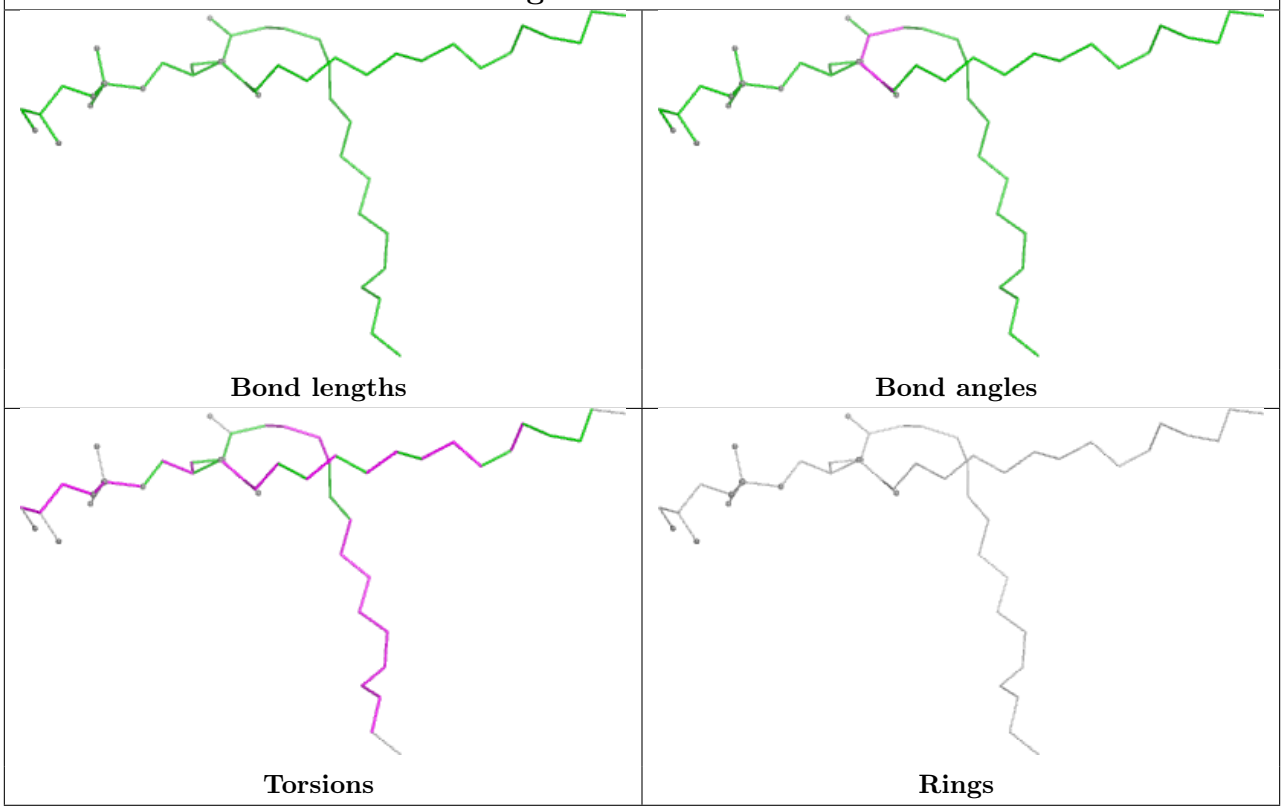
Ligand LMG D 411



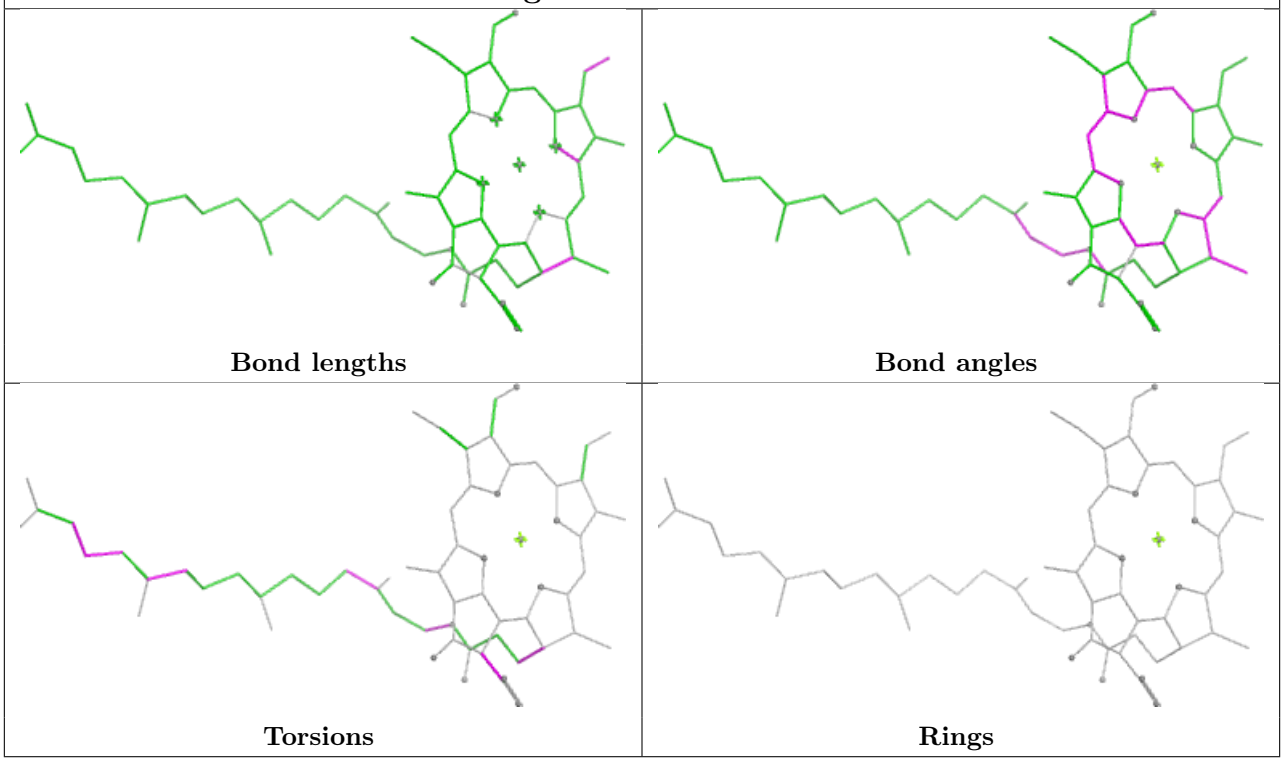
Ligand LHG N 624

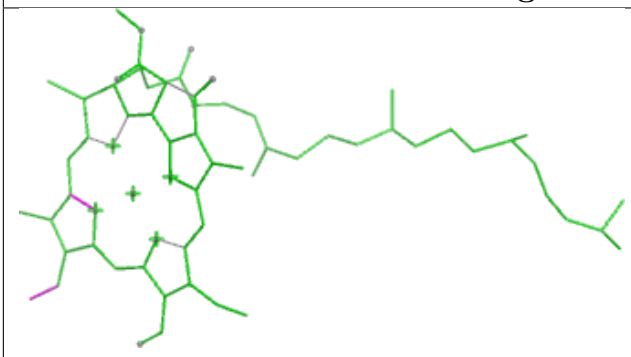
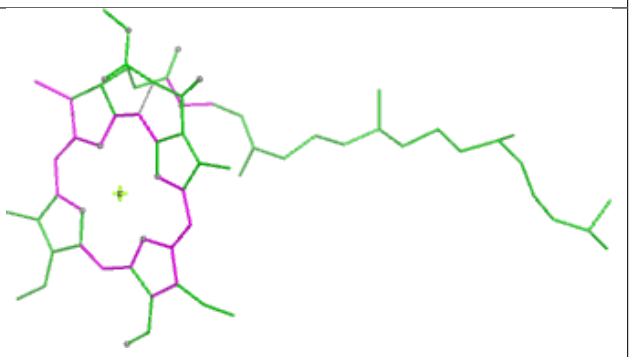
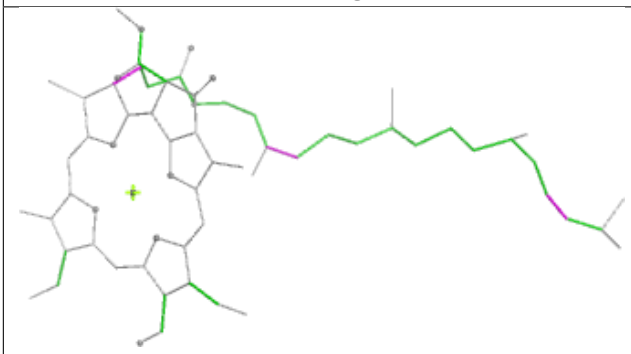
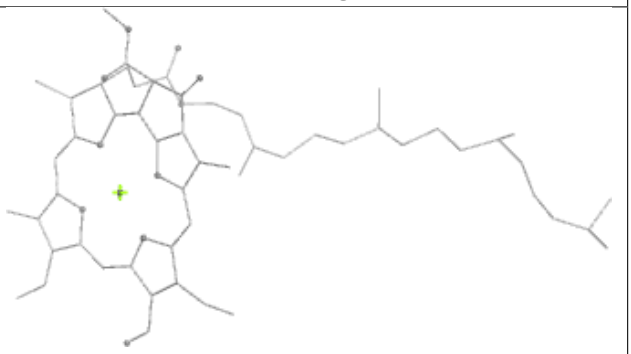


Ligand LHG n 624

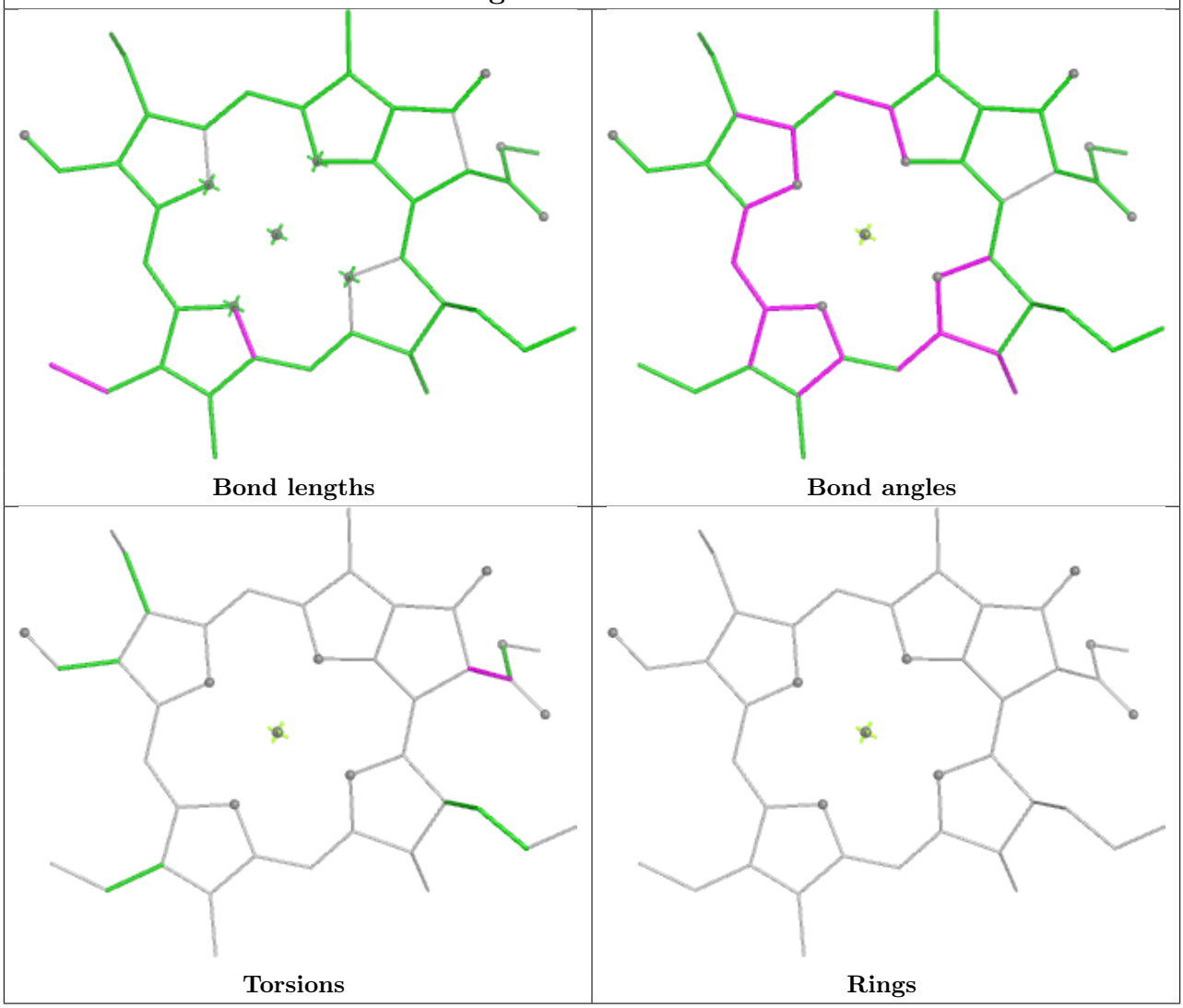


Ligand CHL N 609



Ligand CHL n1 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL r 606



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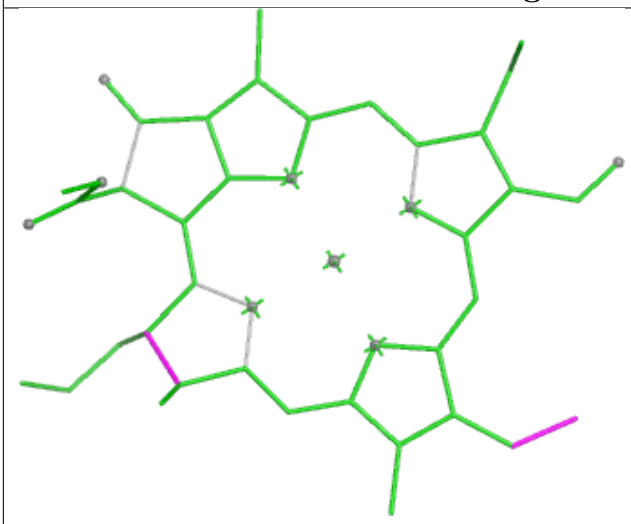
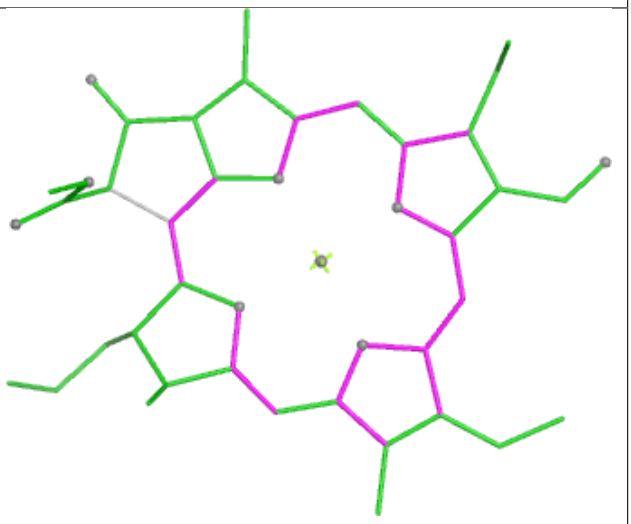
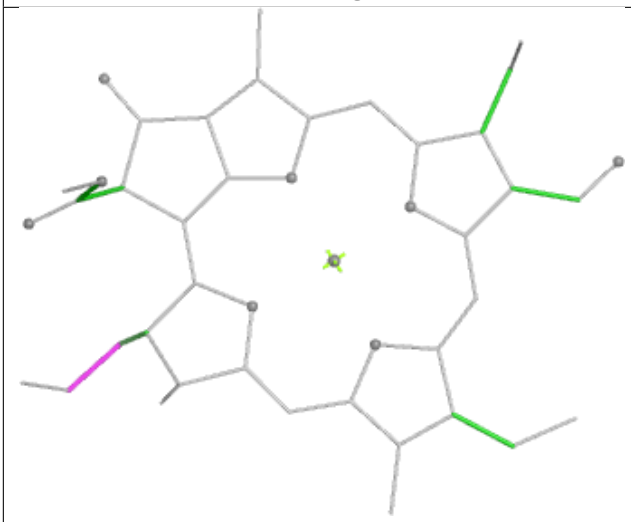


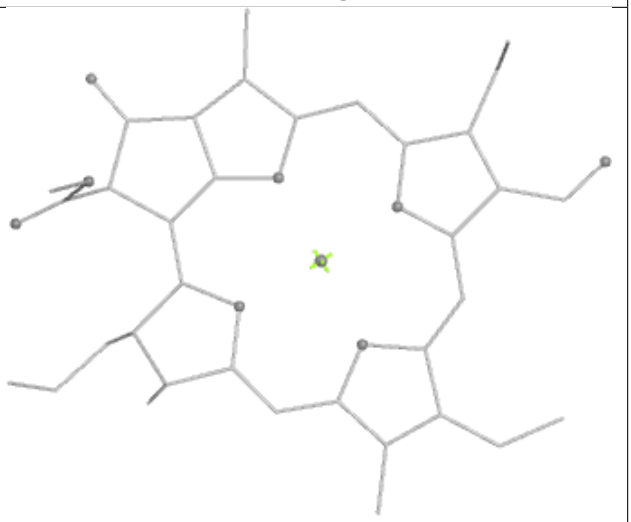
Bond lengths



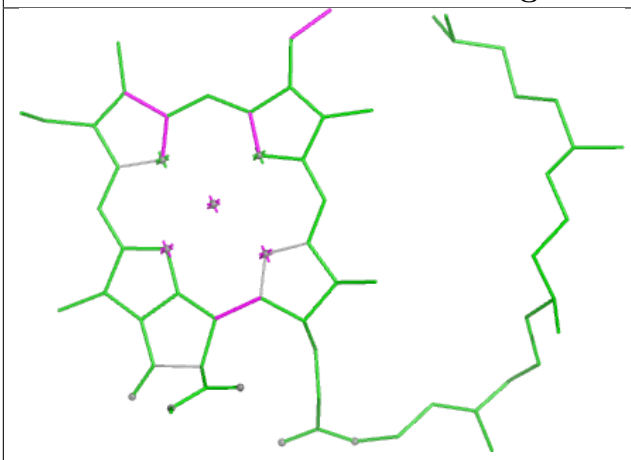
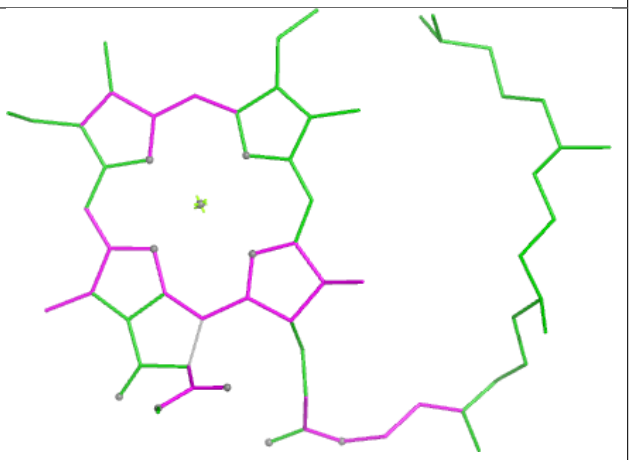
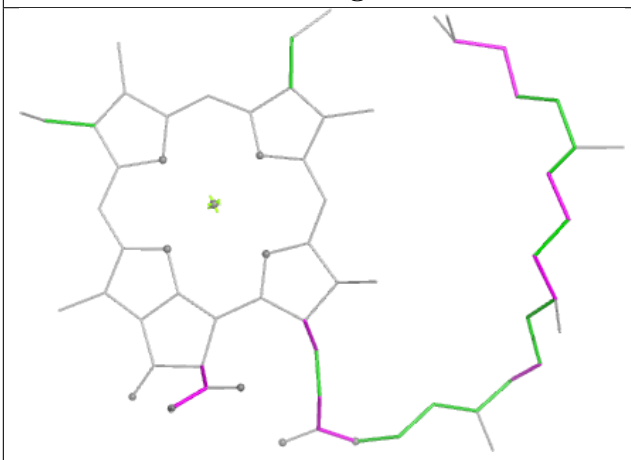
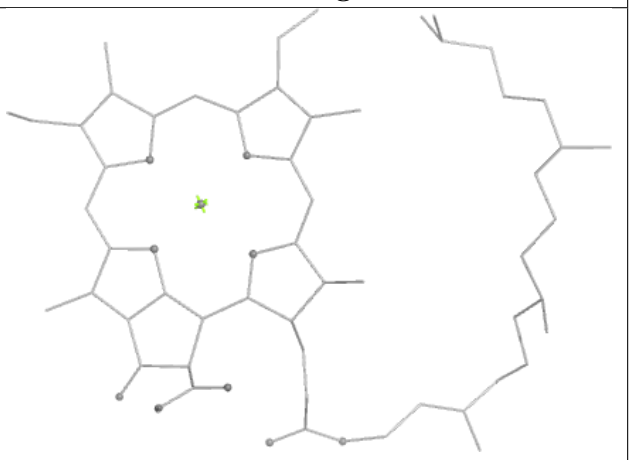
Bond angles



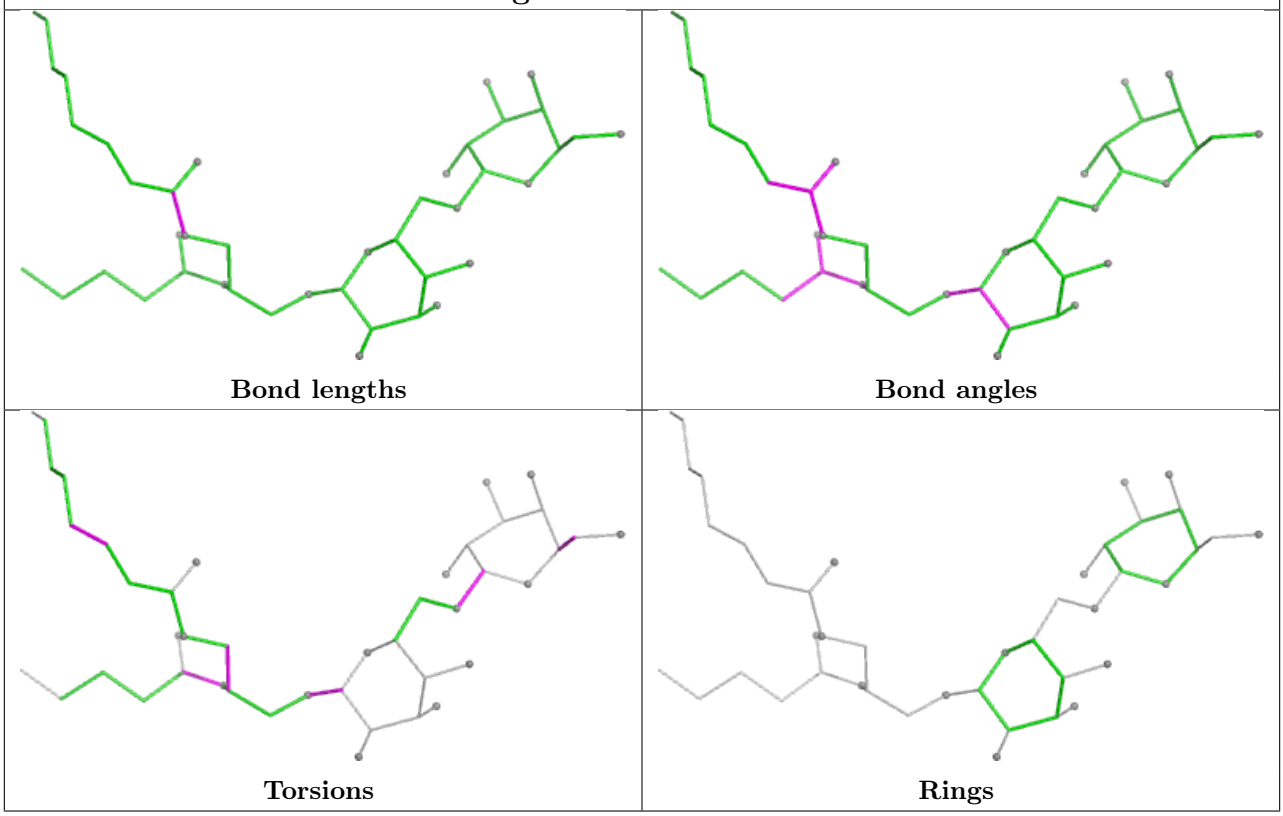
Torsions



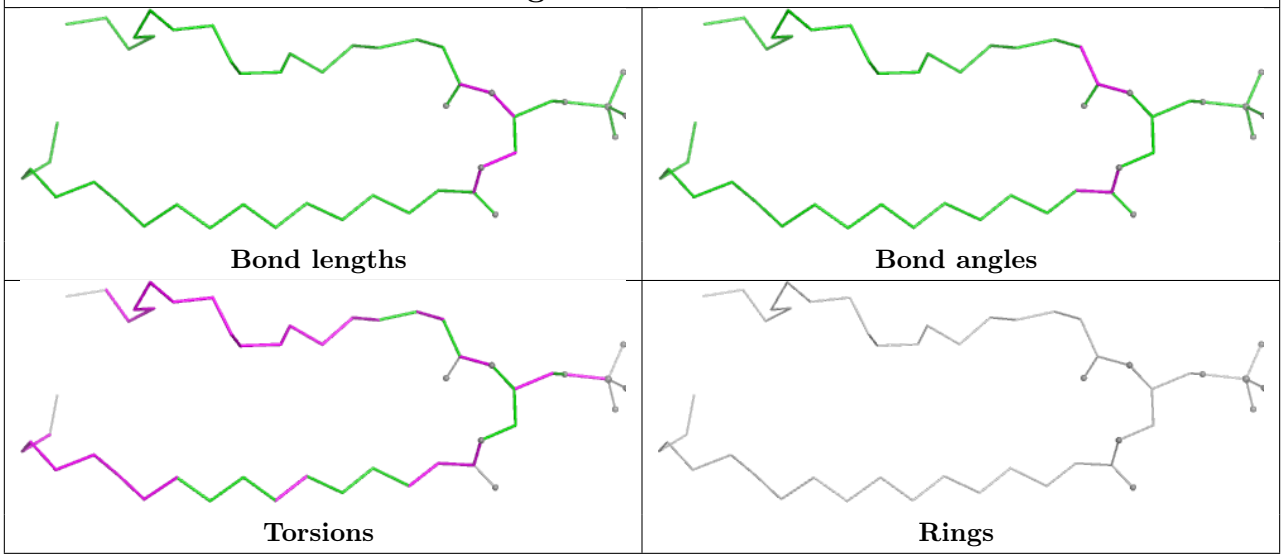
Rings

Ligand CLA c1 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

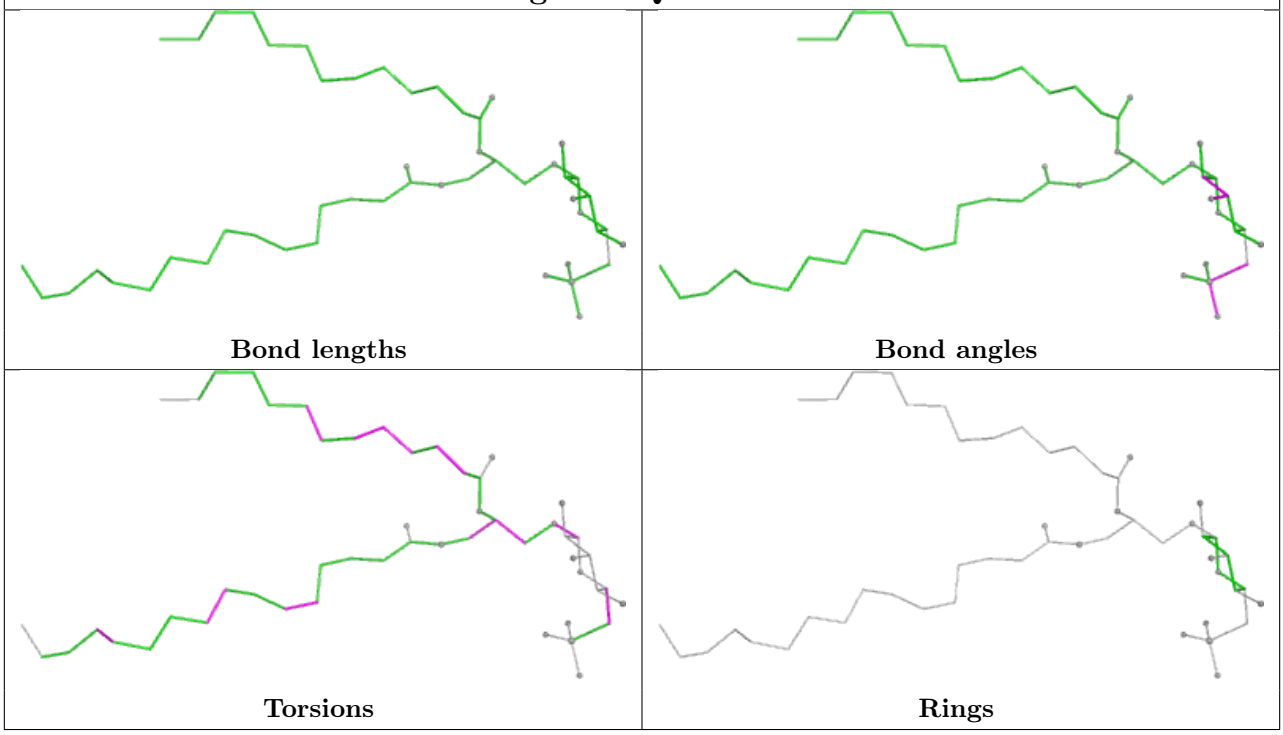
Ligand DGD B1 623



Ligand 3PH B 624



Ligand SQD a 412



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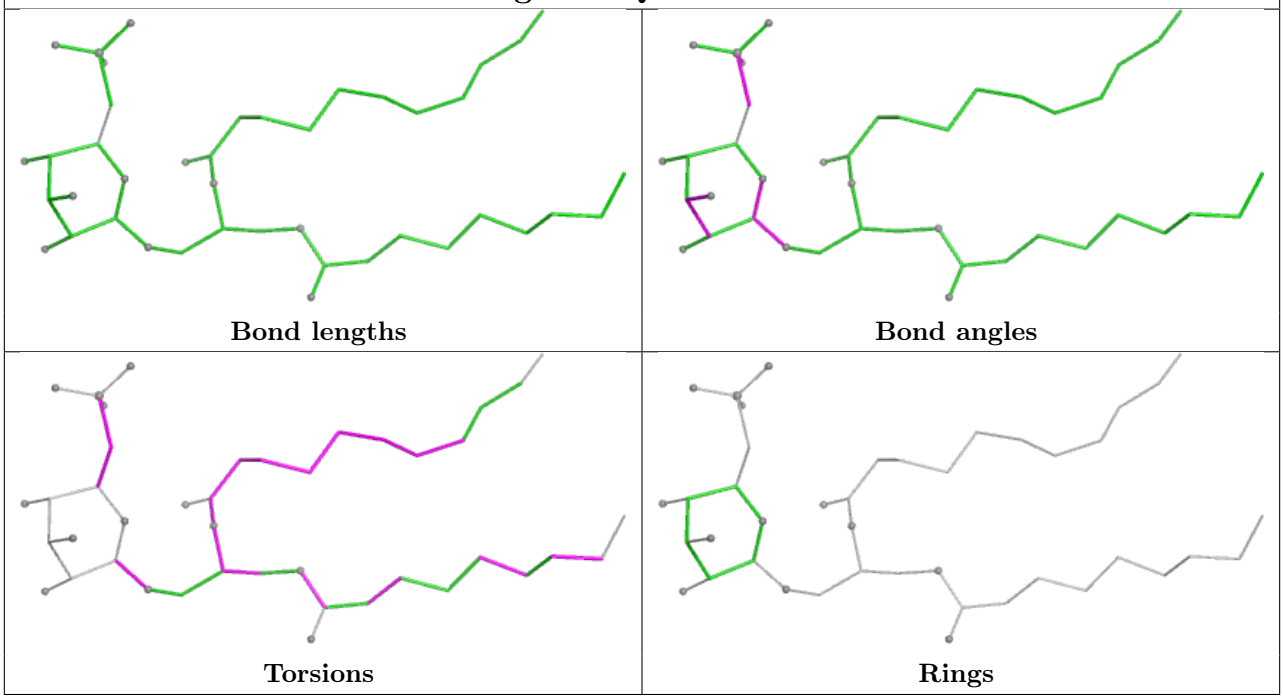

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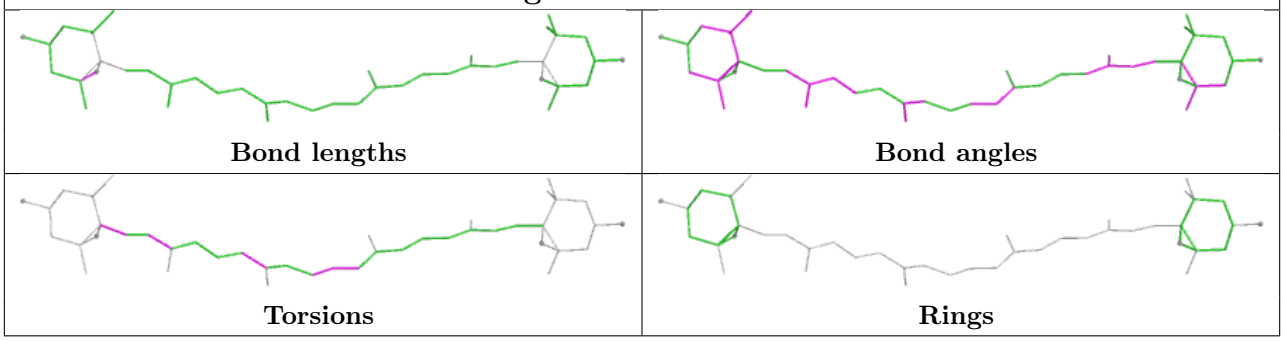

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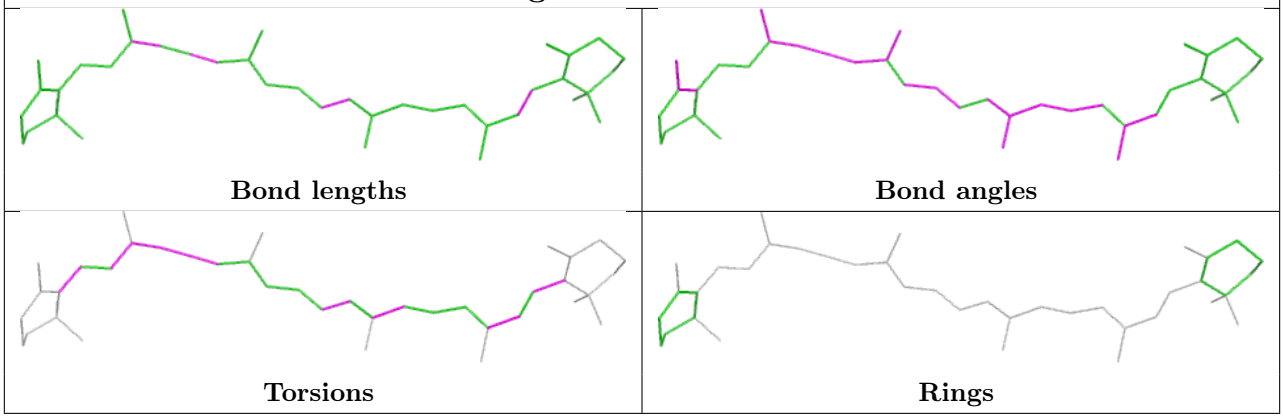

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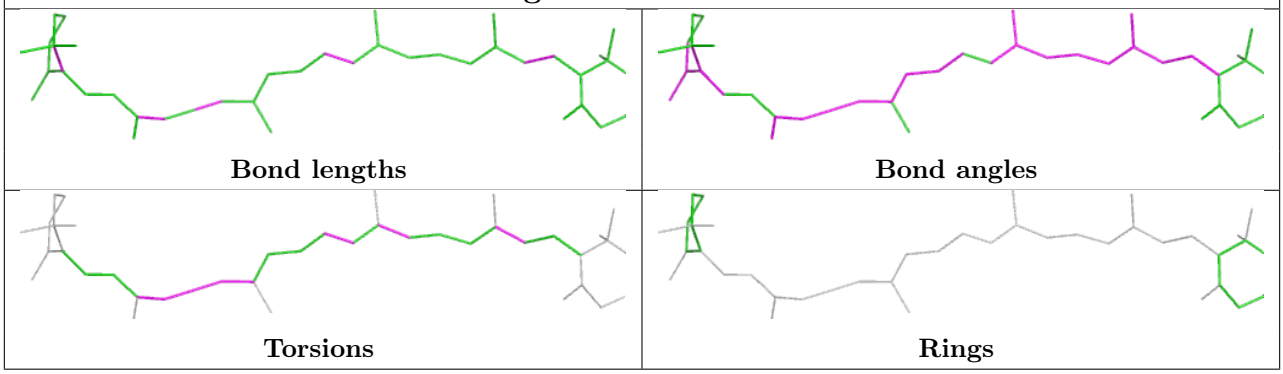

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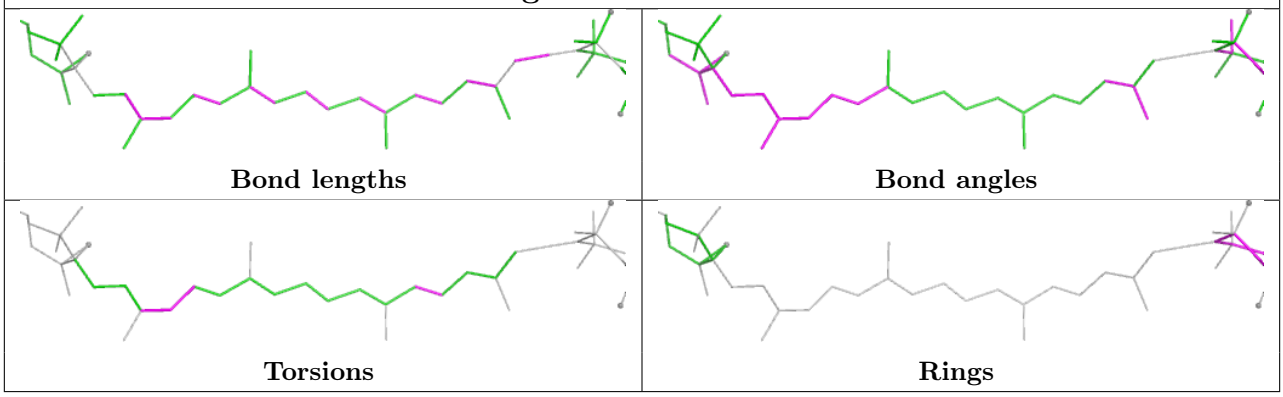

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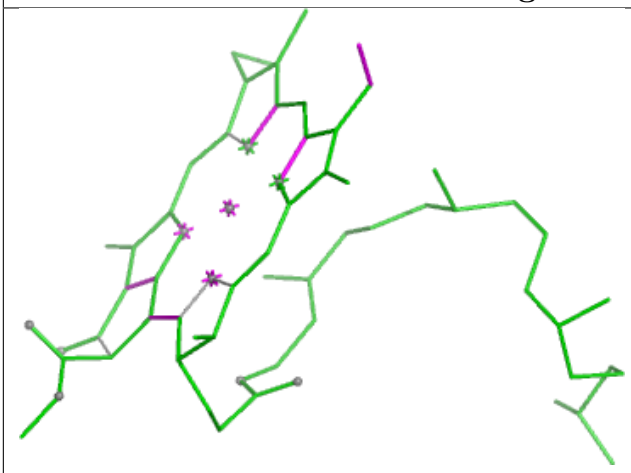
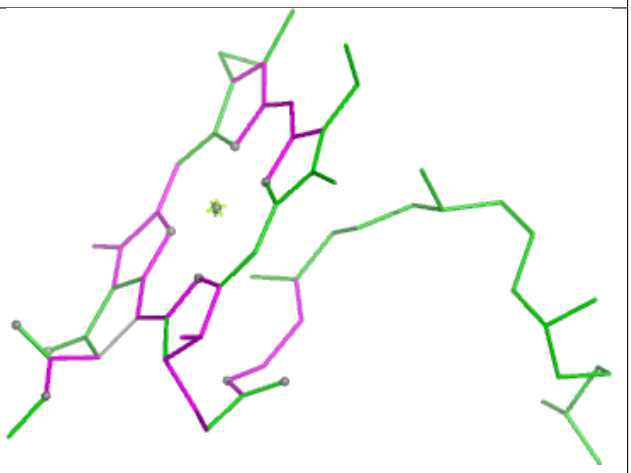
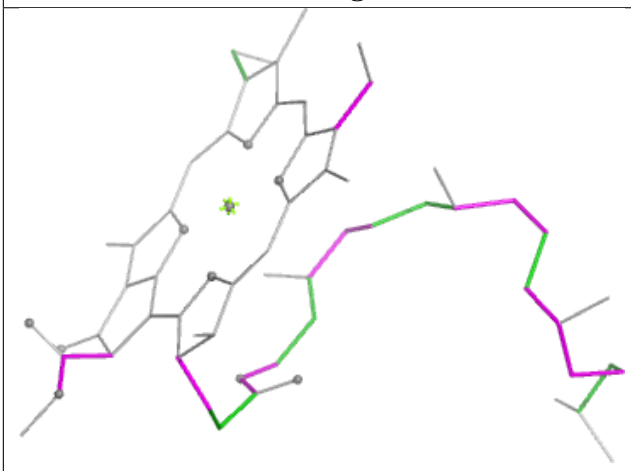
 Bond lengths	 Bond angles
 Torsions	Rings

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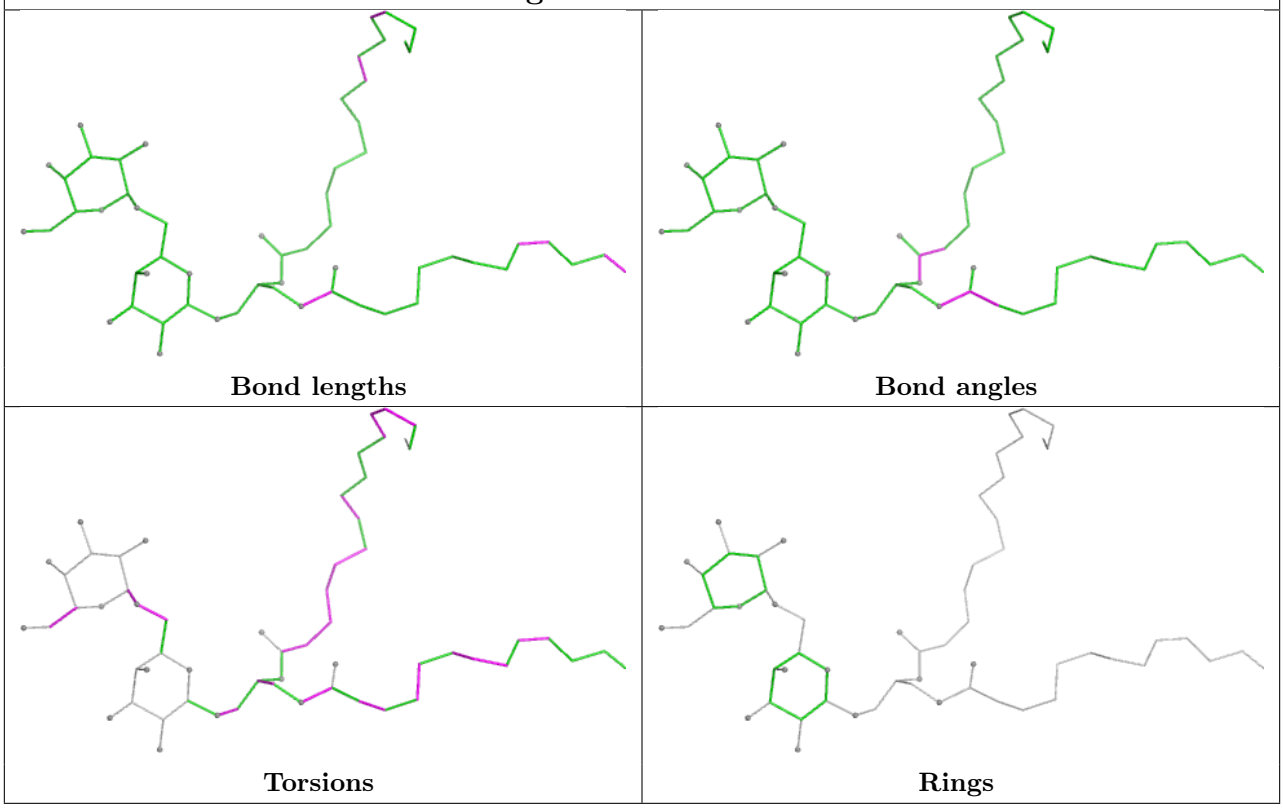

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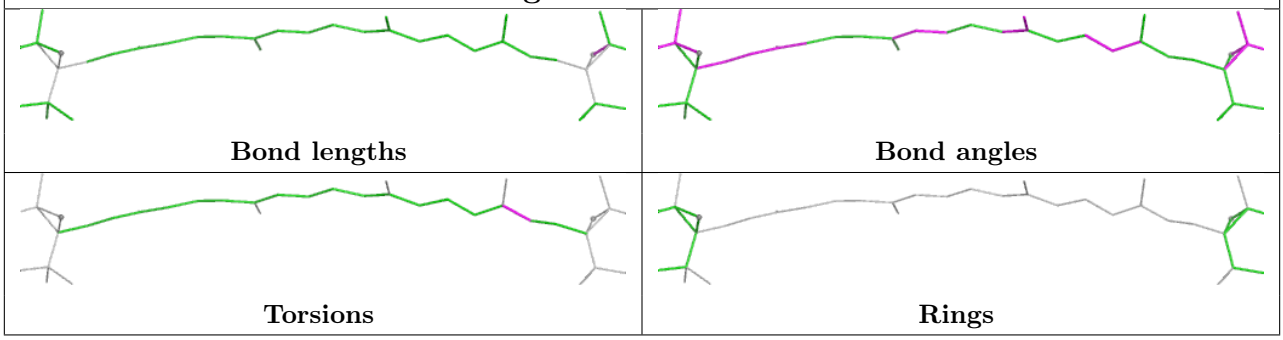

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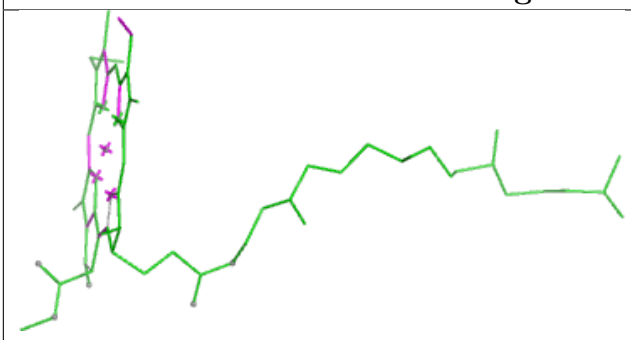
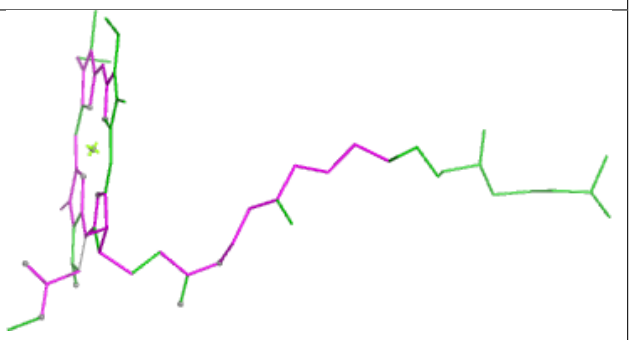
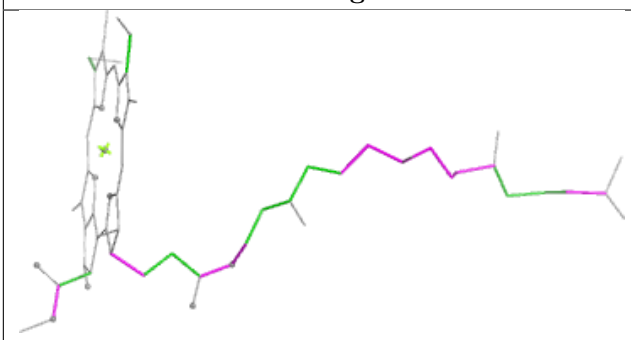
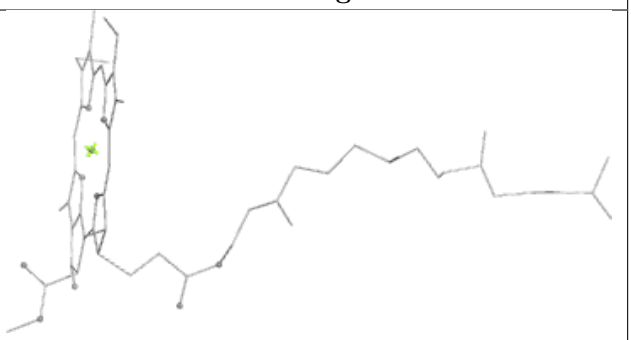
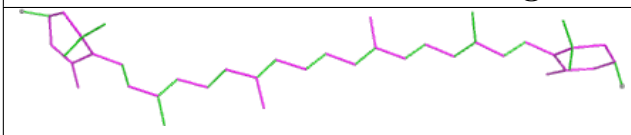
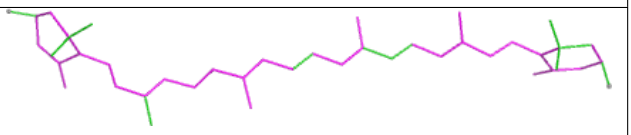
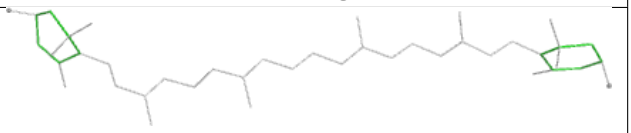
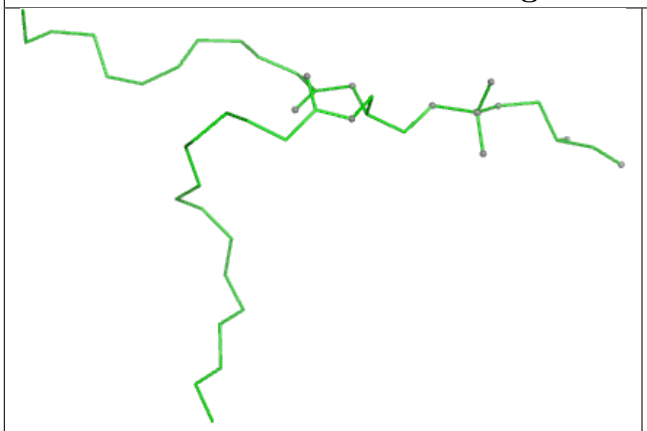
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand C7Z b1 620	
 Bond lengths	 Bond angles
Torsions	 Rings

Ligand LHG s1 624



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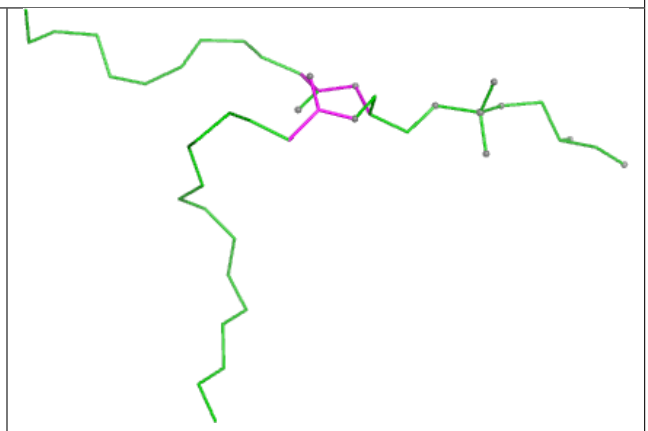

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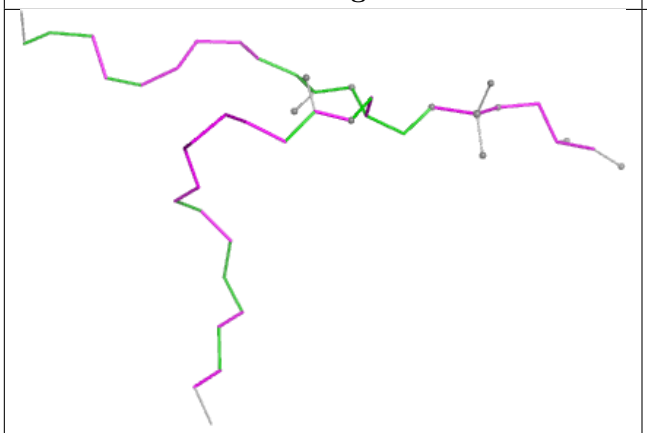

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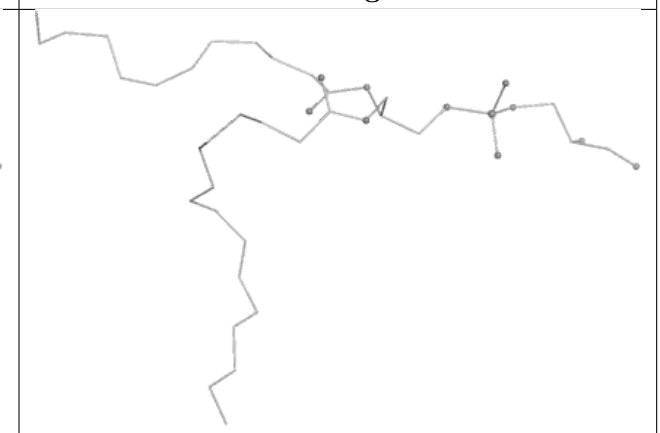
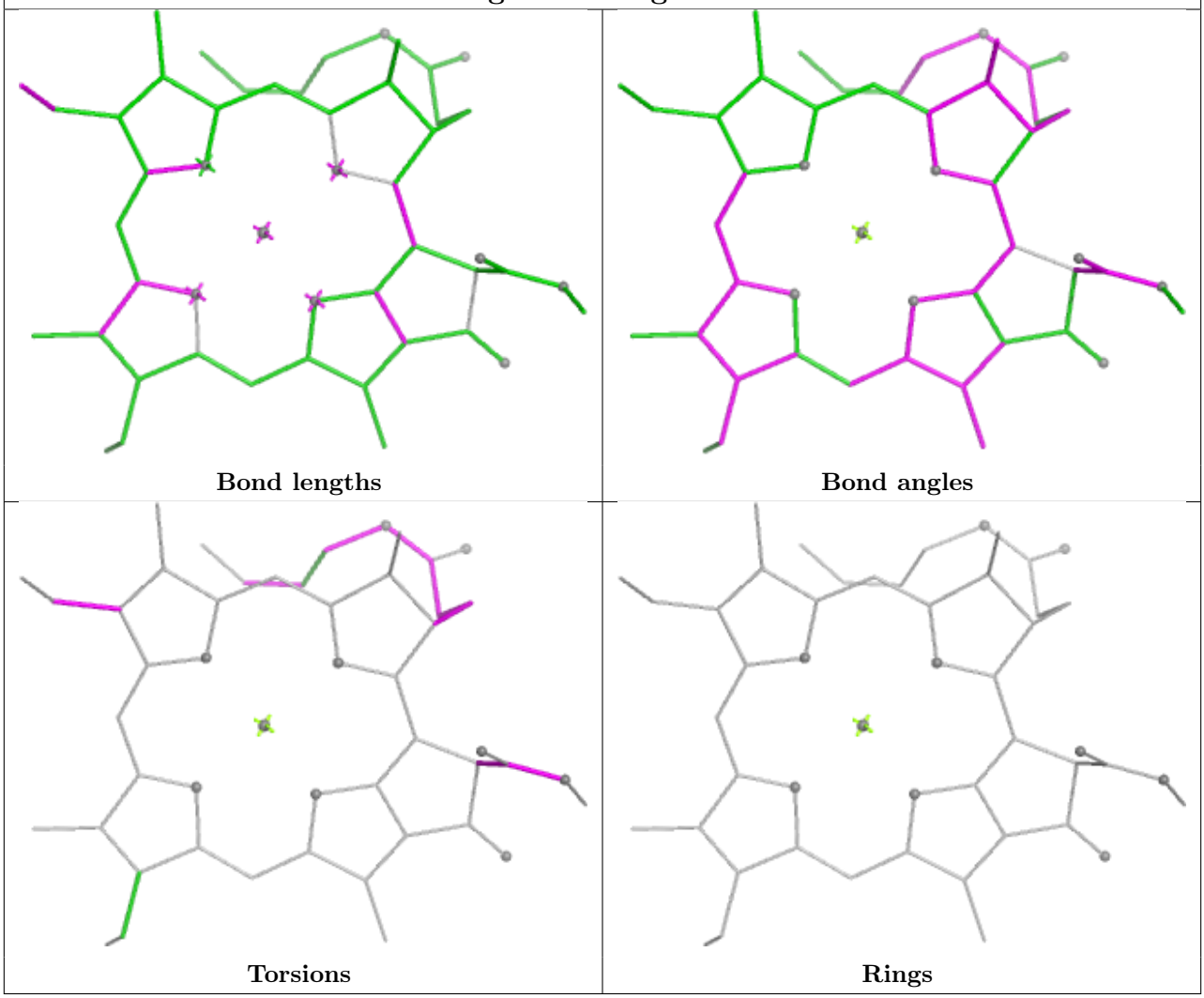
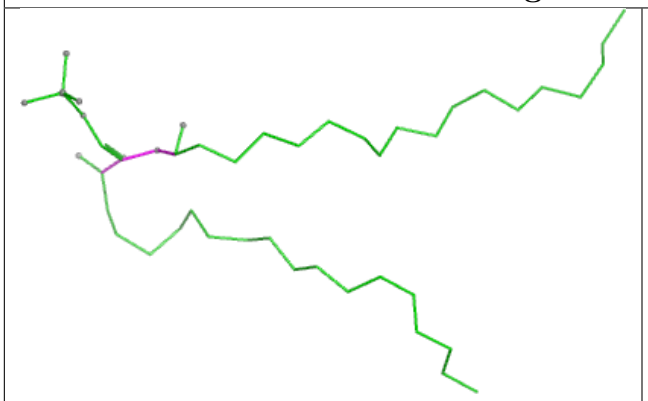


Rings

Ligand CLA g1 614



Ligand 3PH s1 626



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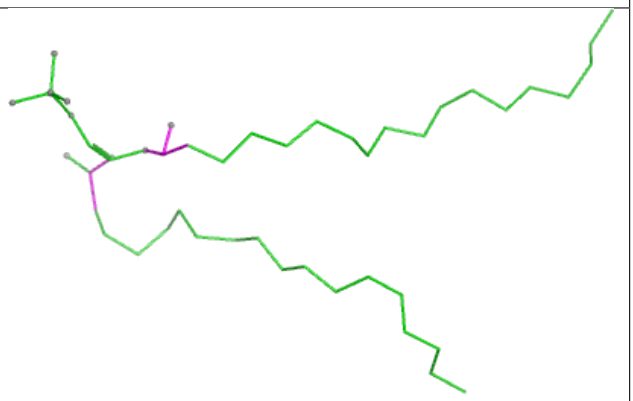
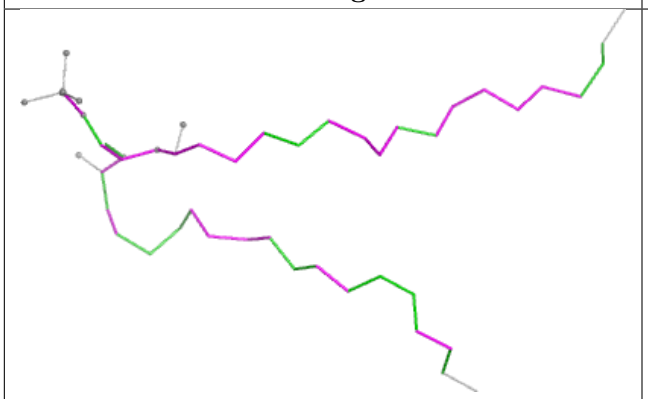


Bond angles



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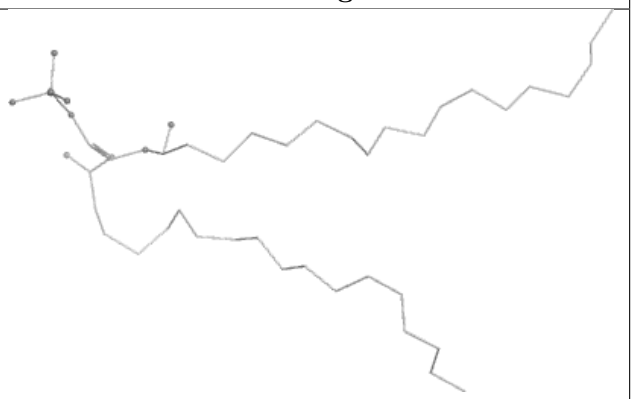
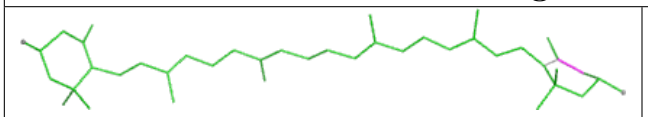


Rings

Ligand LUT r 620



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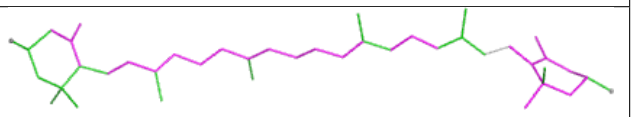

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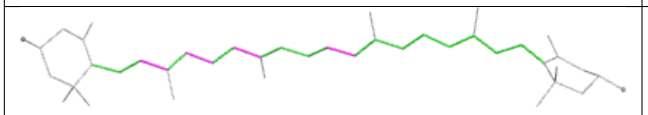

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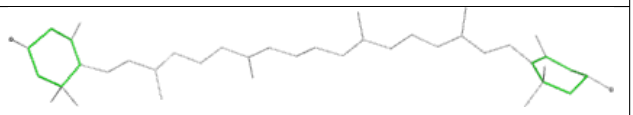

Rings

Ligand LUT s 620

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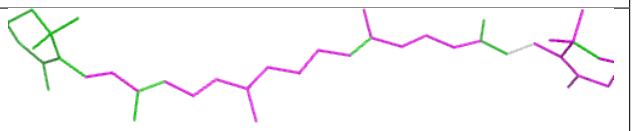

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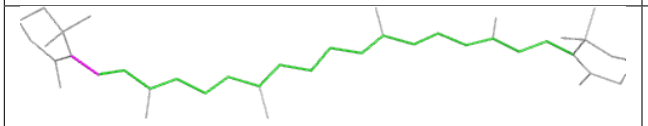

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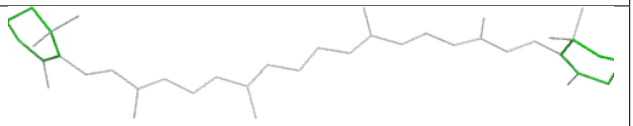
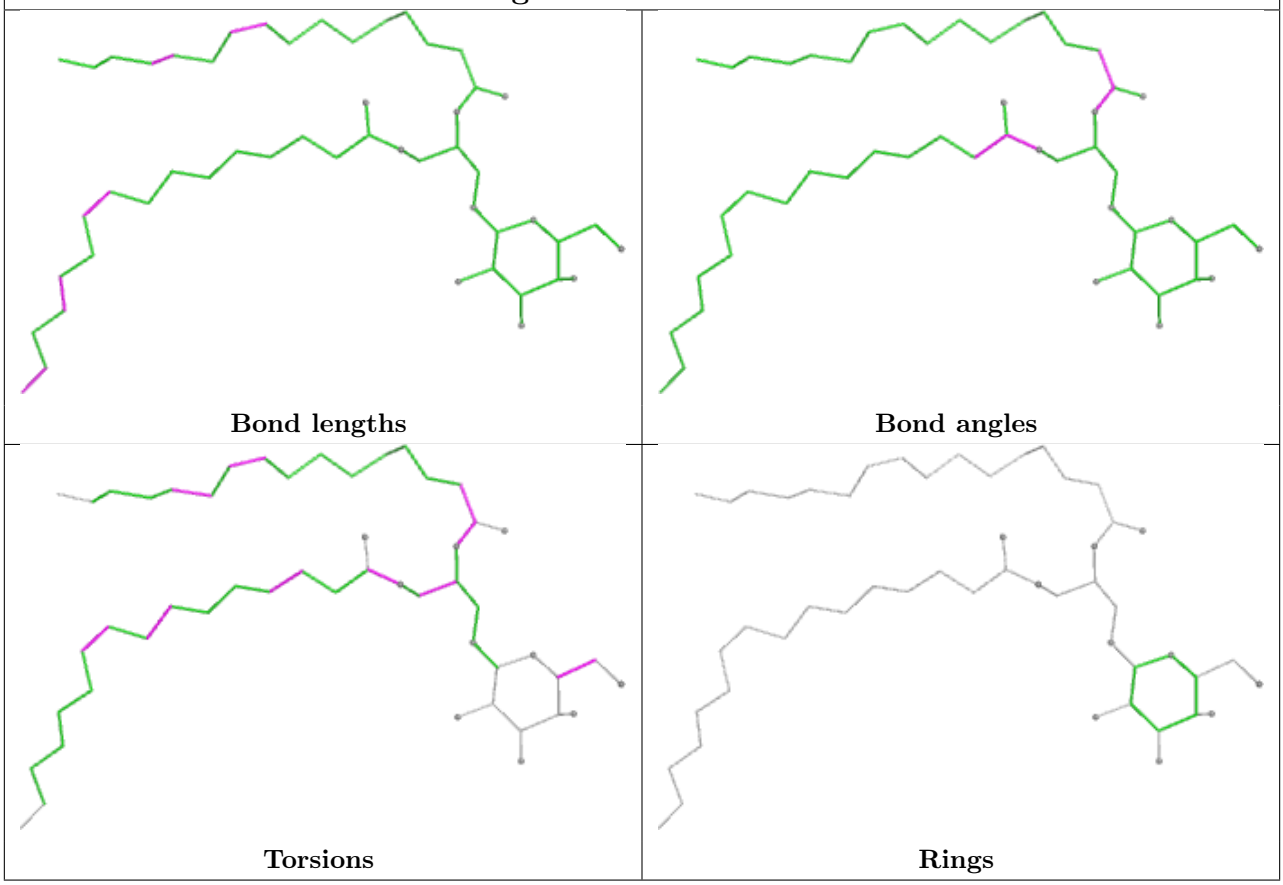
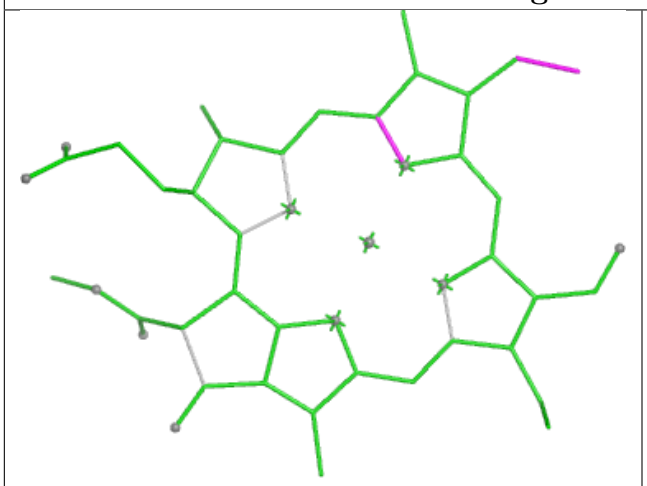


Rings

Ligand LMG C1 521



Ligand CHL s 601



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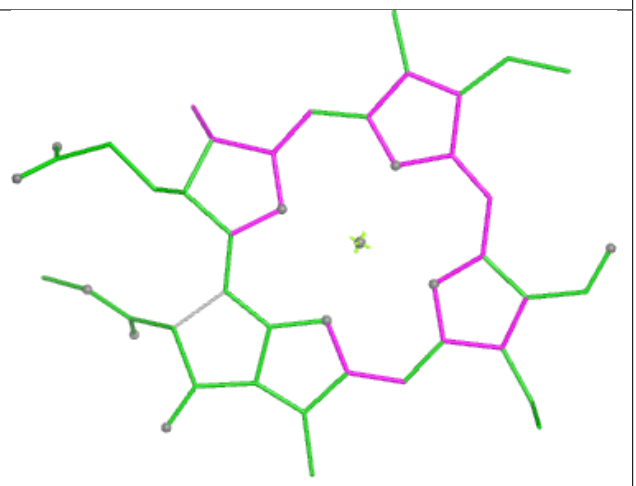

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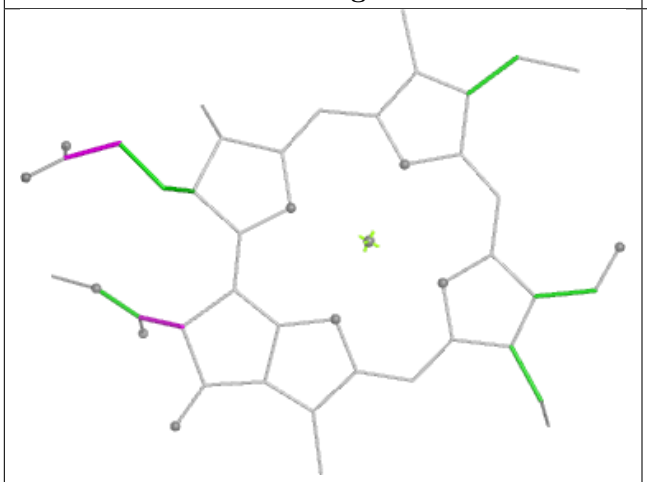

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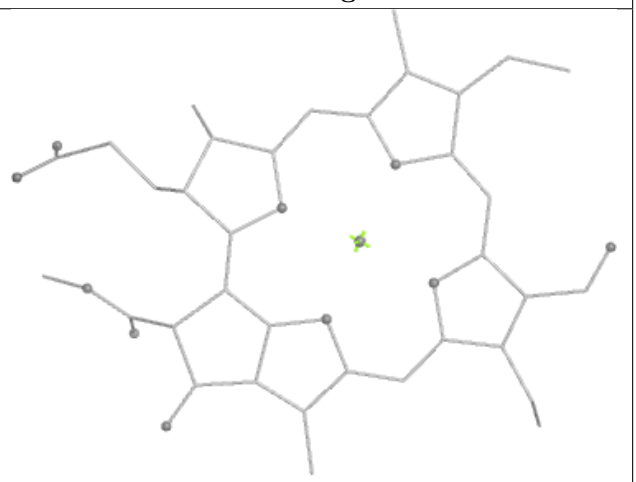
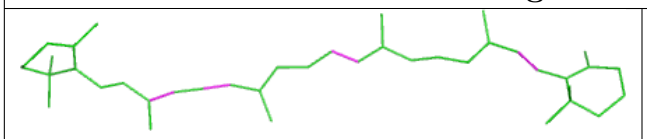


Rings

Ligand BCR d 404



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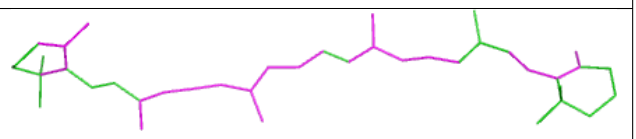

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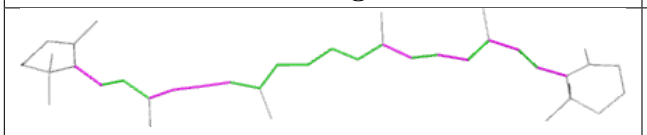

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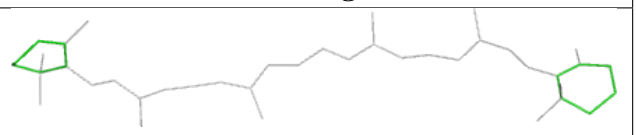
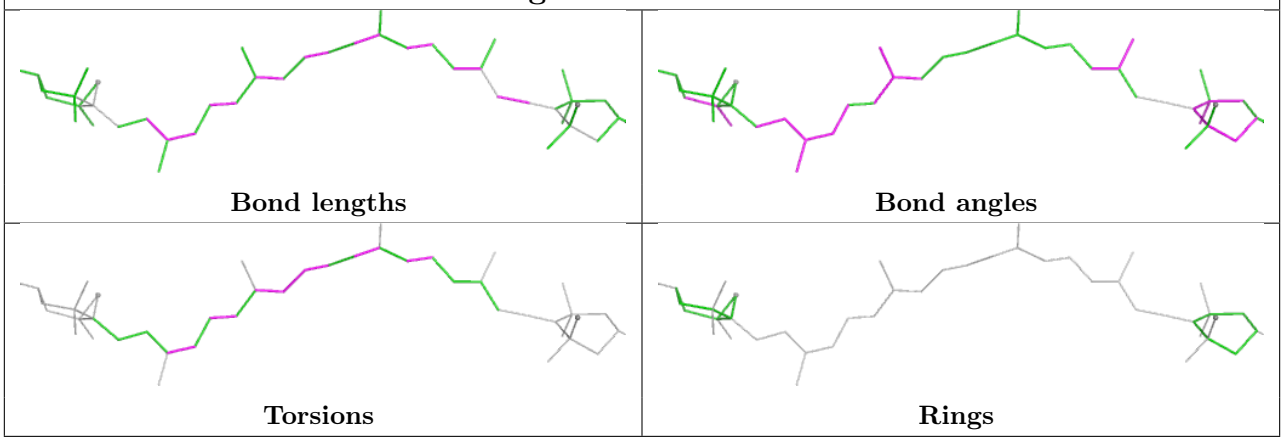
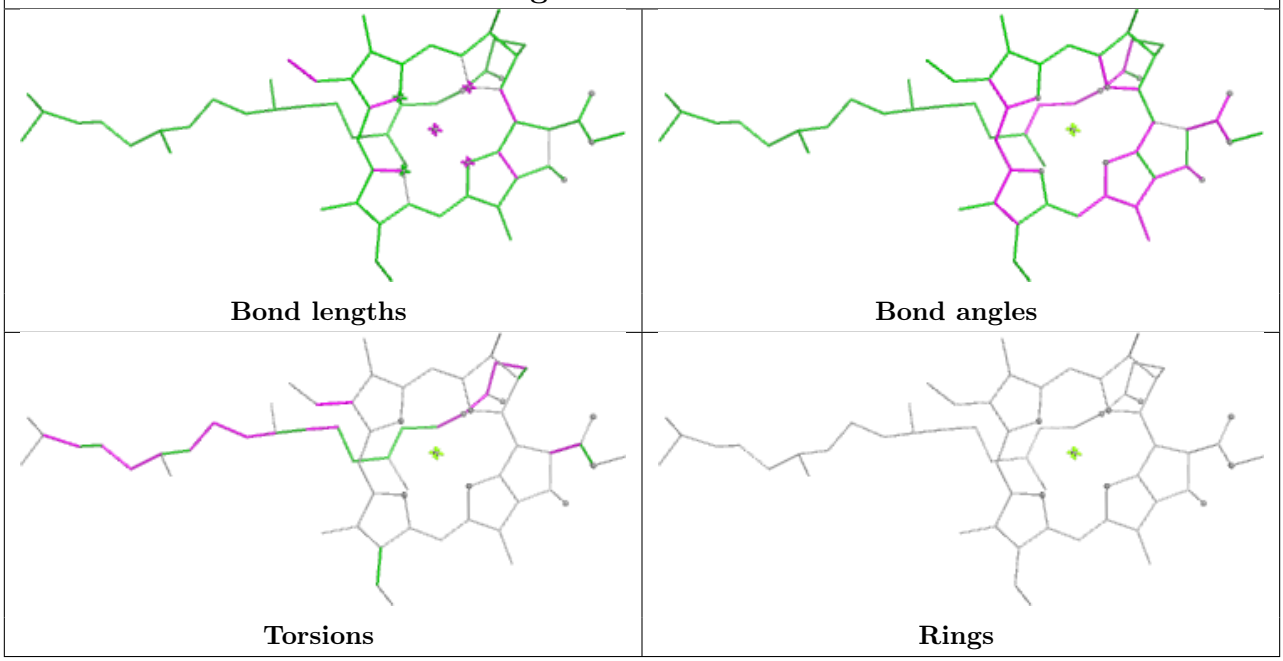


Rings

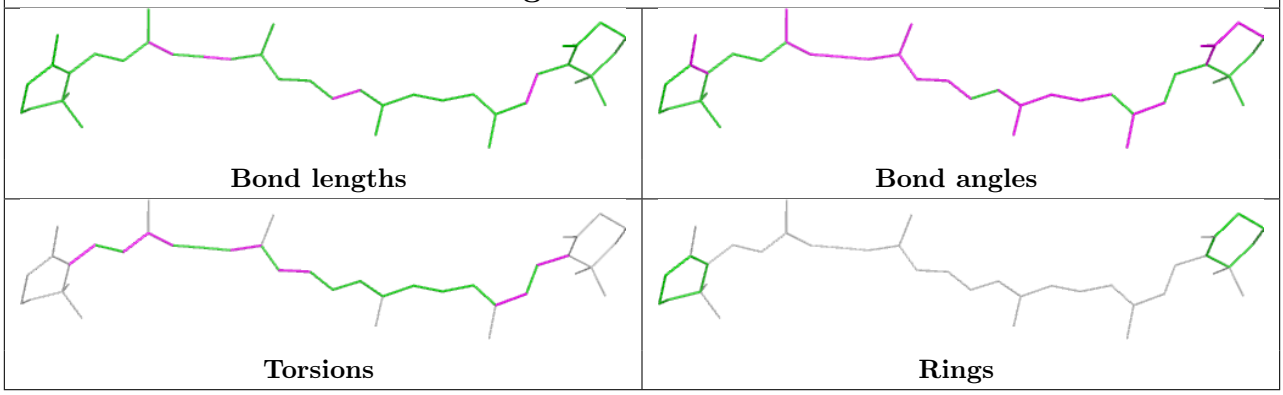
Ligand NEX r 622

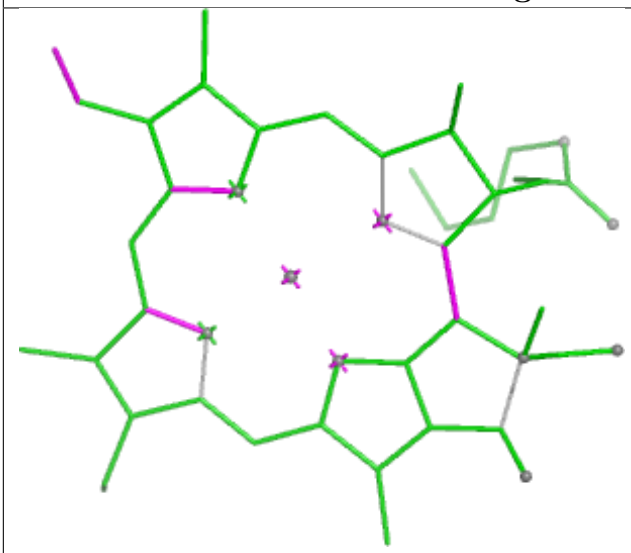
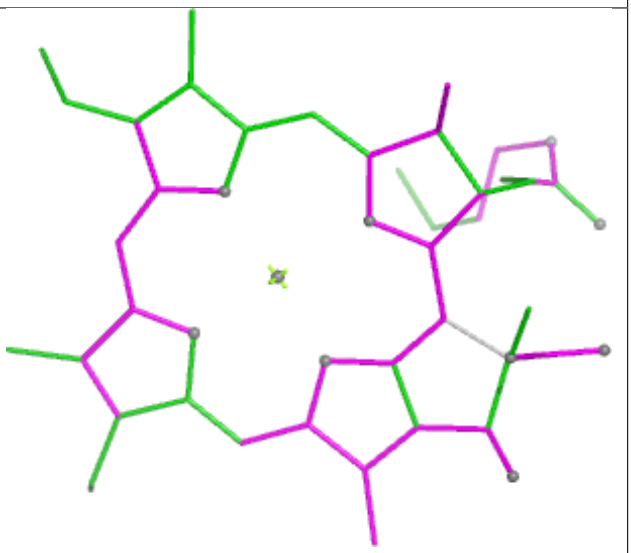
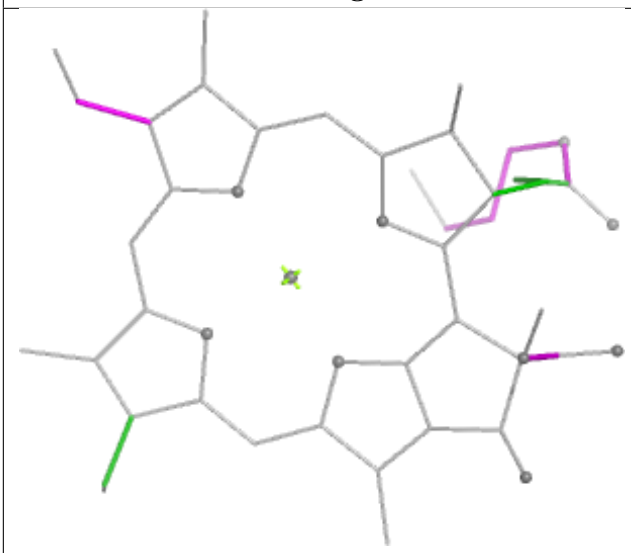
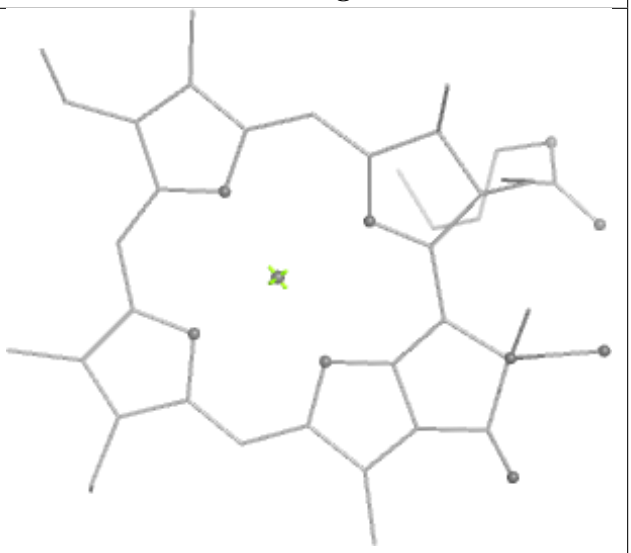


Ligand CLA c 505

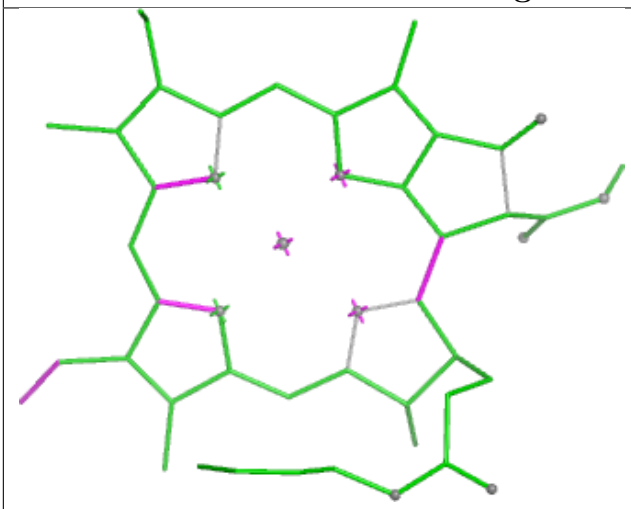


Ligand BCR C 516

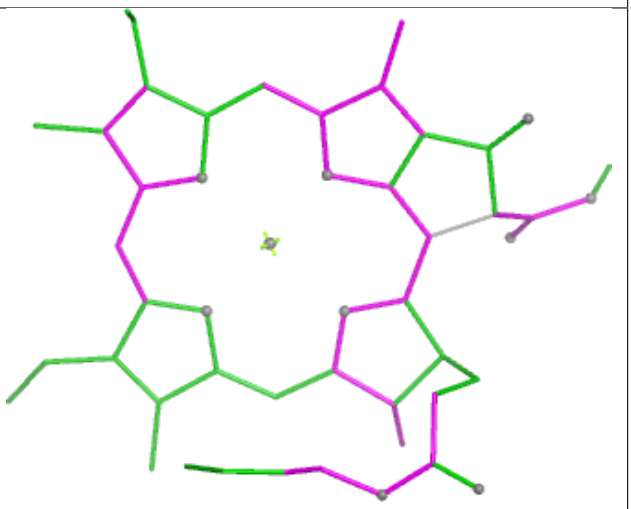


Ligand CLA G1 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

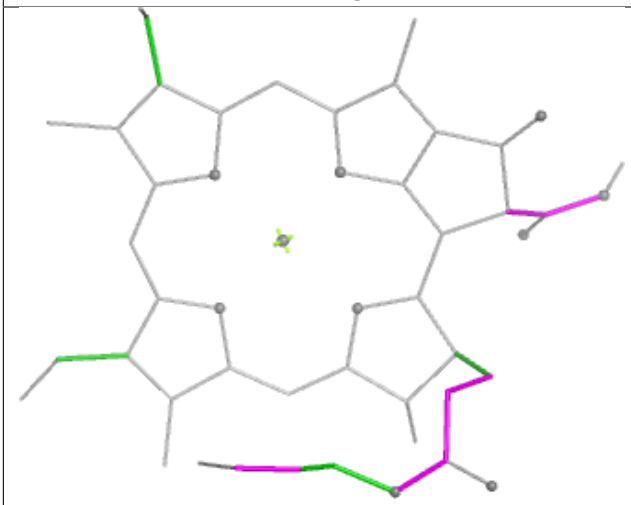
Ligand CLA G1 614



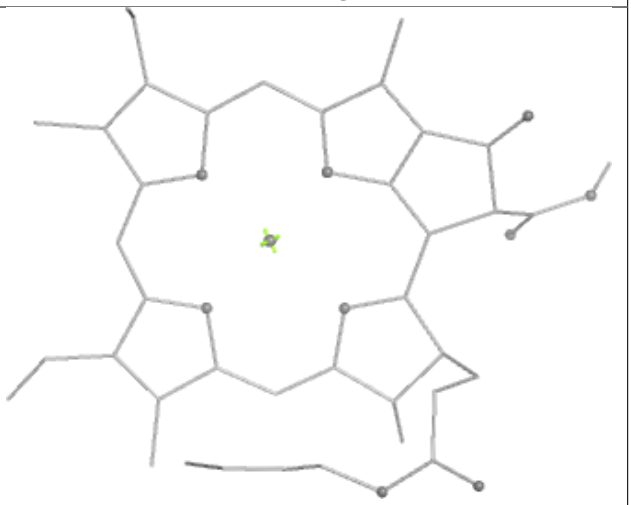
Bond lengths



Bond angles

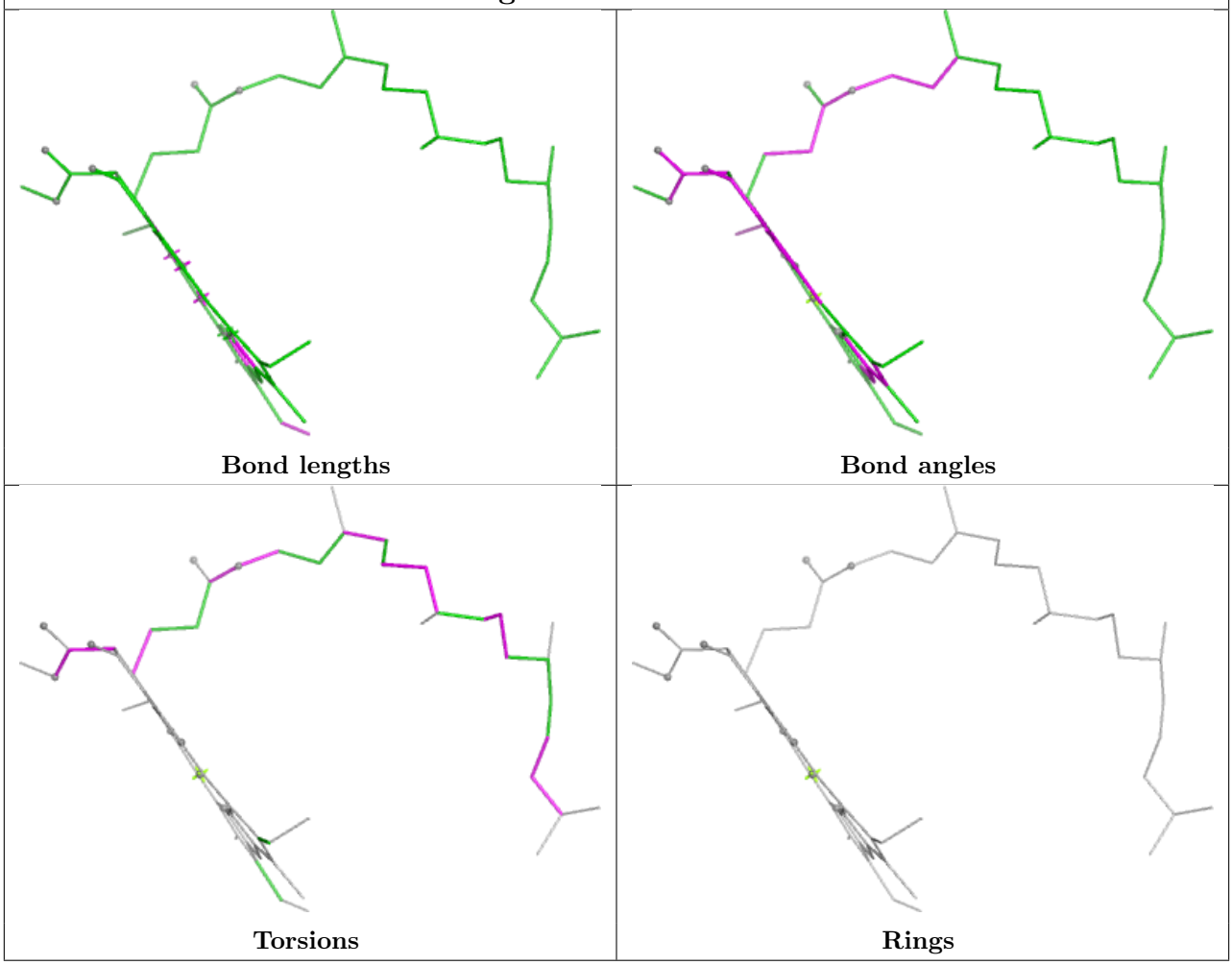


Torsions

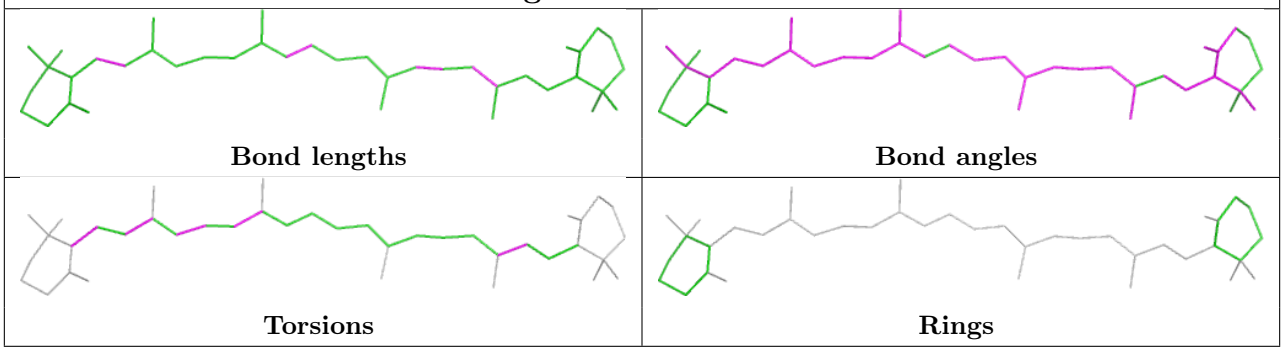


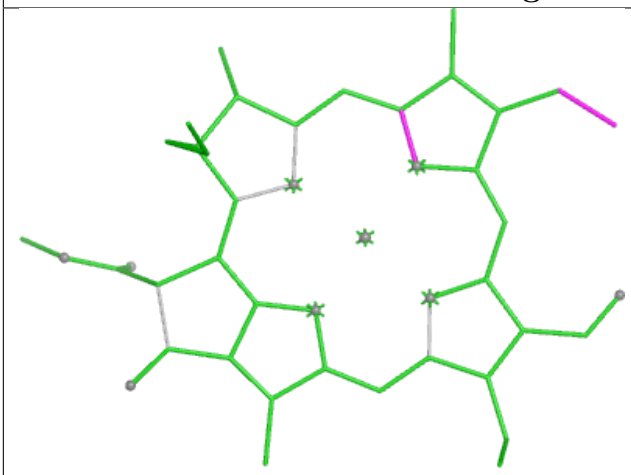
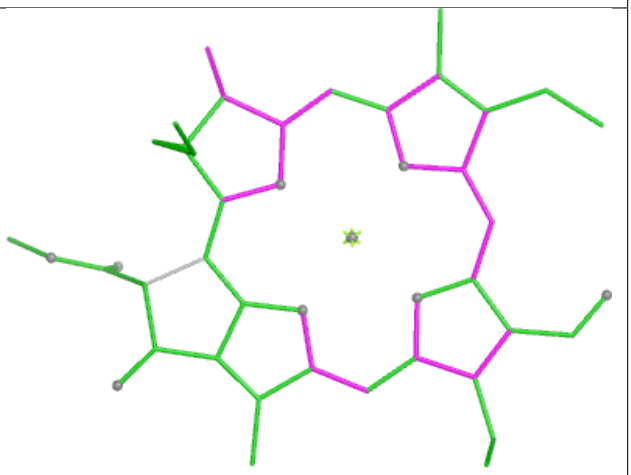
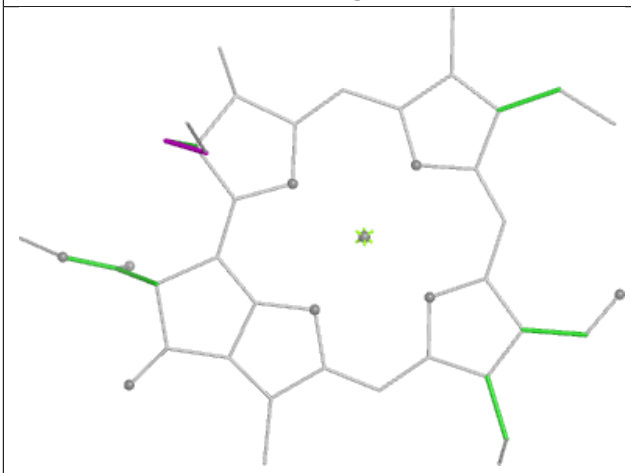
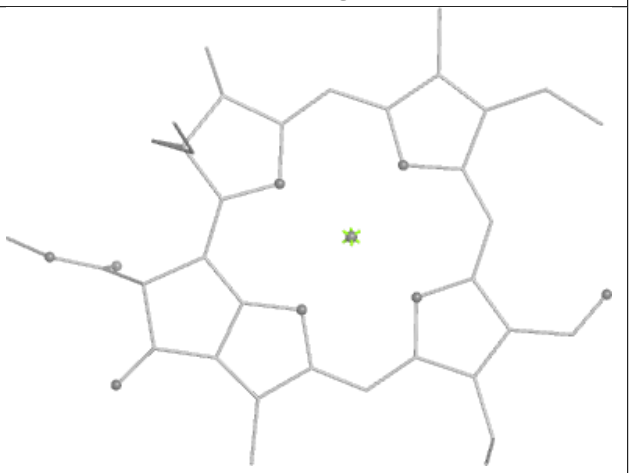
Rings

Ligand CLA b1 612

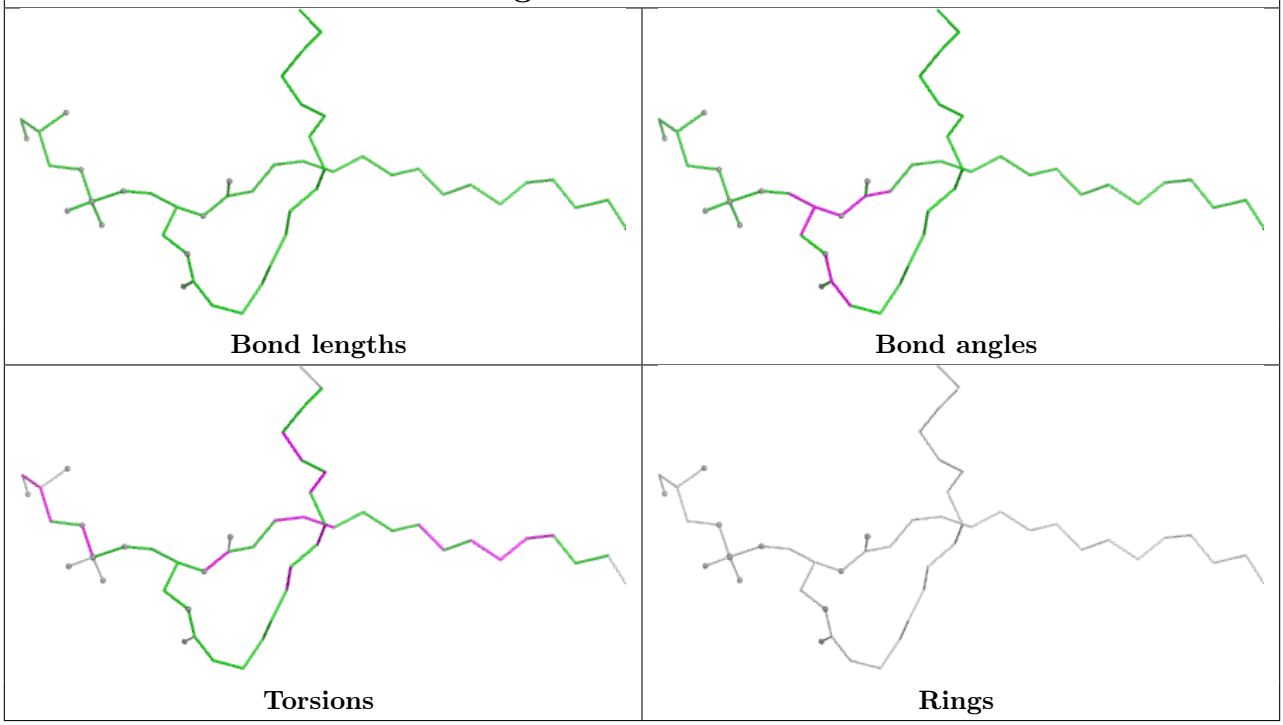


Ligand BCR B 619

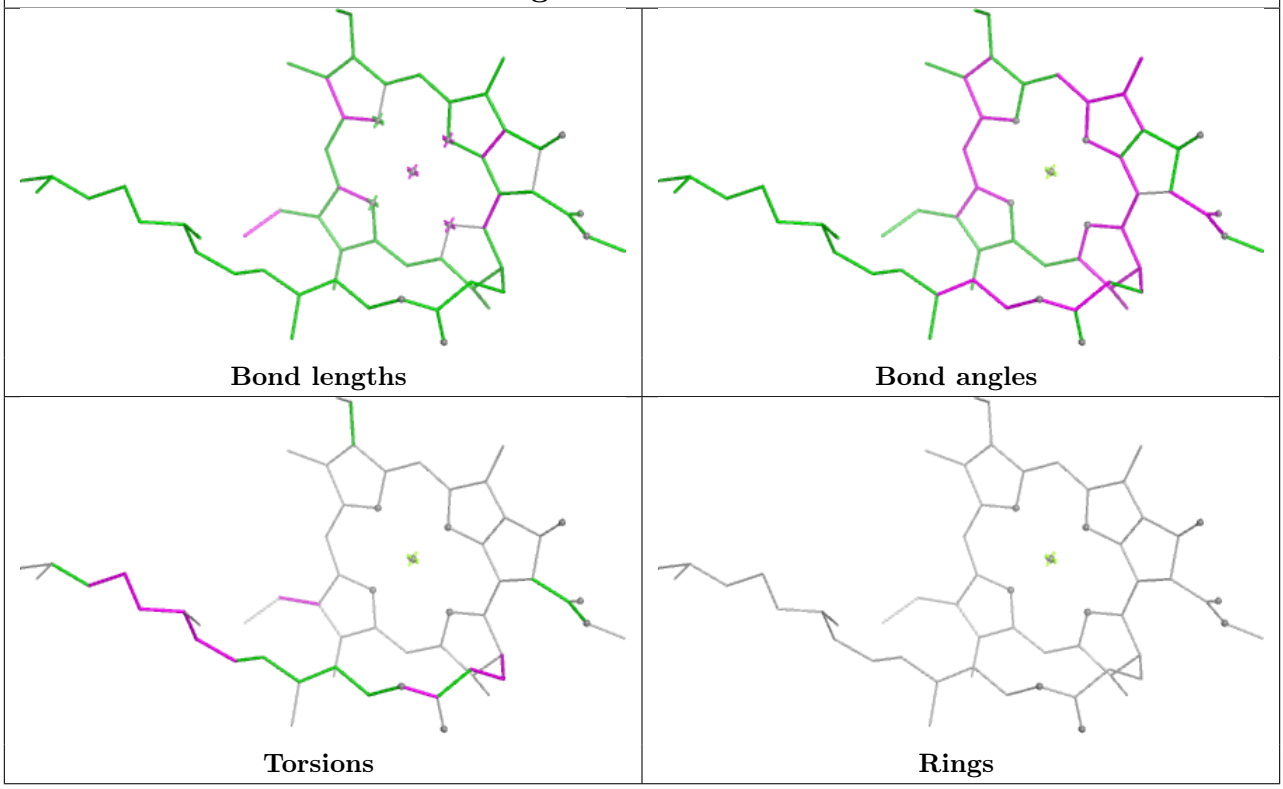


Ligand CHL G 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG Y1 624



Ligand CLA r 610



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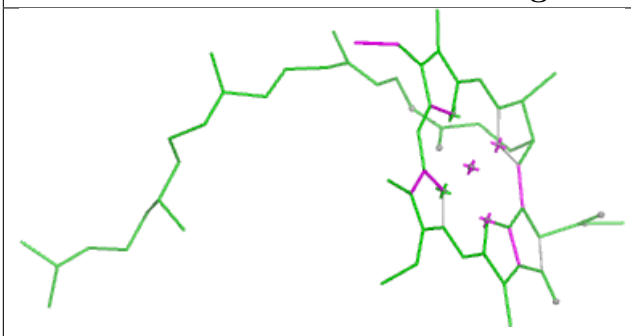
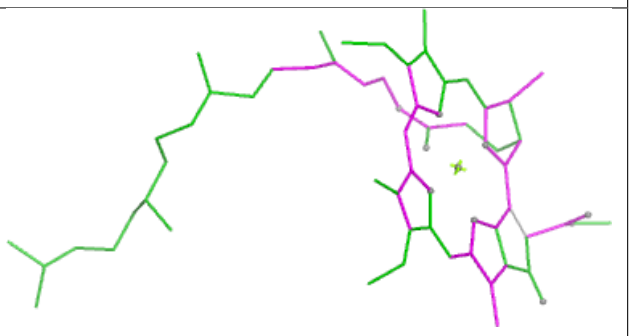
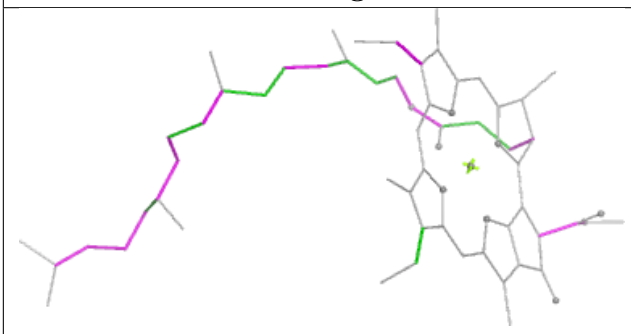
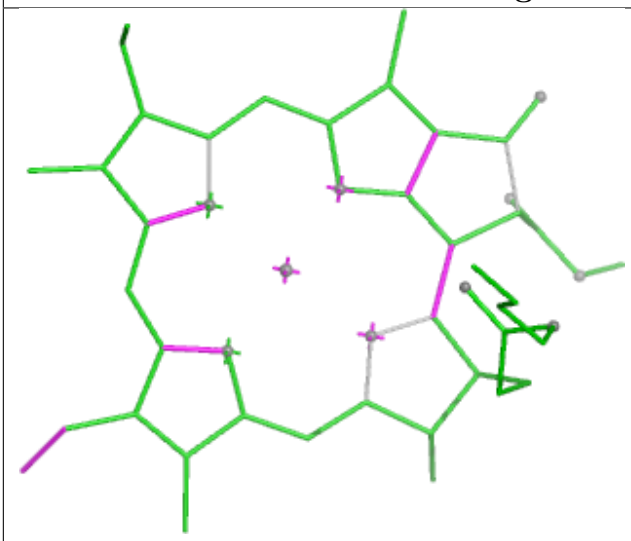
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA R1 604



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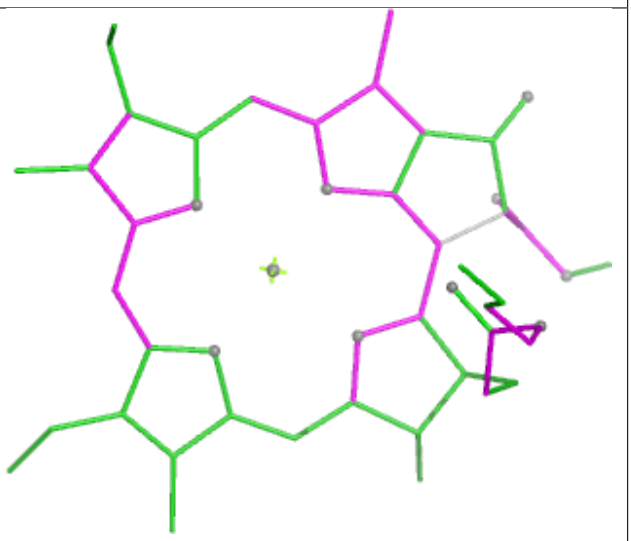
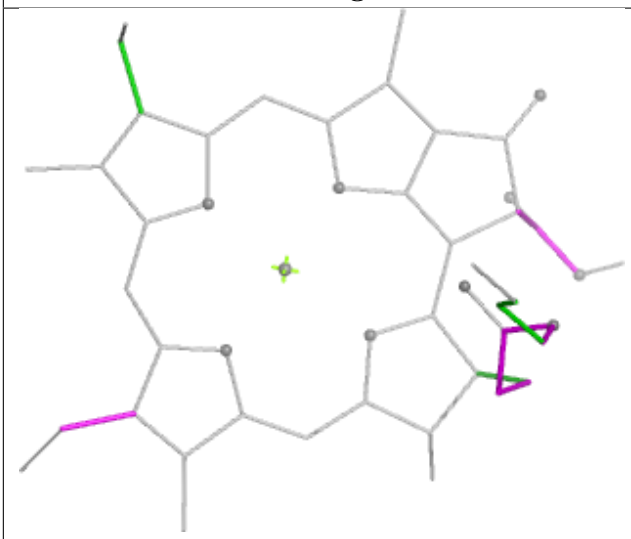
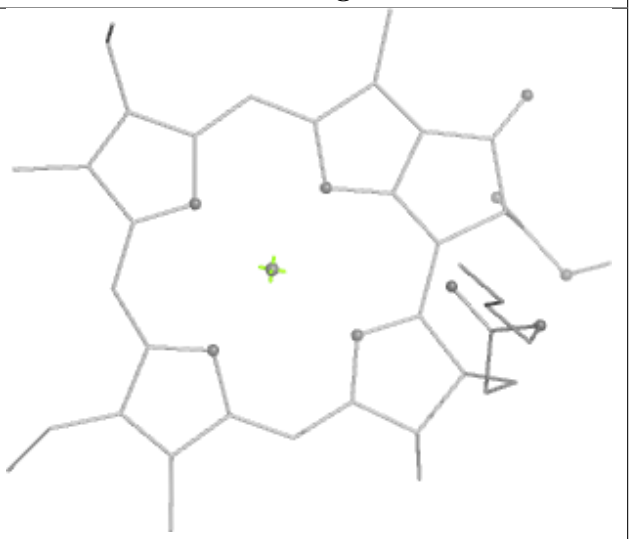


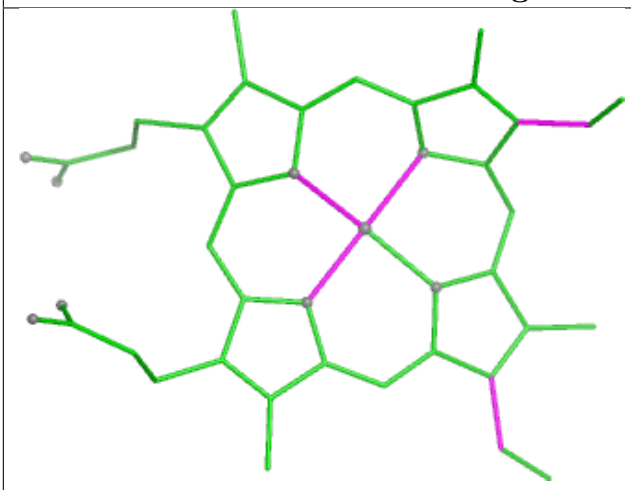
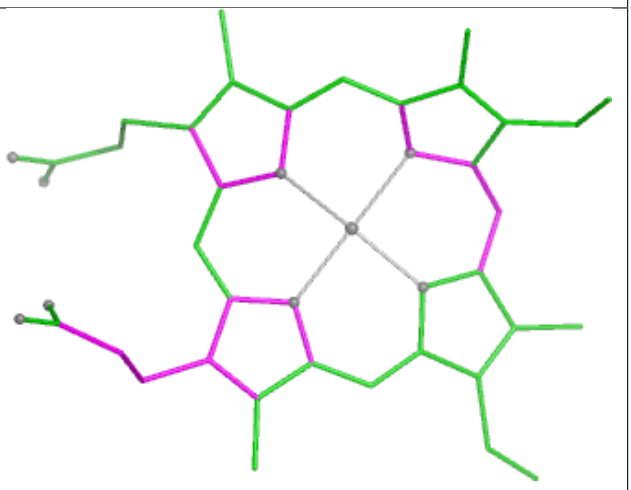
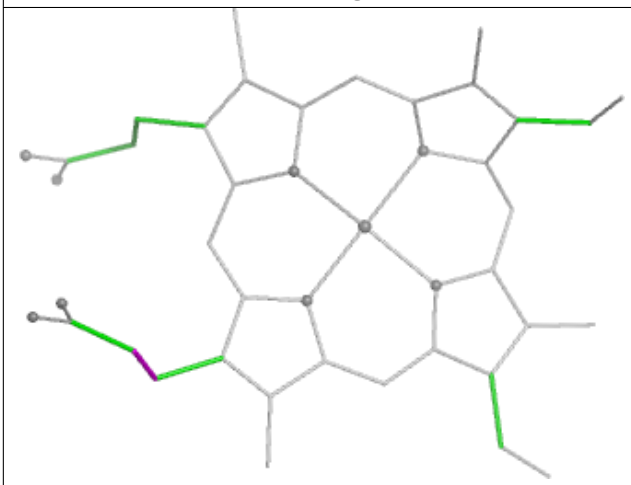
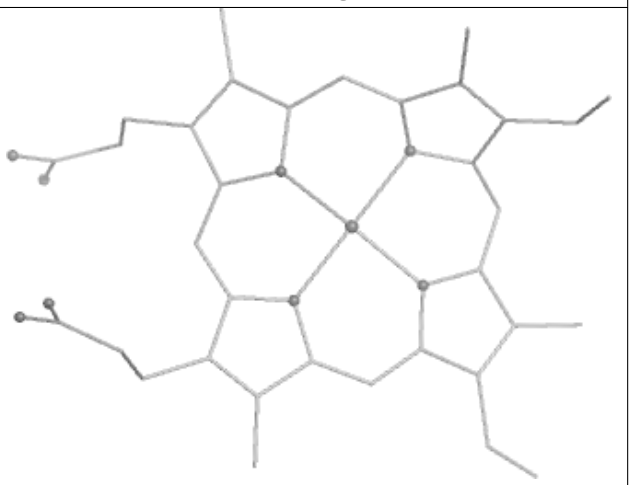
Bond angles

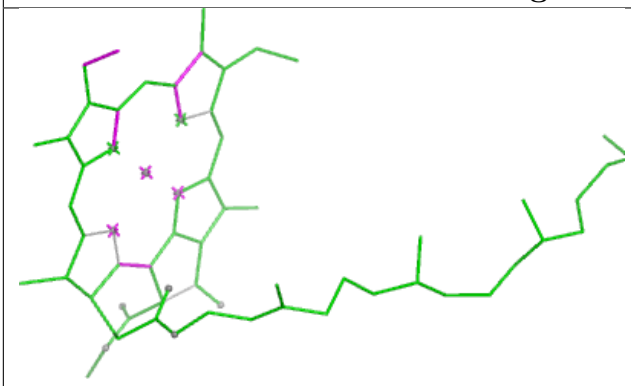
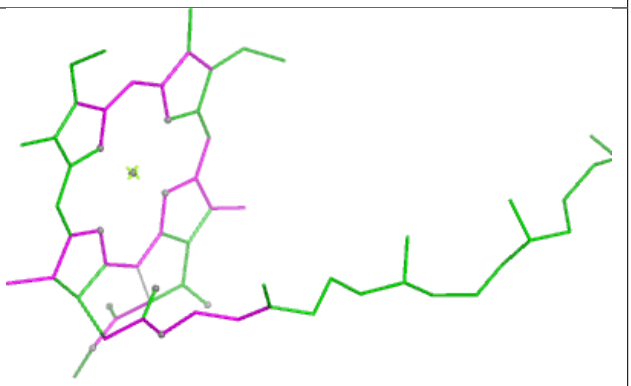
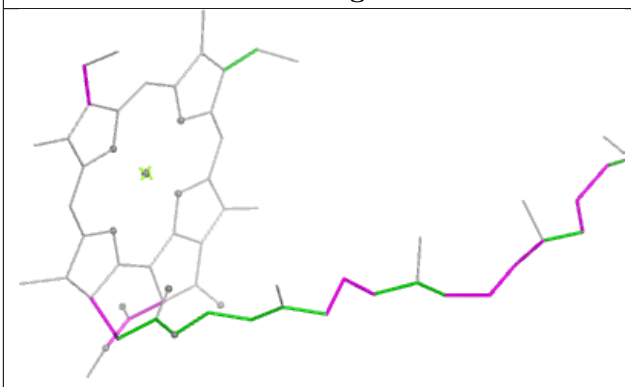
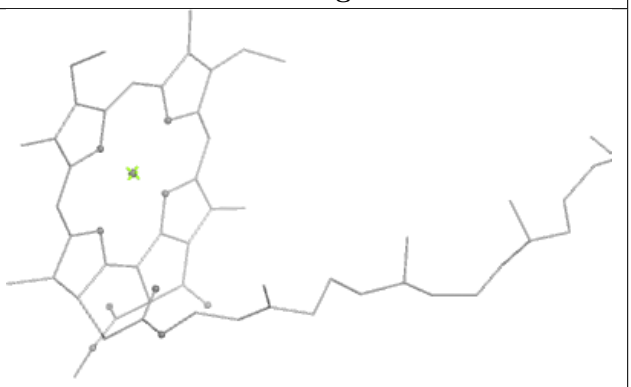


Torsions



Rings

Ligand HEM F1 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

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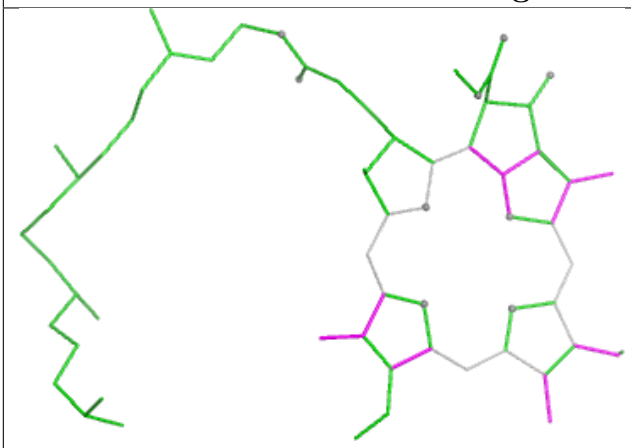
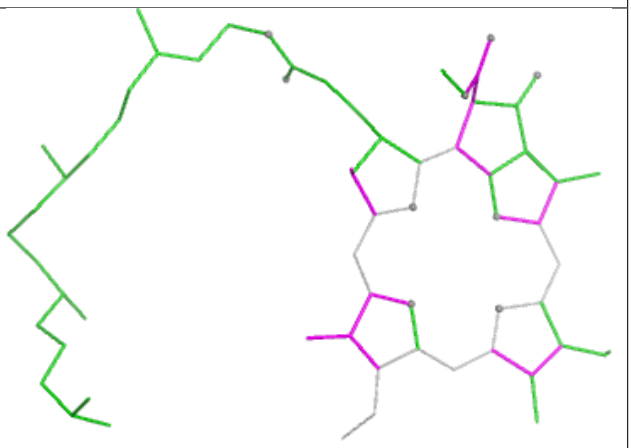
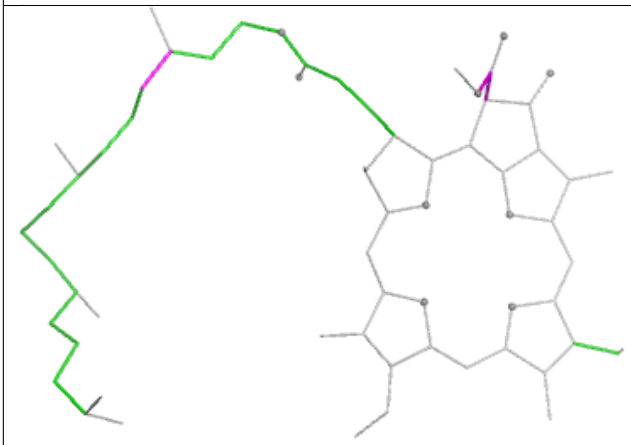
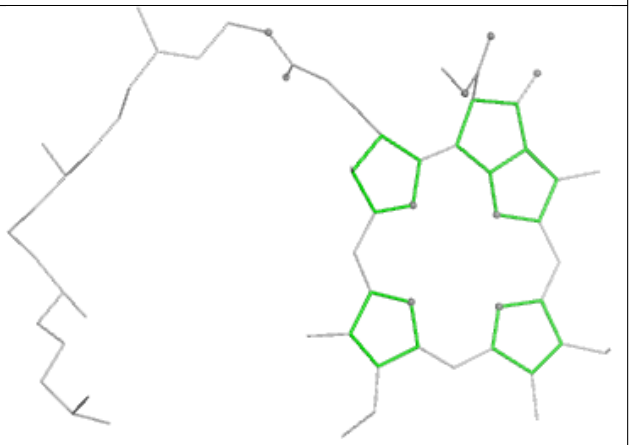
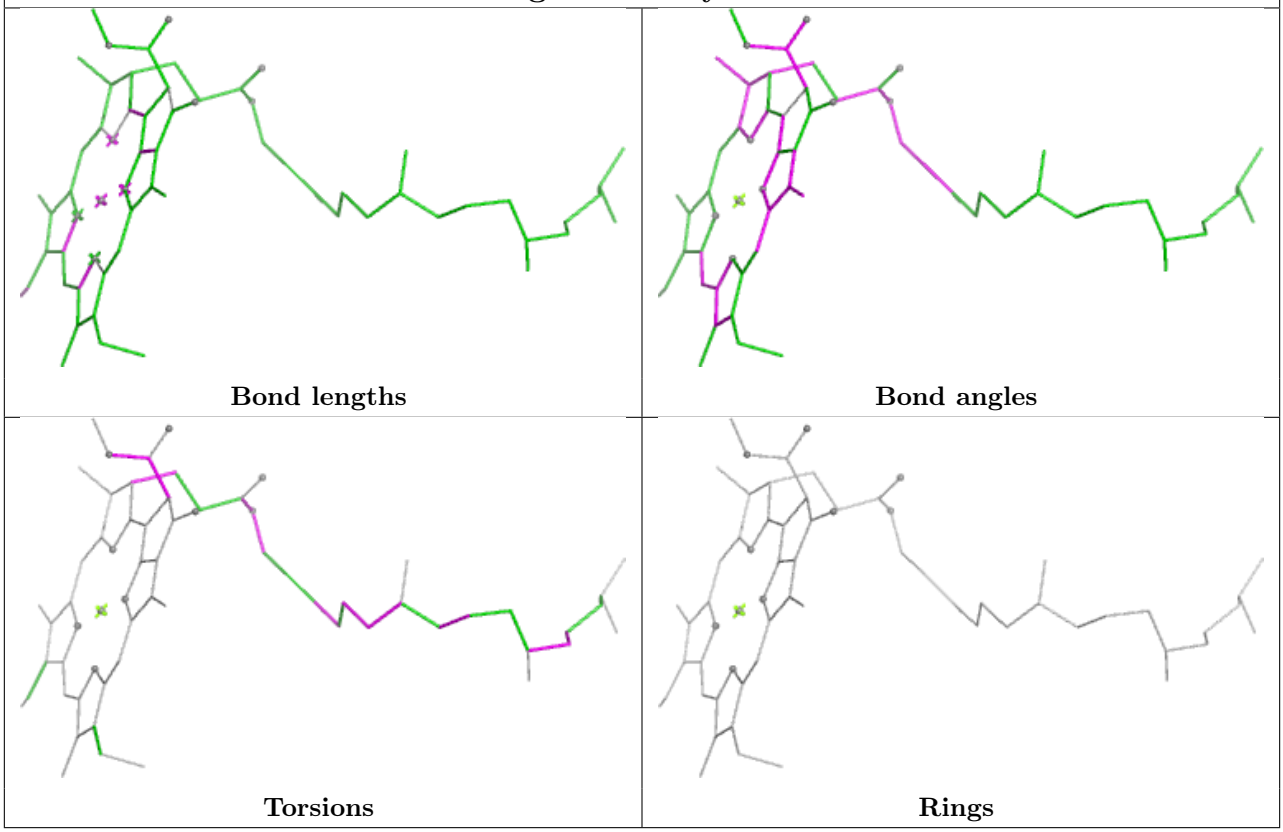
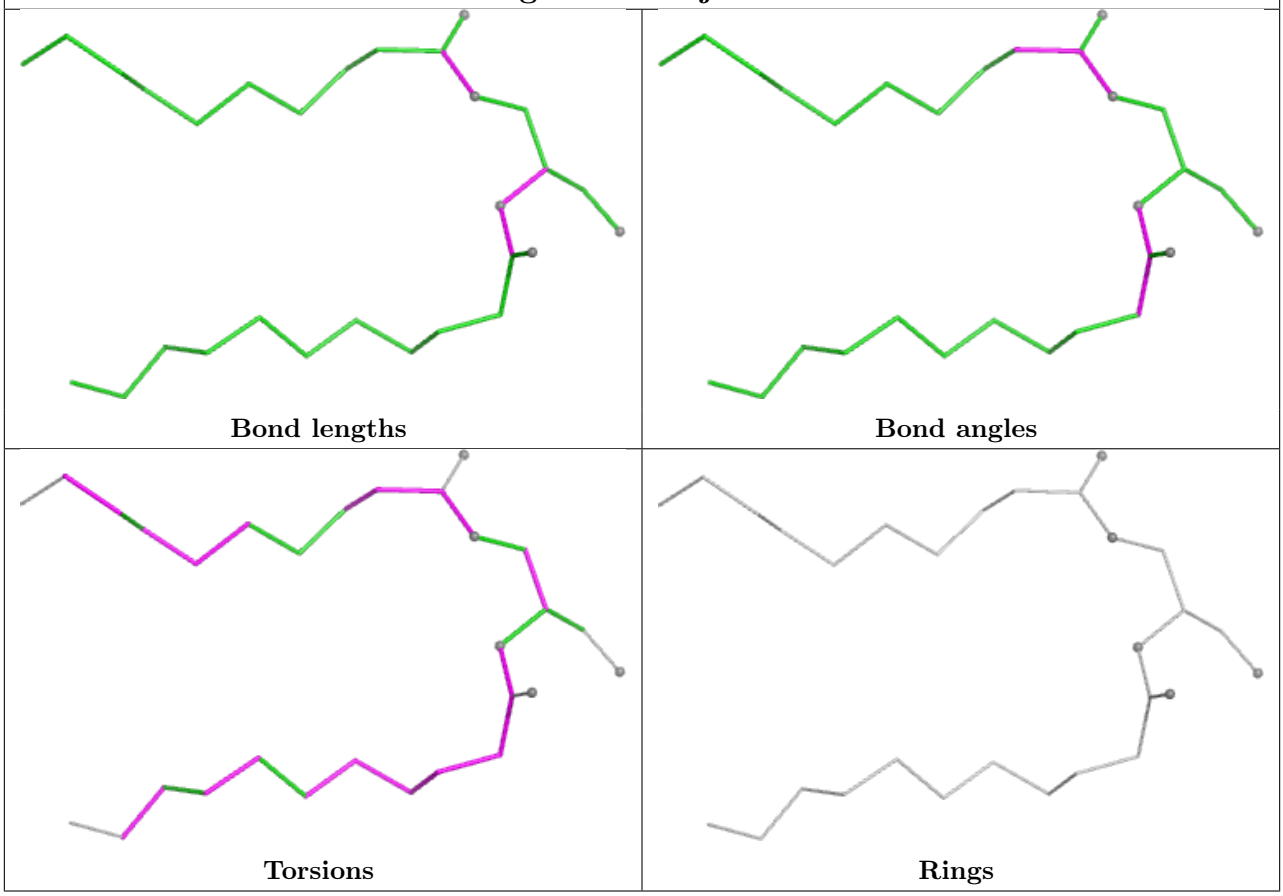
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA y 604



Ligand DGA j1 101



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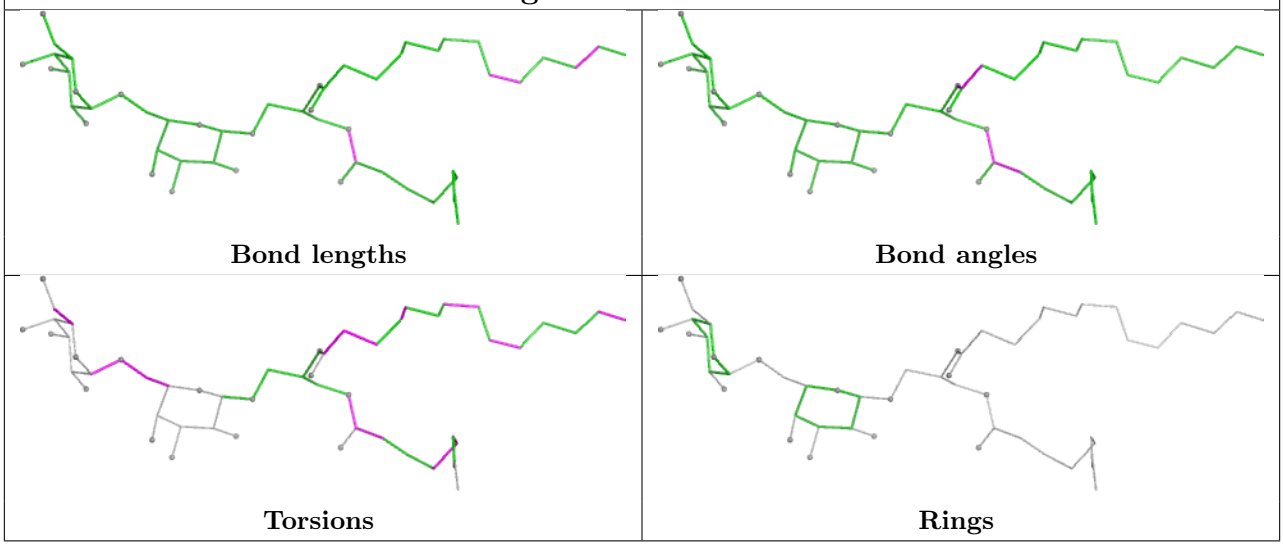
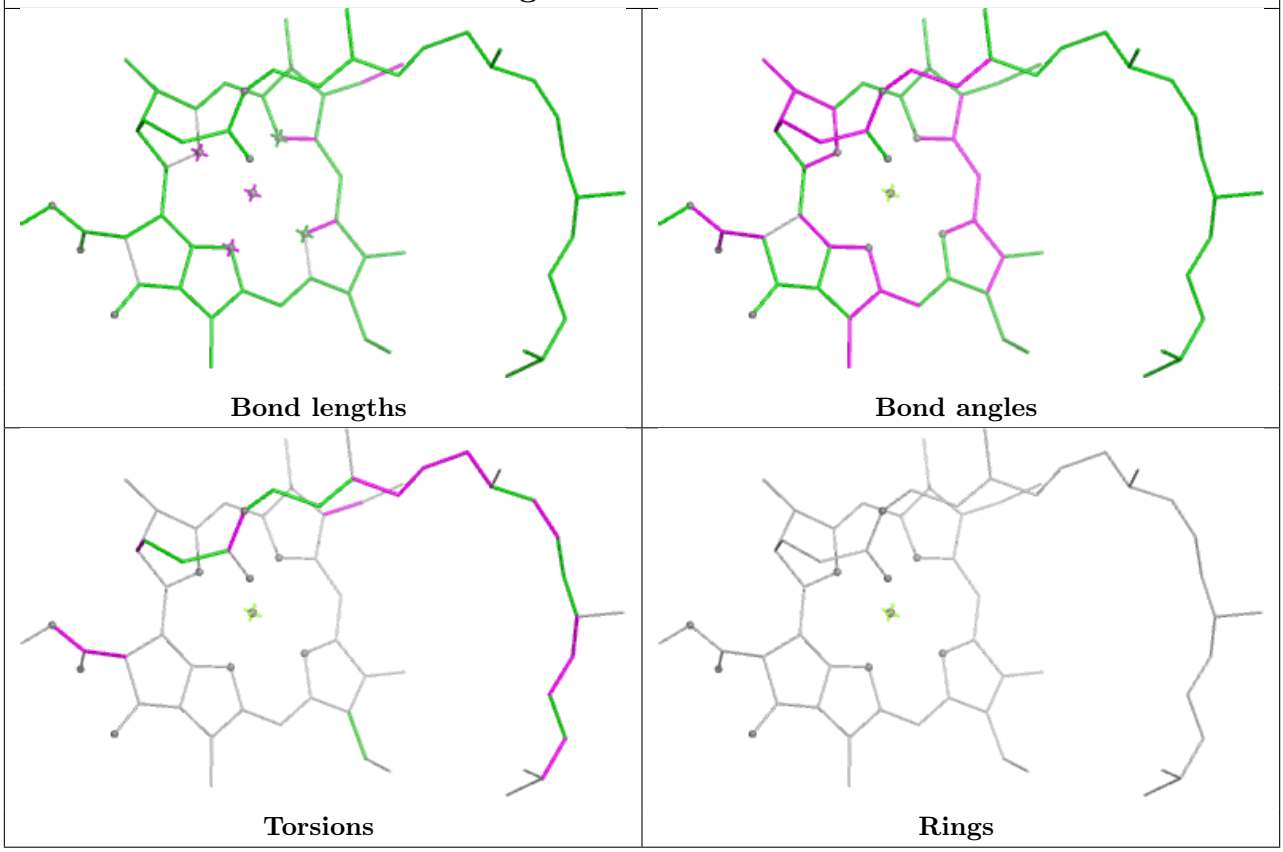


Ligand CLA n1 610



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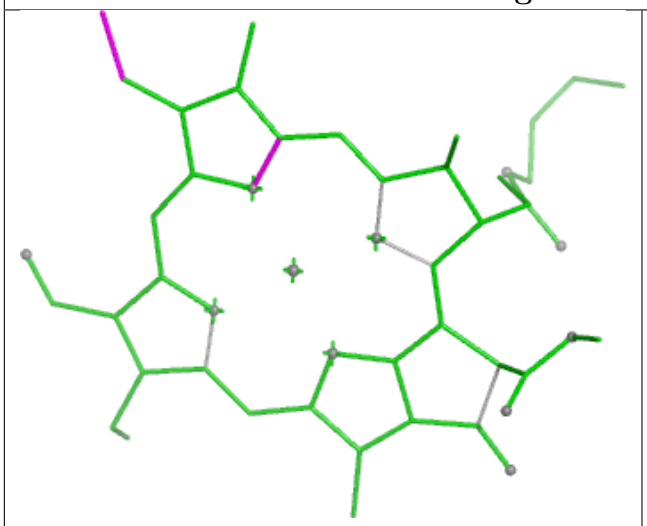
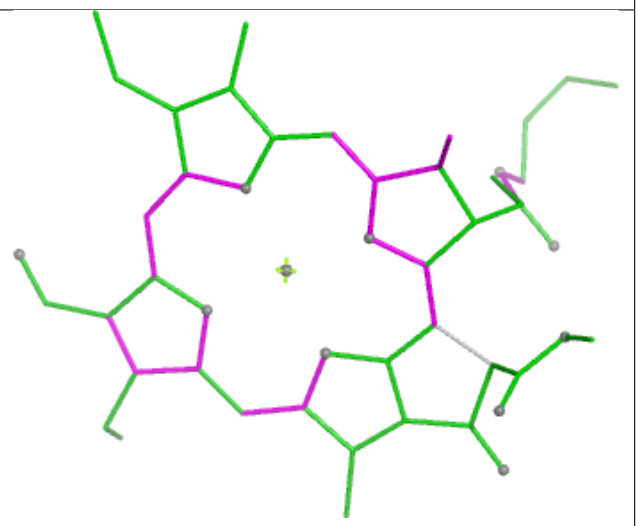
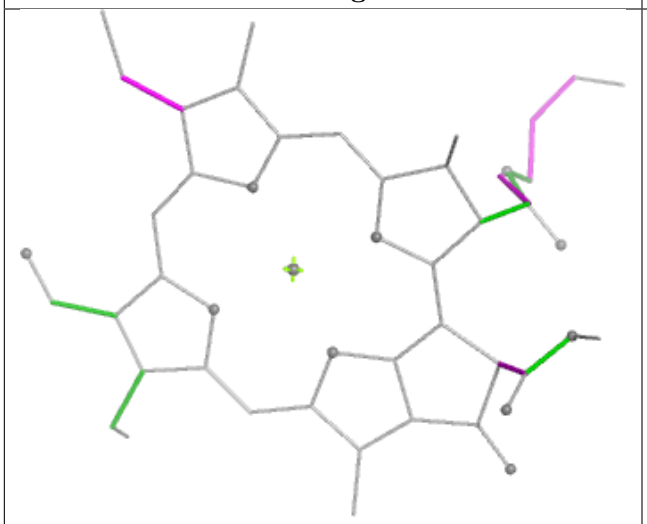


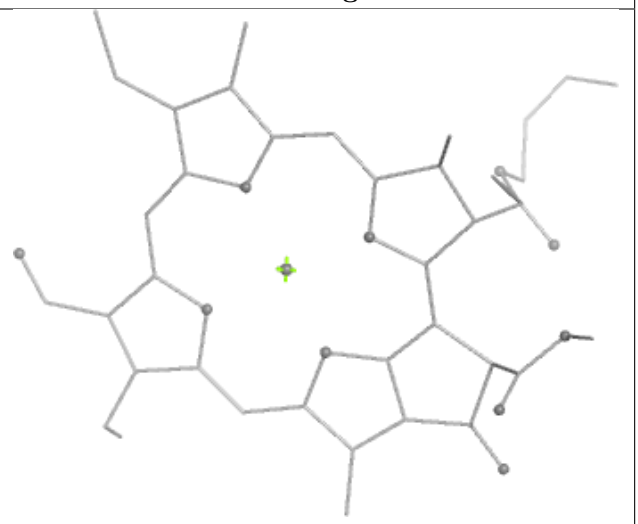
Bond lengths



Bond angles

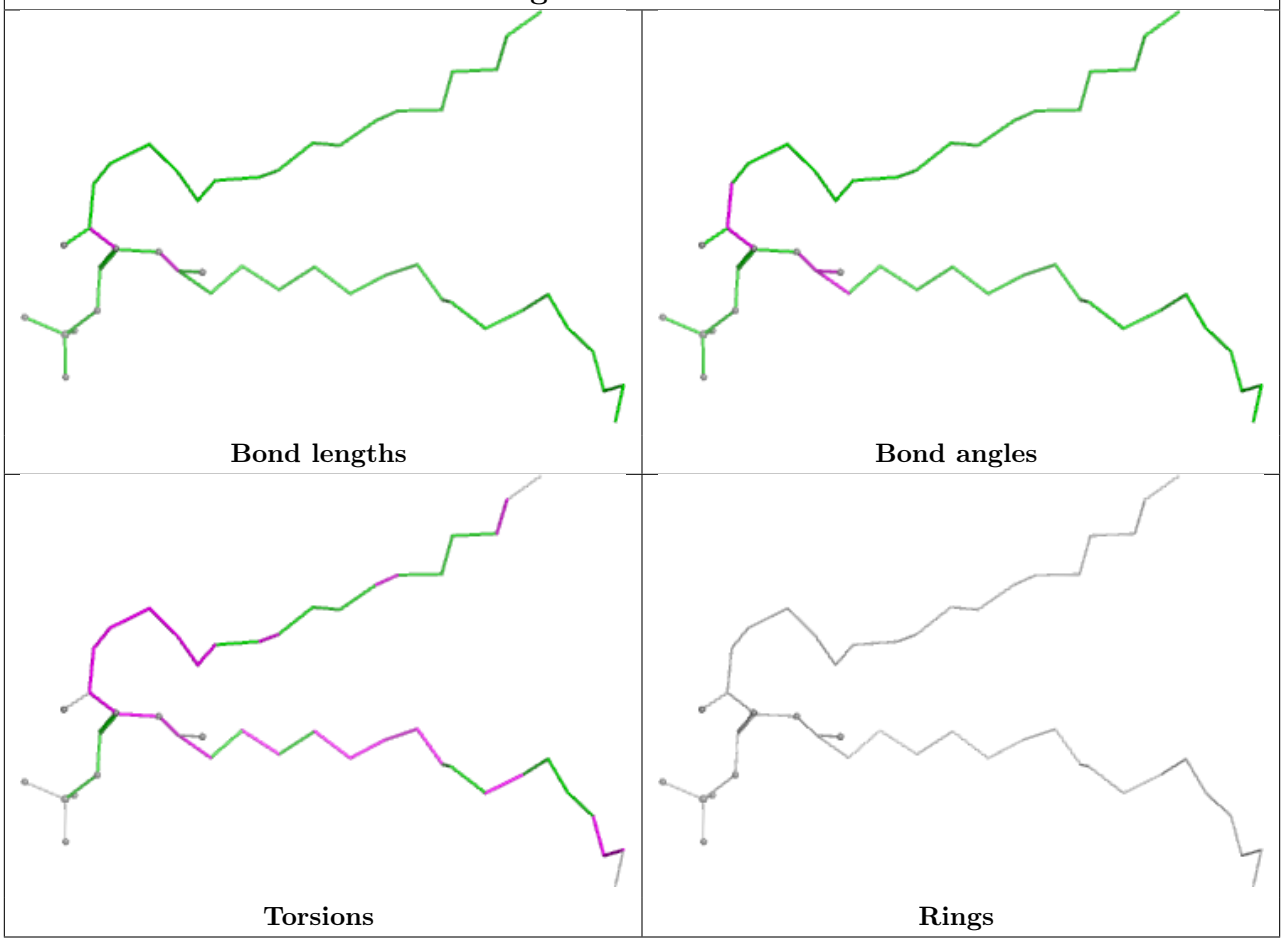


Torsions

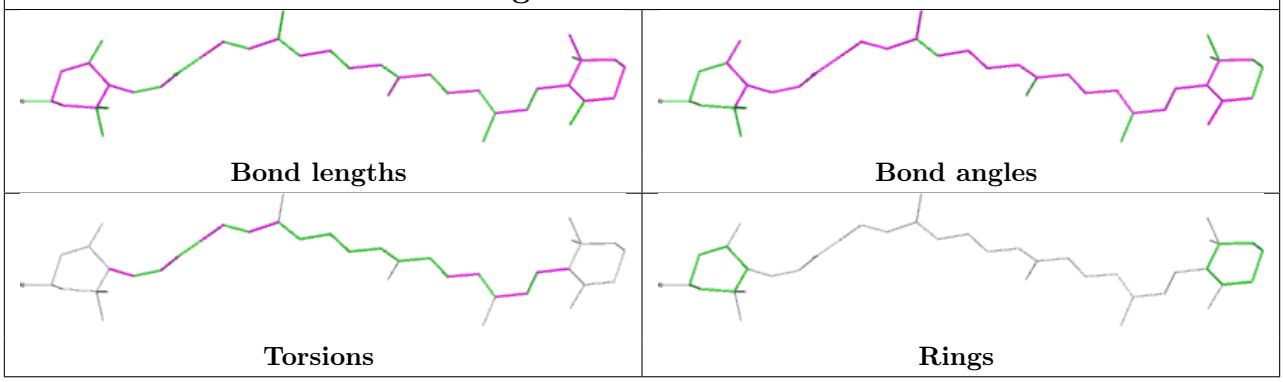


Rings

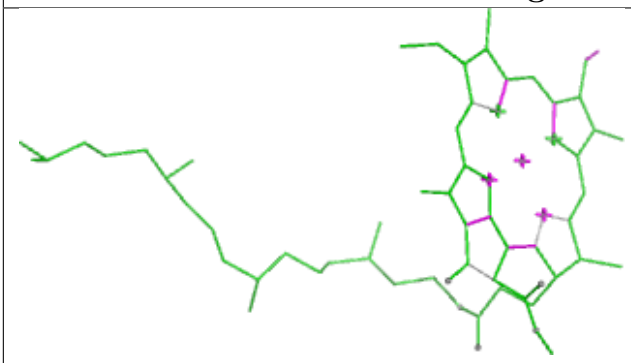
Ligand 3PH S 626



Ligand RRX H1 101



Ligand CLA y 611



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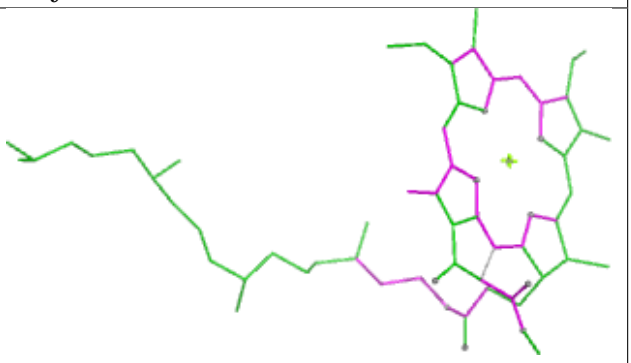

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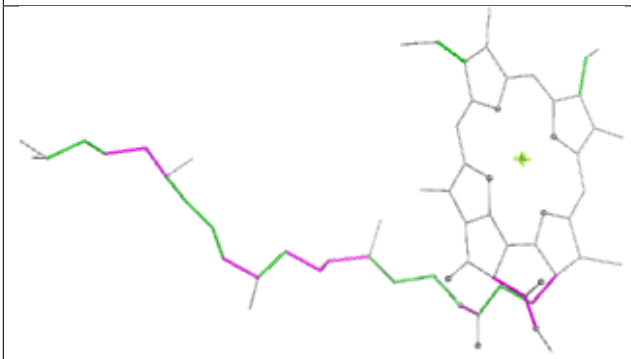

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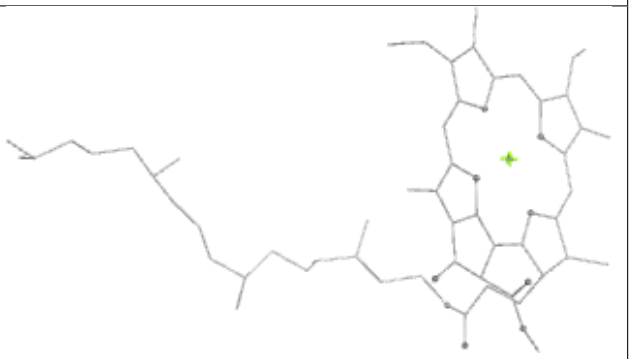
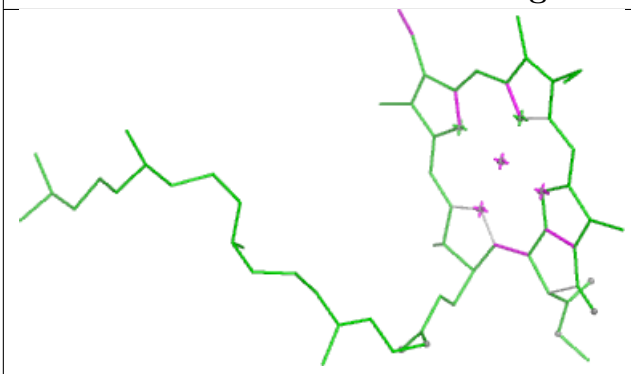


Rings

Ligand CLA c 511



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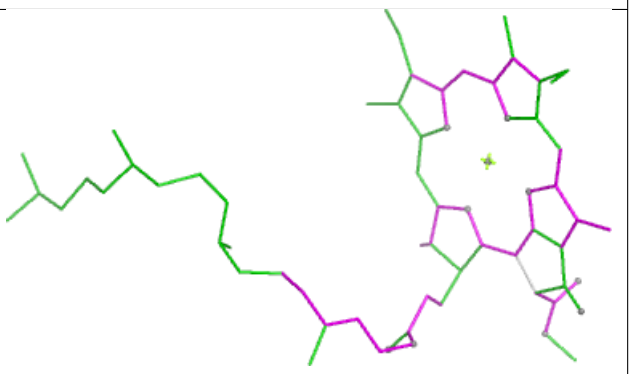
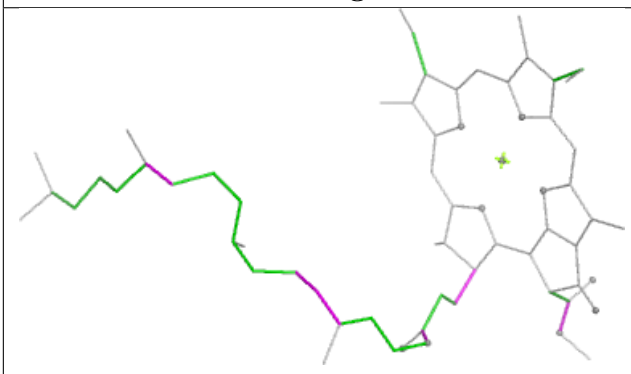


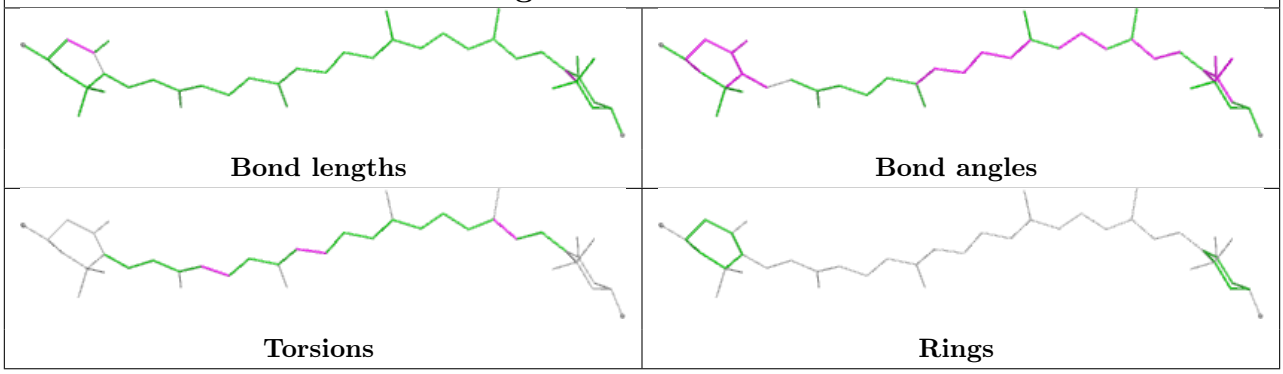
Bond angles



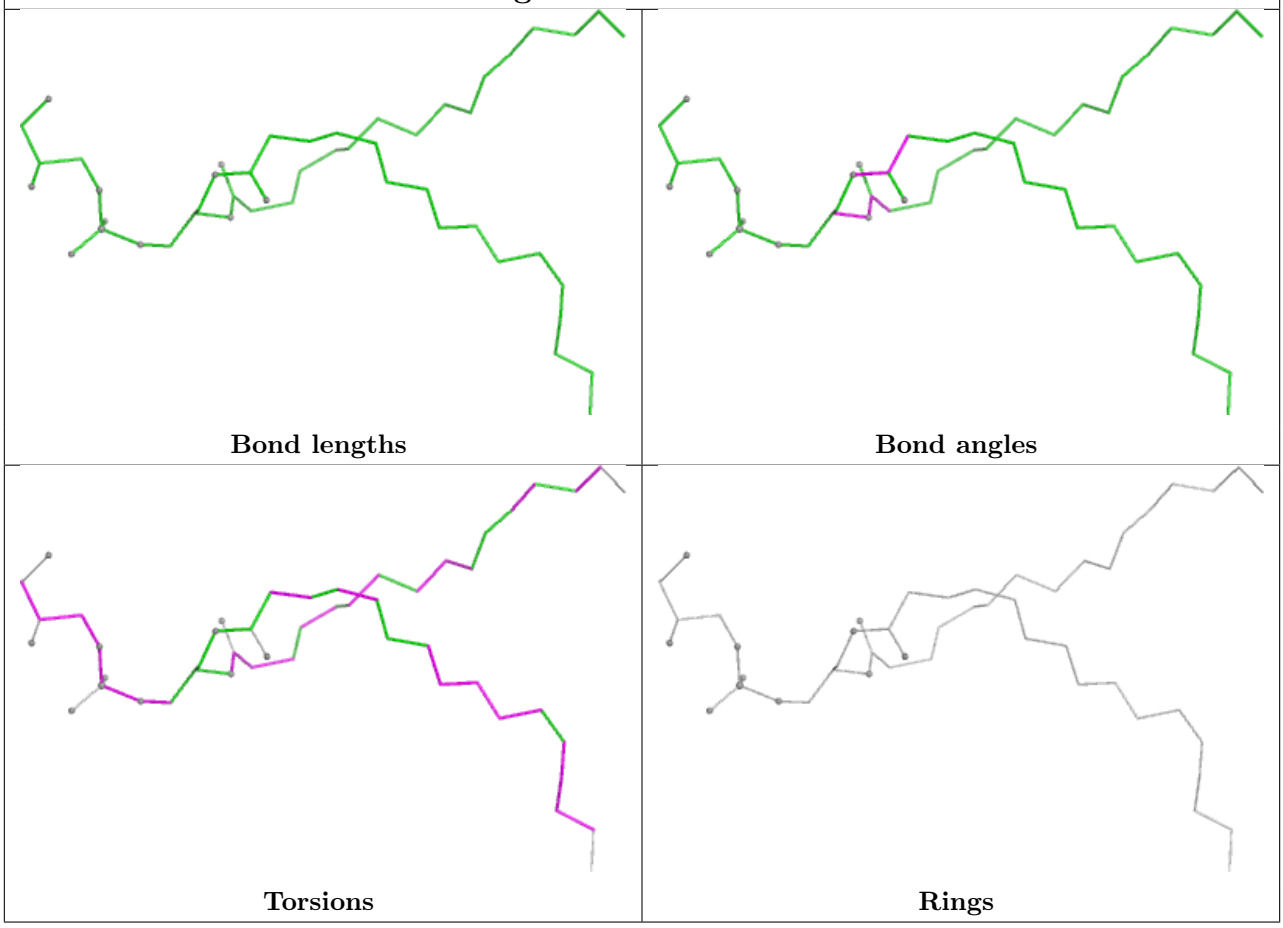
Torsions

Rings

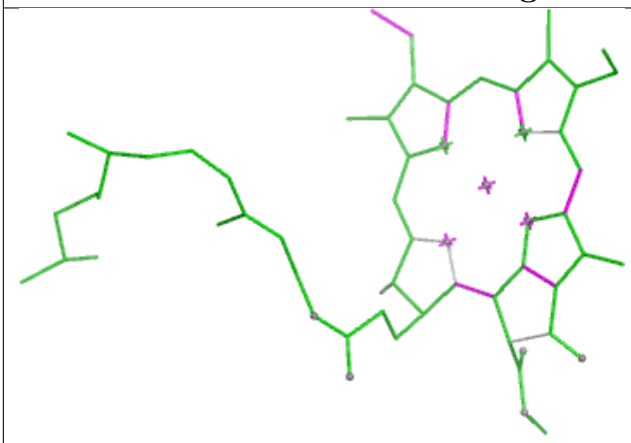
Ligand LUT N1 621



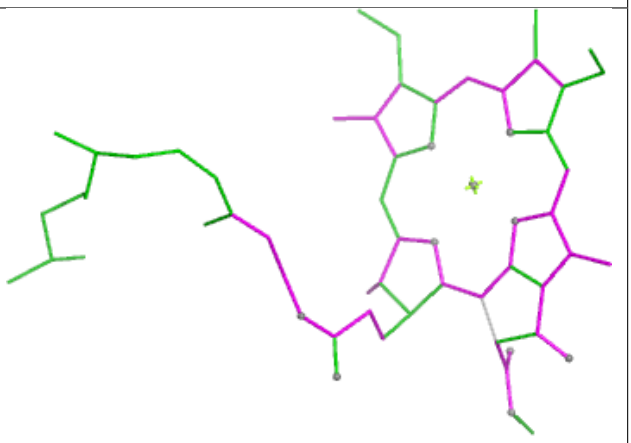
Ligand LHG D1 409



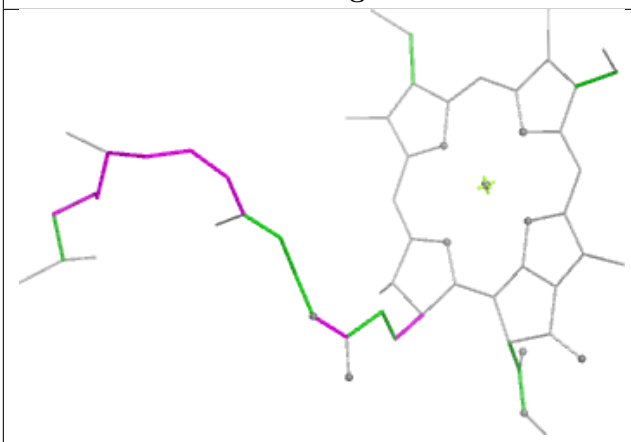
Ligand CLA a1 410



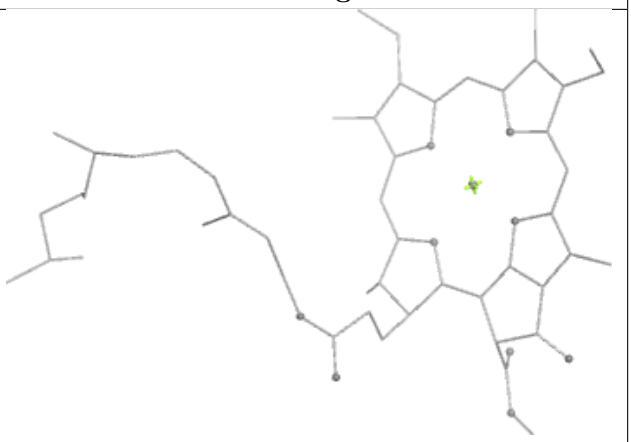
Bond lengths



Bond angles

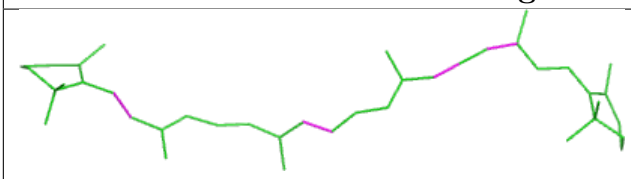


Torsions



Rings

Ligand BCR c1 516



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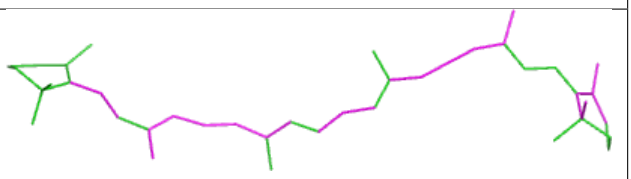
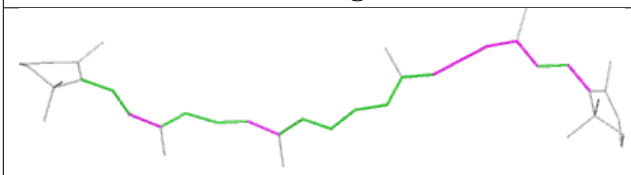
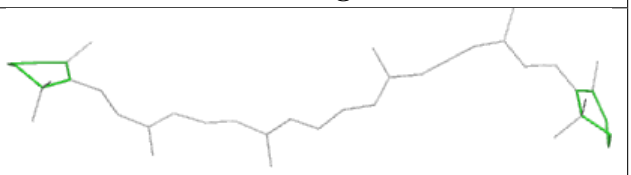


Bond angles

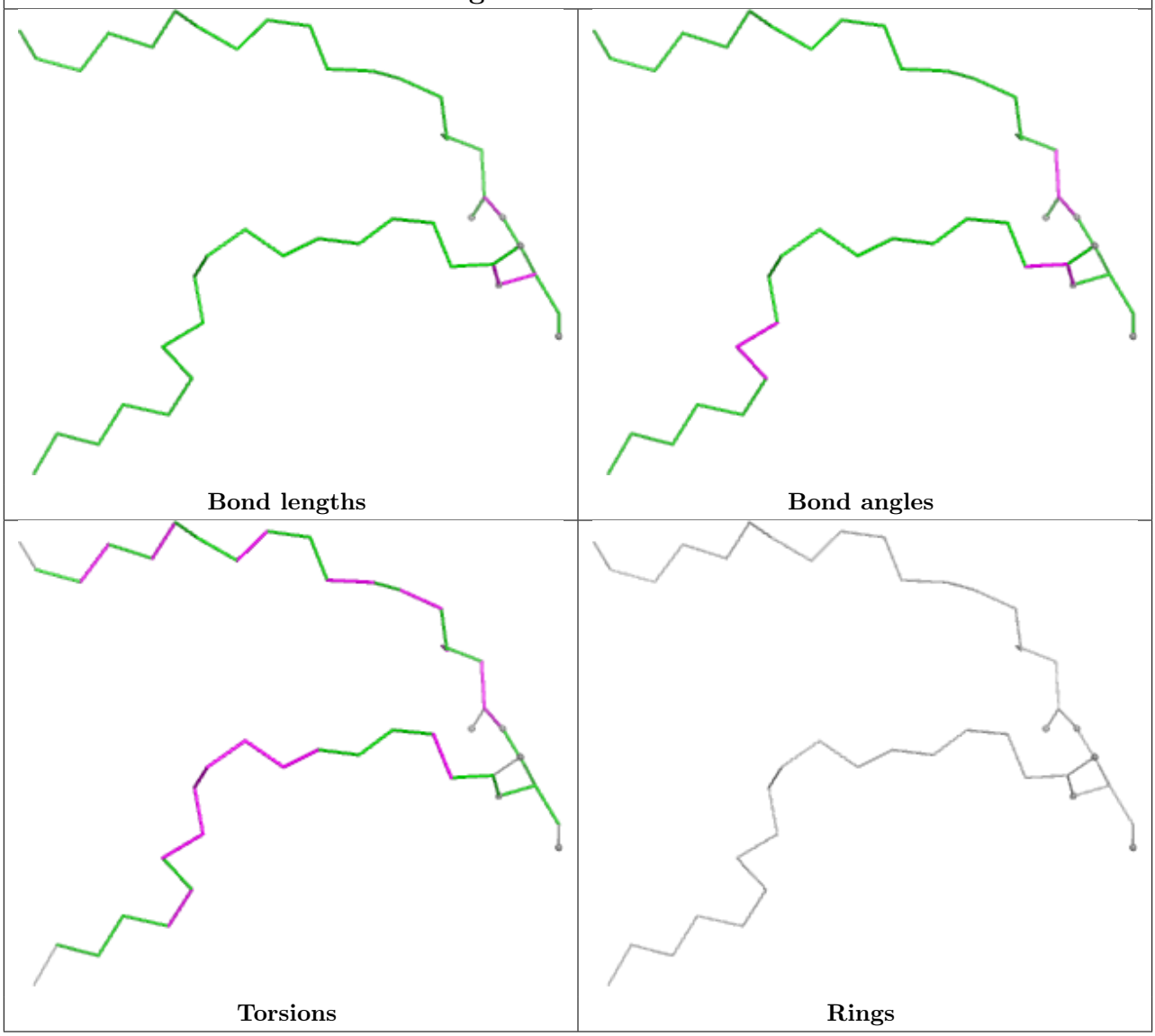


Torsions

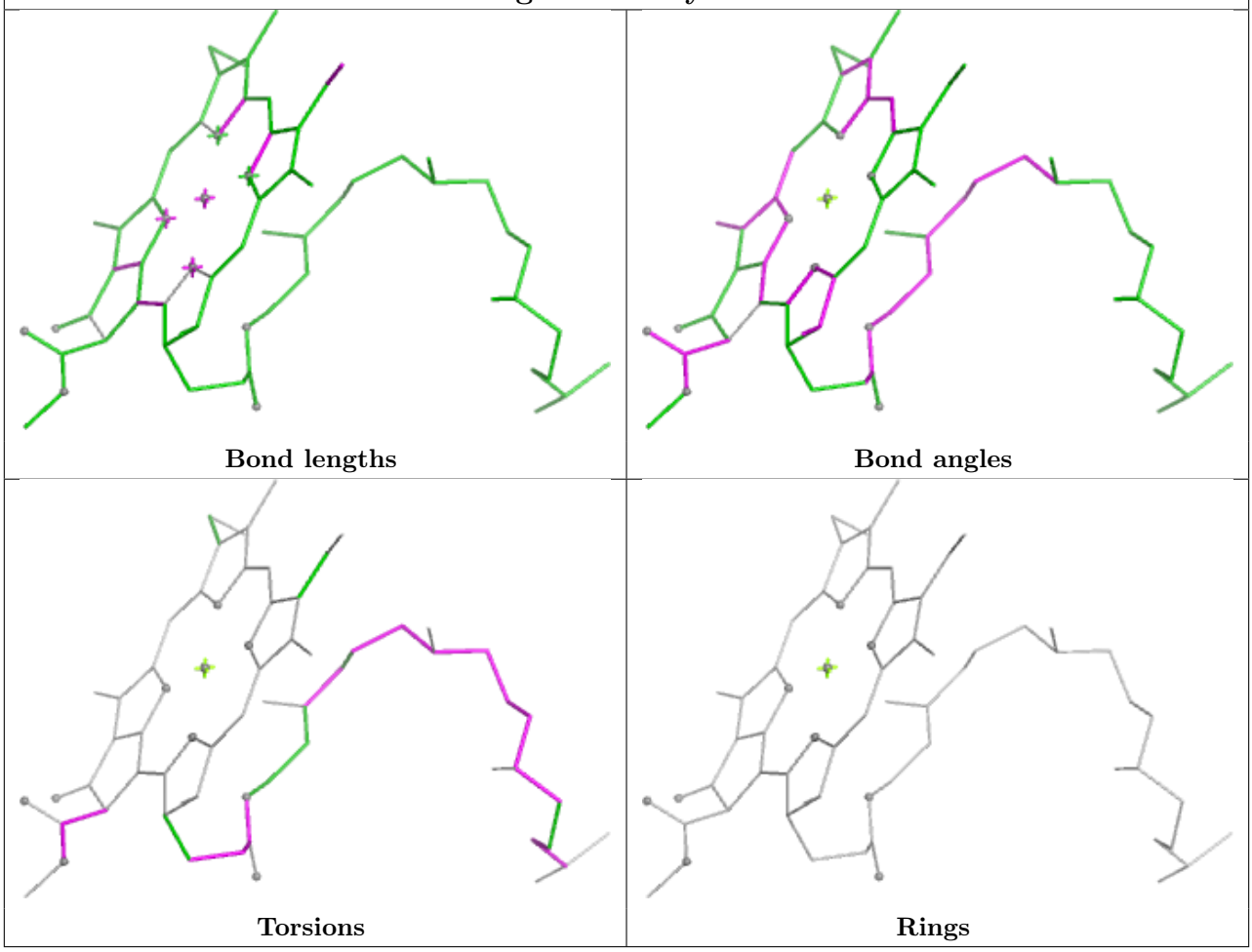


Rings

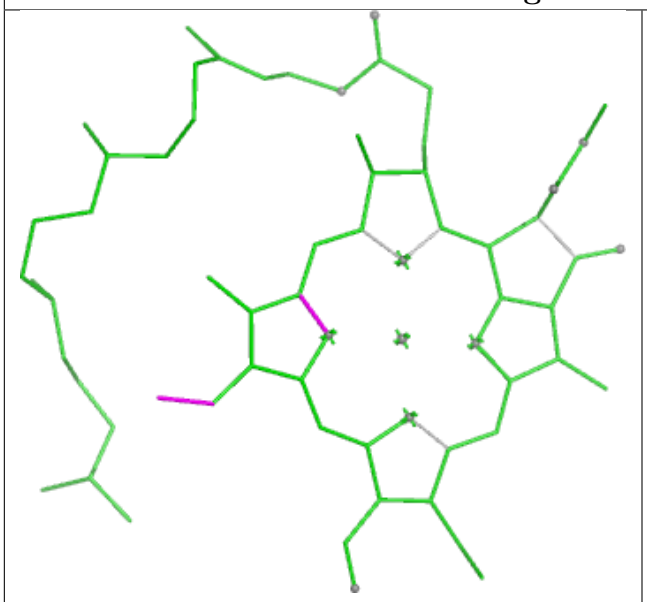
Ligand DGA C 524



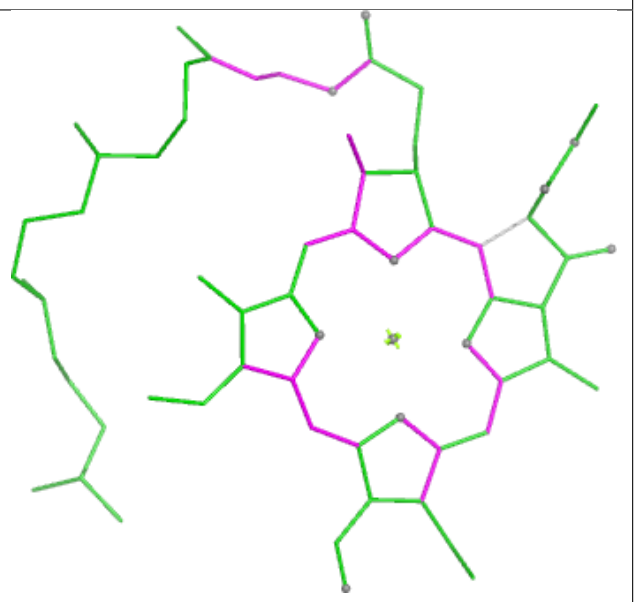
Ligand CLA y 613



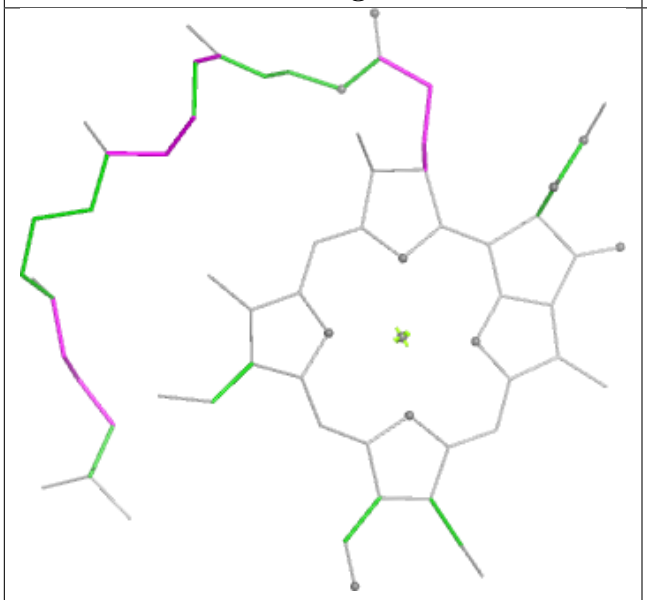
Ligand CHL G 607



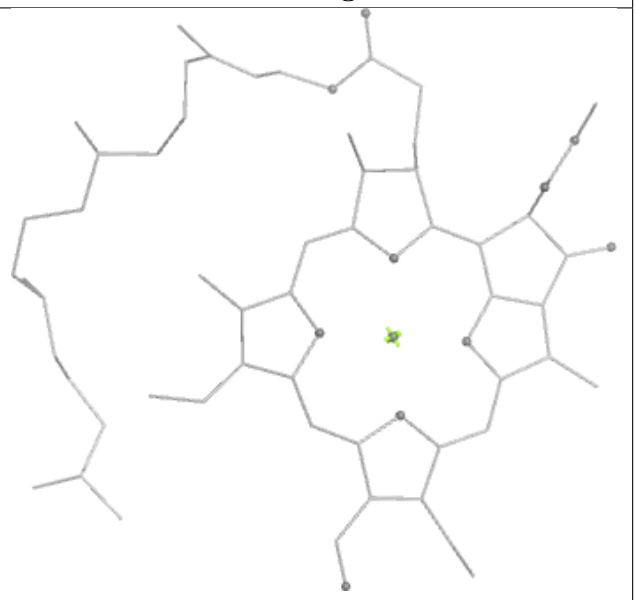
Bond lengths



Bond angles

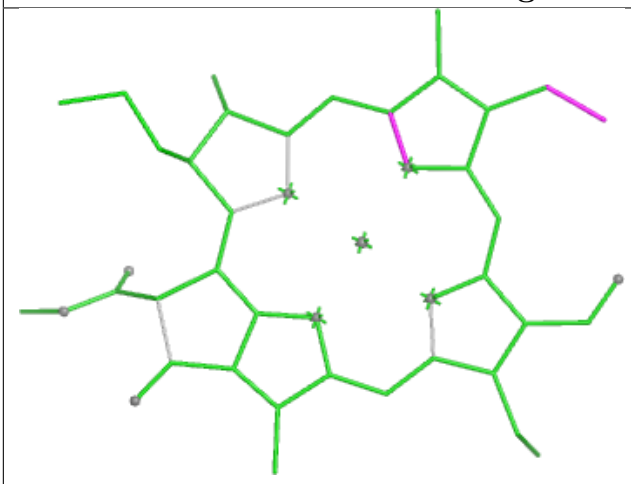


Torsions

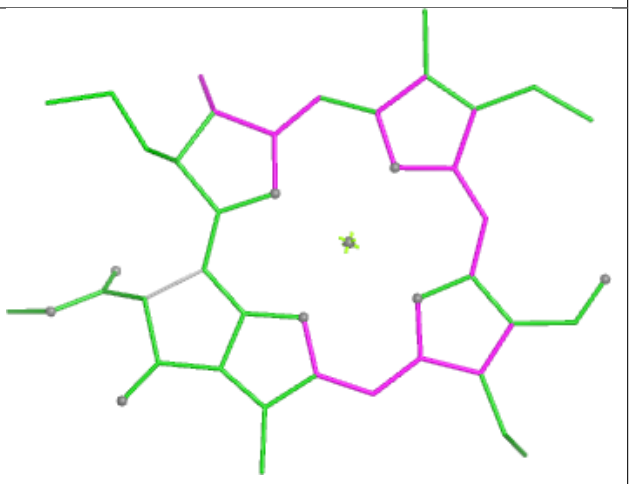


Rings

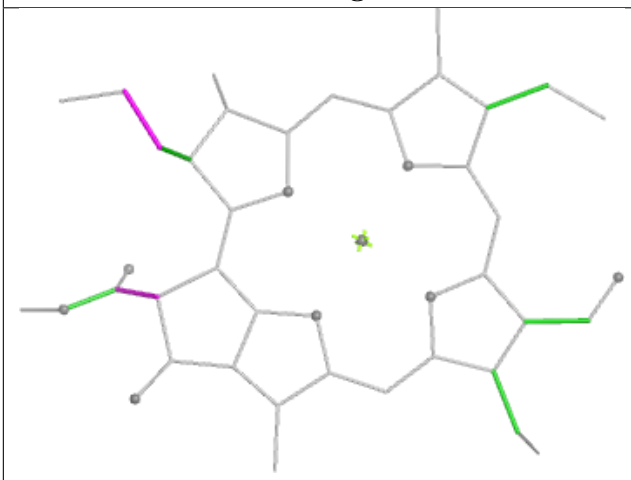
Ligand CHL S1 606



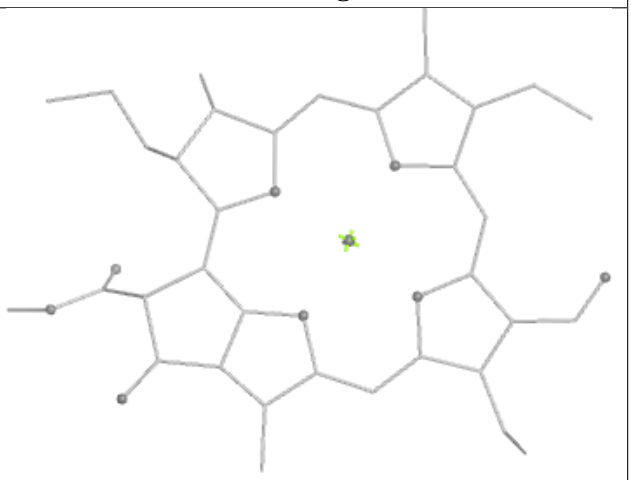
Bond lengths



Bond angles

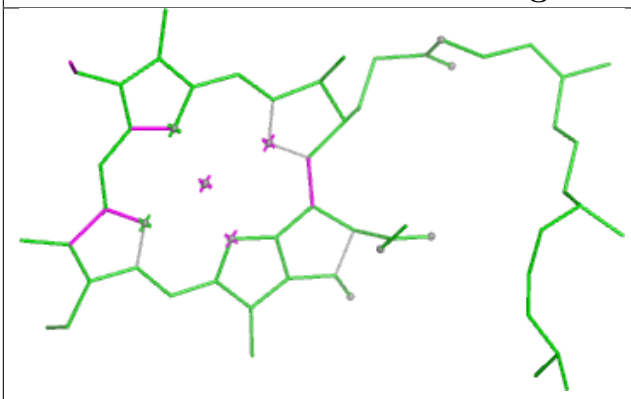


Torsions



Rings

Ligand CLA r 612



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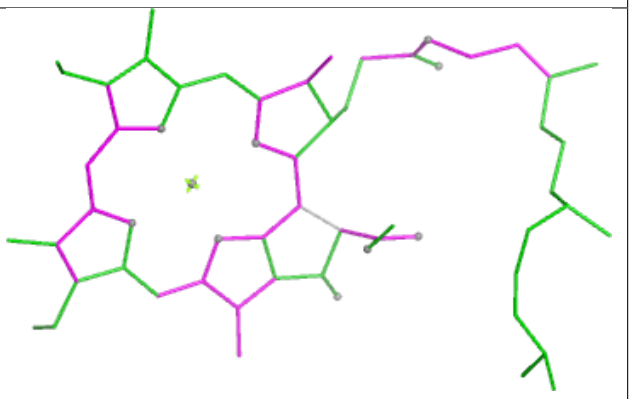
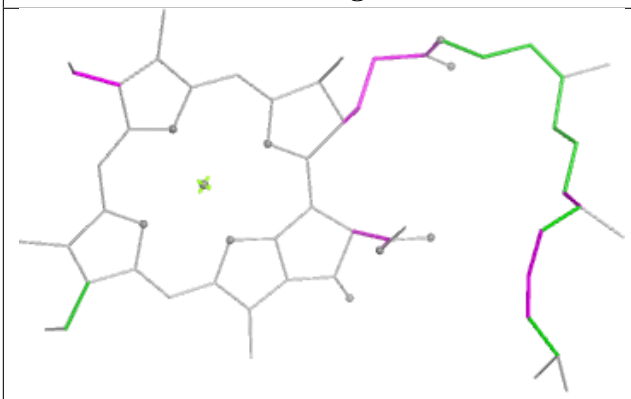


Bond angles



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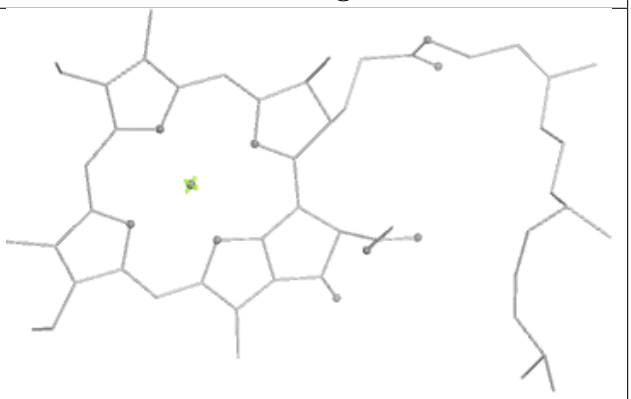
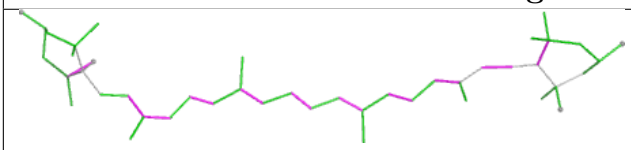


Rings

Ligand NEX g 623



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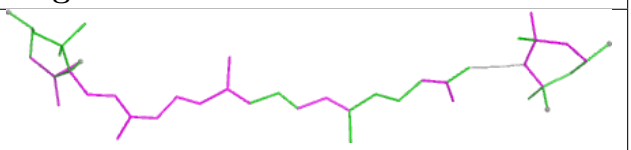

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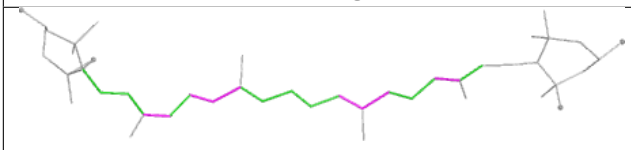

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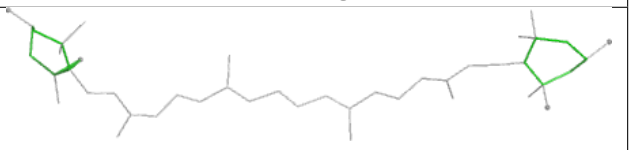
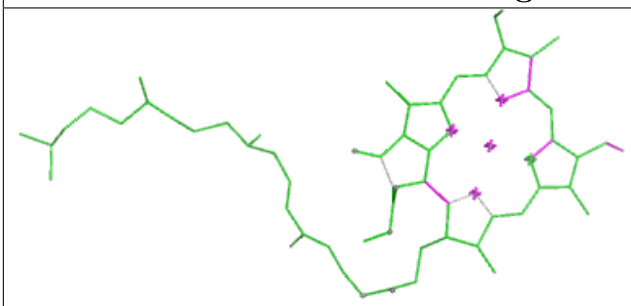
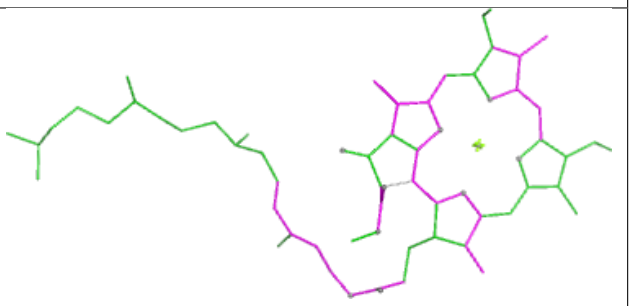
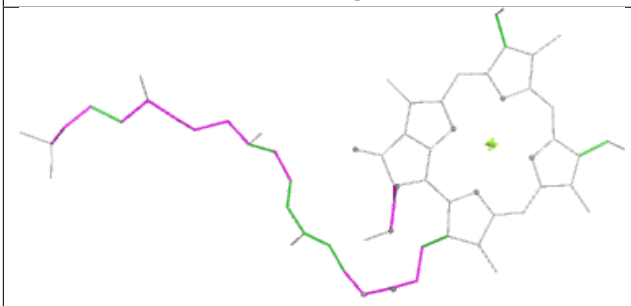
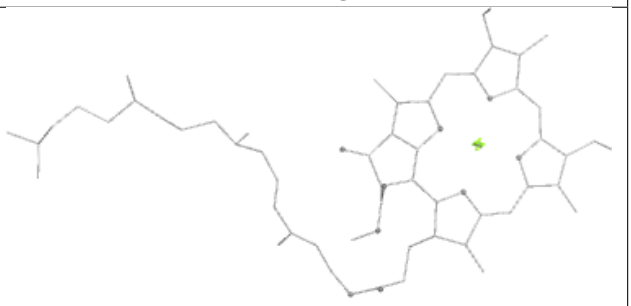


Rings

Ligand CLA B1 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

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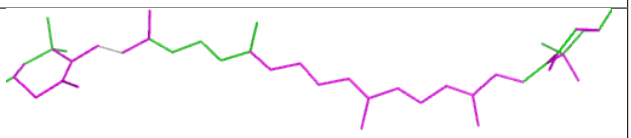
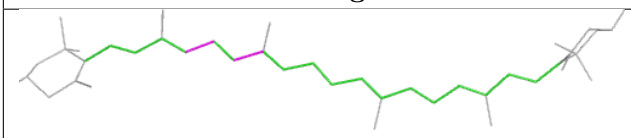
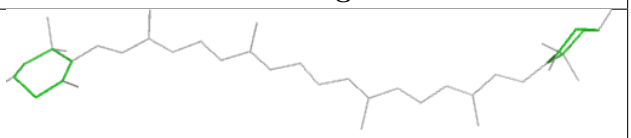
Bond lengths	 Bond angles
 Torsions	 Rings

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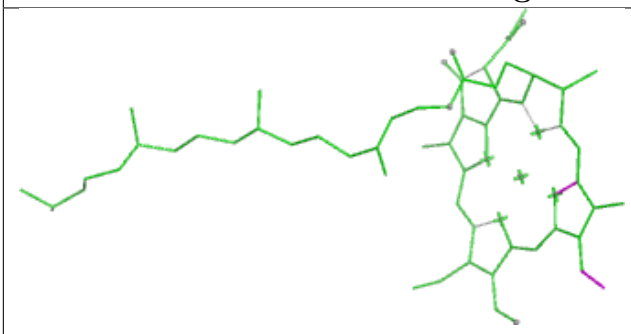
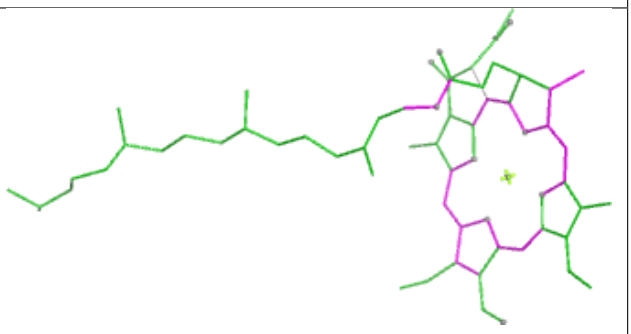
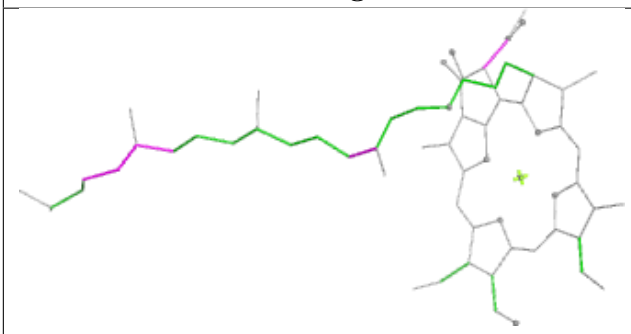
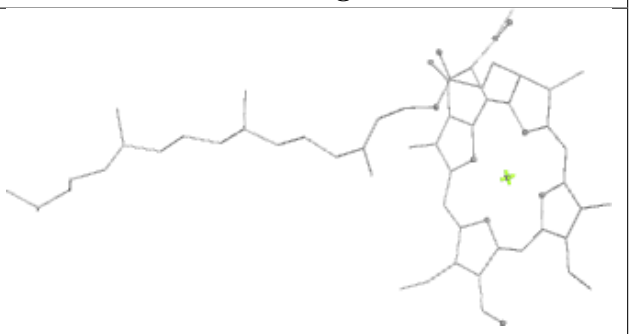
 Bond lengths	 Bond angles
 Torsions	 Rings

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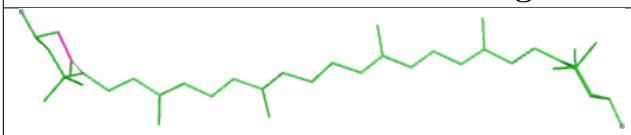
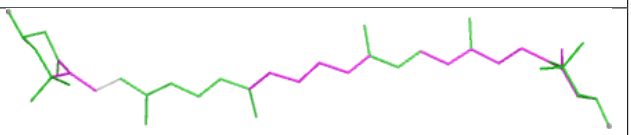
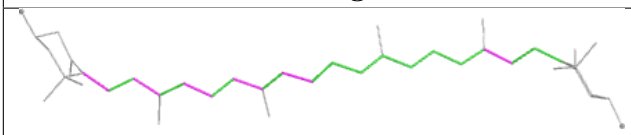
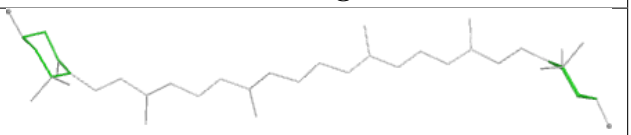
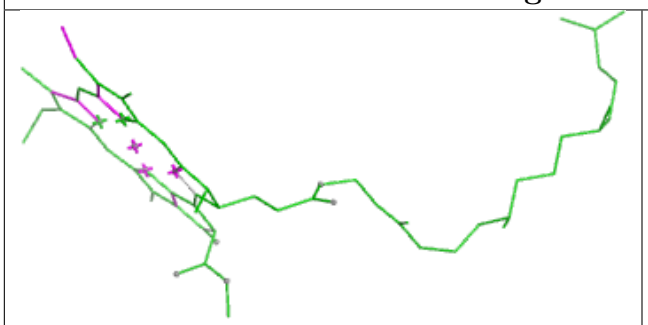
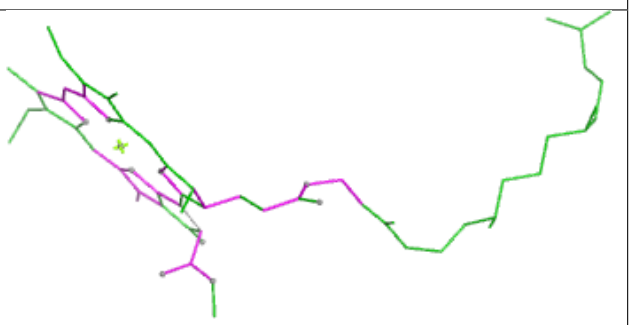
 Bond lengths	 Bond angles
 Torsions	 Rings

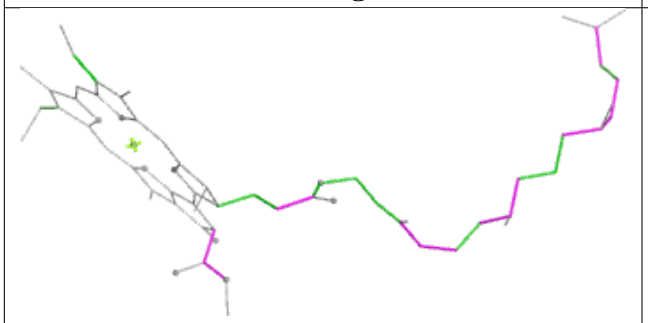
Ligand CLA D 402



Bond lengths



Bond angles



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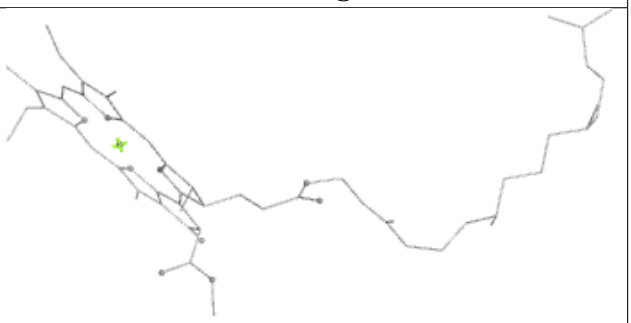
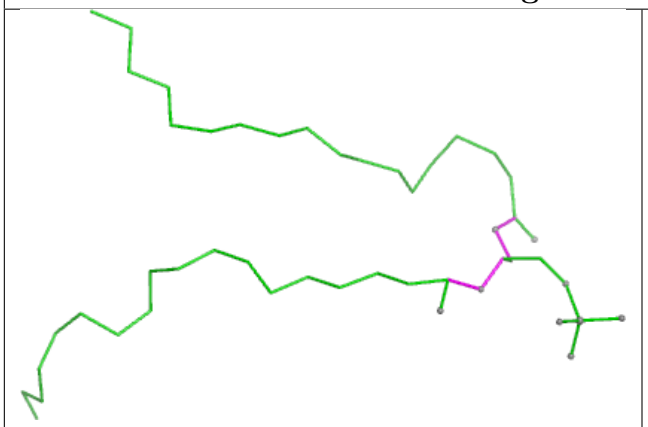
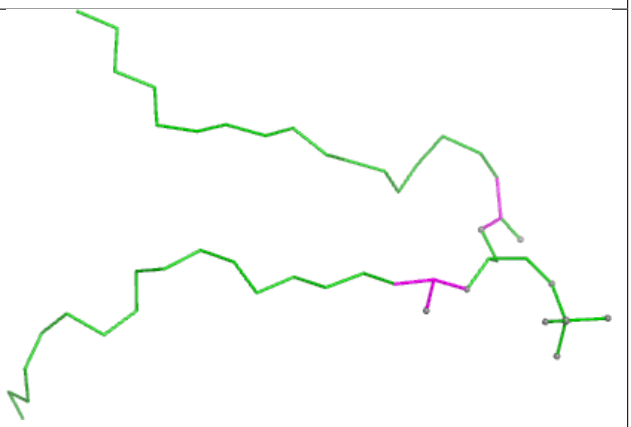


Rings

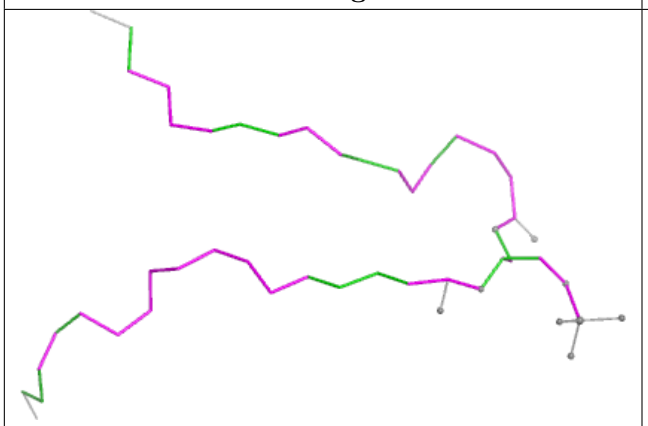
Ligand 3PH S1 626



Bond lengths



Bond angles



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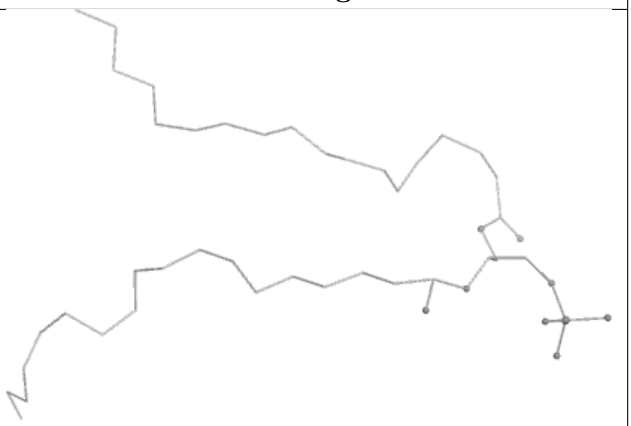
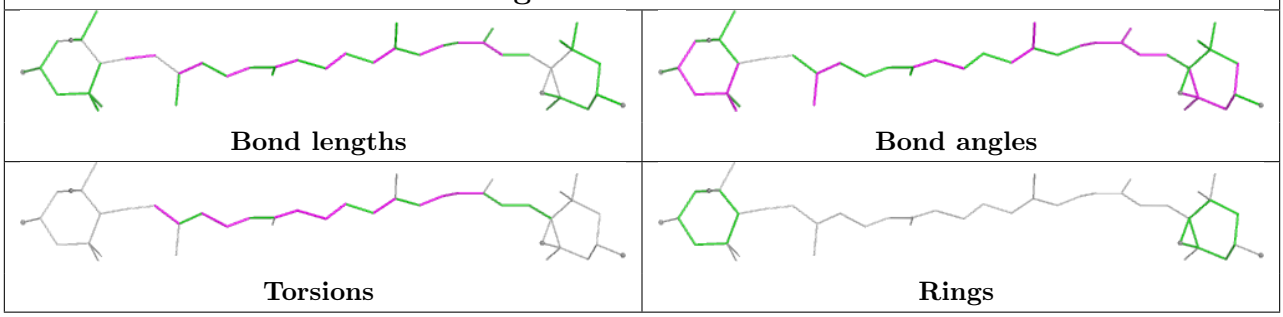
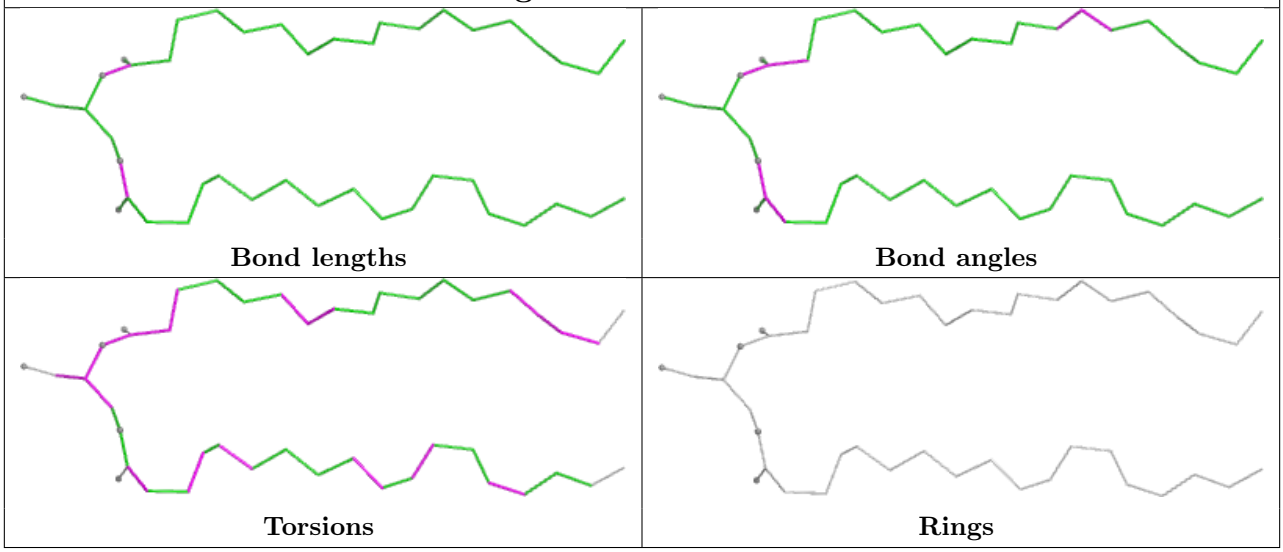


Rings

Ligand NEX R1 622



Ligand DGA b1 625



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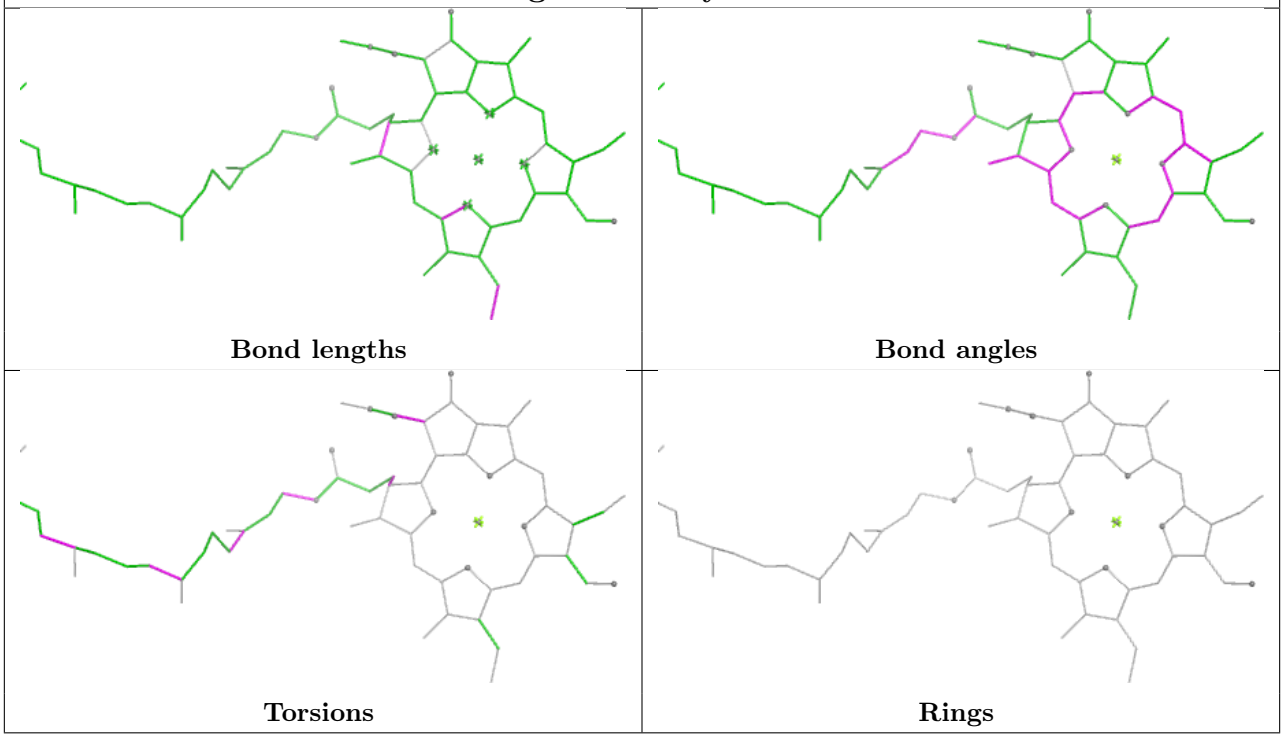
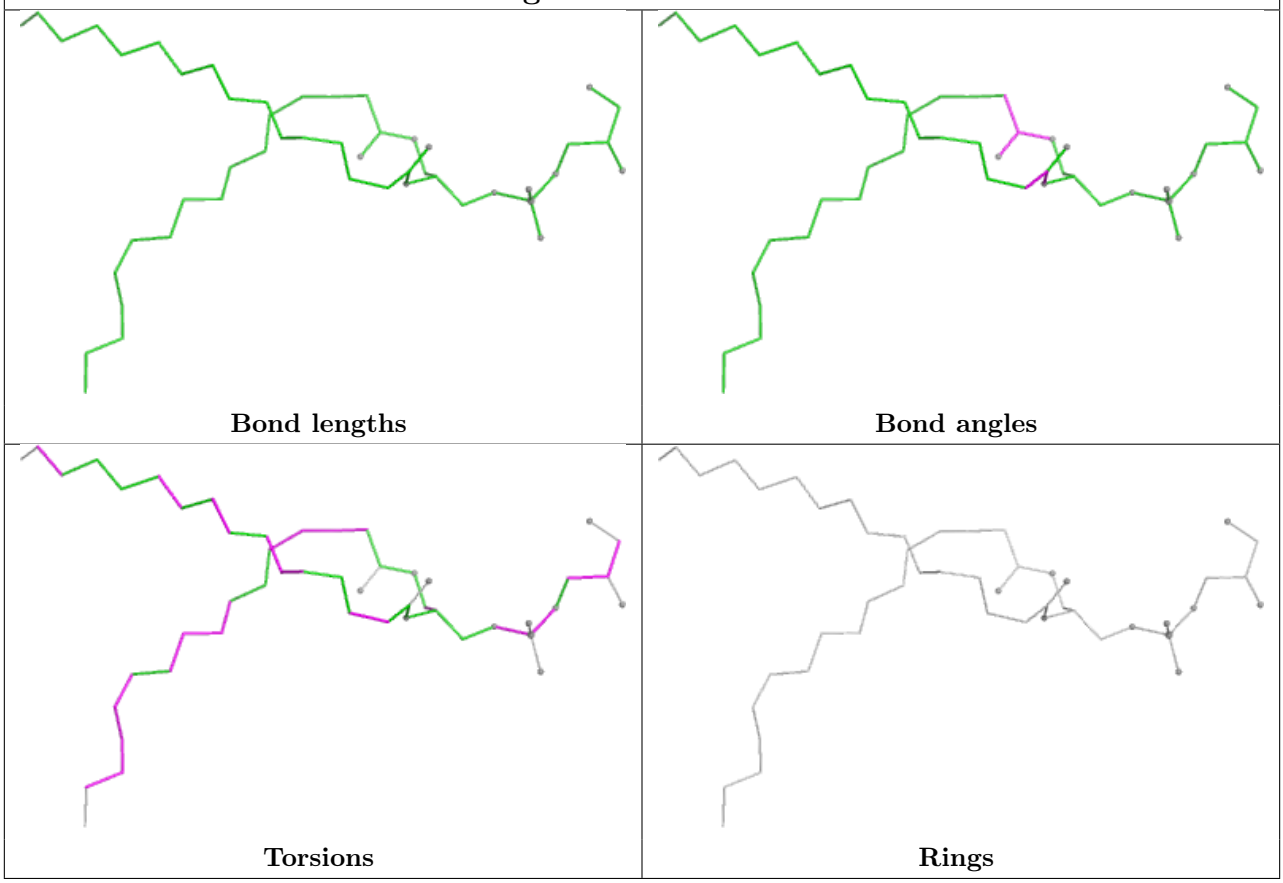
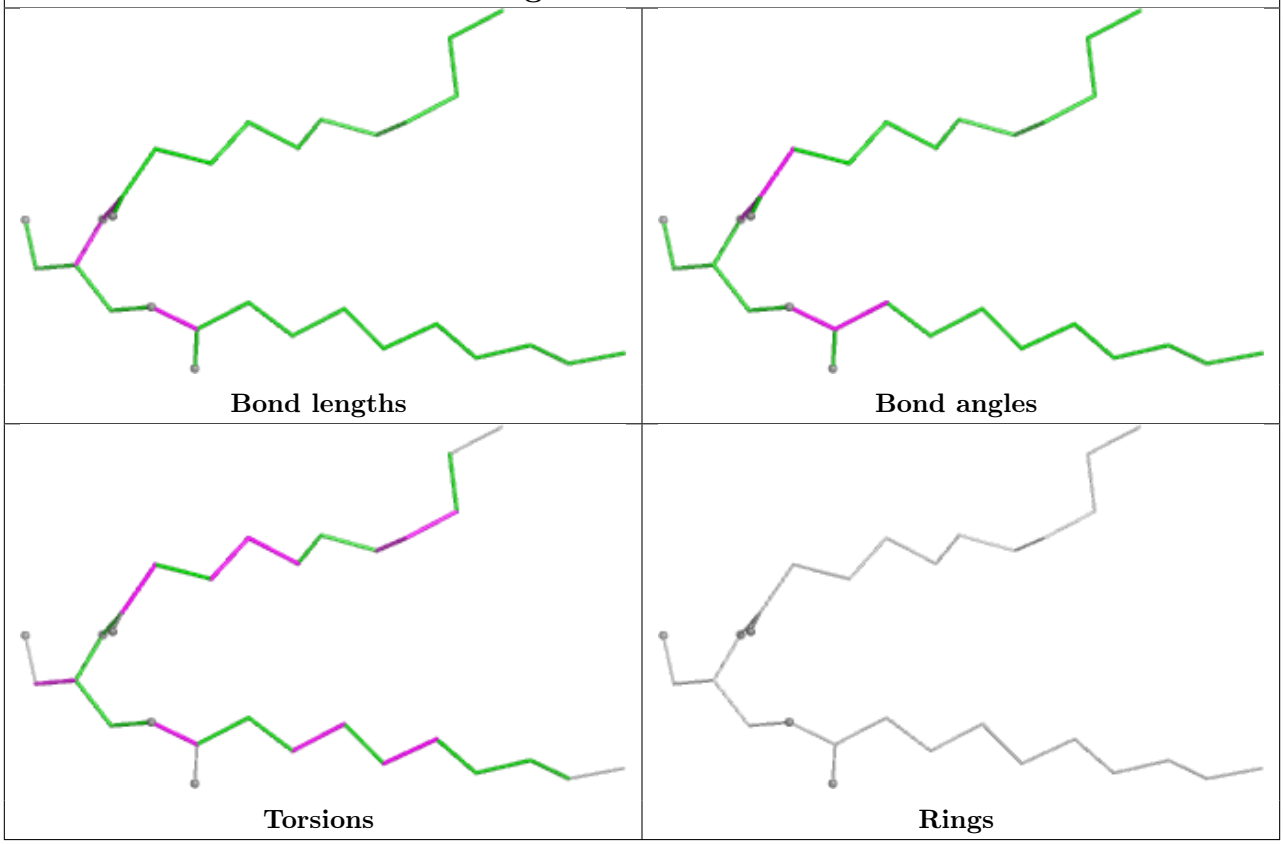


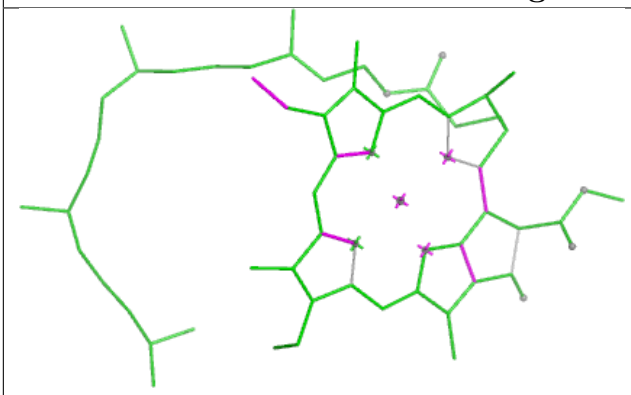
Ligand LHG D 409



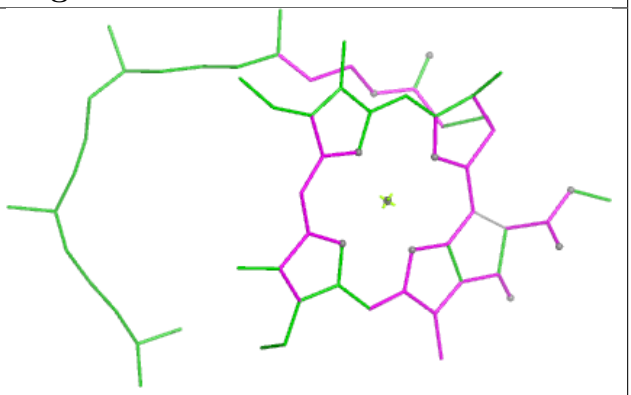
Ligand DGA J 101



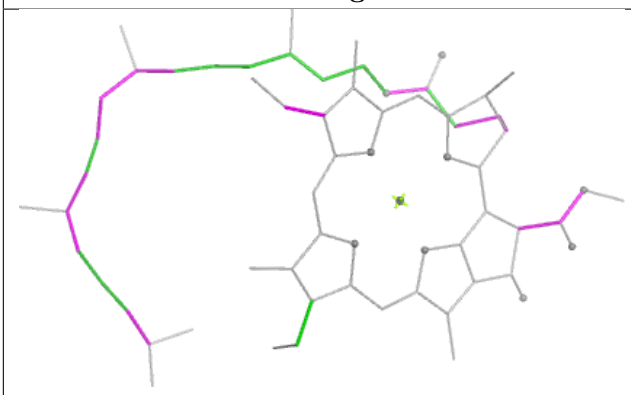
Ligand CLA g 610



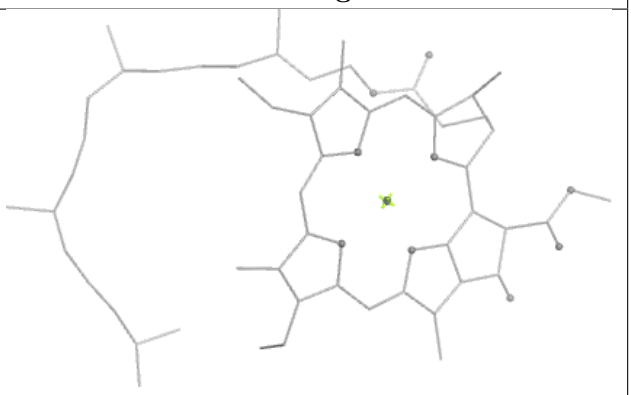
Bond lengths



Bond angles

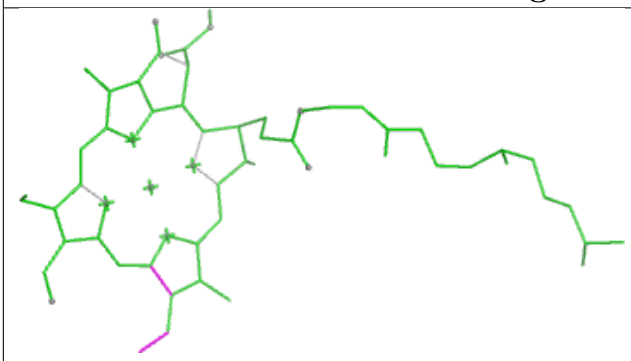


Torsions



Rings

Ligand CHL s 608



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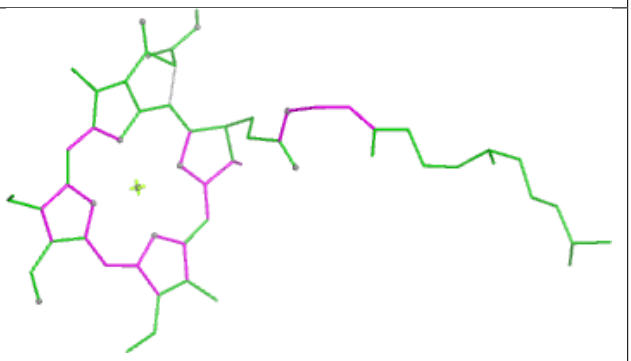
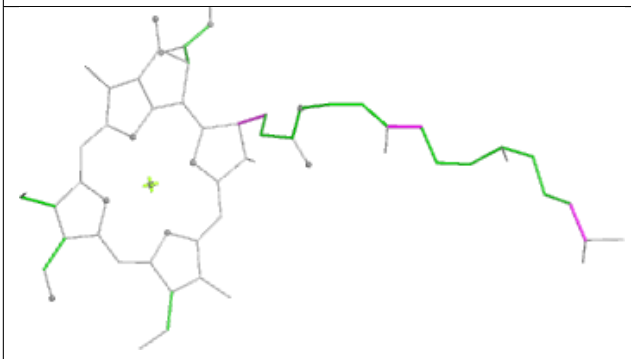
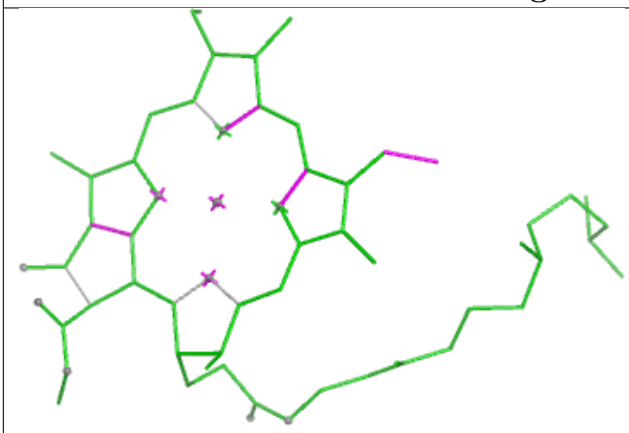
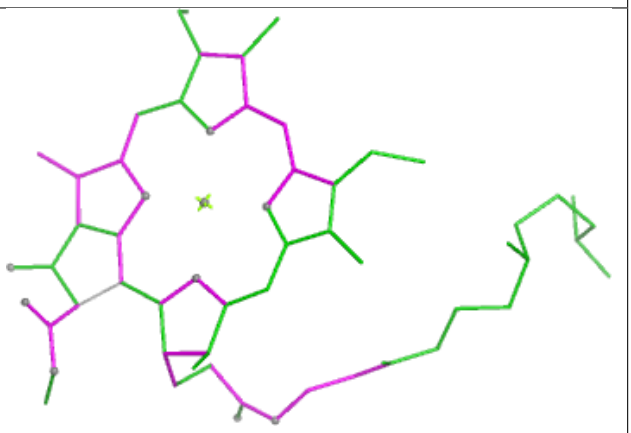
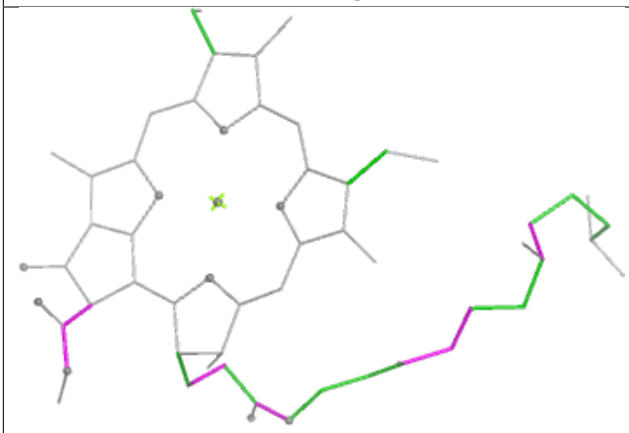
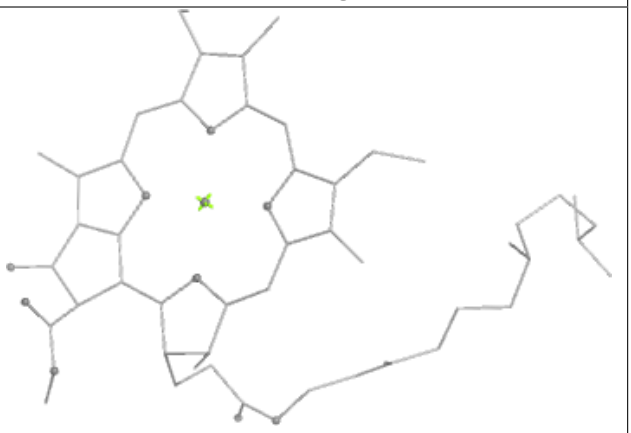


Bond angles

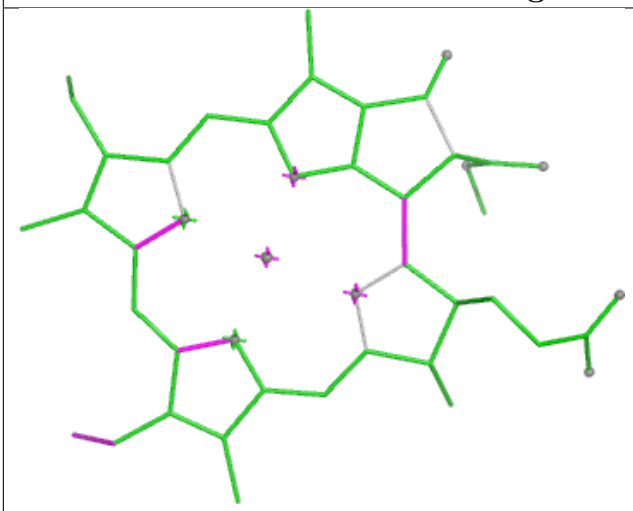


Torsions

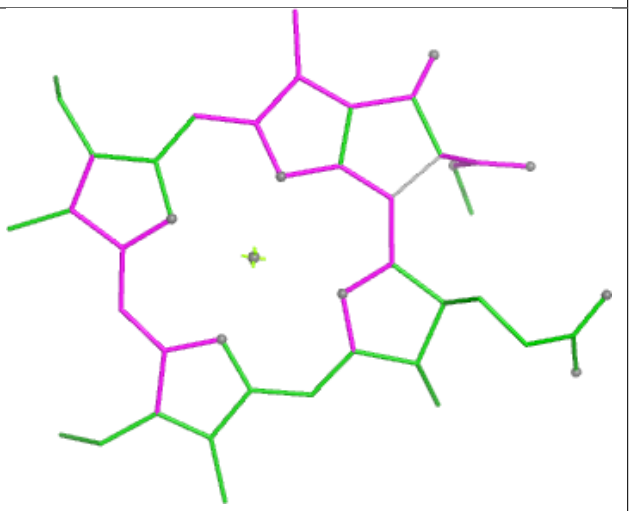
Rings

Ligand CLA r 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

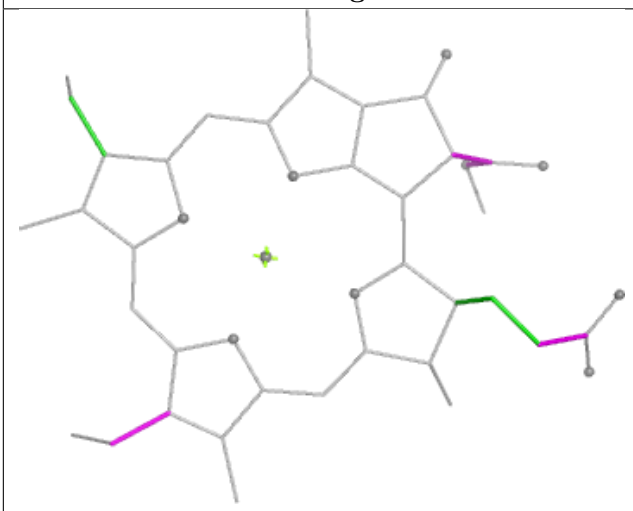
Ligand CLA n 612



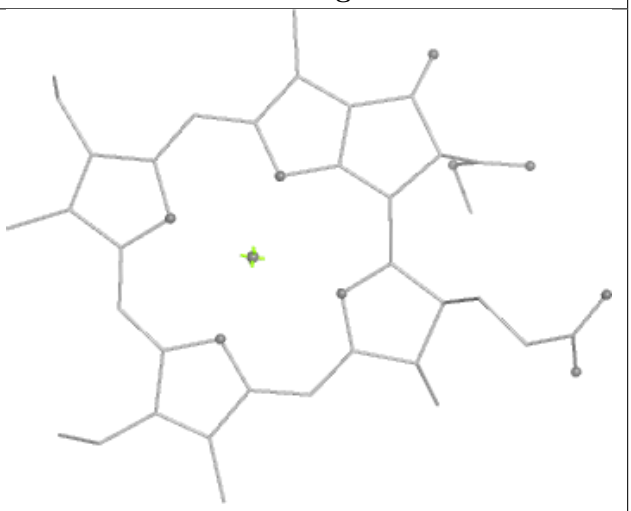
Bond lengths



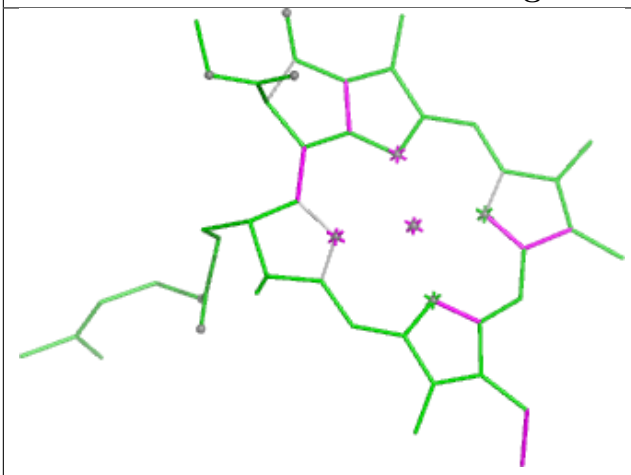
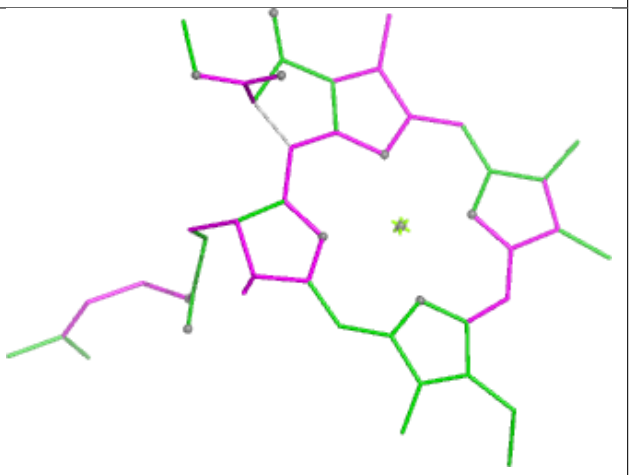
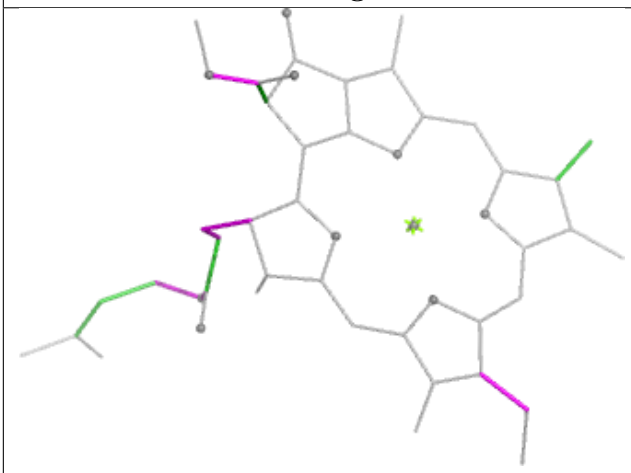
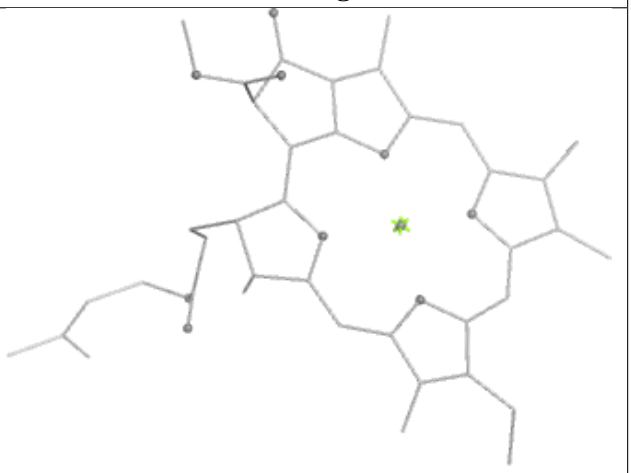
Bond angles



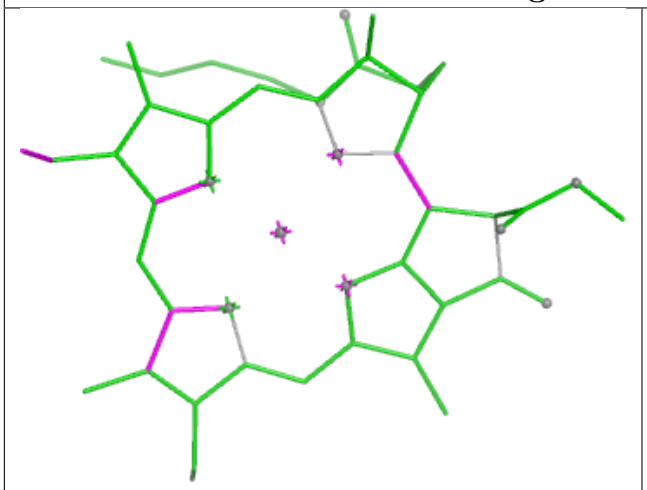
Torsions



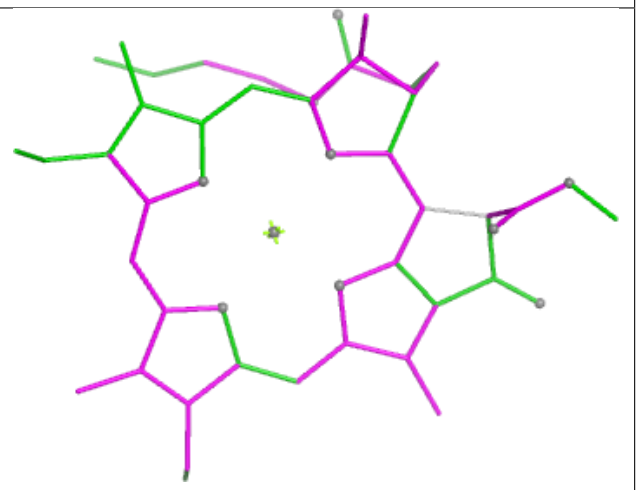
Rings

Ligand CLA Y 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 614



Bond lengths



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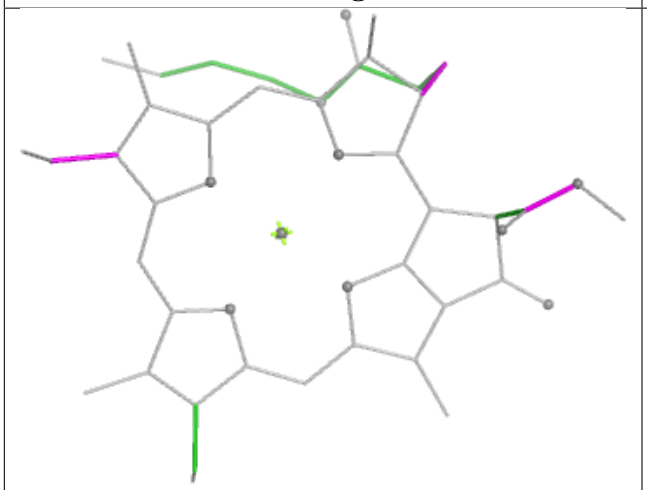
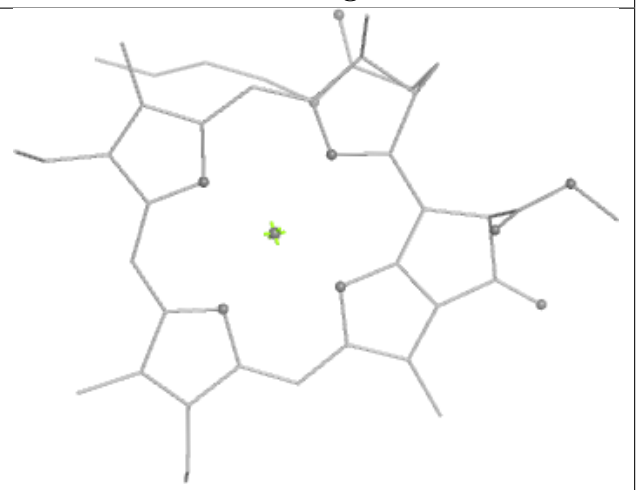
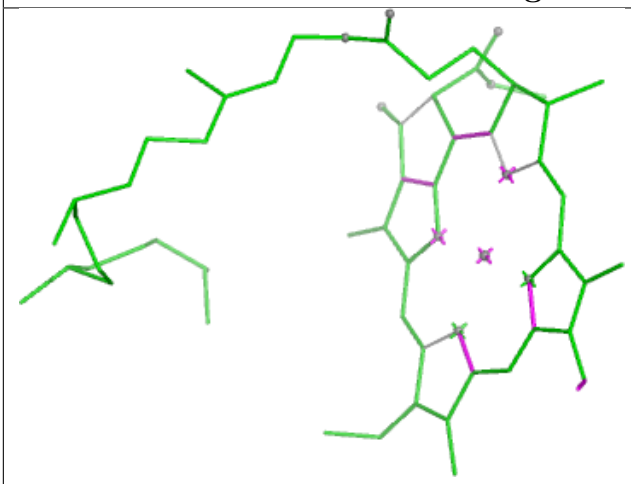
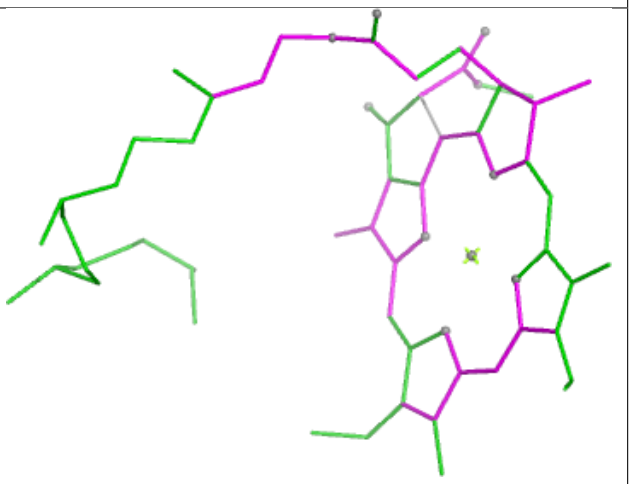
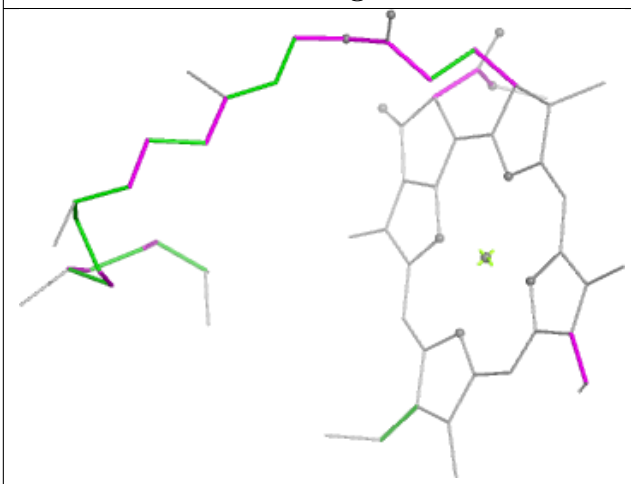
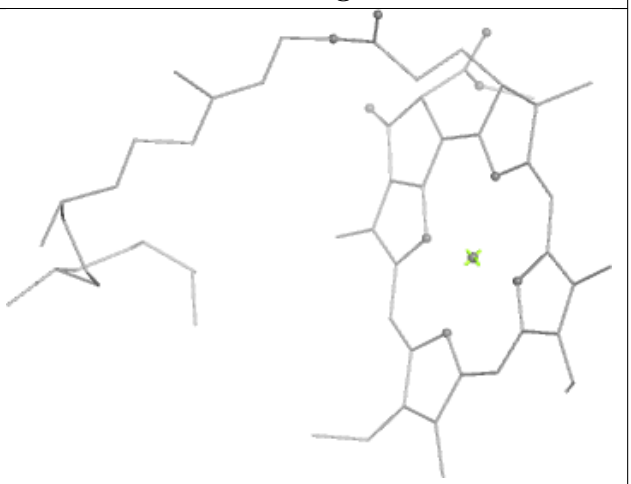


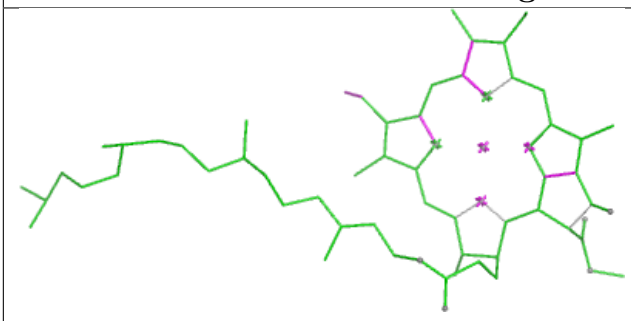
Torsions



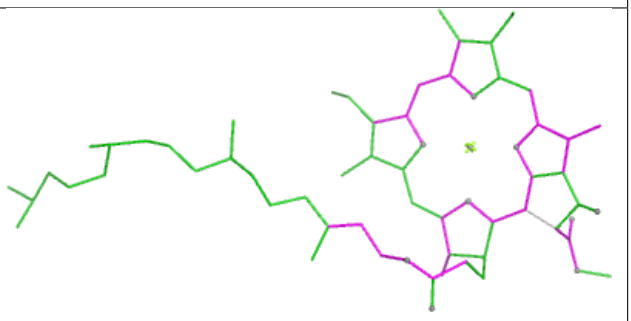
Rings

Ligand CLA C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

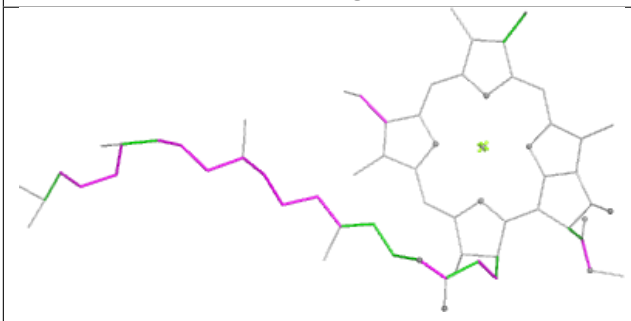
Ligand CLA b1 604



Bond lengths



Bond angles



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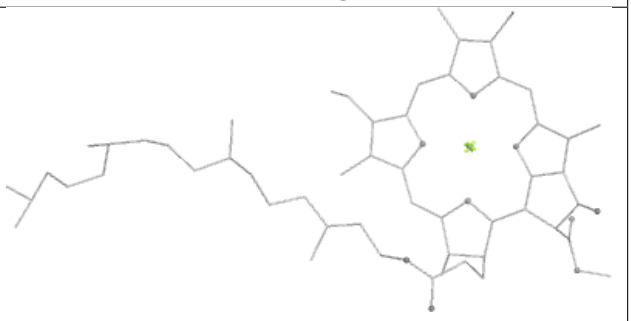
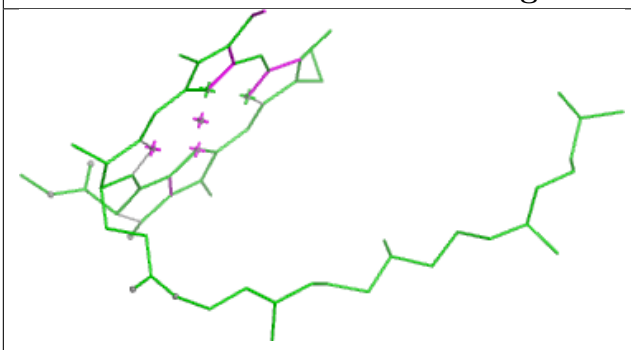


Rings

Ligand CLA c1 508



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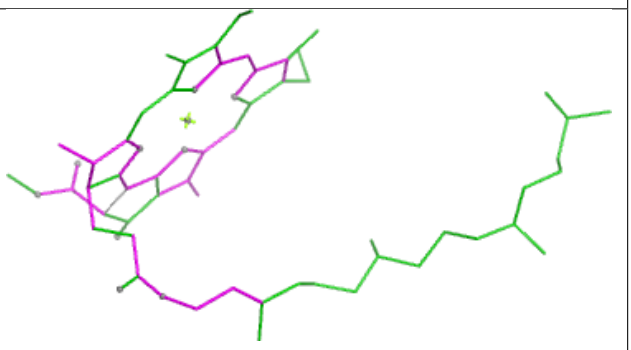
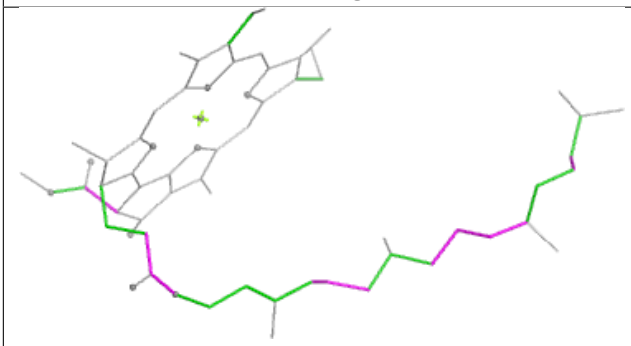
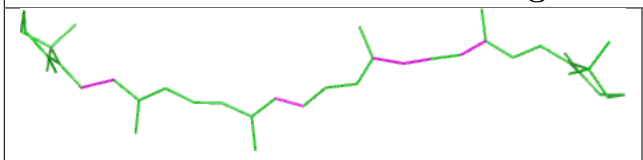
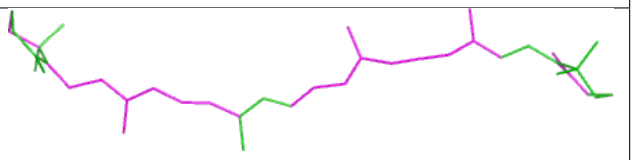
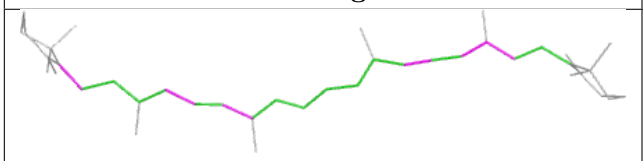
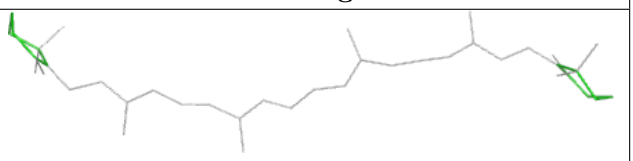


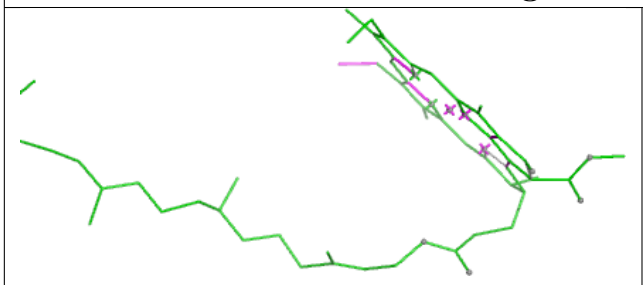
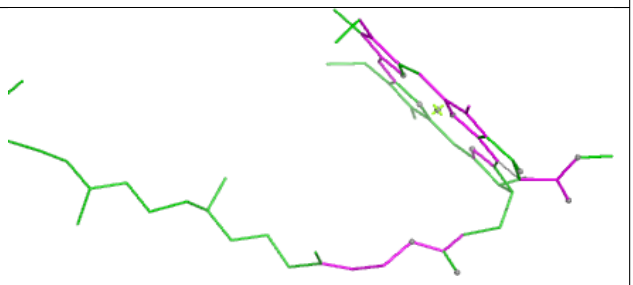
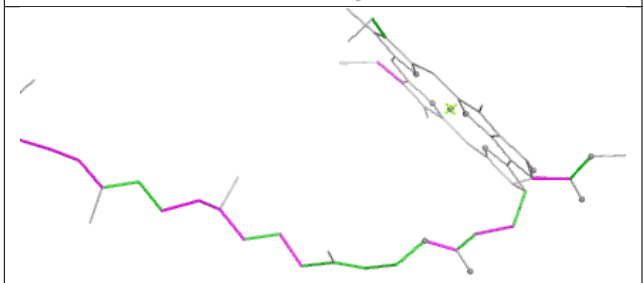
Bond angles



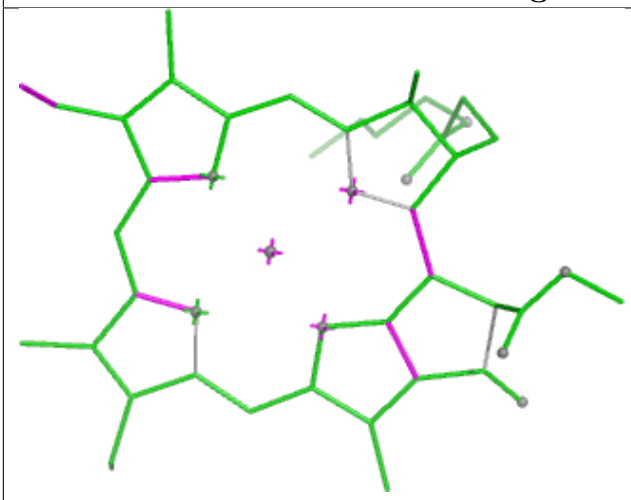
Torsions

Rings

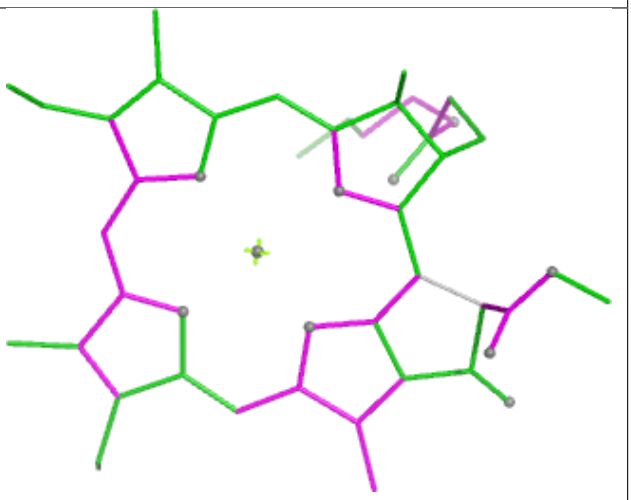
Ligand BCR c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c1 504	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA r 604



Bond lengths



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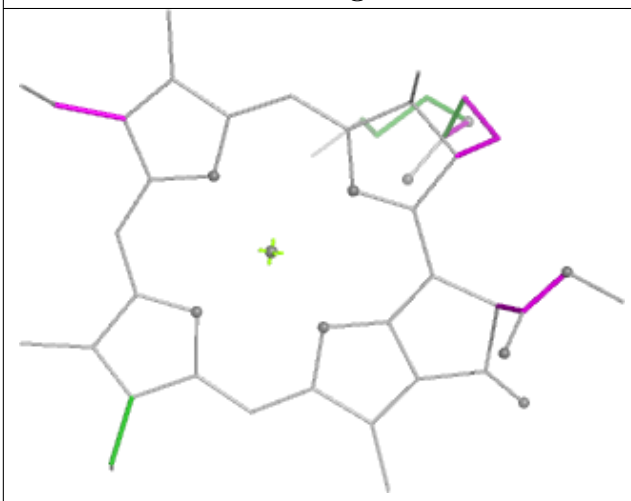

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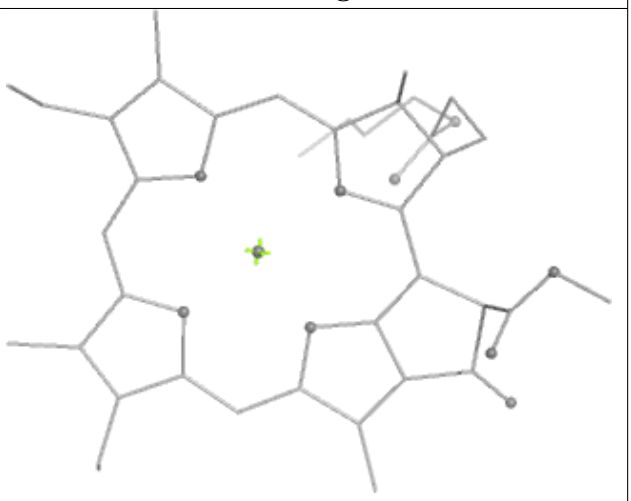
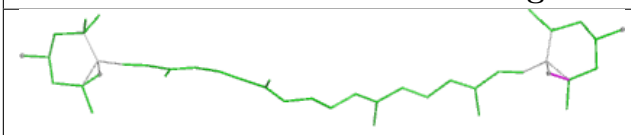


Rings

Ligand XAT y 622



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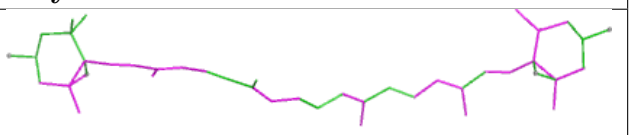

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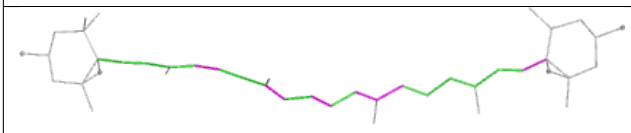

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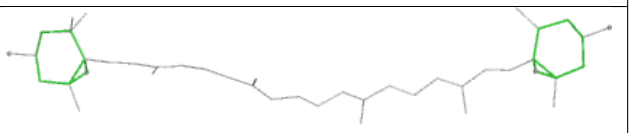
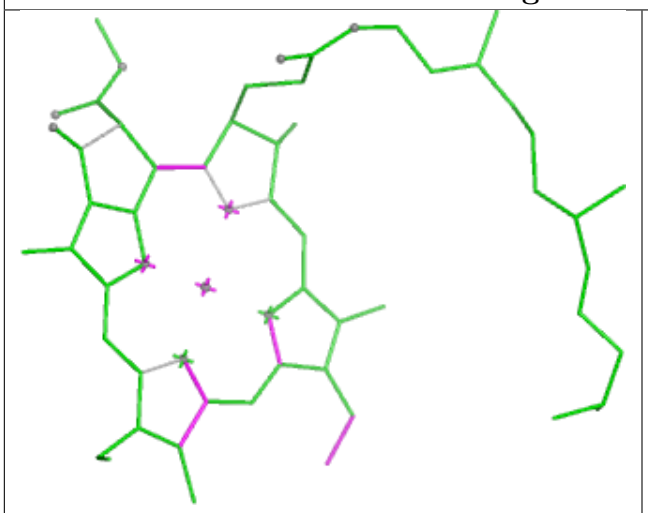


Rings

Ligand CLA r1 603



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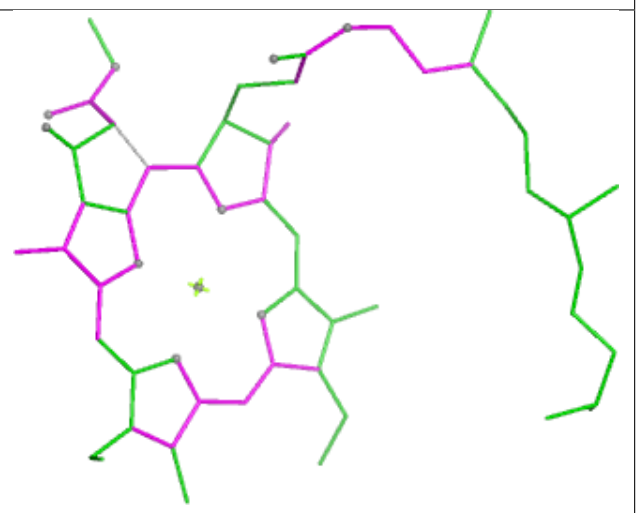

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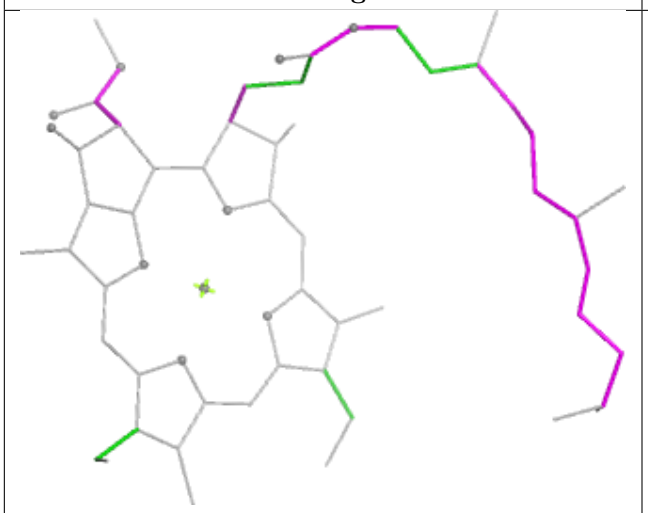
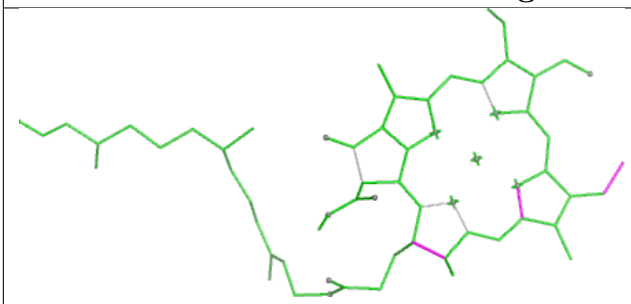


Torsions

Rings

Ligand CHL n1 605



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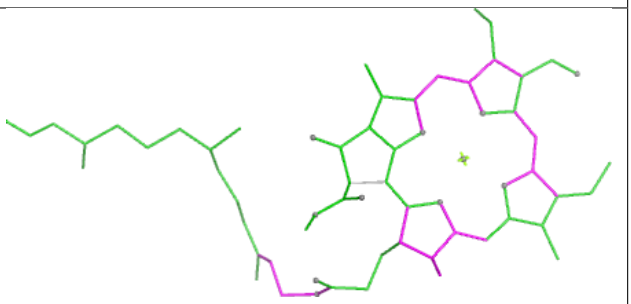
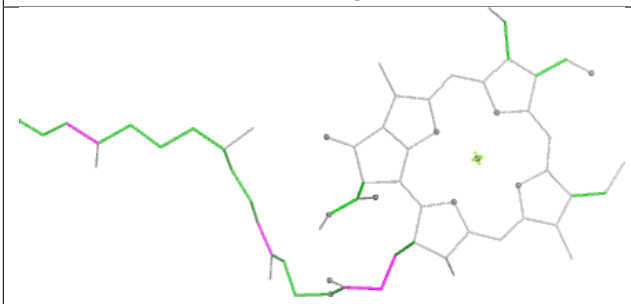


Bond angles



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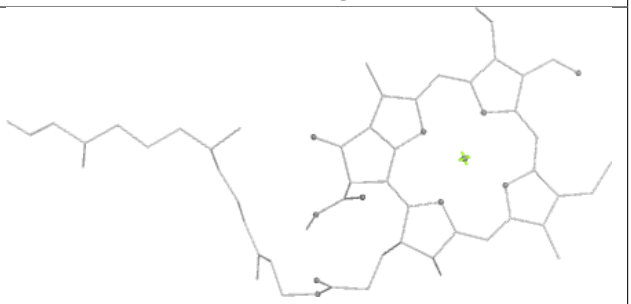

Rings

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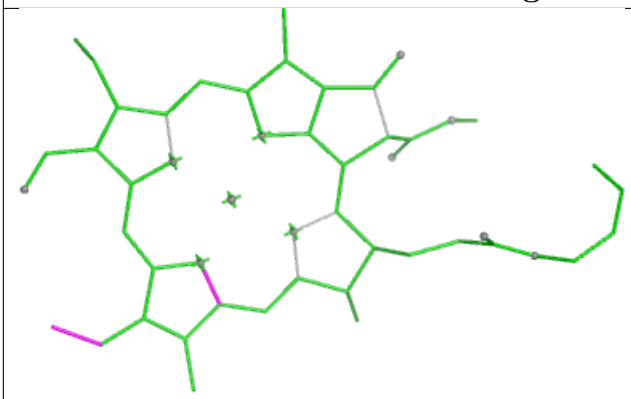

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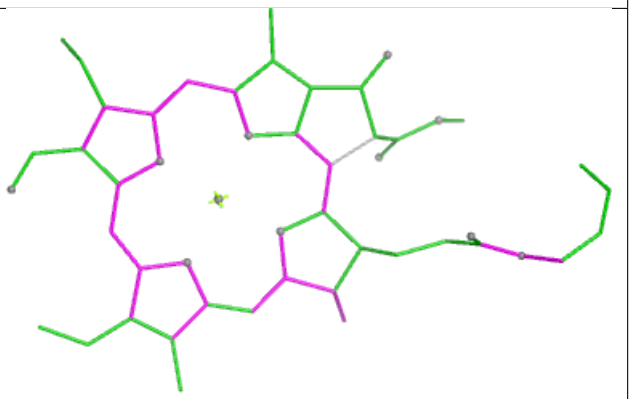

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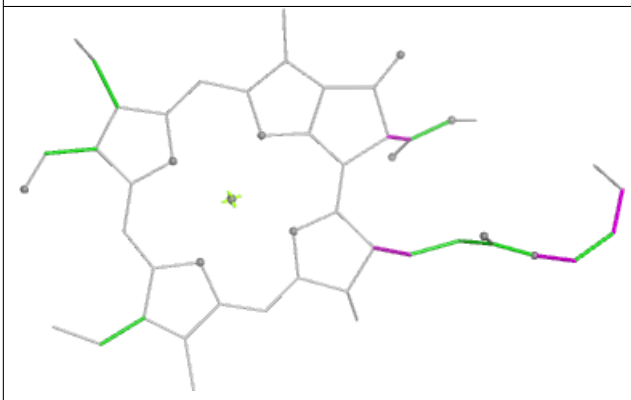

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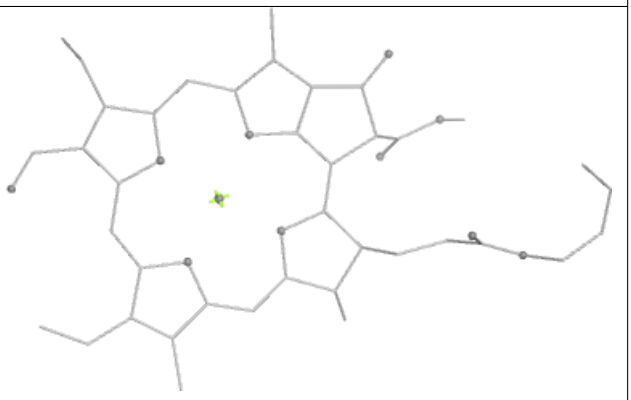
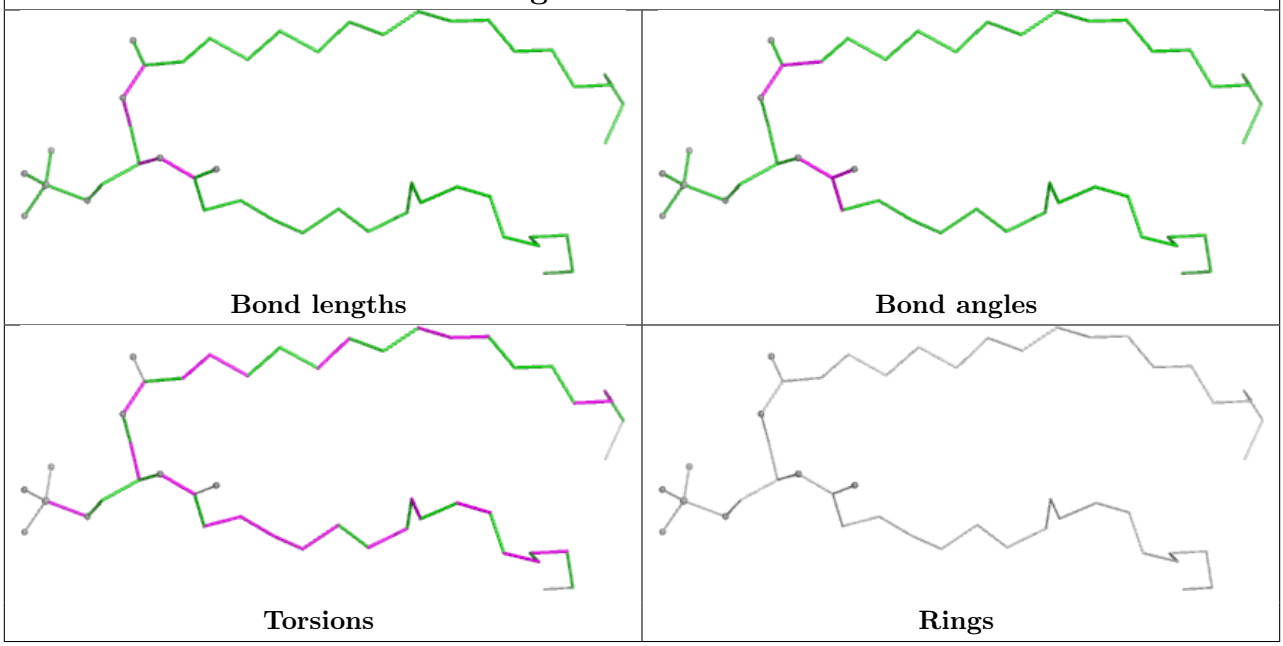


Rings

Ligand 3PH b 624



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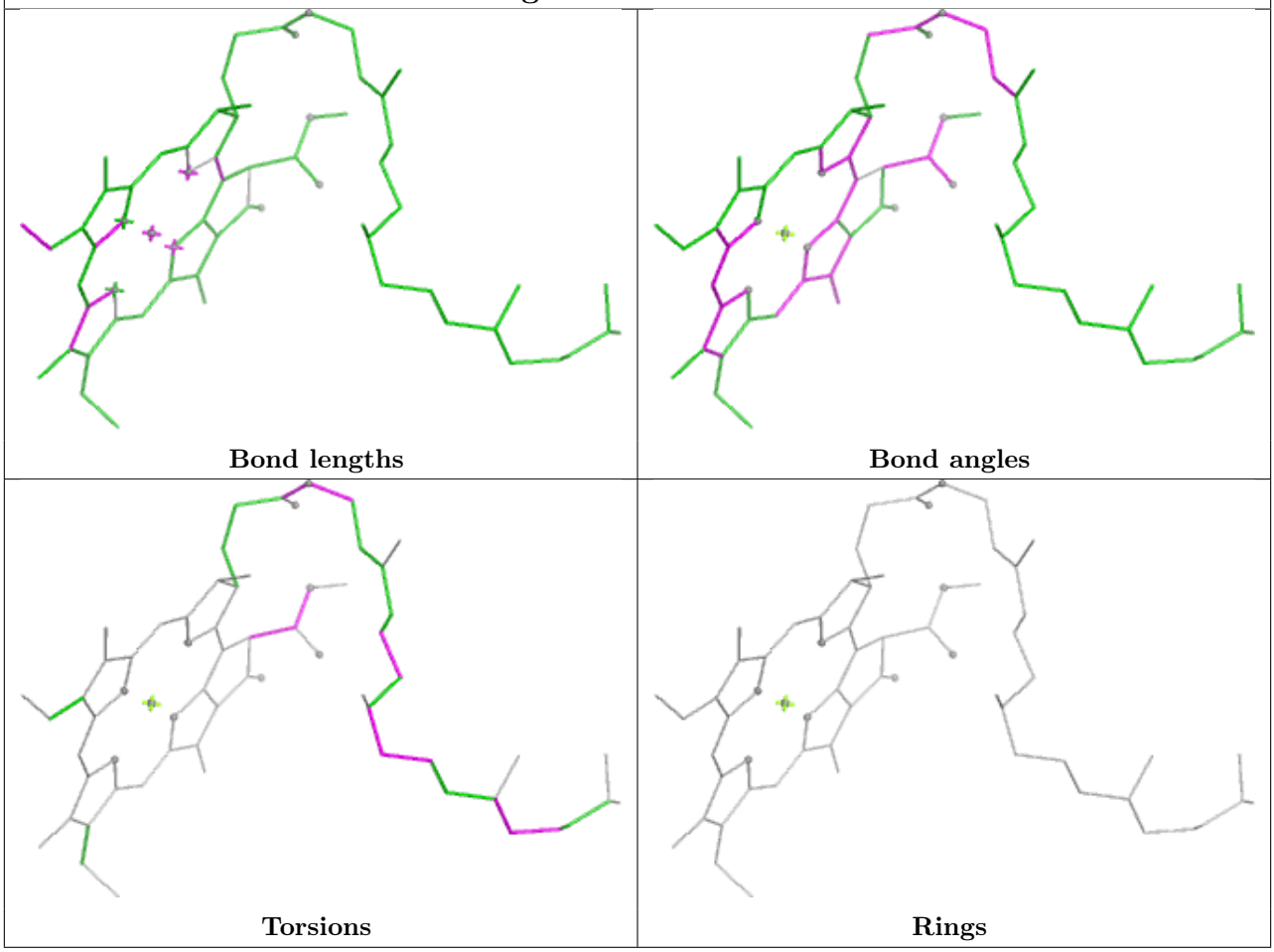
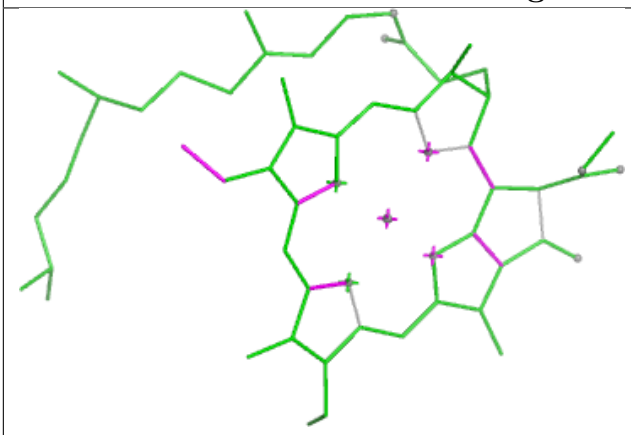
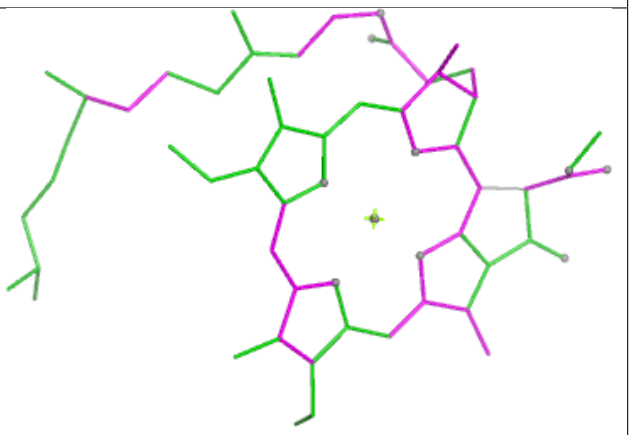
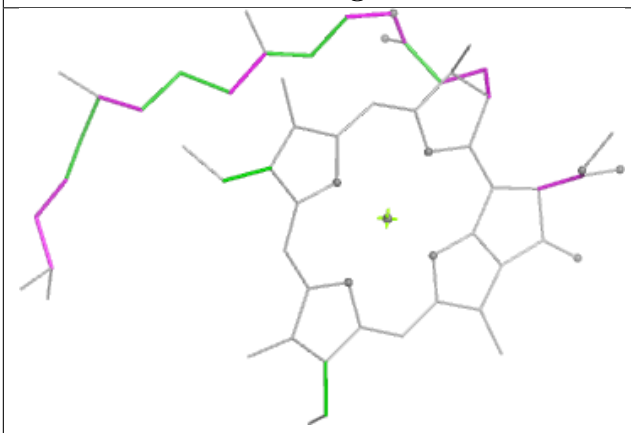
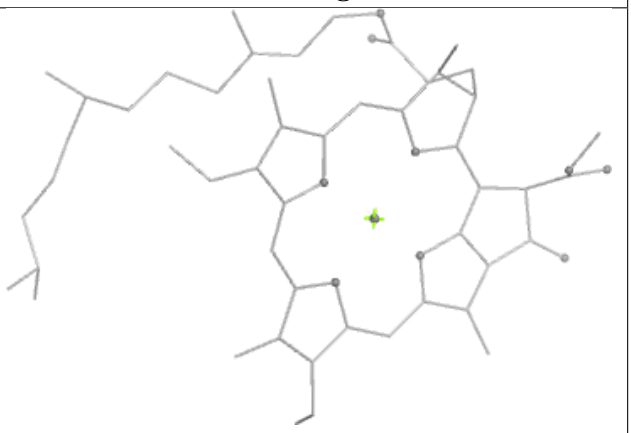
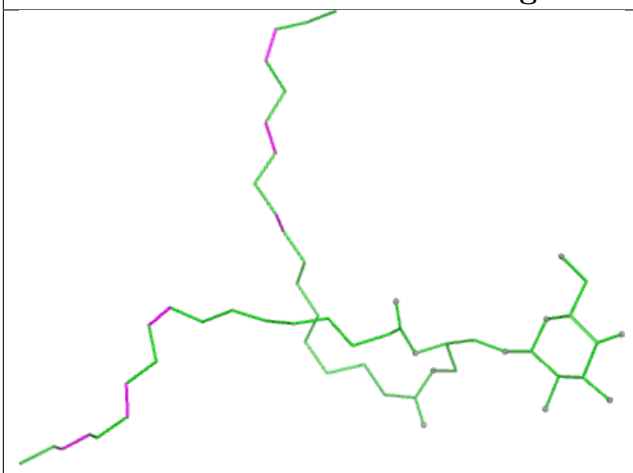
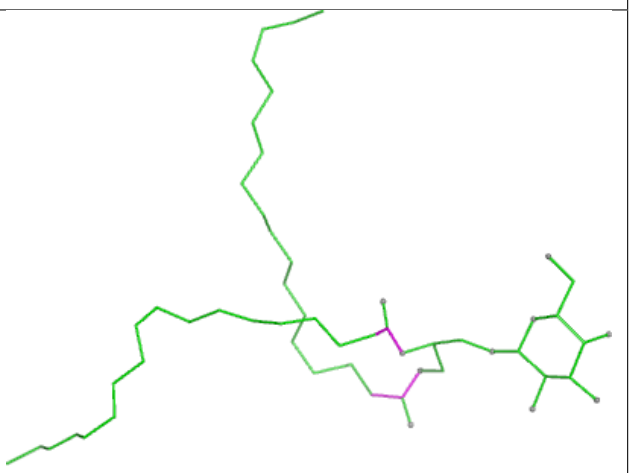


Ligand CLA S 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

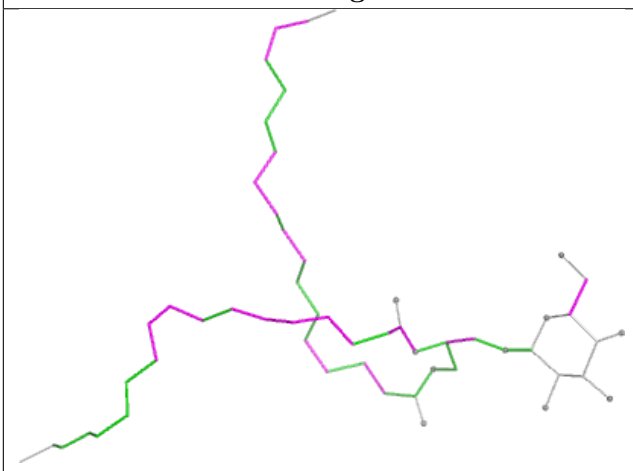
Ligand LMG C 523



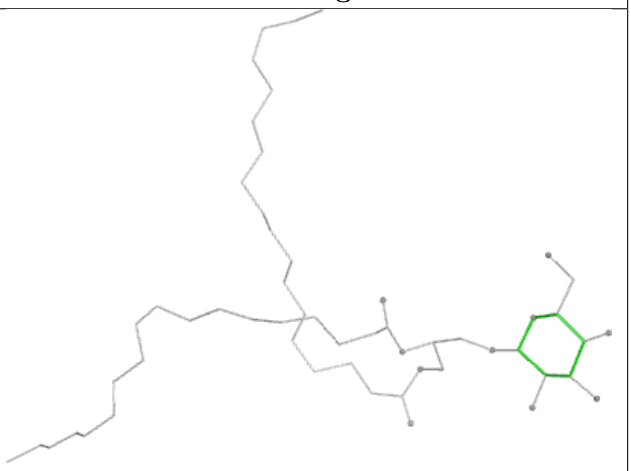
Bond lengths



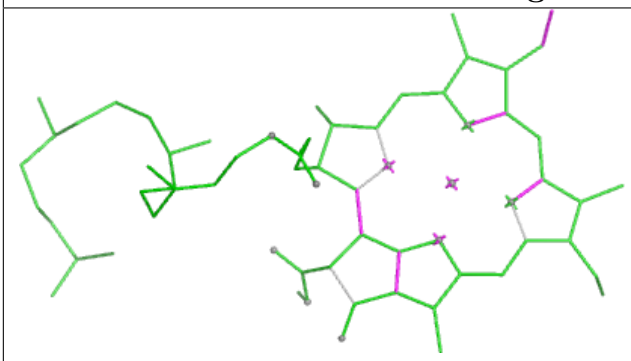
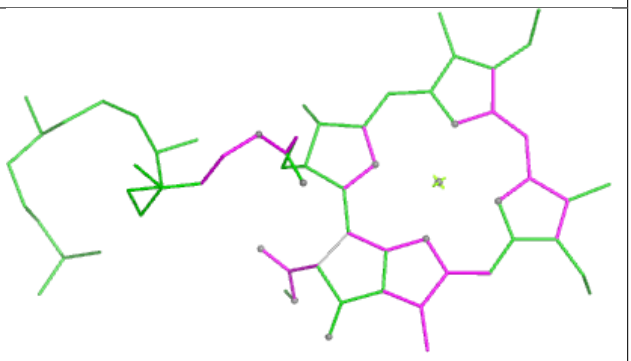
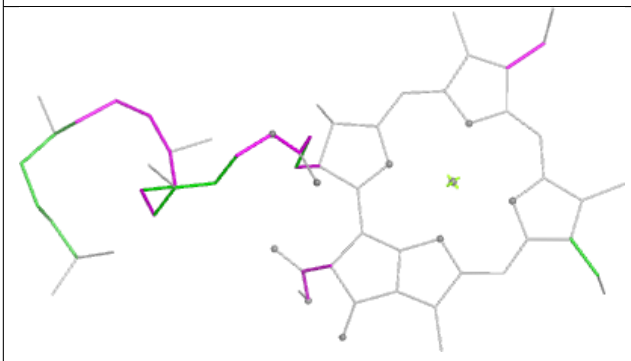
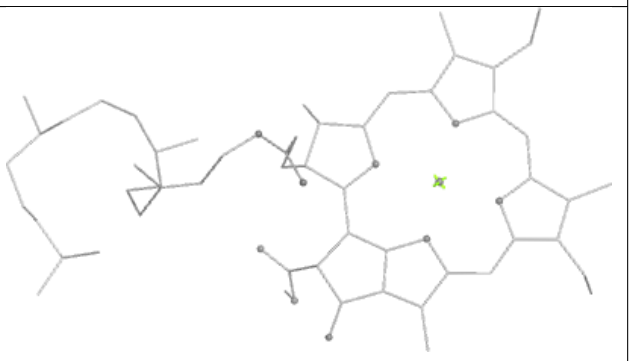
Bond angles



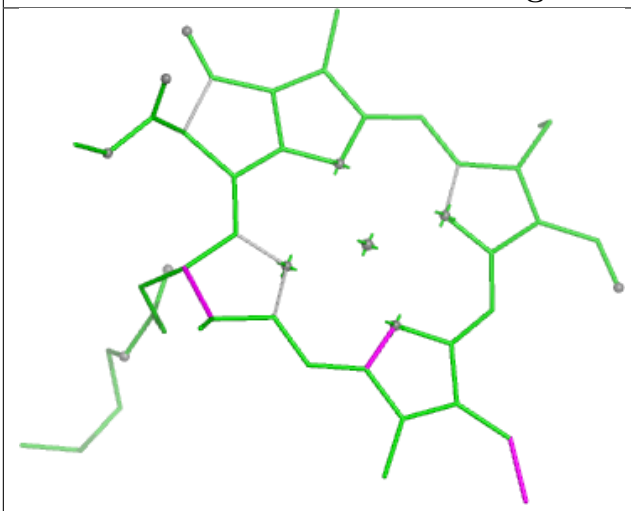
Torsions



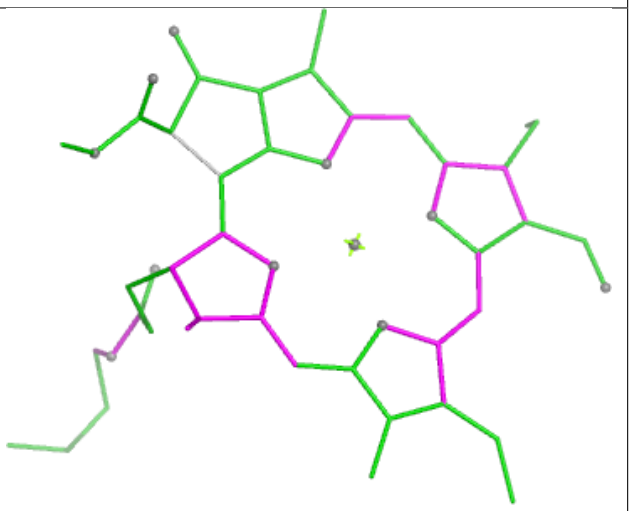
Rings

Ligand CLA b 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

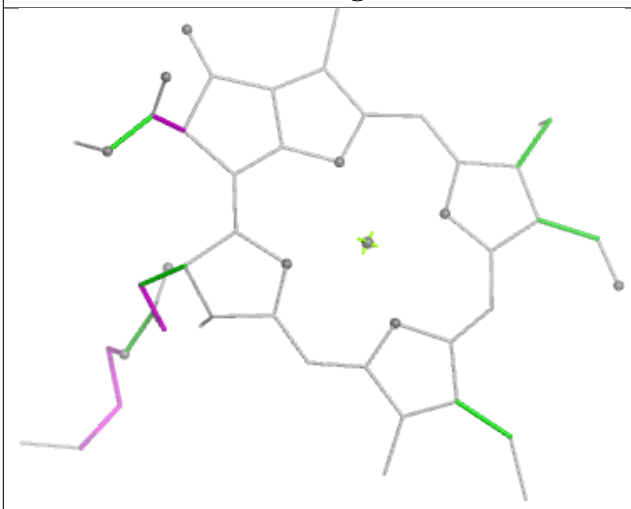
Ligand CHL n 608



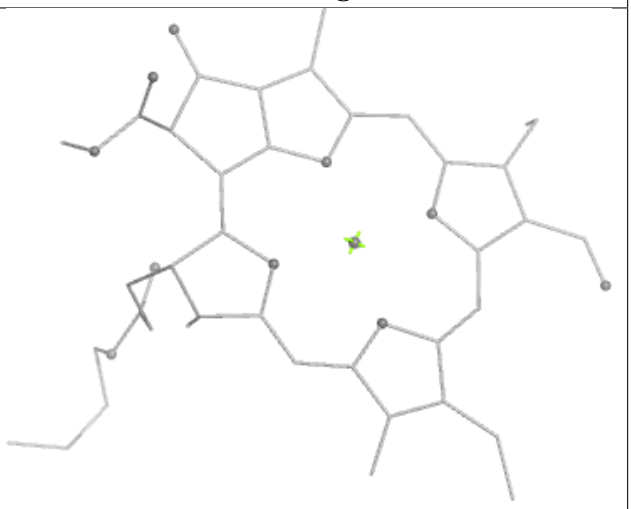
Bond lengths



Bond angles

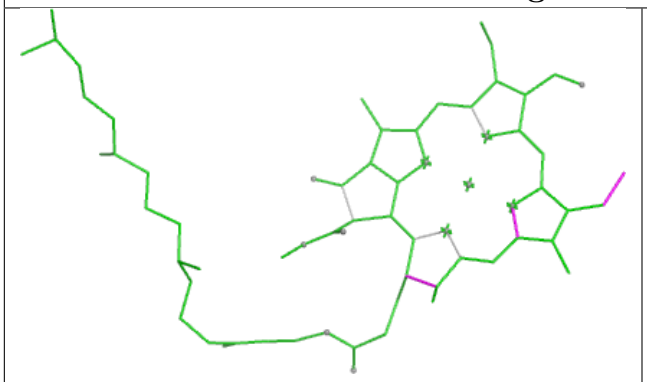


Torsions

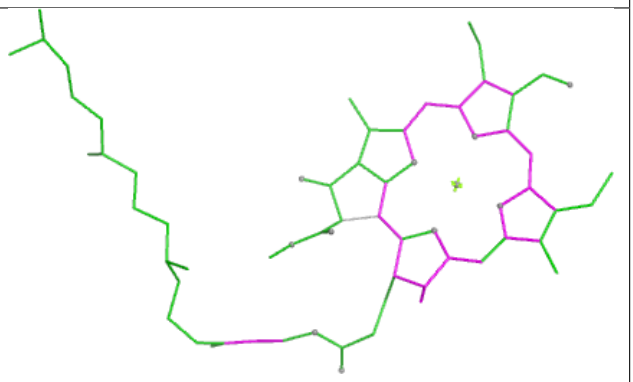


Rings

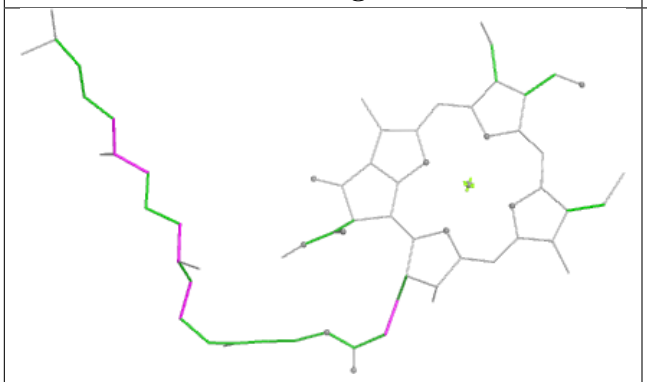
Ligand CHL n 606



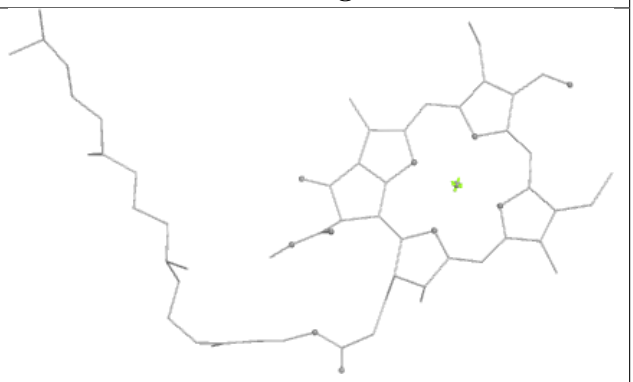
Bond lengths



Bond angles

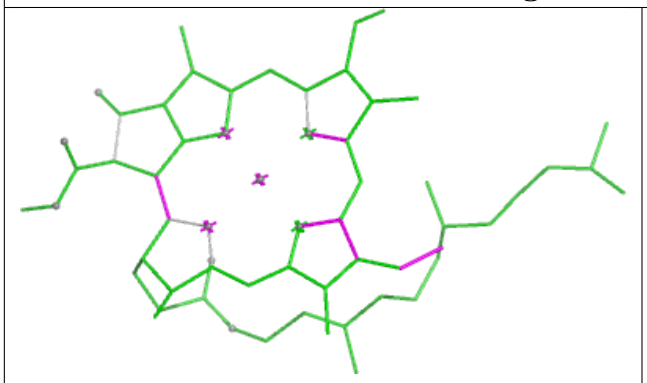


Torsions

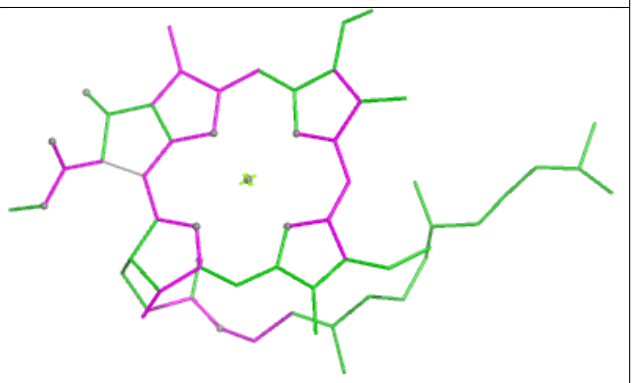


Rings

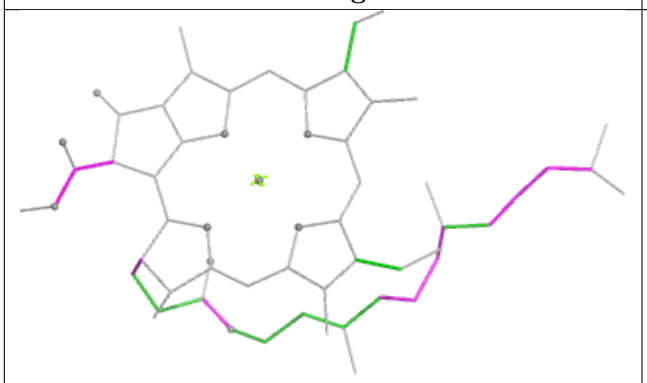
Ligand CLA r1 608



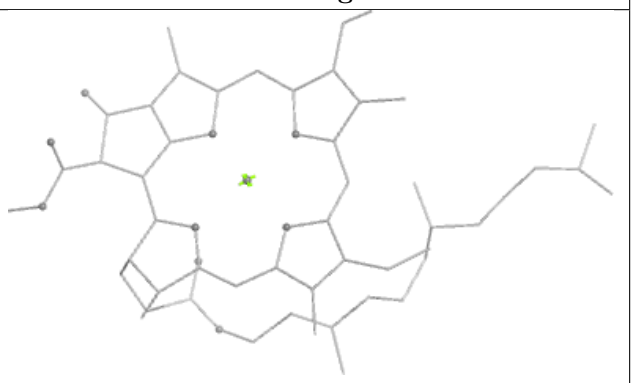
Bond lengths



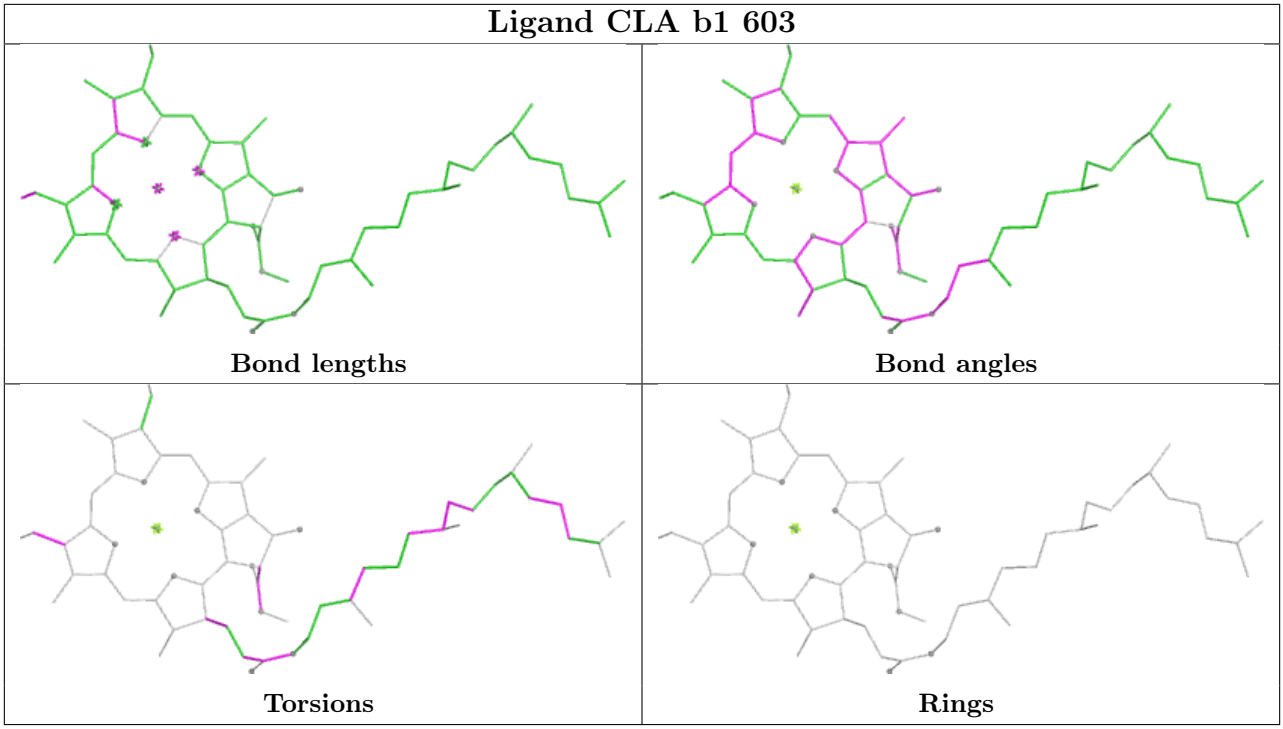
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	r	1
22	r1	1
22	R1	1
22	R	1
20	n1	1
20	n	1
21	G1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	13.15
1	r1	110:PRO	C	126:GLU	N	13.08
1	R1	110:PRO	C	126:GLU	N	12.94
1	R	110:PRO	C	126:GLU	N	12.16

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	n1	57:PRO	C	58:PRO	N	3.54
1	n	57:PRO	C	58:PRO	N	3.28
1	G1	56:GLU	C	57:PHE	N	1.19

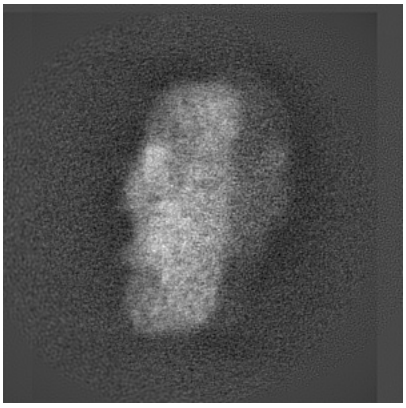
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13444. These allow visual inspection of the internal detail of the map and identification of artifacts.

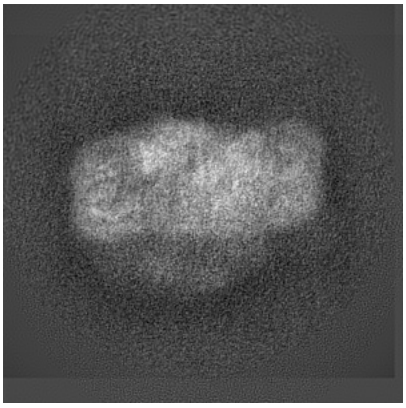
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

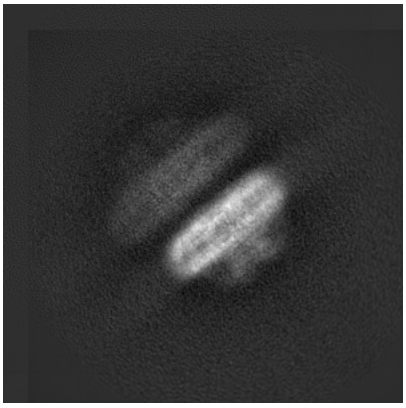
6.1.1 Primary map



X



Y

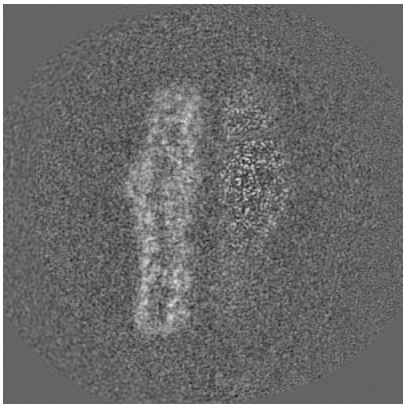


Z

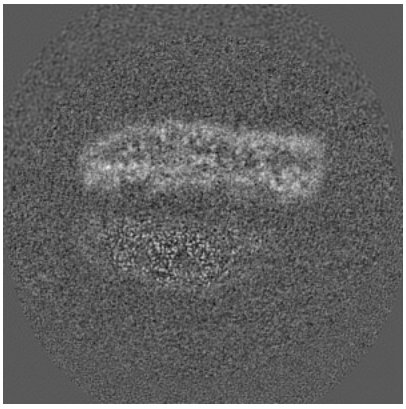
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

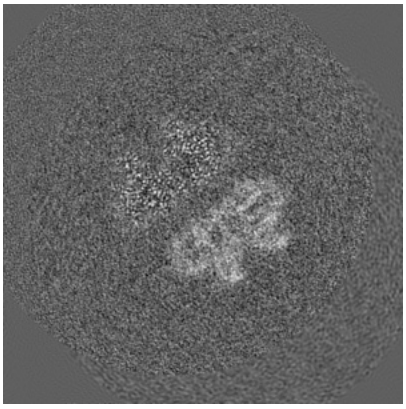
6.2.1 Primary map



X Index: 240



Y Index: 240

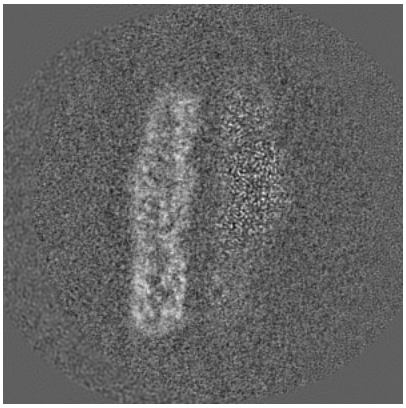


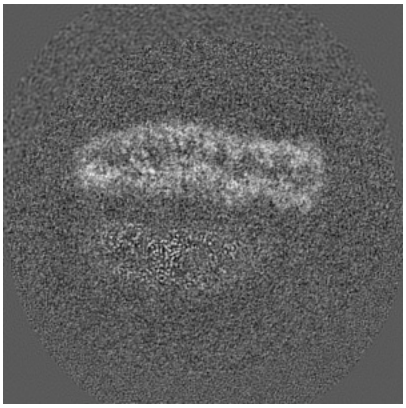
Z Index: 240

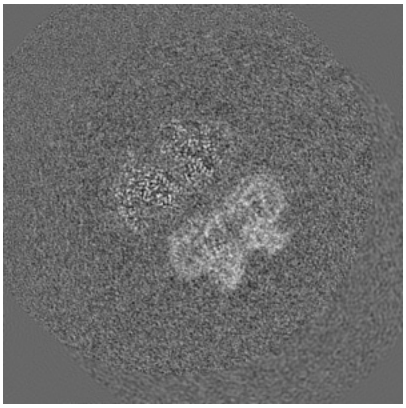
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 232

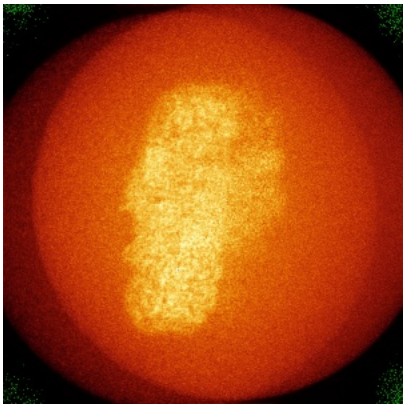

Y Index: 233

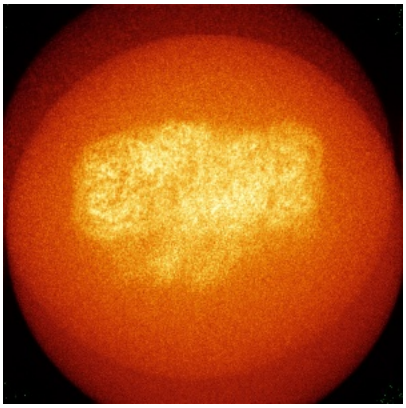

Z Index: 236

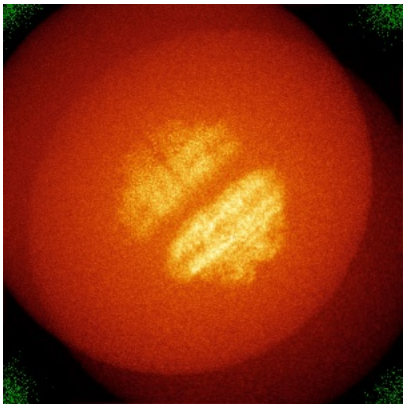
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

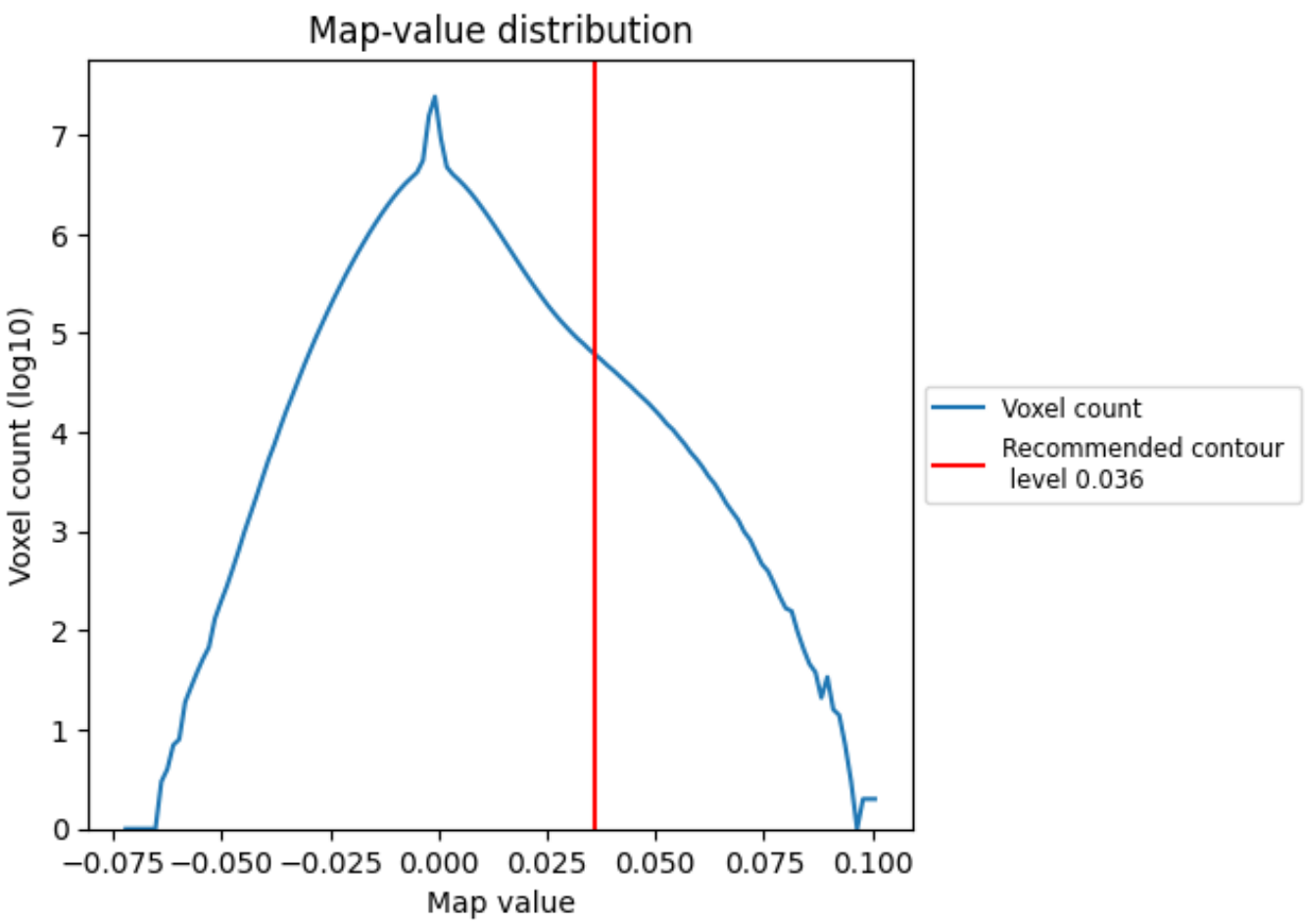
6.6 Mask visualisation (i)

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

7 Map analysis (i)

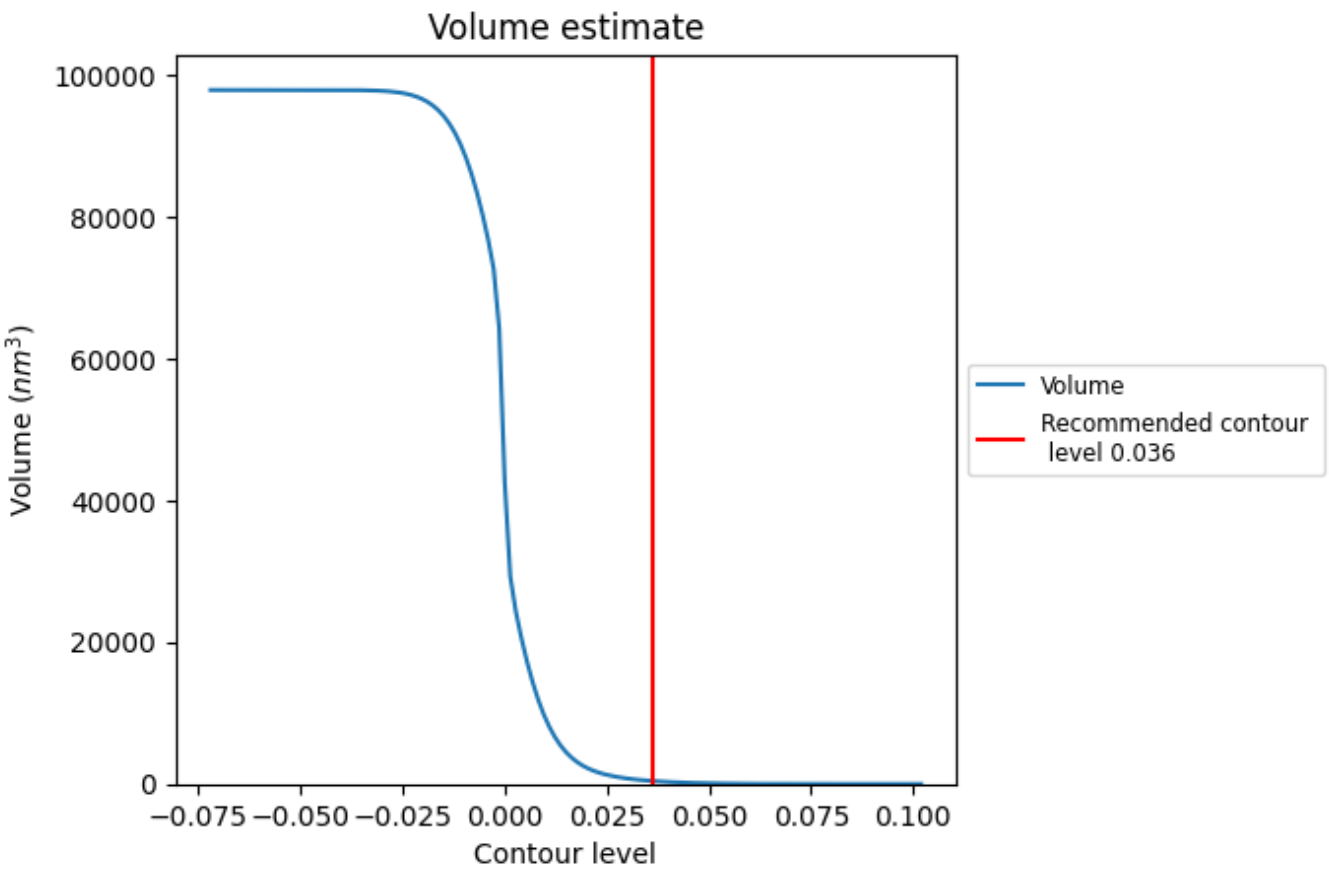
This section contains the results of statistical analysis of the map.

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.

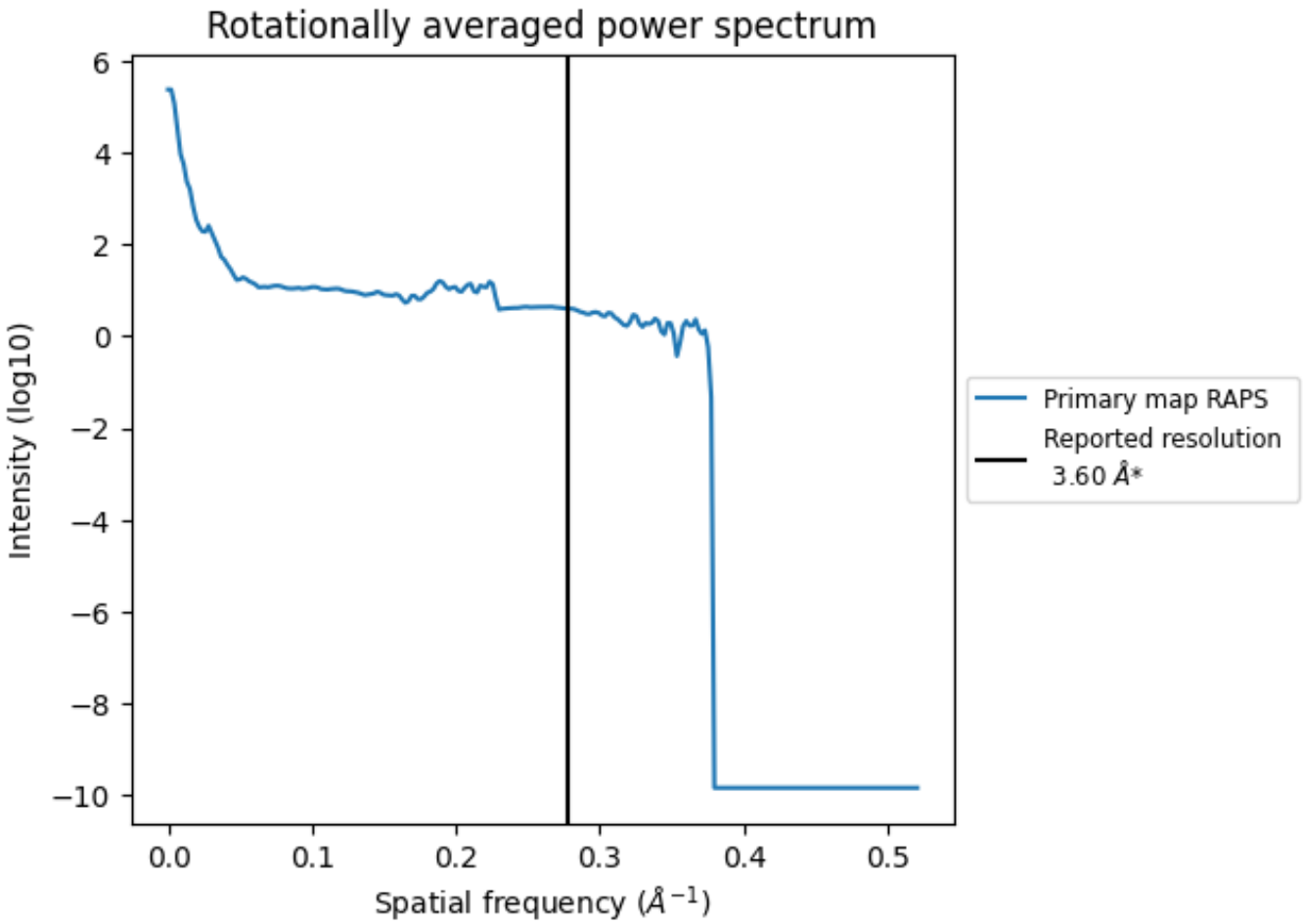
7.2 Volume estimate (i)



The volume at the recommended contour level is 429 nm^3; this corresponds to an approximate mass of 387 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)

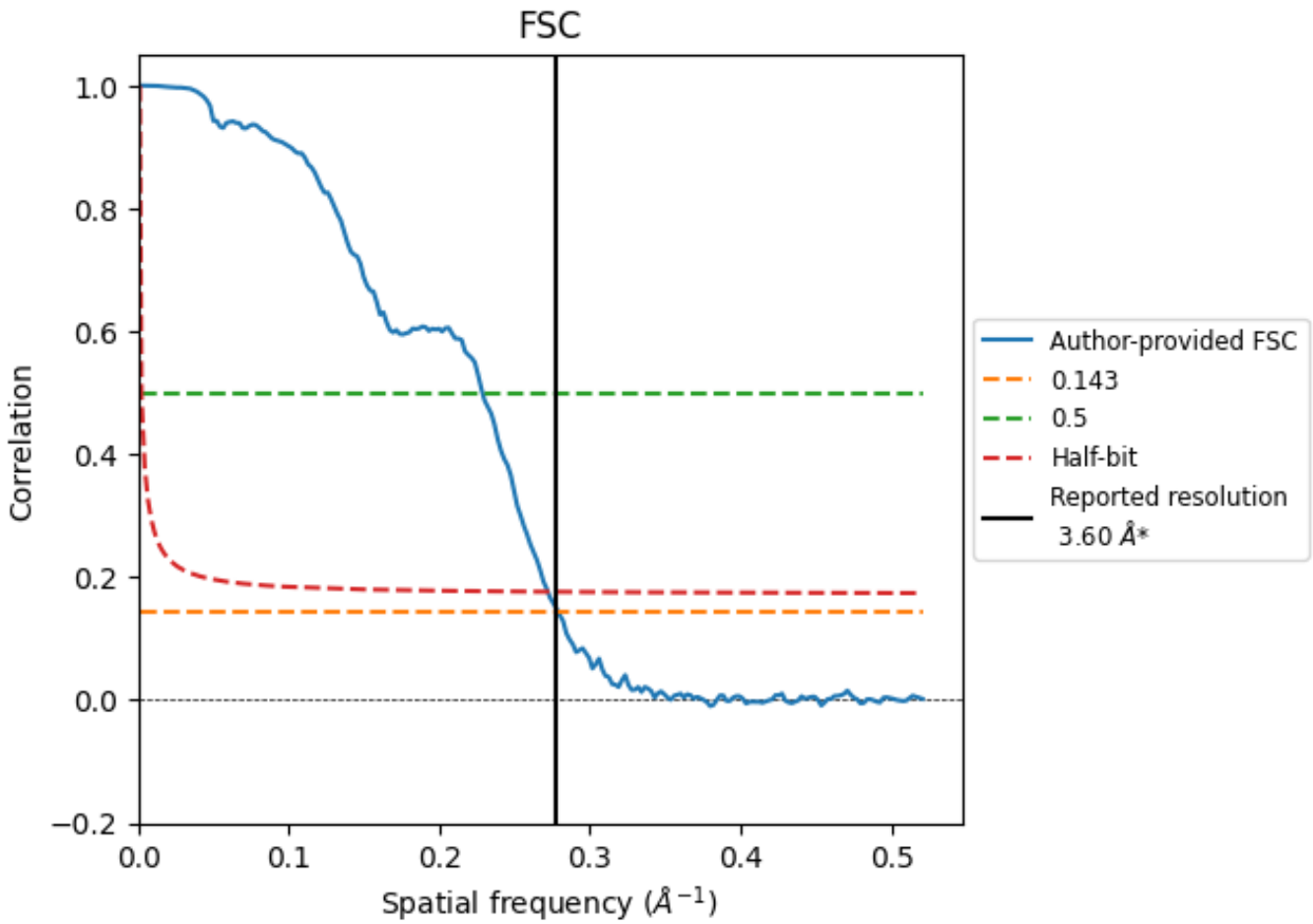


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

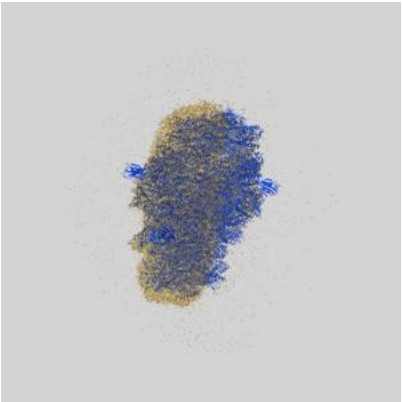
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.37	3.68
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

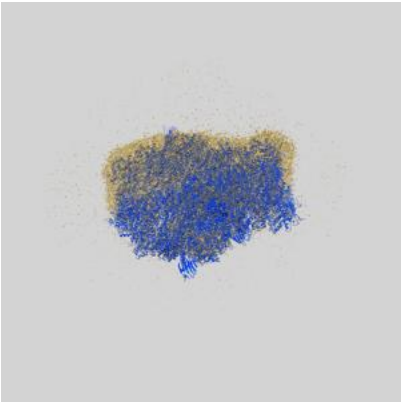
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13444 and PDB model 7PIN. Per-residue inclusion information can be found in section 3 on page 64.

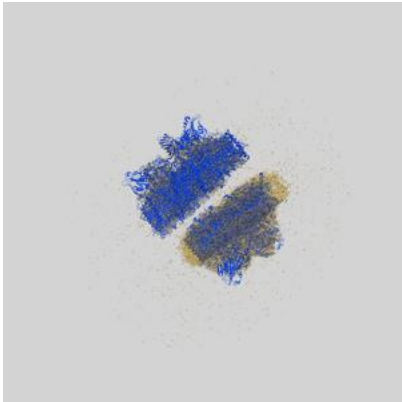
9.1 Map-model overlay (i)



X



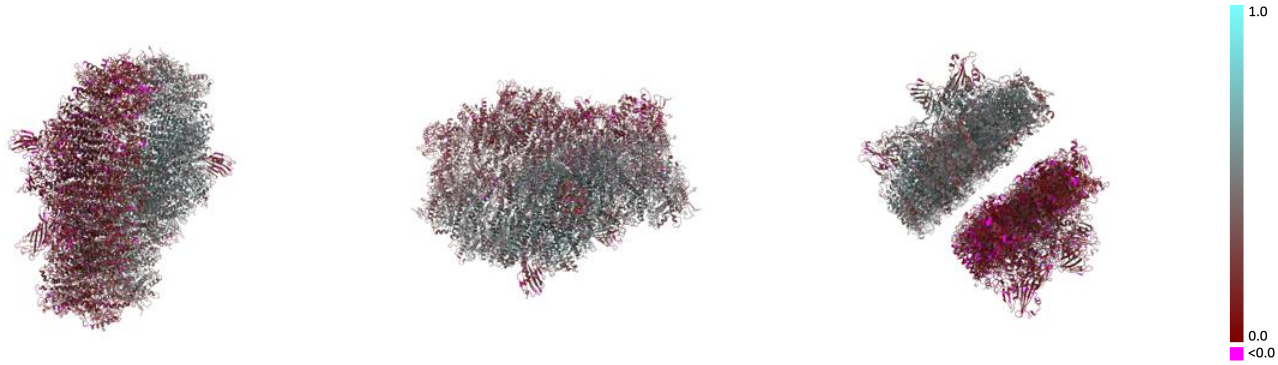
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

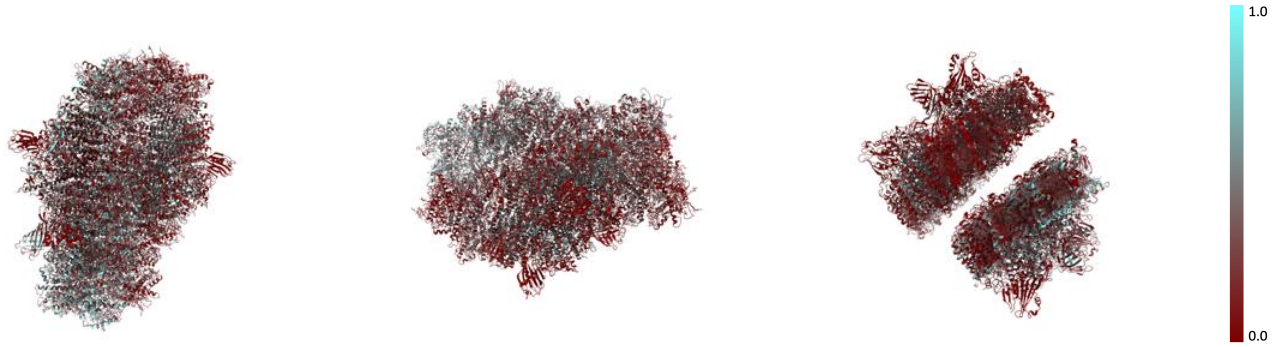
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

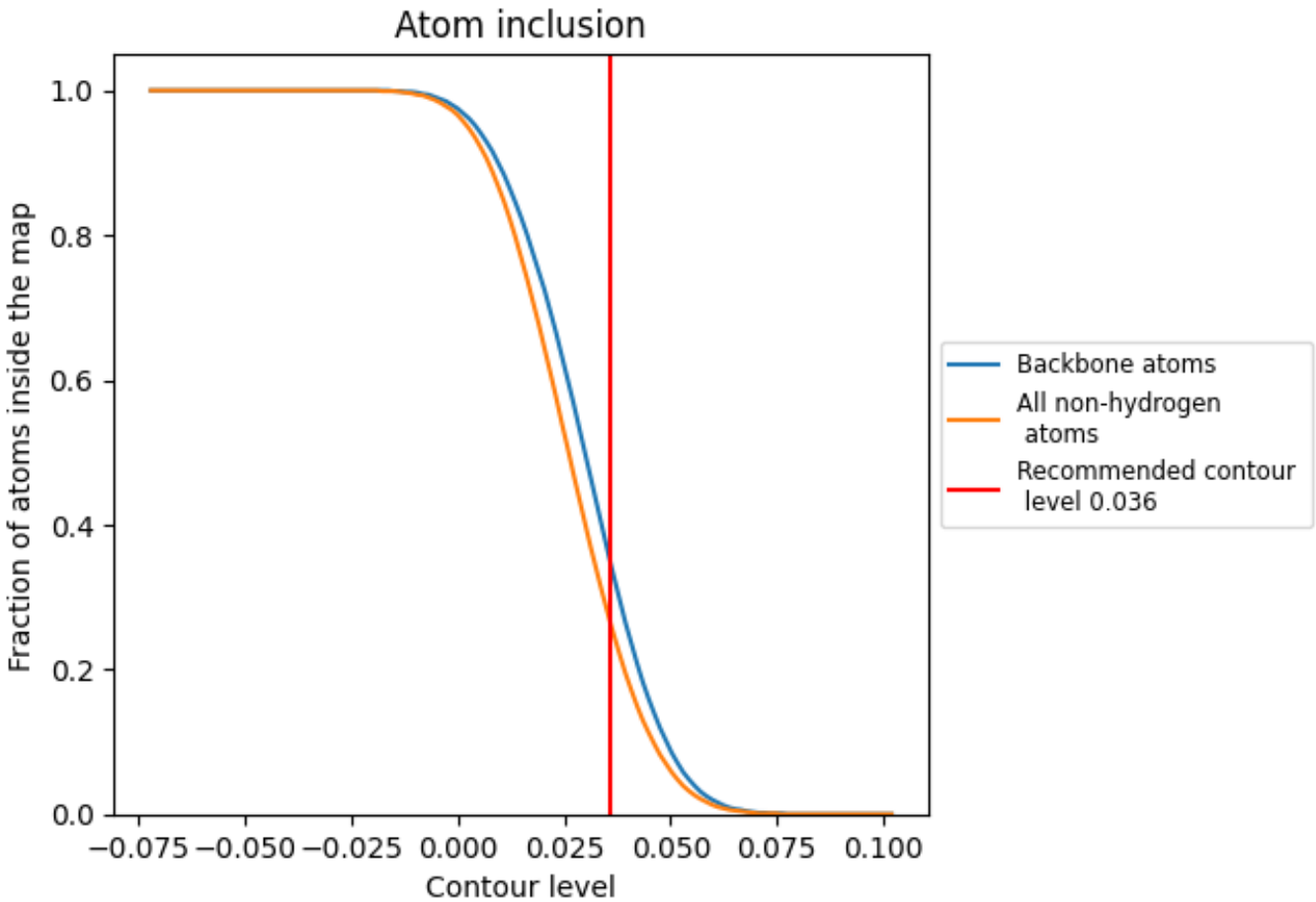
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.036).

9.4 Atom inclusion (i)



At the recommended contour level, 34% of all backbone atoms, 26% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2620	0.3280
A	0.3530	0.5260
A1	0.3490	0.2350
B	0.2800	0.5100
B1	0.2940	0.2060
C	0.3490	0.5370
C1	0.4040	0.2440
D	0.3190	0.5320
D1	0.3360	0.2300
E	0.1680	0.4510
E1	0.3960	0.2140
F	0.2270	0.4540
F1	0.3850	0.1930
G	0.1010	0.4070
G1	0.4160	0.1980
H	0.2160	0.4790
H1	0.2710	0.1950
I	0.2710	0.4970
I1	0.2800	0.2390
J	0.1660	0.4880
J1	0.2520	0.1960
K	0.2340	0.4820
K1	0.3910	0.2320
L	0.2820	0.5100
L1	0.2230	0.2170
M	0.1850	0.4500
M1	0.1740	0.2160
N	0.1410	0.4480
N1	0.4420	0.2080
O	0.1150	0.4130
O1	0.3020	0.2040
P	0.0010	0.2320
P1	0.0250	0.1680
R	0.0980	0.3800
R1	0.2380	0.1720

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Chain	Atom inclusion	Q-score
S	0.1780	0.4500
S1	0.4390	0.2170
T	0.1700	0.4490
T1	0.1940	0.2630
U	0.0830	0.3800
U1	0.2200	0.2430
V	0.1470	0.4630
V1	0.2800	0.2330
W	0.1420	0.4380
W1	0.2650	0.2450
X	0.1290	0.3870
X1	0.3880	0.2580
Y	0.2290	0.4840
Y1	0.4010	0.2140
Z	0.1710	0.4810
Z1	0.3890	0.2370
a	0.3670	0.5310
a1	0.2620	0.1770
b	0.2920	0.5100
b1	0.2540	0.1730
c	0.3480	0.5280
c1	0.2840	0.1760
d	0.3360	0.5210
d1	0.2310	0.1470
e	0.1580	0.4380
e1	0.2260	0.1560
f	0.1640	0.4470
f1	0.2730	0.1240
g	0.0990	0.3840
g1	0.3060	0.1490
h	0.2150	0.4800
h1	0.1890	0.1490
i	0.2940	0.4960
i1	0.2430	0.2320
j	0.2100	0.4710
j1	0.2070	0.1650
k	0.2460	0.4880
k1	0.2370	0.1790
l	0.2790	0.5200
m	0.1820	0.4480
m1	0.2000	0.2000
n	0.1580	0.4320

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Chain	Atom inclusion	Q-score
n1	0.3230	0.1490
o	0.1070	0.4000
o1	0.2650	0.2040
p	0.0010	0.2150
p1	0.0250	0.1470
r	0.0910	0.3850
r1	0.2370	0.1650
s	0.1790	0.4480
s1	0.2430	0.1250
t	0.2150	0.4900
t1	0.1700	0.2200
u	0.0370	0.3030
u1	0.1280	0.1660
v	0.1690	0.4370
v1	0.1470	0.1550
w	0.1640	0.4320
w1	0.2460	0.2170
x	0.0850	0.3690
x1	0.2090	0.1910
y	0.2250	0.4760
y1	0.2950	0.1590
z	0.1690	0.4790
z1	0.1960	0.1480