Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 12:54 PM JST

PDB ID	:	9LE8 / pdb_00009le8
EMDB ID	:	EMD-63018
Title	:	Coordinates of Cryo-EM structure of the Arabidopsis thaliana C2S2M2-type PSII supercomplex
Authors	:	Chen, S.J.B.; Wu, C.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on	:	2025-01-07
Resolution	:	3.37 Å(reported)

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

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

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

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

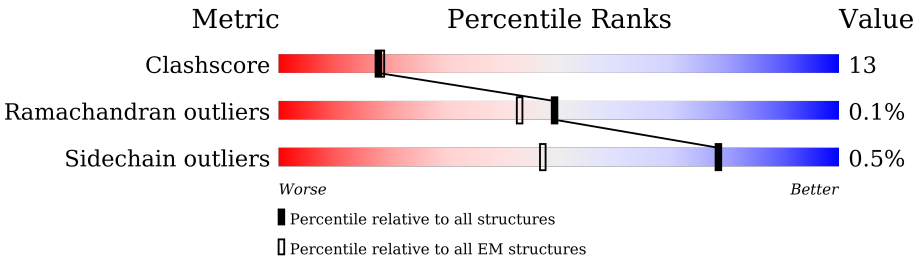
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

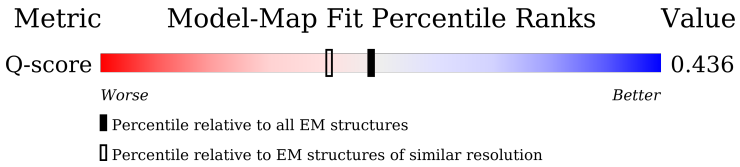
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.37 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	14287 (2.87 - 3.87)

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	9	266	64% 12% 24%
1	AA	266	62% 14% 24%
1	AC	266	60% 15% • 24%
1	AE	266	64% 12% • 24%

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Mol	Chain	Length	Quality of chain
2	0	243	72% 19% 9%
2	AD	243	74% 17% 9%
3	AB	212	62% 28% 9%
3	AF	212	71% 19% 9%
4	AJ	352	81% 11% 8%
4	J	352	78% 14% 8%
5	AK	508	78% 16% 6%
5	O	508	78% 16% 6%
6	AL	459	87% 8% 6%
6	P	459	85% 9% 6%
7	AM	352	84% 13%
7	Q	352	82% 15%
8	E	83	47% 30% 23%
8	e	83	57% 19% 23%
9	F	39	44% 31% 26%
9	f	39	38% 36% 26%
10	AH	232	77% 15% 8%
10	AN	232	72% 17% 11%
10	AQ	232	73% 14% 13%
10	AU	232	75% 17% 8%
10	V	232	74% 15% 11%
10	p	232	73% 14% 13%
11	AO	72	6% 56% 26% 17%
11	j	72	51% 32% 17%
12	I	36	72% 25%

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Mol	Chain	Length	Quality of chain
12	i	36	6% 83% 14%
13	K	37	84% 16%
13	k	37	89% 11%
14	AP	38	61% 29% 8%
14	o	38	58% 32% 8%
15	M	34	9% 74% 18% 6%
15	m	34	9% 65% 26% 6%
16	AR	250	61% 16% 21%
16	q	250	59% 20% 21%
17	AS	232	72% 21% 7%
17	v	232	74% 19% 7%
18	AG	33	76% 12% 12%
18	AT	33	76% 12% 12%
19	U	28	32% 61% 29% 11%
19	u	28	29% 61% 29% 11%
20	W	54	22% 80% 19%
20	w	54	22% 81% 17%
21	X	42	5% 60% 26% 14%
21	x	42	7% 62% 24% 14%
22	AI	62	76% 24%
22	AV	62	89% 11%

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
23	CHL	AN	607	-	-	X	-

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 83915 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	9	202	1537	996	250	286	5	0	0
1	AA	202	1537	996	250	286	5	0	0
1	AC	202	1537	996	250	286	5	0	0
1	AE	202	1537	996	250	286	5	0	0

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

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

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

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

- Molecule 4 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	323	2525	1652	415	445	13	0	0
4	AJ	323	2525	1652	415	445	13	0	0

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	O	479	3757	2462	636	647	12	0	0
5	AK	479	3757	2462	636	647	12	0	0

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	P	433	3373	2221	563	578	11	0	0
6	AL	433	3373	2221	563	578	11	0	0

- Molecule 7 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Q	342	2723	1800	445	466	12	0	0
7	AM	342	2723	1800	445	466	12	0	0

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	E	64	521	342	83	96	0	0
8	e	64	521	342	83	96	0	0

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

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

- Molecule 10 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	V	206	1562	1010	255	292	5	0	0
10	p	202	1536	994	251	286	5	0	0
10	AH	213	1621	1048	266	302	5	0	0
10	AN	206	1562	1010	255	292	5	0	0
10	AQ	202	1536	994	251	286	5	0	0
10	AU	213	1621	1048	266	302	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	j	60	447	293	70	82	2	0	0
11	AO	60	447	293	70	82	2	0	0

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

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

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

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

- Molecule 14 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	o	35	293	195	45	53	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	AP	35	293	195	45	53	0	0

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

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

- Molecule 16 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	q	197	1539	1004	251	281	3	0	0
			Total	C	N	O	S		
16	AR	197	1539	1004	251	281	3	0	0

- Molecule 17 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	v	216	1670	1091	272	303	4	0	0
			Total	C	N	O	S		
17	AS	216	1670	1091	272	303	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	AG	29	239	168	33	37	1	0	0
			Total	C	N	O	S		
18	AT	29	239	168	33	37	1	0	0

- Molecule 19 is a protein called Photosystem II 5 kDa protein, chloroplastic.

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

- Molecule 20 is a protein called Photosystem II reaction center W protein, chloroplastic.

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

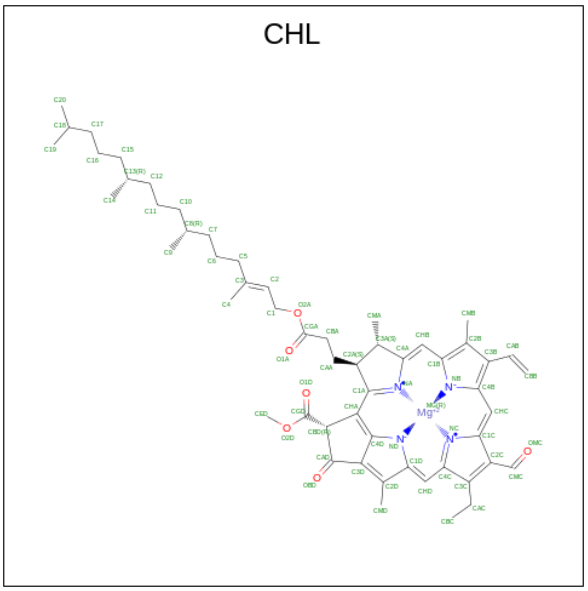
- Molecule 21 is a protein called (thale cress) hypothetical protein.

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

- Molecule 22 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	AI	62	465	313	69	82	1	0	0
22	AV	62	465	313	69	82	1	0	0

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



Mol	Chain	Residues	Atoms					AltConf
23	9	1	Total 41	C 32	Mg 1	N 4	O 4	0
23	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	9	1	Total 63	C 52	Mg 1	N 4	O 6	0
23	9	1	Total 44	C 33	Mg 1	N 4	O 6	0
23	9	1	Total 62	C 51	Mg 1	N 4	O 6	0
23	0	1	Total 64	C 53	Mg 1	N 4	O 6	0
23	0	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	0	1	Total 53	C 42	Mg 1	N 4	O 6	0
23	0	1	Total 44	C 34	Mg 1	N 4	O 5	0
23	0	1	Total 36	C 28	Mg 1	N 4	O 3	0
23	0	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AA	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AA	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AA	1	Total 61	C 50	Mg 1	N 4	O 6	0
23	AA	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AA	1	Total 59	C 48	Mg 1	N 4	O 6	0
23	AA	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AB	1	Total 45	C 34	Mg 1	N 4	O 6	0
23	AB	1	Total 40	C 32	Mg 1	N 4	O 3	0
23	AB	1	Total 44	C 33	Mg 1	N 4	O 6	0
23	AB	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	AB	1	42	33	1	4	4	0
			Total	C	Mg	N	O	
23	AC	1	44	33	1	4	6	0
			Total	C	Mg	N	O	
23	AC	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AC	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AC	1	44	33	1	4	6	0
			Total	C	Mg	N	O	
23	AC	1	62	51	1	4	6	0
			Total	C	Mg	N	O	
23	AD	1	63	52	1	4	6	0
			Total	C	Mg	N	O	
23	AD	1	64	53	1	4	6	0
			Total	C	Mg	N	O	
23	AD	1	53	42	1	4	6	0
			Total	C	Mg	N	O	
23	AD	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AD	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
23	AD	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AE	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AE	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
23	AE	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AE	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
23	AE	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AE	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AF	1	45	34	1	4	6	0
			Total	C	Mg	N	O	
23	AF	1	33	27	1	4	1	0
			Total	C	Mg	N	O	
23	AF	1	35	26	1	4	4	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	AF	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AF	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
23	V	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	V	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	V	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	V	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
23	V	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
23	V	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	p	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	p	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
23	p	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	p	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	p	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	p	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
23	q	1	63	52	1	4	6	0
			Total	C	Mg	N	O	
23	q	1	54	43	1	4	6	0
			Total	C	Mg	N	O	
23	q	1	52	41	1	4	6	0
			Total	C	Mg	N	O	
23	q	1	42	33	1	4	4	0
			Total	C	Mg	N	O	
23	v	1	44	33	1	4	6	0
			Total	C	Mg	N	O	
23	v	1	35	28	1	4	2	0
			Total	C	Mg	N	O	
23	v	1	46	35	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	v	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
23	AH	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	AH	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
23	AH	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	AH	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	AH	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	AN	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	AN	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	AN	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	AN	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	AN	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
23	AN	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
23	AQ	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	AQ	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
23	AQ	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	AQ	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	AQ	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	AQ	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	AR	1	64	53	1	4	6	0
			Total	C	Mg	N	O	
23	AR	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
23	AR	1	53	42	1	4	6	0

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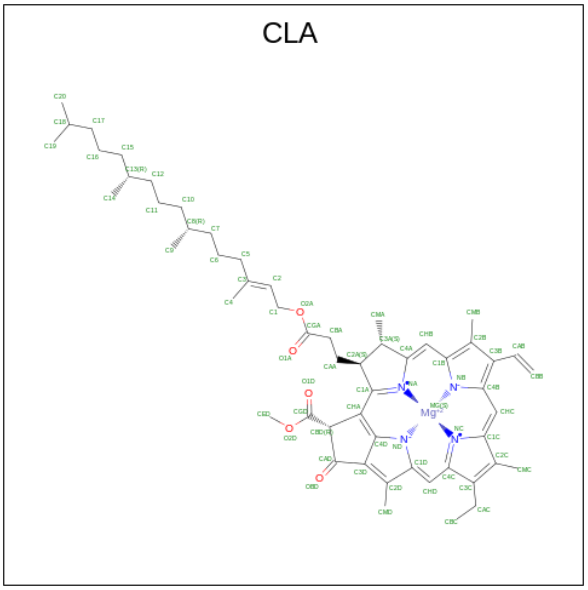
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	AR	1	42	33	1	4	4	0
			Total	C	Mg	N	O	
23	AS	1	44	33	1	4	6	0
			Total	C	Mg	N	O	
23	AS	1	34	27	1	4	2	0
			Total	C	Mg	N	O	
23	AS	1	58	47	1	4	6	0
			Total	C	Mg	N	O	
23	AS	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
23	AU	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	AU	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
23	AU	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
23	AU	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
23	AU	1	66	55	1	4	6	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	9	1	61	51	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	9	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	54	45	1	4	4	0
			Total	C	Mg	N	O	
24	9	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
24	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
24	0	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	0	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	0	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	0	1	58	49	1	4	4	0
			Total	C	Mg	N	O	
24	0	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	0	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	0	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
24	0	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	AA	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
24	AA	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	AA	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AA	1	48	39	1	4	4	0
			Total	C	Mg	N	O	
24	AA	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
24	AA	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	AA	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AA	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AB	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AB	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AB	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AB	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
24	AB	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AB	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AC	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
24	AC	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	AC	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	AC	1	54	45	1	4	4	0
			Total	C	Mg	N	O	
24	AC	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
24	AC	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
24	AC	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
24	AC	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
24	AD	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	AD	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	AD	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AD	1	58	49	1	4	4	0
			Total	C	Mg	N	O	
24	AD	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	AD	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AD	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
24	AD	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	AE	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
24	AE	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	AE	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AE	1	48	39	1	4	4	0
			Total	C	Mg	N	O	
24	AE	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AE	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AE	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AE	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AF	1	39	32	1	4	2	0
			Total	C	Mg	N	O	
24	AF	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AF	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AF	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
24	AF	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AF	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	J	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	J	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	J	1	58	49	1	4	4	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	63	54	1	4	4	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	P	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	P	1	61	52	1	4	4	0
			Total	C	Mg	N	O	
24	Q	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	V	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	V	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	V	1	34	28	1	4	1	0
			Total	C	Mg	N	O	
24	V	1	62	53	1	4	4	0
			Total	C	Mg	N	O	
24	V	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	V	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
24	V	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	K	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	p	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	p	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	p	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	p	1	63	53	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	p	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
24	p	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	p	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
24	p	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	q	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	q	1	58	49	1	4	4	0
			Total	C	Mg	N	O	
24	q	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	q	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	q	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	q	1	63	54	1	4	4	0
			Total	C	Mg	N	O	
24	q	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	q	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	q	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
24	q	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
24	v	1	53	44	1	4	4	0
			Total	C	Mg	N	O	
24	v	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
24	v	1	49	39	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	v	1	53	44	1	4	4	0
			Total	C	Mg	N	O	
24	v	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	AH	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AH	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AH	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	AH	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	AH	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	AH	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	AH	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AH	1	46	37	1	4	4	0
			Total	C	Mg	N	O	
24	AJ	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AJ	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AJ	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	AJ	1	58	49	1	4	4	0
			Total	C	Mg	N	O	
24	AK	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AK	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AK	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AK	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AK	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AK	1	63	54	1	4	4	0
			Total	C	Mg	N	O	
24	AK	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	AK	1	65	55	1	4	5	0
24	AK	1	65	55	1	4	5	0
24	AK	1	65	55	1	4	5	0
24	AK	1	65	55	1	4	5	0
24	AK	1	65	55	1	4	5	0
24	AK	1	65	55	1	4	5	0
24	AK	1	65	55	1	4	5	0
24	AK	1	65	55	1	4	5	0
24	AK	1	65	55	1	4	5	0
24	AL	1	65	55	1	4	5	0
24	AL	1	65	55	1	4	5	0
24	AL	1	65	55	1	4	5	0
24	AL	1	65	55	1	4	5	0
24	AL	1	65	55	1	4	5	0
24	AL	1	65	55	1	4	5	0
24	AL	1	65	55	1	4	5	0
24	AL	1	65	55	1	4	5	0
24	AL	1	65	55	1	4	5	0
24	AL	1	65	55	1	4	5	0
24	AL	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	AL	1	61	52	1	4	4	0
			Total	C	Mg	N	O	
24	AM	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AM	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AN	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AN	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AN	1	37	31	1	4	1	0
			Total	C	Mg	N	O	
24	AN	1	62	53	1	4	4	0
			Total	C	Mg	N	O	
24	AN	1	39	32	1	4	2	0
			Total	C	Mg	N	O	
24	AN	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	AN	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AN	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	AQ	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AQ	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AQ	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	AQ	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AQ	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	AQ	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	AQ	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	AQ	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
24	AR	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	AR	1	58	49	1	4	4	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	AR	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	AR	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	AR	1	39	32	1	4	2	0
			Total	C	Mg	N	O	
24	AR	1	63	54	1	4	4	0
			Total	C	Mg	N	O	
24	AR	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	AR	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	AR	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	AR	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
24	AS	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
24	AS	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	AS	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	AS	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
24	AS	1	53	44	1	4	4	0
			Total	C	Mg	N	O	
24	AS	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
24	AS	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	AS	1	53	44	1	4	4	0
			Total	C	Mg	N	O	
24	AS	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	AU	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AU	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AU	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	AU	1	60	50	1	4	5	0

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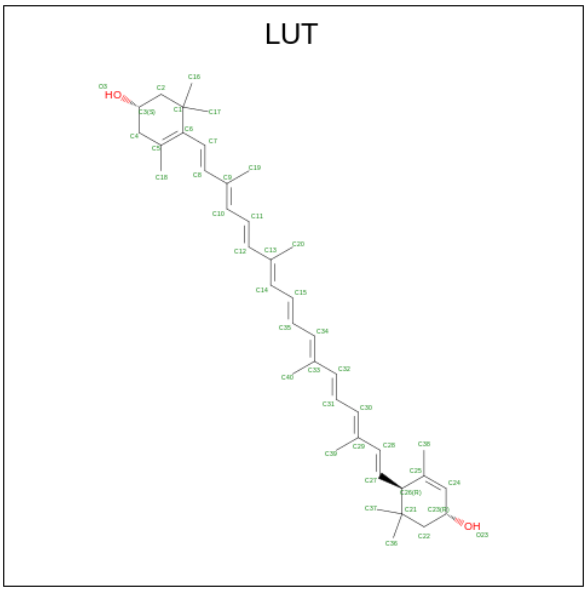
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	AU	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	AU	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	AU	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	AU	1	48	38	1	4	5	0

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



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	9	1	42	40	2	0
			Total	C	O	
25	9	1	42	40	2	0
			Total	C	O	
25	0	1	42	40	2	0
			Total	C	O	
25	0	1	42	40	2	0
			Total	C	O	
25	AA	1	42	40	2	0
			Total	C	O	
25	AA	1	42	40	2	0
			Total	C	O	
25	AC	1	42	40	2	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	AC	1	42	40	2	0
25	AD	1	42	40	2	0
25	AD	1	42	40	2	0
25	AE	1	42	40	2	0
25	AE	1	42	40	2	0
25	AF	1	42	40	2	0
25	V	1	42	40	2	0
25	V	1	42	40	2	0
25	p	1	42	40	2	0
25	p	1	42	40	2	0
25	q	1	42	40	2	0
25	v	1	42	40	2	0
25	v	1	42	40	2	0
25	AH	1	42	40	2	0
25	AH	1	42	40	2	0
25	AN	1	42	40	2	0
25	AN	1	42	40	2	0
25	AQ	1	42	40	2	0
25	AQ	1	42	40	2	0
25	AR	1	42	40	2	0
25	AS	1	42	40	2	0

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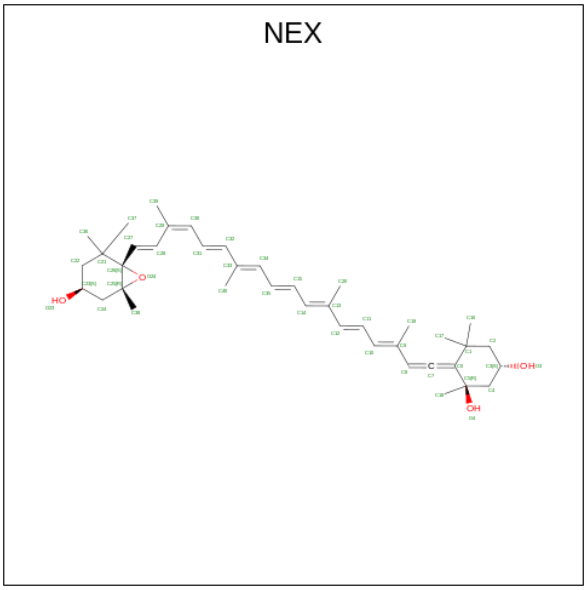
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	AS	1	42	40	2	0
25	AU	1	42	40	2	0
25	AU	1	42	40	2	0

- Molecule 26 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	9	1	44	40	4	0
26	AA	1	44	40	4	0
26	AC	1	44	40	4	0
26	AE	1	44	40	4	0
26	p	1	44	40	4	0
26	q	1	44	40	4	0
26	v	1	44	40	4	0

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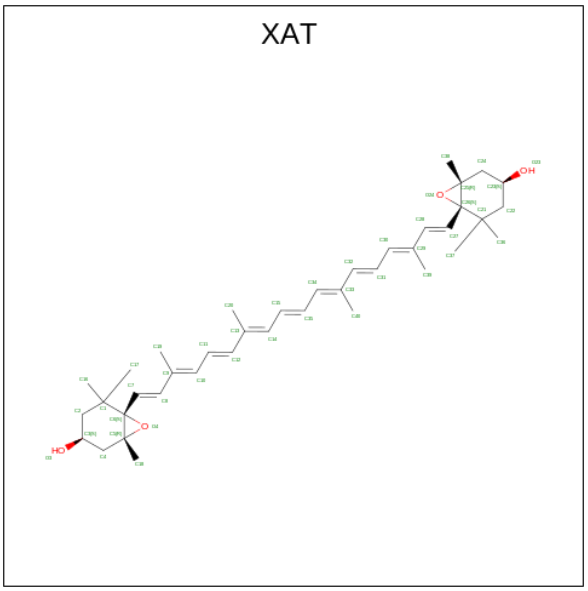
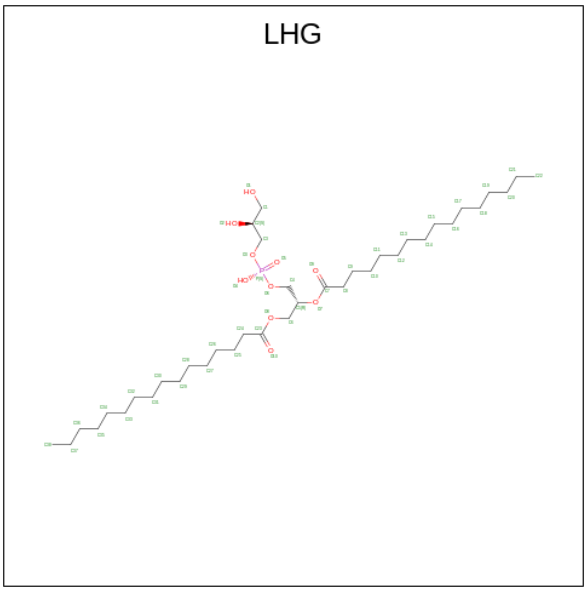
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	AQ	1	44	40	4	0
26	AR	1	44	40	4	0
26	AS	1	44	40	4	0
26	AU	1	44	40	4	0

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



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	9	1	44	40	4	0
27	AB	1	44	40	4	0
27	AF	1	44	40	4	0
27	q	1	44	40	4	0
27	AR	1	44	40	4	0

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
28	0	1	Total	C	O	P	0
			47	36	10	1	
28	AD	1	Total	C	O	P	0
			47	36	10	1	
28	O	1	Total	C	O	P	0
			49	38	10	1	
28	O	1	Total	C	O	P	0
			46	35	10	1	
28	O	1	Total	C	O	P	0
			49	38	10	1	
28	P	1	Total	C	O	P	0
			49	38	10	1	
28	Q	1	Total	C	O	P	0
			49	38	10	1	
28	V	1	Total	C	O	P	0
			49	38	10	1	
28	p	1	Total	C	O		0
			40	35	5		
28	q	1	Total	C	O	P	0
			42	31	10	1	
28	v	1	Total	C	O	P	0
			49	38	10	1	
28	W	1	Total	C	O	P	0
			49	38	10	1	
28	AH	1	Total	C	O	P	0
			49	38	10	1	
28	AK	1	Total	C	O	P	0
			46	35	10	1	

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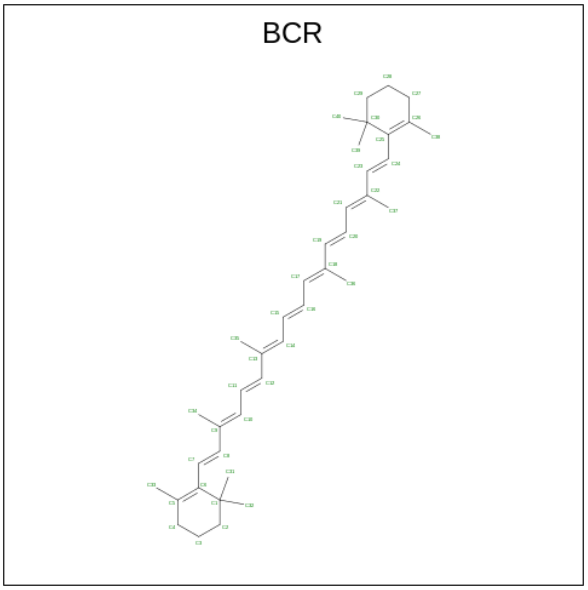
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
28	AK	1	49	38	10	1	0
28	AL	1	49	38	10	1	0
28	AM	1	49	38	10	1	0
28	AN	1	49	38	10	1	0
28	AQ	1	49	38	10	1	0
28	AS	1	49	38	10	1	0
28	w	1	49	38	10	1	0
28	AU	1	49	38	10	1	0

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



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
29	AB	1	40	40	0
29	AF	1	40	40	0
29	J	1	40	40	0

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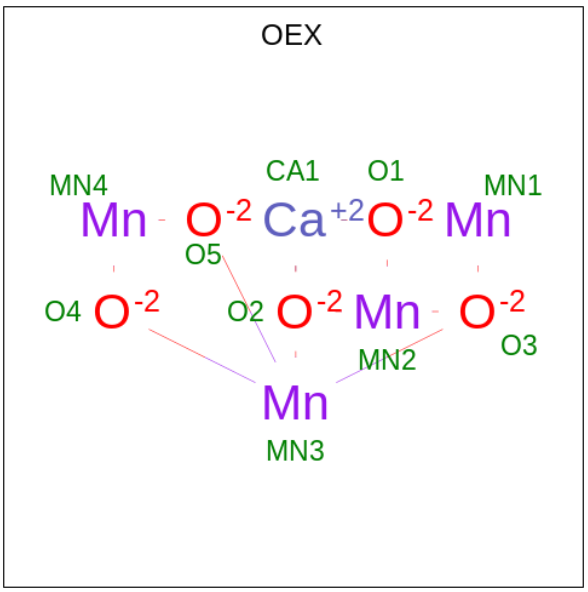
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
29	O	1	40	40	0
			Total	C	
29	O	1	40	40	0
			Total	C	
29	O	1	40	40	0
			Total	C	
29	O	1	40	40	0
			Total	C	
29	P	1	40	40	0
			Total	C	
29	P	1	40	40	0
			Total	C	
29	P	1	40	40	0
			Total	C	
29	F	1	40	40	0
			Total	C	
29	j	1	40	40	0
			Total	C	
29	AI	1	40	40	0
			Total	C	
29	AJ	1	40	40	0
			Total	C	
29	AK	1	40	40	0
			Total	C	
29	AK	1	40	40	0
			Total	C	
29	AK	1	40	40	0
			Total	C	
29	AK	1	40	40	0
			Total	C	
29	AL	1	40	40	0
			Total	C	
29	AL	1	40	40	0
			Total	C	
29	f	1	40	40	0
			Total	C	
29	AO	1	40	40	0
			Total	C	
29	k	1	40	40	0
			Total	C	
29	AV	1	40	40	0

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).

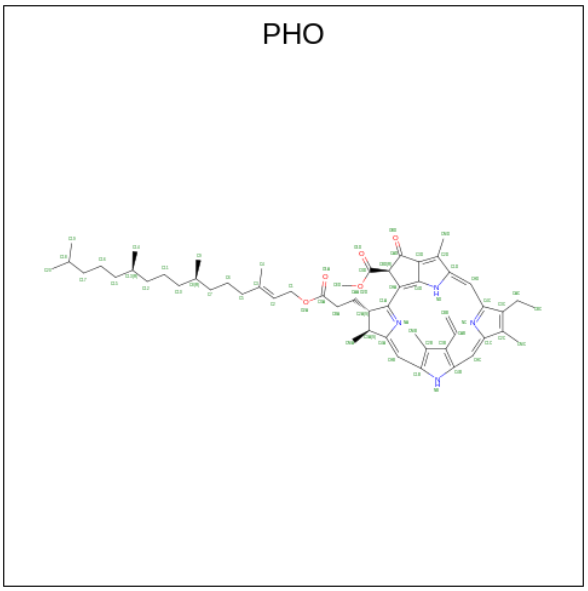


Mol	Chain	Residues	Atoms				AltConf
30	J	1	Total 10	Ca 1	Mn 4	O 5	0
30	AJ	1	Total 10	Ca 1	Mn 4	O 5	0

- Molecule 31 is FE (II) ION (CCD ID: FE2) (formula: Fe).

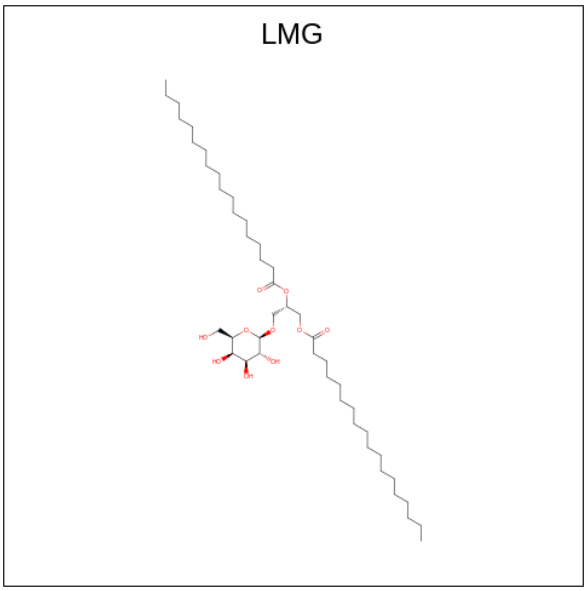
Mol	Chain	Residues	Atoms		AltConf
31	J	1	Total 1	Fe 1	0
31	AJ	1	Total 1	Fe 1	0

- Molecule 32 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



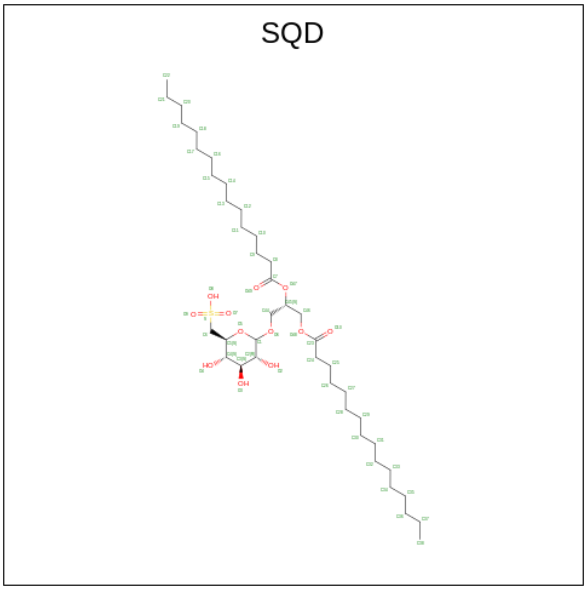
Mol	Chain	Residues	Atoms				AltConf
32	J	1	Total	C	N	O	0
			64	55	4	5	
32	J	1	Total	C	N	O	0
			64	55	4	5	
32	AJ	1	Total	C	N	O	0
			64	55	4	5	
32	AJ	1	Total	C	N	O	0
			64	55	4	5	

- 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	J	1	48	38	10		0
33	O	1	51	41	10		0
33	O	1	40	30	10		0
33	P	1	51	41	10		0
33	Q	1	46	36	10		0
33	AK	1	40	30	10		0
33	AK	1	51	41	10		0
33	AL	1	48	38	10		0
33	AL	1	51	41	10		0
33	AM	1	46	36	10		0

- Molecule 34 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	
34	J	1	54	41	12	1	0

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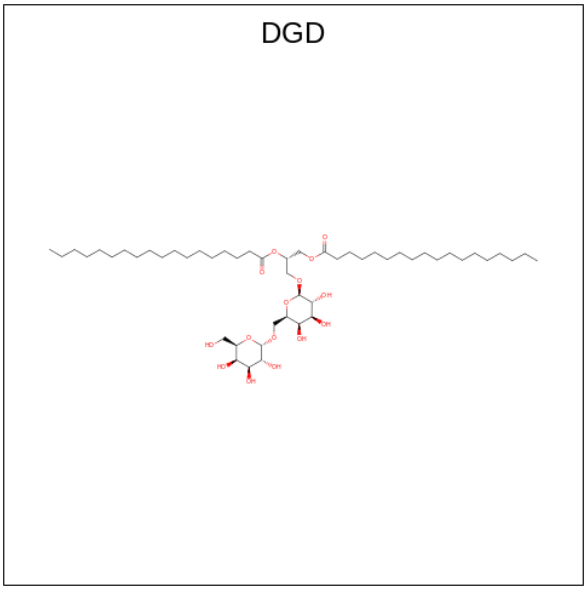
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
34	Q	1	50	37	12	1	0
34	o	1	42	29	12	1	0
34	M	1	54	41	12	1	0
34	AJ	1	54	41	12	1	0
34	AM	1	50	37	12	1	0
34	AP	1	42	29	12	1	0
34	m	1	54	41	12	1	0

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	J	1	60	45	15	0
35	J	1	59	44	15	0
35	P	1	55	40	15	0
35	j	1	62	47	15	0

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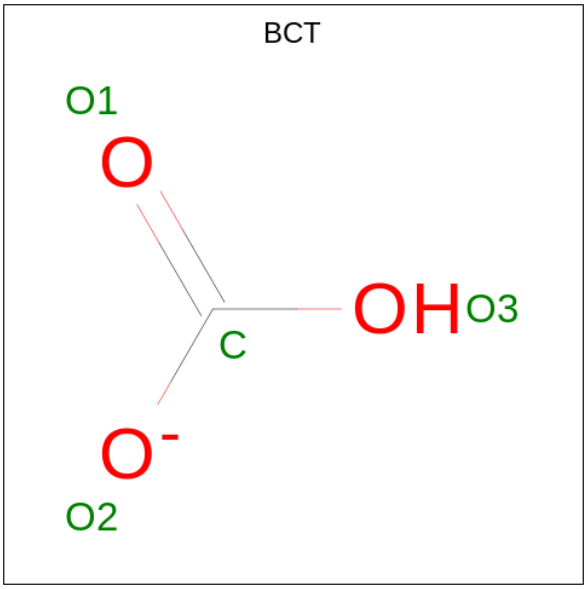
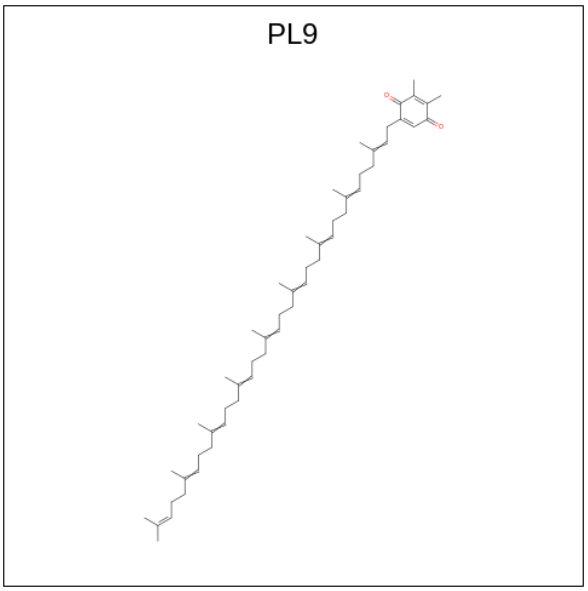
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	AJ	1	59	44	15	0
35	AJ	1	60	45	15	0
35	AL	1	55	40	15	0
35	AL	1	62	47	15	0
35	AO	1	62	47	15	0

- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



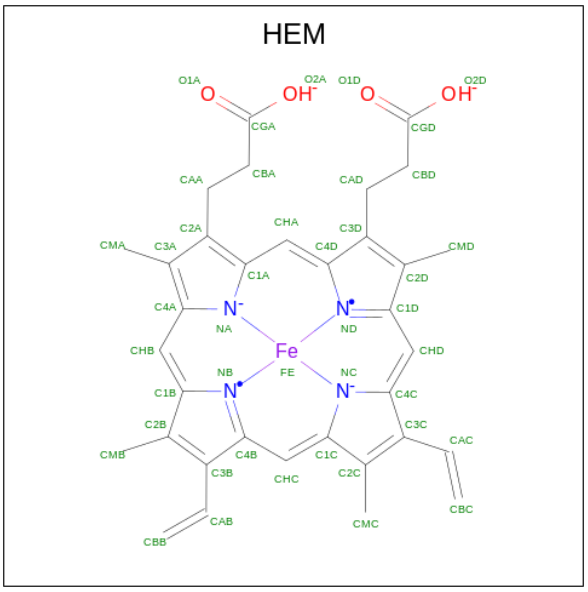
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	J	1	4	1	3	0
36	AM	1	4	1	3	0

- Molecule 37 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
37	Q	1	Total 52	C 50	O 2	0
37	AM	1	Total 52	C 50	O 2	0

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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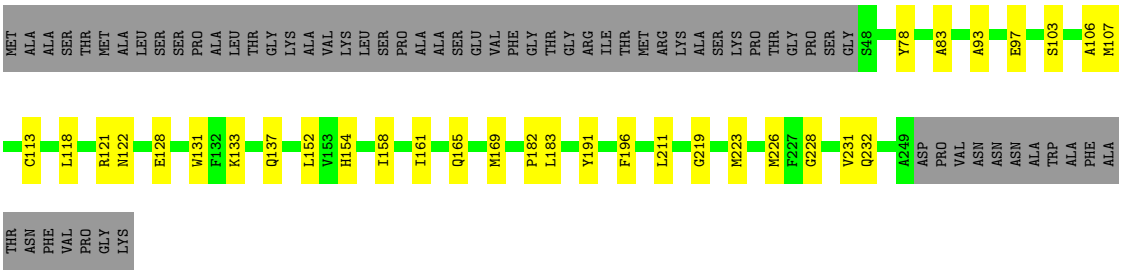
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
38	f	1	43	34	1	4	4	0

3 Residue-property plots (i)

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

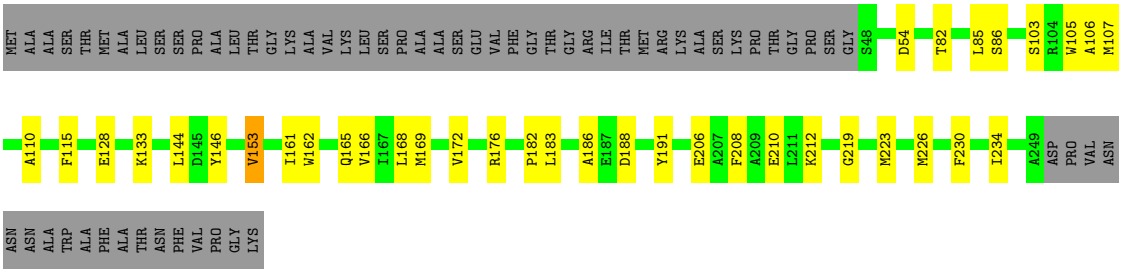
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 9: 64% 12% 24%



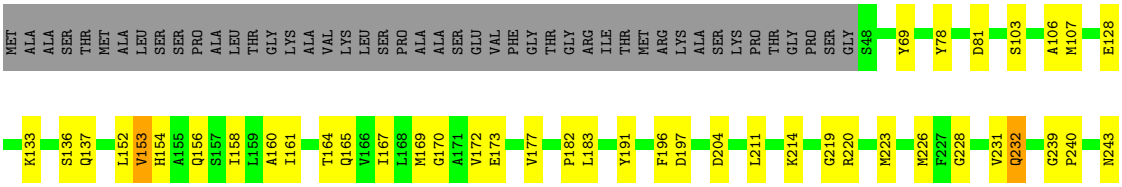
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain AA: 62% 14% 24%



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

Chain AC: 60% 15% • 24%



A249 ASP PRO VAL ASN ASN ASN ALA TRP ALA PHE ALA THR ASN PHE VAL PRO GLY LYS

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

Chain AE: 64% 12% • 24%

MET ALA ALA SER THR MET ALA LEU SER SER PRO ALA LEU THR GLY LYS ALA VAL LYS LEU SER PRO ALA ALA SER GLU VAL PHE GLY THR GLY ARG ILE THR MET ARG LYS ALA SER LYS PRO THR GLY PRO SER GLY S48 D54 L59 S63 S103 R104 W105 A106 M107

E128 A129 V130 L152 V153 H154 W162 V166 I167 L168 M169 G170 A171 V172 R176 P182 L183 A186 D197 E206 E210 G219 M223 M226 Q232 T236 G237 K238 E242 N243 A249 ASP PRO VAL ASN ASN ASN ALA TRP ALA PHE ALA THR ASN

PHE VAL PRO GLY LYS

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

Chain 0: 72% 19% 9%

ALA SER SER PHE ASN PRO LEU ARG ASP VAL VAL SER LEU GLY SER PRO LYS TYR THR MET G43 N44 D45 L46 G49 R52 V53 K54 Y66 L67 T68 G69 D78 A94 R101 W102 A103 F108 T112 K118 W119 V120 R121 E126 P127 V128 K131 G141

L142 Q154 V159 L160 Q163 V164 M167 V170 L178 D179 E183 L187 L197 A200 E208 L209 I214 G217 R218 M221 G226 F227 F228 V229 Q230 N253 G264 ALA

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

Chain AD: 74% 17% 9%

ALA SER SER PHE ASN PRO LEU ARG ASP VAL VAL SER LEU GLY SER PRO LYS TYR THR MET G43 R52 V61 Q62 L67 Y75 S83 F89 A90 K91 A94 R101 W102 A103 M104 T112 K118 K125 K131 Q135 E139 G140 G141 L142 Q154

S155 I156 V159 M167 G168 L169 V170 R174 E183 L187 L209 G217 M221 F227 G235 K236 G237 E240 V250 N253 G264 ALA

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

Chain AB: 62% 28% 9%

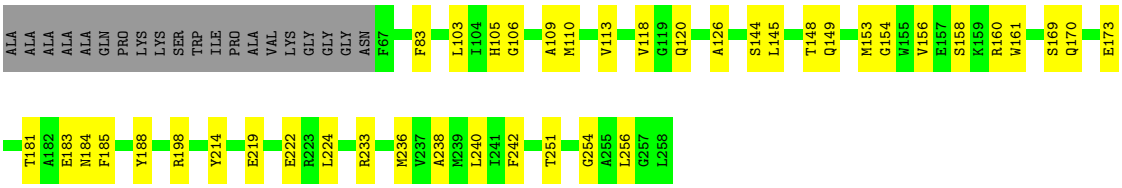
ALA ALA ALA ALA ALA GLN PRO LYS LYS SER TRP ILE PRO ALA VAL LYS GLY GLY GLY ASN F67 P70 L73 L77 P78 G82 F83 L95 R99 L103 I104 H105 G106 A109 A112 V113 L114 G115 I116 F117 V118 G119 Q120 V125 A126 A130 Q133

S144 T148 Q149 L150 L151 V156 E157 W161 V162 D163 P167 Q170 E173 T176 T181 A182 E183 N184 F185 Q192 R198 L203 A206 G207 K208 N209 R210 V213 Y214 E219 K220 L221 L224 K225 I229 S232 R233 L234 M239 L240 I241

E245 T251 P252 L258

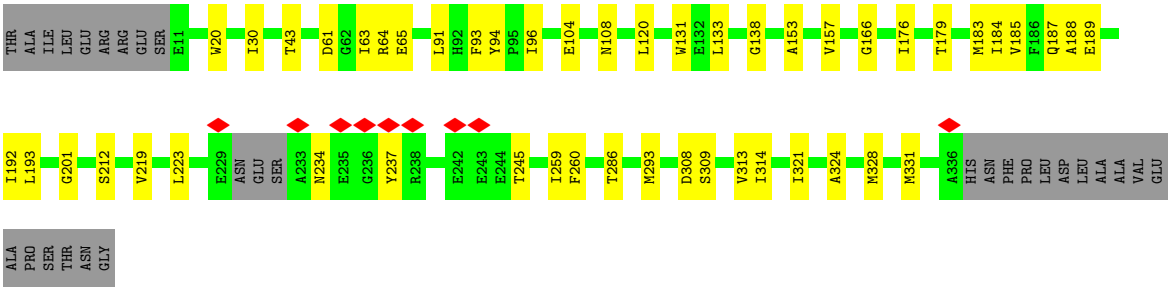
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain AF: 71% 19% 9%



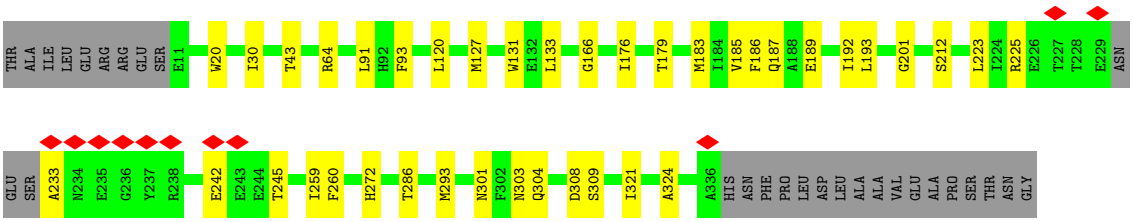
• Molecule 4: Photosystem II protein D1

Chain J: 78% 14% 8%



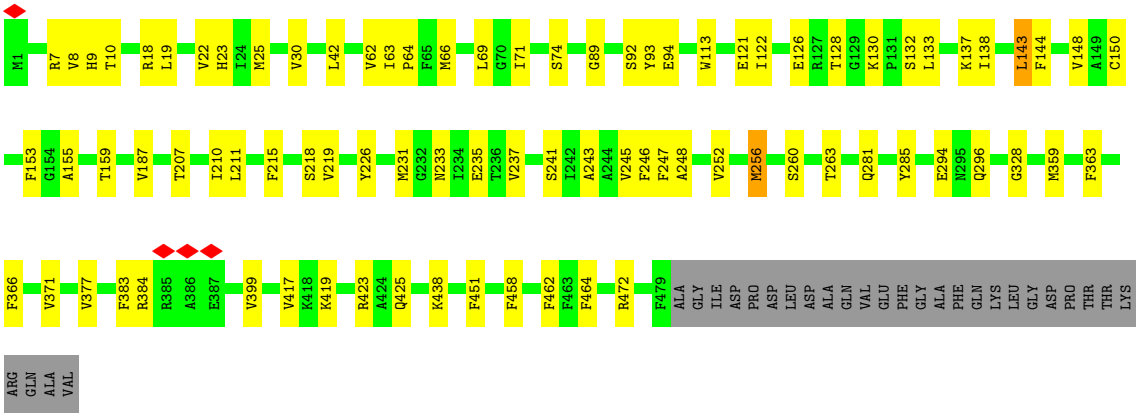
• Molecule 4: Photosystem II protein D1

Chain AJ: 81% 11% 8%



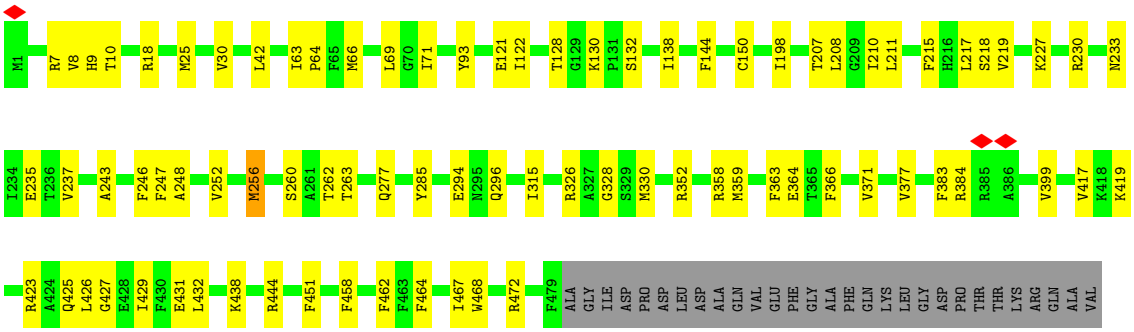
• Molecule 5: Photosystem II CP47 reaction center protein

Chain O: 78% 16% 6%



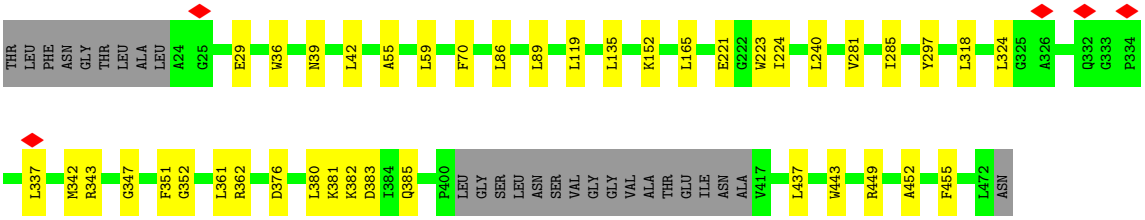
• Molecule 5: Photosystem II CP47 reaction center protein

Chain AK:



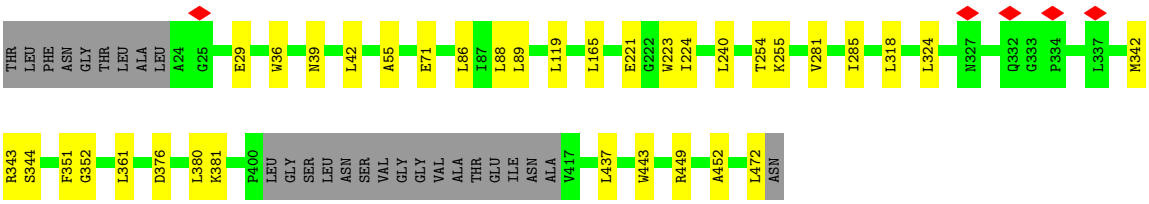
- Molecule 6: Photosystem II CP43 reaction center protein

Chain P:



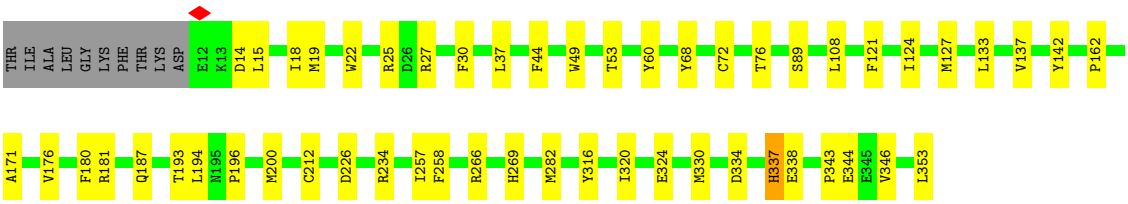
- Molecule 6: Photosystem II CP43 reaction center protein

Chain AL:



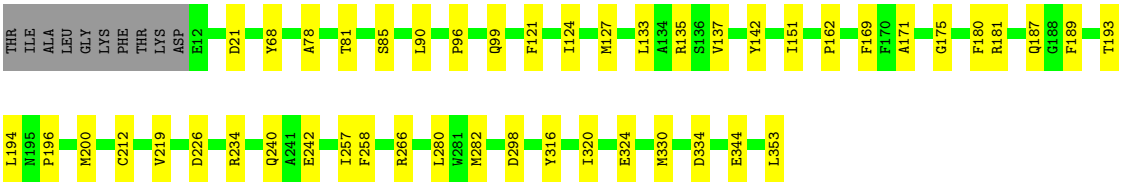
- Molecule 7: Photosystem II D2 protein

Chain Q:



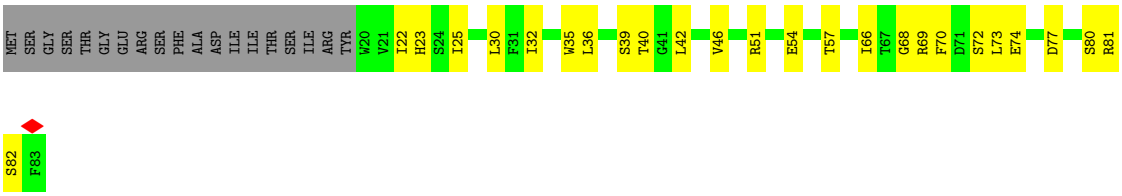
- Molecule 7: Photosystem II D2 protein

Chain AM:



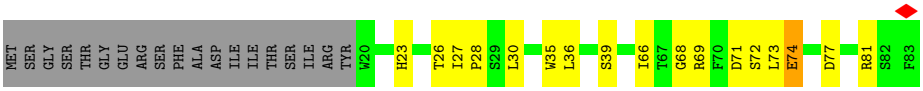
• Molecule 8: Cytochrome b559 subunit alpha

Chain E:



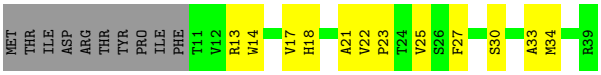
• Molecule 8: Cytochrome b559 subunit alpha

Chain e:



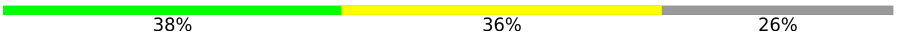
• Molecule 9: Cytochrome b559 subunit beta

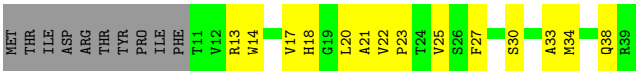
Chain F:



• Molecule 9: Cytochrome b559 subunit beta

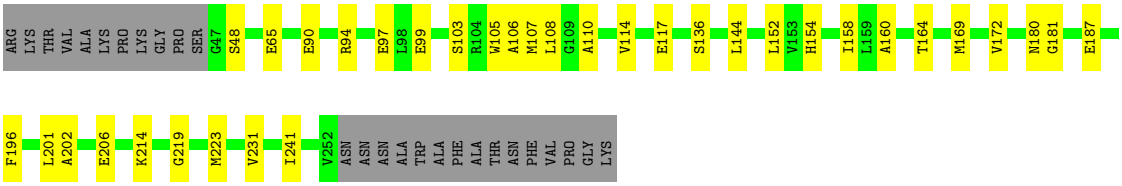
Chain f:





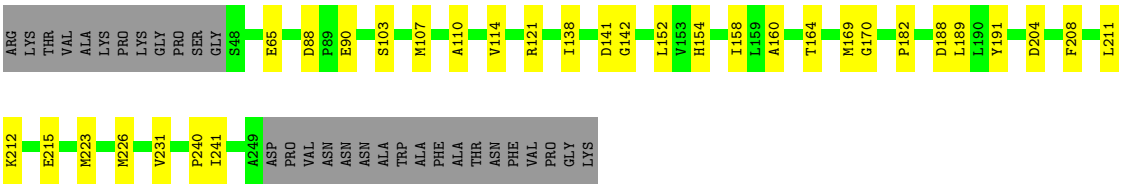
• Molecule 10: Chlorophyll a-b binding protein 1, chloroplastic

Chain V:



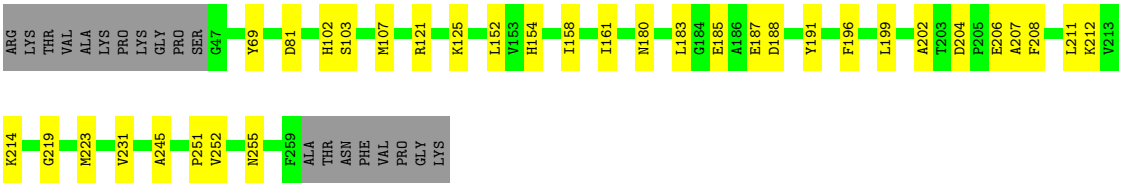
• Molecule 10: Chlorophyll a-b binding protein 1, chloroplastic

Chain p: 73% 14% 13%



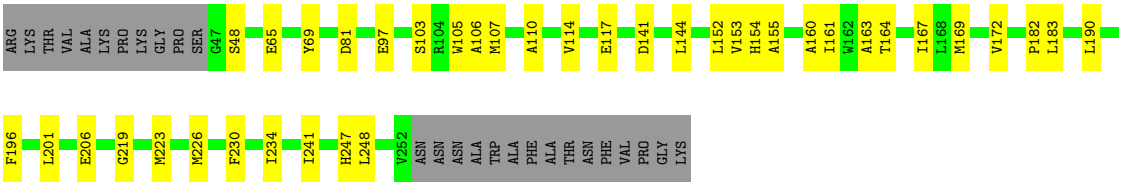
• Molecule 10: Chlorophyll a-b binding protein 1, chloroplastic

Chain AH: 77% 15% 8%



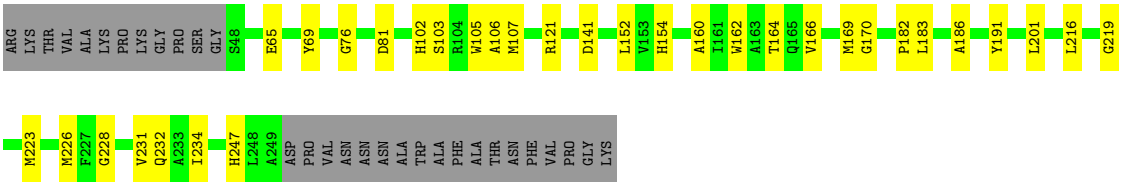
• Molecule 10: Chlorophyll a-b binding protein 1, chloroplastic

Chain AN: 72% 17% 11%



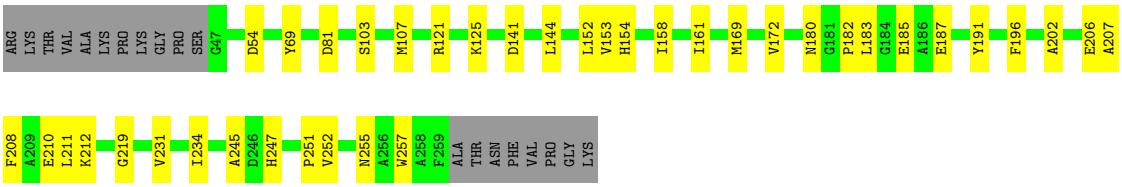
• Molecule 10: Chlorophyll a-b binding protein 1, chloroplastic

Chain AQ: 73% 14% 13%



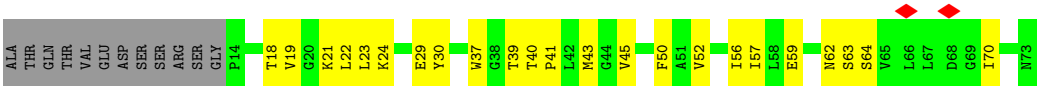
• Molecule 10: Chlorophyll a-b binding protein 1, chloroplastic

Chain AU: 75% 17% 8%



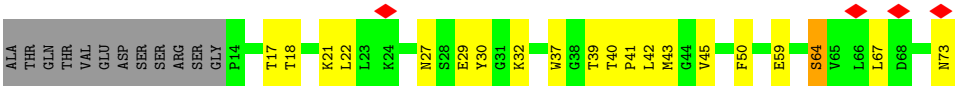
• Molecule 11: Photosystem II reaction center protein H

Chain j:



- Molecule 11: Photosystem II reaction center protein H

Chain AO:

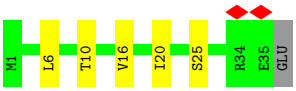


- Molecule 12: Photosystem II reaction center protein I

Chain I:

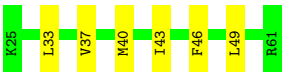
- Molecule 12: Photosystem II reaction center protein I

Chain i:



- Molecule 13: Photosystem II reaction center protein K

Chain K:



- Molecule 13: Photosystem II reaction center protein K

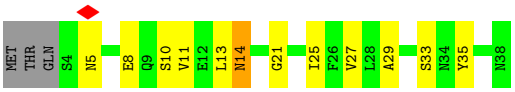
Chain k:

- Molecule 14: Photosystem II reaction center protein L

Chain o:

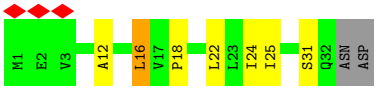
- Molecule 14: Photosystem II reaction center protein L

Chain AP:



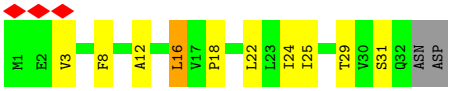
• Molecule 15: Photosystem II reaction center protein M

Chain M:



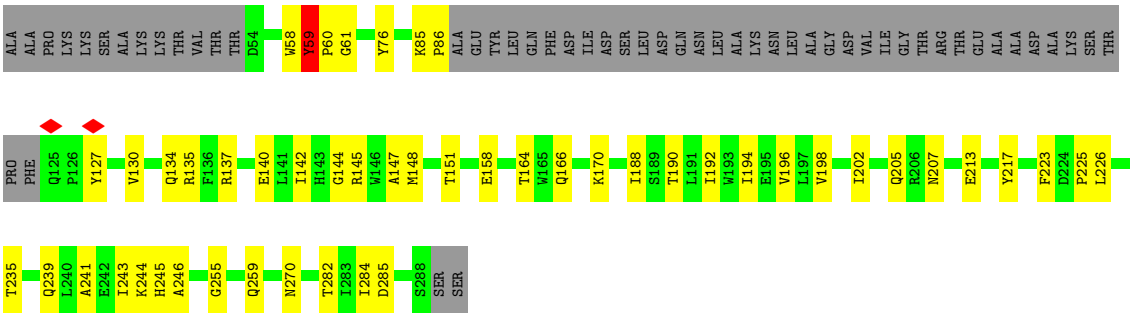
• Molecule 15: Photosystem II reaction center protein M

Chain m:



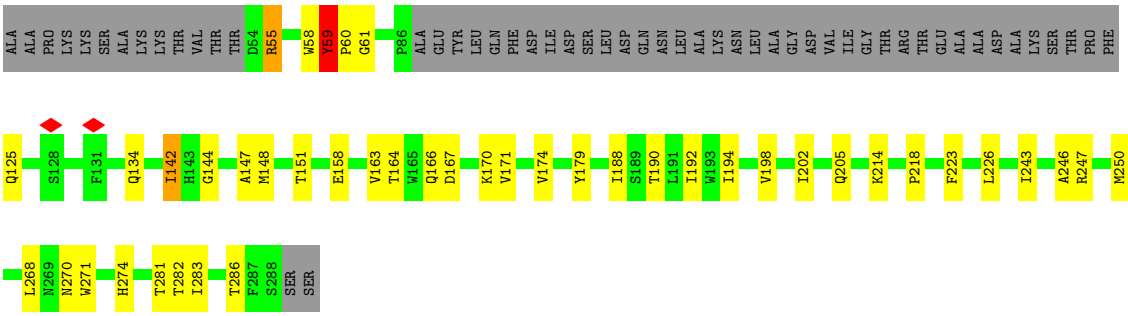
• Molecule 16: Chlorophyll a-b binding protein CP29.1, chloroplastic

Chain q:



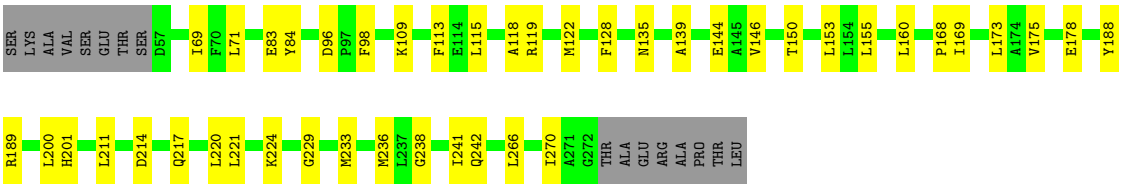
• Molecule 16: Chlorophyll a-b binding protein CP29.1, chloroplastic

Chain AR:



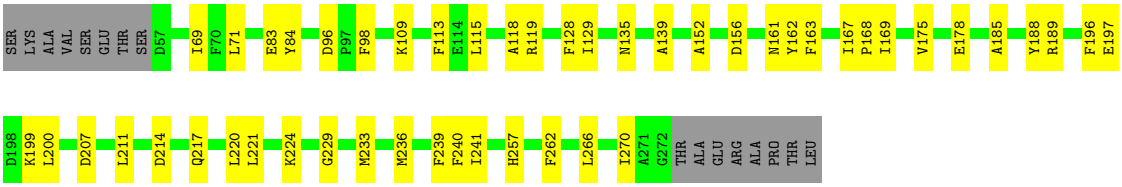
• Molecule 17: Chlorophyll a-b binding protein CP26, chloroplastic

Chain v: 74% 19% 7%



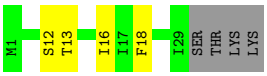
• Molecule 17: Chlorophyll a-b binding protein CP26, chloroplastic

Chain AS: 72% 21% 7%



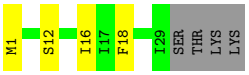
• Molecule 18: Photosystem II reaction center protein T

Chain AG: 76% 12% 12%



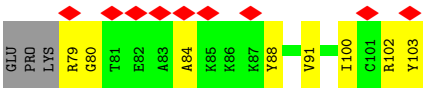
• Molecule 18: Photosystem II reaction center protein T

Chain AT: 76% 12% 12%



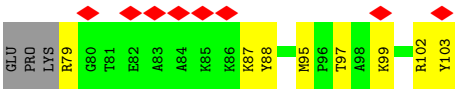
• Molecule 19: Photosystem II 5 kDa protein, chloroplastic

Chain U: 32% 61% 29% 11%



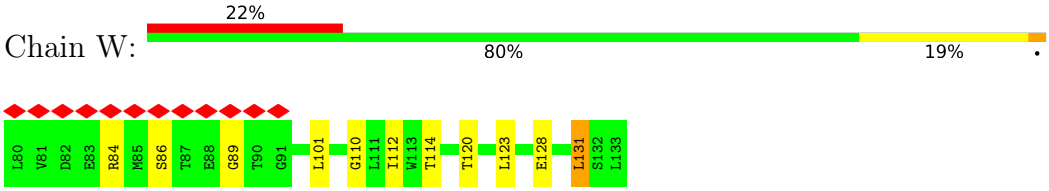
• Molecule 19: Photosystem II 5 kDa protein, chloroplastic

Chain u: 29% 61% 29% 11%



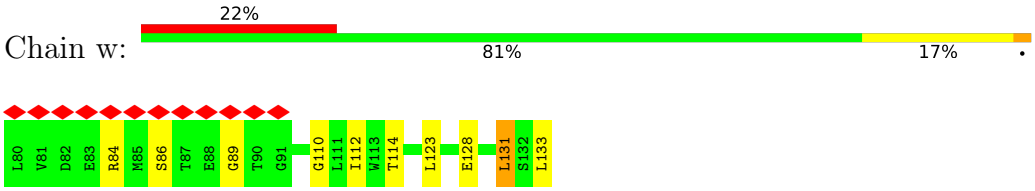
• Molecule 20: Photosystem II reaction center W protein, chloroplastic

Chain W:



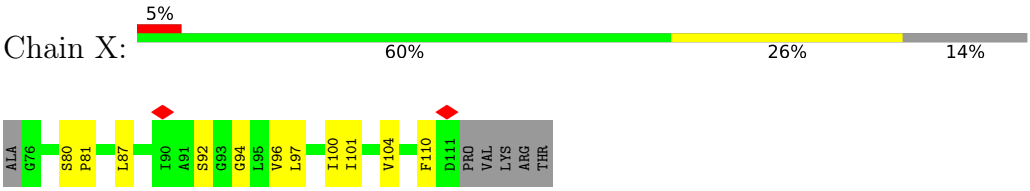
• Molecule 20: Photosystem II reaction center W protein, chloroplastic

Chain w:



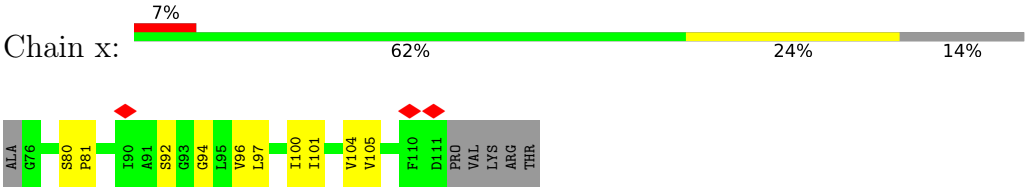
• Molecule 21: (thale cress) hypothetical protein

Chain X:



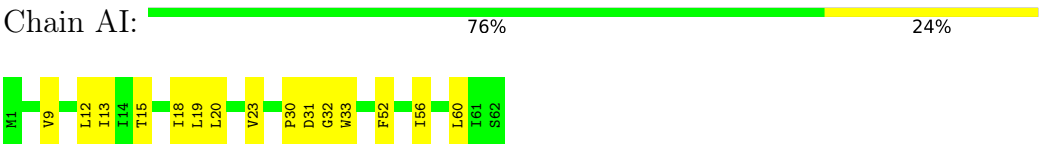
• Molecule 21: (thale cress) hypothetical protein

Chain x:



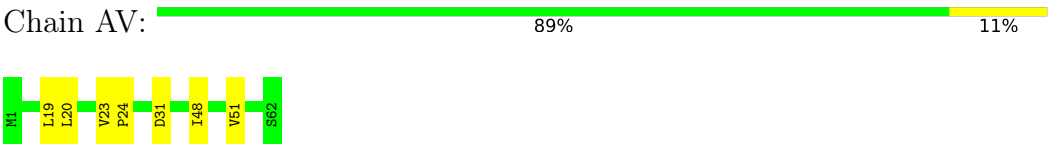
• Molecule 22: Photosystem II reaction center protein Z

Chain AI:



• Molecule 22: Photosystem II reaction center protein Z

Chain AV:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38544	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	57.686	Depositor
Minimum map value	-23.601	Depositor
Average map value	0.027	Depositor
Map value standard deviation	1.343	Depositor
Recommended contour level	4.62	Depositor
Map size (Å)	583.2, 583.2, 583.2	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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: BCT, LHG, PHO, LUT, PL9, OEX, NEX, DGD, BCR, CLA, HEM, XAT, SQD, LMG, CHL, FE2

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	9	0.15	0/1582	0.35	0/2150
1	AA	0.17	0/1582	0.41	0/2150
1	AC	0.15	0/1582	0.38	0/2150
1	AE	0.16	0/1582	0.39	0/2150
2	0	0.18	0/1768	0.45	0/2405
2	AD	0.19	0/1768	0.42	0/2405
3	AB	0.18	0/1564	0.46	0/2123
3	AF	0.22	0/1564	0.54	0/2123
4	AJ	0.14	0/2602	0.35	0/3546
4	J	0.15	0/2602	0.36	0/3546
5	AK	0.15	0/3886	0.36	1/5293 (0.0%)
5	O	0.16	0/3886	0.38	1/5293 (0.0%)
6	AL	0.14	0/3487	0.34	0/4750
6	P	0.13	0/3487	0.33	0/4750
7	AM	0.15	0/2816	0.39	0/3837
7	Q	0.16	0/2816	0.40	0/3837
8	E	0.19	0/538	0.48	0/731
8	e	0.21	0/538	0.56	1/731 (0.1%)
9	F	0.18	0/230	0.41	0/311
9	f	0.19	0/230	0.39	0/311
10	AH	0.17	0/1669	0.40	0/2270
10	AN	0.17	0/1607	0.40	0/2184
10	AQ	0.15	0/1580	0.35	0/2146
10	AU	0.15	0/1669	0.39	0/2270
10	V	0.16	0/1607	0.38	0/2184
10	p	0.16	0/1580	0.38	0/2146
11	AO	0.19	0/456	0.52	0/619
11	j	0.22	0/456	0.54	0/619
12	I	0.21	0/294	0.55	0/397
12	i	0.19	0/294	0.45	0/397
13	K	0.18	0/313	0.46	0/428
13	k	0.20	0/313	0.41	0/428

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
14	AP	0.19	0/301	0.36	0/409
14	o	0.16	0/301	0.34	0/409
15	M	0.25	0/254	0.52	0/347
15	m	0.27	0/254	0.52	0/347
16	AR	0.22	0/1585	0.51	0/2161
16	q	0.20	0/1585	0.48	0/2161
17	AS	0.16	0/1715	0.39	0/2328
17	v	0.15	0/1715	0.35	0/2328
18	AG	0.18	0/246	0.43	0/333
18	AT	0.14	0/246	0.27	0/333
19	U	0.26	0/197	0.59	0/261
19	u	0.24	0/197	0.50	0/261
20	W	0.16	0/439	0.42	0/594
20	w	0.15	0/439	0.36	0/594
21	X	0.20	0/250	0.40	0/339
21	x	0.17	0/250	0.39	0/339
22	AI	0.21	0/475	0.47	0/649
22	AV	0.18	0/475	0.42	0/649
All	All	0.17	0/62872	0.40	3/85522 (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
11	AO	0	1
16	AR	0	2
16	q	0	2
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	e	74	GLU	CA-CB-CG	5.70	125.50	114.10
5	O	256	MET	CB-CG-SD	5.45	129.05	112.70
5	AK	256	MET	CB-CG-SD	5.39	128.87	112.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AO	64	SER	Peptide
16	AR	58	TRP	Peptide
16	AR	59	TYR	Peptide
16	q	58	TRP	Peptide
16	q	59	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	9	1537	0	1480	28	0
1	AA	1537	0	1480	36	0
1	AC	1537	0	1480	37	0
1	AE	1537	0	1480	32	0
2	0	1716	0	1658	49	0
2	AD	1716	0	1658	33	0
3	AB	1512	0	1444	49	0
3	AF	1512	0	1444	48	0
4	AJ	2525	0	2443	35	0
4	J	2525	0	2443	39	0
5	AK	3757	0	3641	76	0
5	O	3757	0	3641	81	0
6	AL	3373	0	3302	30	0
6	P	3373	0	3302	37	0
7	AM	2723	0	2615	42	0
7	Q	2723	0	2615	55	0
8	E	521	0	497	23	0
8	e	521	0	497	12	0
9	F	225	0	233	15	0
9	f	225	0	233	14	0
10	AH	1621	0	1550	31	0
10	AN	1562	0	1503	33	0
10	AQ	1536	0	1480	36	0
10	AU	1621	0	1550	34	0
10	V	1562	0	1503	29	0
10	p	1536	0	1480	33	0
11	AO	447	0	471	21	0
11	j	447	0	471	25	0
12	I	286	0	295	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	i	286	0	295	3	0
13	K	302	0	313	4	0
13	k	302	0	313	3	0
14	AP	293	0	283	11	0
14	o	293	0	283	12	0
15	M	250	0	279	10	0
15	m	250	0	279	11	0
16	AR	1539	0	1502	45	0
16	q	1539	0	1502	48	0
17	AS	1670	0	1649	42	0
17	v	1670	0	1649	43	0
18	AG	239	0	255	4	0
18	AT	239	0	255	3	0
19	U	195	0	206	14	0
19	u	195	0	206	14	0
20	W	428	0	405	9	0
20	w	428	0	405	8	0
21	X	248	0	266	14	0
21	x	248	0	266	7	0
22	AI	465	0	495	12	0
22	AV	465	0	495	5	0
23	0	289	0	216	33	0
23	9	302	0	234	30	0
23	AA	304	0	233	27	0
23	AB	217	0	138	15	0
23	AC	242	0	175	20	0
23	AD	331	0	281	42	0
23	AE	306	0	238	35	0
23	AF	203	0	118	14	0
23	AH	296	0	280	47	0
23	AN	353	0	332	59	0
23	AQ	362	0	350	51	0
23	AR	215	0	180	16	0
23	AS	180	0	126	17	0
23	AU	296	0	280	47	0
23	V	349	0	328	55	0
23	p	360	0	347	52	0
23	q	211	0	169	17	0
23	v	163	0	97	14	0
24	0	424	0	369	15	0
24	9	399	0	333	23	0
24	AA	387	0	308	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	AB	265	0	192	11	0
24	AC	388	0	315	30	0
24	AD	424	0	370	20	0
24	AE	370	0	281	13	0
24	AF	259	0	186	18	0
24	AH	471	0	465	30	0
24	AJ	238	0	239	13	0
24	AK	1038	0	1149	79	0
24	AL	841	0	930	33	0
24	AM	130	0	144	5	0
24	AN	441	0	427	23	0
24	AQ	465	0	460	27	0
24	AR	518	0	451	29	0
24	AS	459	0	384	19	0
24	AU	473	0	468	29	0
24	J	188	0	200	12	0
24	K	65	0	72	2	0
24	O	1038	0	1149	77	0
24	P	776	0	858	29	0
24	Q	180	0	183	9	0
24	V	375	0	353	24	0
24	p	427	0	396	22	0
24	q	524	0	458	34	0
24	v	459	0	384	21	0
25	0	84	0	112	4	0
25	9	84	0	112	13	0
25	AA	84	0	112	8	0
25	AC	84	0	112	14	0
25	AD	84	0	112	6	0
25	AE	84	0	112	16	0
25	AF	42	0	56	7	0
25	AH	84	0	112	11	0
25	AN	84	0	112	16	0
25	AQ	84	0	112	6	0
25	AR	42	0	56	12	0
25	AS	84	0	112	8	0
25	AU	84	0	112	12	0
25	V	84	0	112	13	0
25	p	84	0	112	7	0
25	q	42	0	56	10	0
25	v	84	0	112	10	0
26	9	44	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	AA	44	0	56	1	0
26	AC	44	0	56	4	0
26	AE	44	0	56	1	0
26	AQ	44	0	56	2	0
26	AR	44	0	56	6	0
26	AS	44	0	56	1	0
26	AU	44	0	56	1	0
26	p	44	0	56	2	0
26	q	44	0	56	3	0
26	v	44	0	56	1	0
27	9	44	0	56	2	0
27	AB	44	0	56	7	0
27	AF	44	0	56	7	0
27	AR	44	0	56	0	0
27	q	44	0	56	1	0
28	0	47	0	67	3	0
28	AD	47	0	67	0	0
28	AH	49	0	74	0	0
28	AK	95	0	139	3	0
28	AL	49	0	74	2	0
28	AM	49	0	74	2	0
28	AN	49	0	74	2	0
28	AQ	49	0	74	1	0
28	AS	49	0	74	1	0
28	AU	49	0	74	0	0
28	O	144	0	213	7	0
28	P	49	0	74	2	0
28	Q	49	0	74	2	0
28	V	49	0	74	2	0
28	W	49	0	74	2	0
28	p	40	0	67	1	0
28	q	42	0	57	2	0
28	v	49	0	74	1	0
28	w	49	0	74	2	0
29	AB	40	0	56	4	0
29	AF	40	0	56	2	0
29	AI	40	0	56	2	0
29	AJ	40	0	56	4	0
29	AK	160	0	224	11	0
29	AL	80	0	112	5	0
29	AO	40	0	56	3	0
29	AV	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	F	40	0	56	2	0
29	J	40	0	56	4	0
29	O	160	0	224	15	0
29	P	120	0	168	10	0
29	f	40	0	56	3	0
29	j	40	0	56	5	0
29	k	40	0	56	4	0
30	AJ	10	0	0	0	0
30	J	10	0	0	0	0
31	AJ	1	0	0	0	0
31	J	1	0	0	0	0
32	AJ	128	0	148	8	0
32	J	128	0	148	7	0
33	AK	91	0	122	2	0
33	AL	99	0	138	2	0
33	AM	46	0	62	0	0
33	J	48	0	66	0	0
33	O	91	0	122	2	0
33	P	51	0	72	2	0
33	Q	46	0	62	0	0
34	AJ	54	0	78	6	0
34	AM	50	0	67	2	0
34	AP	42	0	48	5	0
34	J	54	0	78	7	0
34	M	54	0	78	3	0
34	Q	50	0	67	2	0
34	m	54	0	78	3	0
34	o	42	0	48	5	0
35	AJ	119	0	154	3	0
35	AL	117	0	150	2	0
35	AO	62	0	82	3	0
35	J	119	0	154	3	0
35	P	55	0	68	1	0
35	j	62	0	82	2	0
36	AM	4	0	1	0	0
36	J	4	0	1	0	0
37	AM	52	0	73	0	0
37	Q	52	0	73	0	0
38	F	43	0	30	4	0
38	f	43	0	30	3	0
All	All	83915	0	83064	2237	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 13.

All (2237) 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)
23:V:607:CHL:H121	23:V:607:CHL:C9	1.34	1.49
23:AU:608:CHL:H121	23:AU:608:CHL:C9	1.38	1.46
23:AH:601:CHL:H52	23:AH:601:CHL:C9	1.36	1.46
23:AH:608:CHL:H121	23:AH:608:CHL:C9	1.37	1.43
23:AN:607:CHL:C9	23:AN:607:CHL:H121	1.37	1.40
23:AU:601:CHL:H52	23:AU:601:CHL:C9	1.31	1.36
23:AH:601:CHL:H92	23:AH:601:CHL:C5	1.45	1.34
23:p:608:CHL:H121	23:p:608:CHL:C9	1.51	1.32
23:AU:601:CHL:H92	23:AU:601:CHL:C5	1.43	1.31
23:AH:608:CHL:C9	23:AH:608:CHL:C12	2.15	1.24
23:AN:607:CHL:H91	23:AN:607:CHL:C12	1.69	1.20
23:AN:607:CHL:C9	23:AN:607:CHL:C12	2.20	1.16
23:AU:608:CHL:C9	23:AU:608:CHL:C12	2.14	1.16
23:AU:608:CHL:C12	23:AU:608:CHL:H91	1.70	1.15
23:V:607:CHL:H91	23:V:607:CHL:C12	1.68	1.15
23:AD:302:CHL:H91	23:AD:302:CHL:C14	1.76	1.14
23:V:607:CHL:C9	23:V:607:CHL:C12	2.18	1.13
23:AH:608:CHL:C12	23:AH:608:CHL:H91	1.72	1.12
23:0:601:CHL:H142	23:0:601:CHL:C9	1.80	1.11
23:AN:608:CHL:HBB1	23:AQ:601:CHL:H2	1.26	1.11
23:0:601:CHL:H91	23:0:601:CHL:C14	1.83	1.07
23:V:607:CHL:H121	23:V:607:CHL:H93	1.35	1.07
23:AN:607:CHL:H121	23:AN:607:CHL:H93	1.39	1.05
23:AQ:608:CHL:C9	23:AQ:608:CHL:H121	1.86	1.04
23:AD:302:CHL:H91	23:AD:302:CHL:H142	1.05	1.03
23:p:608:CHL:H91	23:p:608:CHL:C12	1.84	1.03
23:AQ:608:CHL:H121	23:AQ:608:CHL:H91	1.37	1.03
23:AH:608:CHL:H121	23:AH:608:CHL:H93	1.37	1.03
10:AQ:107:MET:HE1	24:AQ:610:CLA:HAB	1.41	1.00
8:E:69:ARG:HB3	19:U:102:ARG:HH22	1.27	1.00
24:O:602:CLA:HAA1	11:j:57:ILE:HD11	1.45	0.98
23:0:601:CHL:C9	23:0:601:CHL:C14	2.40	0.98
23:AD:302:CHL:H142	23:AD:302:CHL:C9	1.94	0.98
23:0:601:CHL:H142	23:0:601:CHL:H91	0.99	0.98
23:AD:302:CHL:H121	23:AD:302:CHL:H93	1.42	0.97
23:p:608:CHL:C9	23:p:608:CHL:C12	2.35	0.97
23:AU:608:CHL:H121	23:AU:608:CHL:H93	1.41	0.97
23:p:608:CHL:H121	23:p:608:CHL:H91	1.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AD:302:CHL:C14	23:AD:302:CHL:C9	2.42	0.96
23:AU:607:CHL:HMB2	23:AU:607:CHL:H91	1.47	0.96
6:P:165:LEU:HD21	24:P:506:CLA:HAB	1.48	0.96
23:AH:607:CHL:HMB2	23:AH:607:CHL:H91	1.46	0.95
23:AD:301:CHL:H121	23:AD:301:CHL:H91	1.49	0.95
9:F:14:TRP:O	9:F:18:HIS:ND1	1.99	0.95
23:AU:608:CHL:C12	23:AU:608:CHL:H93	1.93	0.94
10:AN:226:MET:HG2	25:AN:615:LUT:H12	1.50	0.93
23:AE:605:CHL:H92	23:AE:605:CHL:HMB1	1.51	0.93
23:AH:608:CHL:C12	23:AH:608:CHL:H93	1.92	0.93
23:AQ:608:CHL:H93	23:AQ:608:CHL:H11	1.51	0.90
24:AF:603:CLA:HBC3	27:AF:613:XAT:H12	1.50	0.90
23:p:608:CHL:H121	23:p:608:CHL:H93	1.51	0.90
6:AL:165:LEU:HD21	24:AL:507:CLA:HAB	1.54	0.89
16:q:130:VAL:HG13	24:q:618:CLA:HED2	1.52	0.89
16:AR:214:LYS:HD3	16:AR:218:PRO:HA	1.52	0.89
23:AH:608:CHL:H121	23:AH:608:CHL:H91	0.90	0.88
23:AH:601:CHL:C9	23:AH:601:CHL:C5	2.13	0.88
23:V:607:CHL:H121	23:V:607:CHL:H91	0.87	0.87
23:V:606:CHL:H201	23:p:601:CHL:H91	1.57	0.86
23:AN:607:CHL:H121	23:AN:607:CHL:H91	0.88	0.86
5:O:226:TYR:HA	5:O:231:MET:HG3	1.57	0.86
5:AK:122:ILE:O	11:AO:27:ASN:ND2	2.10	0.85
23:AU:608:CHL:H121	23:AU:608:CHL:H91	0.87	0.85
23:AN:606:CHL:H201	23:AQ:601:CHL:H91	1.58	0.84
10:AU:183:LEU:HG	23:AU:608:CHL:HBB1	1.57	0.84
24:p:618:CLA:HBB1	24:p:618:CLA:HHC	1.61	0.83
23:AQ:607:CHL:H201	23:AU:601:CHL:H91	1.60	0.82
15:M:24:ILE:HD13	15:m:24:ILE:HD13	1.62	0.81
4:AJ:233:ALA:O	7:AM:266:ARG:NH1	2.14	0.81
23:AD:302:CHL:HBB1	23:AD:302:CHL:HHC	1.63	0.80
23:AU:601:CHL:C9	23:AU:601:CHL:C5	2.11	0.80
2:AD:159:VAL:HG22	23:AD:317:CHL:HAC1	1.61	0.80
4:AJ:308:ASP:OD1	4:AJ:309:SER:N	2.15	0.80
23:p:607:CHL:H201	23:AH:601:CHL:H91	1.63	0.80
23:9:607:CHL:HBA2	27:9:618:XAT:H41	1.62	0.79
23:p:608:CHL:H93	23:p:608:CHL:H11	1.65	0.79
5:AK:294:GLU:HB2	5:AK:296:GLN:HE21	1.48	0.79
24:AF:610:CLA:HBA2	24:AF:610:CLA:HBD	1.65	0.79
23:0:606:CHL:HHC	23:0:606:CHL:HBB1	1.65	0.78
5:AK:217:LEU:HD23	24:AR:617:CLA:HBA2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AB:130:ALA:HA	3:AB:133:GLN:HE22	1.46	0.78
23:AD:302:CHL:C9	23:AD:302:CHL:H121	2.14	0.78
10:AN:107:MET:HE1	24:AN:609:CLA:HAB	1.64	0.78
10:AH:183:LEU:HG	23:AH:608:CHL:HBB1	1.64	0.78
2:AD:125:LYS:HB2	2:AD:135:GLN:HE22	1.46	0.78
24:9:610:CLA:H2	25:9:615:LUT:H26	1.66	0.77
17:v:153:LEU:HD22	17:v:160:LEU:HD13	1.67	0.77
4:AJ:301:ASN:OD1	4:AJ:303:ASN:ND2	2.16	0.77
16:AR:144:GLY:HA3	16:AR:246:ALA:HB1	1.66	0.77
24:AB:603:CLA:HBC3	27:AB:613:XAT:H12	1.66	0.77
24:P:512:CLA:HBA1	24:P:512:CLA:HBD	1.67	0.76
23:AE:605:CHL:HMB1	23:AE:605:CHL:C9	2.14	0.76
24:AL:514:CLA:HBA1	24:AL:514:CLA:HBD	1.68	0.76
1:9:133:LYS:HA	23:9:607:CHL:HED1	1.68	0.75
23:AA:608:CHL:HHC	23:AA:608:CHL:HBB1	1.69	0.75
23:V:607:CHL:H92	23:V:607:CHL:H41	1.68	0.75
17:v:224:LYS:HE2	24:v:311:CLA:HED1	1.66	0.75
17:AS:224:LYS:HE2	24:AS:311:CLA:HED1	1.68	0.75
10:p:226:MET:HG2	25:p:615:LUT:H12	1.69	0.74
8:e:30:LEU:HD11	9:f:22:VAL:HG13	1.69	0.74
10:p:182:PRO:HB2	23:p:608:CHL:HBB2	1.70	0.74
10:AN:161:ILE:HG12	23:AN:617:CHL:HAC1	1.68	0.74
24:AC:609:CLA:H2	25:AC:614:LUT:H26	1.68	0.74
23:AN:607:CHL:H92	23:AN:607:CHL:H41	1.68	0.74
2:0:159:VAL:HG22	23:0:617:CHL:HAC1	1.69	0.74
23:V:607:CHL:C12	23:V:607:CHL:H93	2.02	0.74
17:v:233:MET:HE1	24:v:303:CLA:HAB	1.69	0.74
5:O:294:GLU:HB2	5:O:296:GLN:HE21	1.51	0.73
2:0:167:MET:HE3	23:0:608:CHL:HAC2	1.69	0.73
23:AA:605:CHL:HHC	23:AA:605:CHL:HBB1	1.69	0.73
25:AS:316:LUT:H8	25:AS:316:LUT:H171	1.71	0.73
4:J:308:ASP:OD1	4:J:309:SER:N	2.21	0.73
10:AQ:183:LEU:HG	23:AQ:608:CHL:HBB1	1.70	0.73
16:AR:144:GLY:O	16:AR:148:MET:HG3	1.88	0.73
8:E:69:ARG:HB3	19:U:102:ARG:NH2	2.03	0.73
2:AD:253:ASN:HB2	24:AD:313:CLA:HED1	1.70	0.73
23:AQ:609:CHL:HBB1	23:AU:601:CHL:H51	1.70	0.73
23:AD:302:CHL:C9	23:AD:302:CHL:C12	2.67	0.73
23:p:609:CHL:HBB1	23:AH:601:CHL:H51	1.72	0.72
24:AF:603:CLA:HHC	24:AF:603:CLA:HBB1	1.71	0.72
4:J:104:GLU:OE2	4:J:108:ASN:ND2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:183:LEU:HG	23:AC:607:CHL:HBB1	1.71	0.72
10:V:206:GLU:OE1	10:V:206:GLU:N	2.19	0.72
23:AQ:608:CHL:C3	23:AQ:608:CHL:H92	2.20	0.72
1:AE:176:ARG:HH12	23:AE:607:CHL:HED1	1.54	0.72
1:AC:133:LYS:HA	23:AD:301:CHL:HED1	1.72	0.72
23:AU:601:CHL:HHC	23:AU:601:CHL:HBB1	1.72	0.72
26:p:616:NEX:H192	26:p:616:NEX:H183	1.73	0.71
17:v:175:VAL:HG22	23:v:307:CHL:HBC1	1.72	0.71
23:9:607:CHL:H121	23:9:607:CHL:H91	1.70	0.71
10:V:196:PHE:HA	23:V:607:CHL:H51	1.72	0.71
23:AQ:608:CHL:H92	23:AQ:608:CHL:C2	2.20	0.71
1:9:183:LEU:HG	23:9:608:CHL:HBB1	1.71	0.71
24:V:610:CLA:HBB1	24:V:610:CLA:HHC	1.73	0.71
24:AN:603:CLA:H193	23:AN:608:CHL:C9	2.19	0.71
7:Q:187:GLN:HB2	24:Q:403:CLA:HBC1	1.72	0.71
1:9:161:ILE:HD11	23:9:606:CHL:C2D	2.21	0.71
24:O:601:CLA:HBD	24:O:601:CLA:HBA1	1.73	0.71
2:0:253:ASN:HB2	24:0:613:CLA:HED1	1.71	0.71
1:AC:182:PRO:HB2	23:AC:607:CHL:HBB2	1.73	0.71
1:AA:169:MET:HA	1:AA:172:VAL:HG22	1.72	0.70
25:AE:614:LUT:H161	23:AE:617:CHL:HBB1	1.73	0.70
3:AF:219:GLU:OE1	3:AF:219:GLU:N	2.24	0.70
7:AM:187:GLN:HB2	24:AM:403:CLA:HBC1	1.72	0.70
5:O:285:TYR:HE2	19:U:88:TYR:HA	1.54	0.70
23:AQ:607:CHL:H121	23:AU:601:CHL:H18	1.73	0.70
24:V:603:CLA:H193	23:V:608:CHL:C9	2.21	0.70
16:q:194:ILE:O	16:q:198:VAL:HG22	1.91	0.70
24:AR:604:CLA:H12	26:AR:615:NEX:H382	1.73	0.70
1:AE:223:MET:HE3	24:AE:602:CLA:HMC2	1.74	0.70
24:O:601:CLA:H102	29:j:101:BCR:H402	1.73	0.70
5:O:281:GLN:HE21	19:U:91:VAL:HG22	1.57	0.70
23:V:616:CHL:HHC	23:V:616:CHL:HBB1	1.72	0.70
10:AN:206:GLU:N	10:AN:206:GLU:OE2	2.25	0.70
24:AK:603:CLA:HBD	24:AK:603:CLA:HBA1	1.73	0.70
4:J:184:ILE:HG23	4:J:328:MET:HE2	1.74	0.70
6:P:29:GLU:OE1	6:P:29:GLU:N	2.24	0.70
10:AN:196:PHE:HA	23:AN:607:CHL:H51	1.74	0.70
5:O:92:SER:OG	5:O:94:GLU:OE1	2.07	0.69
8:E:30:LEU:HD11	9:F:22:VAL:HG13	1.73	0.69
23:AN:606:CHL:C20	23:AQ:601:CHL:H91	2.22	0.69
24:q:608:CLA:HHC	24:q:608:CLA:HBB1	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:v:169:ILE:HD12	17:v:173:LEU:HD23	1.73	0.69
2:AD:101:ARG:NH1	23:AD:307:CHL:OBD	2.25	0.69
16:q:255:GLY:O	16:q:259:GLN:HG3	1.92	0.69
5:AK:472:ARG:HH22	24:AK:613:CLA:CGD	2.04	0.69
23:AQ:608:CHL:H91	23:AQ:608:CHL:C12	2.13	0.69
1:9:182:PRO:HB2	23:9:608:CHL:HBB2	1.74	0.69
1:AC:220:ARG:HH12	24:AC:602:CLA:HED2	1.57	0.69
23:p:607:CHL:H121	23:AH:601:CHL:H18	1.73	0.69
10:AN:183:LEU:HG	23:AN:607:CHL:HBB1	1.75	0.69
23:AQ:608:CHL:H93	23:AQ:608:CHL:C1	2.21	0.69
1:AA:161:ILE:HD12	23:AA:617:CHL:HAC1	1.75	0.69
16:AR:194:ILE:O	16:AR:198:VAL:HG22	1.93	0.69
3:AB:161:TRP:HB2	23:AB:608:CHL:HMA2	1.74	0.69
24:O:604:CLA:H41	24:O:604:CLA:H92	1.73	0.69
5:AK:468:TRP:HE1	5:AK:472:ARG:HH21	1.39	0.69
24:AK:603:CLA:H102	29:AO:101:BCR:H402	1.75	0.69
10:AU:103:SER:HB2	10:AU:219:GLY:HA3	1.75	0.69
3:AF:120:GLN:HE22	3:AF:126:ALA:HA	1.58	0.69
23:AH:601:CHL:HHC	23:AH:601:CHL:HBB1	1.75	0.69
3:AB:112:ALA:O	3:AB:116:ILE:HG13	1.93	0.69
4:J:131:TRP:HZ2	6:P:449:ARG:HD2	1.57	0.69
2:AD:94:ALA:HA	2:AD:187:LEU:HD21	1.73	0.68
1:AA:219:GLY:O	1:AA:223:MET:HG3	1.94	0.68
24:AK:606:CLA:H41	24:AK:606:CLA:H92	1.73	0.68
23:AN:607:CHL:C12	23:AN:607:CHL:H93	2.07	0.68
24:AR:608:CLA:HHC	24:AR:608:CLA:HBB1	1.76	0.68
1:AA:223:MET:HE1	24:AA:602:CLA:HAB	1.75	0.68
10:AH:103:SER:HB2	10:AH:219:GLY:HA3	1.75	0.68
10:AN:153:VAL:H	23:AN:617:CHL:HED2	1.59	0.68
3:AF:160:ARG:HH22	23:AF:608:CHL:CGD	2.07	0.68
23:AQ:608:CHL:C9	23:AQ:608:CHL:C2	2.72	0.68
10:AU:158:ILE:O	10:AU:161:ILE:HG22	1.93	0.68
29:O:617:BCR:H383	34:m:101:SQD:H122	1.76	0.68
4:AJ:131:TRP:HZ2	6:AL:449:ARG:HD2	1.58	0.68
5:O:42:LEU:HD11	5:O:93:TYR:HB2	1.75	0.68
23:p:606:CHL:HMC	23:p:607:CHL:C4C	2.24	0.68
23:p:608:CHL:C2	23:p:608:CHL:H92	2.24	0.68
17:AS:233:MET:HE1	24:AS:303:CLA:HAB	1.75	0.68
1:9:128:GLU:N	1:9:137:GLN:OE1	2.27	0.68
1:AC:107:MET:HE1	24:AC:609:CLA:HAB	1.76	0.68
4:J:94:TYR:OH	4:J:104:GLU:OE1	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:M:101:SQD:H122	29:AK:619:BCR:H383	1.76	0.68
17:AS:83:GLU:OE1	17:AS:83:GLU:N	2.25	0.68
10:p:65:GLU:OE1	10:p:65:GLU:N	2.26	0.67
23:v:308:CHL:HHC	23:v:308:CHL:HBB1	1.76	0.67
23:AQ:608:CHL:H121	23:AQ:608:CHL:H93	1.76	0.67
1:AA:206:GLU:OE1	1:AA:206:GLU:N	2.25	0.67
10:V:164:THR:HG21	23:V:616:CHL:HBC1	1.74	0.67
23:AU:601:CHL:C5	23:AU:601:CHL:H93	2.20	0.67
16:q:207:ASN:HD22	24:q:618:CLA:HHD	1.59	0.67
10:p:231:VAL:HG11	24:p:613:CLA:HAC2	1.77	0.67
16:q:144:GLY:O	16:q:148:MET:HG3	1.95	0.67
5:O:137:LYS:NZ	11:j:29:GLU:OE2	2.27	0.67
5:AK:30:VAL:HG12	24:AK:607:CLA:HHD	1.77	0.67
23:AR:605:CHL:HMC	23:AR:606:CHL:C2C	2.24	0.67
24:AR:609:CLA:H2	25:AR:614:LUT:H373	1.77	0.67
1:AE:167:ILE:HG23	1:AE:168:LEU:HD22	1.76	0.67
23:q:605:CHL:HMC	23:q:606:CHL:C2C	2.25	0.67
10:AN:103:SER:OG	10:AN:219:GLY:HA3	1.95	0.67
1:9:231:VAL:HG11	24:9:613:CLA:HAC2	1.76	0.66
23:0:601:CHL:C14	23:0:601:CHL:H93	2.24	0.66
23:AQ:608:CHL:HBD	23:AQ:608:CHL:HBA1	1.75	0.66
24:q:604:CLA:H12	26:q:615:NEX:H382	1.77	0.66
26:AQ:617:NEX:H192	26:AQ:617:NEX:H183	1.77	0.66
11:j:29:GLU:OE1	11:j:29:GLU:N	2.28	0.66
23:AH:608:CHL:H41	23:AH:608:CHL:H92	1.77	0.66
24:9:610:CLA:H72	24:9:610:CLA:HBB1	1.75	0.66
2:0:102:TRP:NE1	23:0:608:CHL:O1D	2.28	0.66
3:AB:78:PRO:HB2	3:AB:229:ILE:HD12	1.77	0.66
20:W:110:GLY:O	20:W:114:THR:HG23	1.96	0.66
24:9:611:CLA:HBB1	24:9:611:CLA:HHC	1.78	0.66
16:AR:188:ILE:O	16:AR:192:ILE:HD12	1.96	0.66
3:AB:144:SER:O	3:AB:148:THR:HG23	1.95	0.66
23:AD:302:CHL:C9	23:AD:302:CHL:H143	2.23	0.66
3:AF:169:SER:OG	3:AF:170:GLN:OE1	2.13	0.66
23:AH:608:CHL:HBD	23:AH:608:CHL:HBA1	1.78	0.66
4:AJ:176:ILE:HD13	24:AJ:405:CLA:HED1	1.78	0.66
24:v:310:CLA:H52	25:v:315:LUT:H28	1.76	0.66
23:AN:606:CHL:HMB2	23:AN:606:CHL:H91	1.77	0.66
1:AE:182:PRO:HB2	23:AE:606:CHL:HBB2	1.78	0.65
17:v:221:LEU:HD23	17:v:224:LYS:HD2	1.78	0.65
16:AR:158:GLU:HB3	16:AR:268:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:131:LYS:HE2	2:0:131:LYS:HA	1.77	0.65
17:v:115:LEU:HD13	17:v:200:LEU:HD12	1.77	0.65
9:f:14:TRP:O	9:f:18:HIS:ND1	2.28	0.65
10:V:90:GLU:OE1	10:V:90:GLU:N	2.25	0.65
23:p:608:CHL:HBD	23:p:608:CHL:HBA1	1.78	0.65
21:x:100:ILE:O	21:x:104:VAL:HG23	1.96	0.65
17:v:229:GLY:O	17:v:233:MET:HG3	1.96	0.65
9:f:13:ARG:O	9:f:17:VAL:HG22	1.97	0.65
2:0:101:ARG:NH1	23:0:607:CHL:OBD	2.30	0.65
8:e:69:ARG:O	8:e:72:SER:OG	2.14	0.65
16:AR:166:GLN:OE1	16:AR:166:GLN:N	2.22	0.65
21:x:92:SER:O	21:x:96:VAL:HG23	1.97	0.65
23:0:601:CHL:H93	23:0:601:CHL:H121	1.77	0.65
10:AH:161:ILE:HD11	23:AH:606:CHL:C2D	2.27	0.65
2:0:118:LYS:HG3	2:0:119:TRP:HD1	1.62	0.65
3:AB:181:THR:OG1	3:AB:184:ASN:OD1	2.14	0.65
10:AU:161:ILE:HD11	23:AU:606:CHL:C2D	2.27	0.65
7:Q:18:ILE:HG22	21:X:110:PHE:CE2	2.32	0.65
7:Q:200:MET:HE2	7:Q:282:MET:HG3	1.79	0.65
16:q:205:GLN:HB3	23:q:607:CHL:CMC	2.27	0.65
25:AN:615:LUT:H181	25:AN:615:LUT:H8	1.77	0.65
24:AR:608:CLA:HMA2	24:AR:617:CLA:CHD	2.27	0.65
24:AF:610:CLA:HBA2	24:AF:610:CLA:CBD	2.26	0.65
5:O:419:LYS:HE2	5:O:423:ARG:HH22	1.60	0.65
11:j:18:THR:HA	11:j:21:LYS:HD2	1.79	0.65
5:AK:10:THR:HG21	24:AK:613:CLA:HED1	1.79	0.65
23:AU:608:CHL:H92	23:AU:608:CHL:H41	1.79	0.65
1:AA:162:TRP:O	1:AA:166:VAL:HG23	1.97	0.64
3:AB:133:GLN:OE1	3:AB:133:GLN:N	2.29	0.64
19:u:97:THR:O	19:u:99:LYS:NZ	2.27	0.64
3:AB:183:GLU:N	3:AB:183:GLU:OE1	2.28	0.64
5:O:30:VAL:HG12	24:O:605:CLA:HHD	1.79	0.64
10:p:211:LEU:HD22	24:p:610:CLA:H2	1.79	0.64
25:AE:614:LUT:H163	23:AE:617:CHL:HMC	1.79	0.64
16:AR:147:ALA:O	16:AR:151:THR:HG23	1.97	0.64
10:AU:231:VAL:HG11	24:AU:612:CLA:HAC2	1.78	0.64
1:AA:165:GLN:HE22	23:AA:606:CHL:HMC	1.61	0.64
32:J:405:PHO:H41	34:J:410:SQD:H223	1.80	0.64
6:P:297:TYR:OH	24:P:501:CLA:O1A	2.15	0.64
1:AA:176:ARG:HH12	23:AA:608:CHL:HED1	1.63	0.64
4:J:176:ILE:HD13	24:J:404:CLA:HED1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AS:221:LEU:HD23	17:AS:224:LYS:HD2	1.80	0.64
1:AC:228:GLY:O	1:AC:232:GLN:NE2	2.30	0.64
24:AC:604:CLA:HMB2	25:AC:615:LUT:H162	1.78	0.64
3:AF:183:GLU:OE1	3:AF:183:GLU:N	2.30	0.64
16:q:170:LYS:HZ1	23:q:606:CHL:CAD	2.10	0.64
16:AR:190:THR:O	16:AR:194:ILE:HG12	1.97	0.64
5:O:247:PHE:HB2	24:O:608:CLA:HBC1	1.80	0.64
7:Q:337:HIS:CE1	7:Q:338:GLU:HG2	2.33	0.64
10:p:160:ALA:O	10:p:164:THR:HG23	1.98	0.64
4:J:237:TYR:HB2	7:Q:266:ARG:HH21	1.62	0.64
17:AS:115:LEU:HD13	17:AS:200:LEU:HD12	1.79	0.64
1:AC:231:VAL:HG11	24:AC:612:CLA:HAC2	1.80	0.64
23:AC:601:CHL:HHD	23:AC:601:CHL:HBC2	1.78	0.64
2:0:94:ALA:HA	2:0:187:LEU:HD21	1.79	0.64
23:AD:301:CHL:H121	23:AD:301:CHL:C9	2.26	0.64
24:AJ:404:CLA:HBD	24:AJ:405:CLA:HAC2	1.79	0.64
23:AN:607:CHL:H192	23:AN:607:CHL:HBA2	1.80	0.64
24:AR:604:CLA:HBA1	24:AR:604:CLA:HBD	1.80	0.64
1:AA:128:GLU:HG2	1:AA:133:LYS:HG2	1.79	0.63
10:p:114:VAL:HG13	10:p:241:ILE:HD11	1.79	0.63
21:X:100:ILE:O	21:X:104:VAL:HG23	1.98	0.63
5:AK:248:ALA:O	5:AK:252:VAL:HG23	1.98	0.63
10:AQ:160:ALA:O	10:AQ:164:THR:HG23	1.98	0.63
24:AE:611:CLA:HBD	24:AE:611:CLA:HBA1	1.80	0.63
2:AD:52:ARG:NH2	2:AD:67:LEU:O	2.31	0.63
3:AF:118:VAL:HG11	24:AF:604:CLA:HAC2	1.80	0.63
5:O:472:ARG:HH12	24:O:611:CLA:CGD	2.10	0.63
23:V:606:CHL:H91	23:V:606:CHL:HMB2	1.78	0.63
1:9:158:ILE:O	1:9:161:ILE:HG22	1.98	0.63
24:AC:610:CLA:HHC	24:AC:610:CLA:HBB1	1.79	0.63
5:O:248:ALA:O	5:O:252:VAL:HG23	1.98	0.63
25:V:614:LUT:H181	25:V:614:LUT:H8	1.81	0.63
10:AN:65:GLU:OE1	10:AN:65:GLU:N	2.21	0.63
6:P:119:LEU:HD21	13:K:40:MET:HE1	1.80	0.63
7:Q:22:TRP:HB2	21:X:110:PHE:CZ	2.34	0.63
4:J:96:ILE:HG12	12:I:1:MET:HE1	1.80	0.63
24:q:612:CLA:HMB2	25:q:614:LUT:H162	1.80	0.63
23:AN:606:CHL:H201	23:AQ:601:CHL:C9	2.29	0.63
10:AH:231:VAL:HG11	24:AH:612:CLA:HAC2	1.80	0.63
7:AM:200:MET:HE2	7:AM:282:MET:HG3	1.81	0.63
16:AR:134:GLN:OE1	16:AR:134:GLN:N	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:219:GLY:O	10:V:223:MET:HG3	1.99	0.63
16:q:144:GLY:HA3	16:q:246:ALA:HB1	1.80	0.63
7:AM:85:SER:HB2	19:u:102:ARG:NH2	2.13	0.63
16:AR:270:ASN:OD1	24:AR:612:CLA:HED1	1.99	0.63
23:AA:606:CHL:H92	23:AA:606:CHL:HMB1	1.81	0.62
10:V:65:GLU:OE1	10:V:65:GLU:N	2.20	0.62
24:AD:303:CLA:HED2	24:AD:303:CLA:H2A	1.81	0.62
23:V:601:CHL:H52	23:V:601:CHL:H92	1.80	0.62
5:AK:419:LYS:HE2	5:AK:423:ARG:HH22	1.64	0.62
24:9:602:CLA:H12	24:9:602:CLA:H3A	1.80	0.62
23:AD:302:CHL:H93	23:AD:302:CHL:C12	2.20	0.62
9:F:27:PHE:HE2	29:F:101:BCR:H12C	1.65	0.62
21:X:92:SER:O	21:X:96:VAL:HG23	2.00	0.62
23:AN:601:CHL:H52	23:AN:601:CHL:H92	1.81	0.62
10:p:223:MET:HE1	24:p:602:CLA:HAB	1.79	0.62
8:E:51:ARG:NH1	8:E:54:GLU:OE2	2.32	0.62
6:AL:318:LEU:HD23	6:AL:351:PHE:HE1	1.65	0.62
24:AL:508:CLA:HMA2	24:AL:508:CLA:H2	1.81	0.62
23:V:606:CHL:H201	23:p:601:CHL:C9	2.29	0.62
24:AK:603:CLA:HAC1	29:AO:101:BCR:H383	1.81	0.62
24:AQ:603:CLA:H152	23:AQ:609:CHL:H91	1.81	0.62
3:AB:104:ILE:HG23	23:AB:608:CHL:HMD1	1.81	0.62
24:J:403:CLA:HBD	24:J:404:CLA:HAC2	1.82	0.62
8:E:70:PHE:HB2	19:U:103:TYR:HE2	1.64	0.62
23:AR:606:CHL:HED2	23:AR:606:CHL:H11	1.81	0.62
25:AS:316:LUT:H8	25:AS:316:LUT:C17	2.30	0.62
23:AU:608:CHL:HBD	23:AU:608:CHL:HBA1	1.82	0.62
2:0:183:GLU:OE1	2:0:183:GLU:N	2.32	0.62
10:p:241:ILE:H	10:p:241:ILE:HD12	1.63	0.62
24:AF:602:CLA:HMC1	27:AF:613:XAT:H31	1.81	0.62
9:f:22:VAL:HB	9:f:23:PRO:HD3	1.82	0.62
23:AN:601:CHL:HED1	28:AN:616:LHG:H141	1.82	0.62
10:AQ:231:VAL:HG11	24:AQ:613:CLA:HAC2	1.81	0.62
3:AF:109:ALA:O	3:AF:113:VAL:HG13	2.00	0.61
5:O:74:SER:HA	5:O:92:SER:HB2	1.81	0.61
9:F:22:VAL:HB	9:F:23:PRO:HD3	1.82	0.61
16:AR:179:TYR:HH	26:AR:615:NEX:H1	1.48	0.61
26:AU:616:NEX:H192	26:AU:616:NEX:H183	1.82	0.61
7:Q:344:GLU:CD	7:Q:344:GLU:H	2.08	0.61
10:p:107:MET:HE1	24:p:610:CLA:CAB	2.30	0.61
16:q:190:THR:O	16:q:194:ILE:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AN:182:PRO:HB2	23:AN:607:CHL:HBB2	1.81	0.61
3:AB:99:ARG:NH2	24:AB:602:CLA:HED1	2.15	0.61
3:AB:114:LEU:O	3:AB:118:VAL:HG12	2.00	0.61
3:AF:236:MET:HE2	24:AF:602:CLA:HMC2	1.80	0.61
15:M:31:SER:OG	15:m:31:SER:OG	1.95	0.61
17:AS:241:ILE:HG21	24:AS:313:CLA:HAC2	1.82	0.61
6:P:318:LEU:HD23	6:P:351:PHE:HE1	1.65	0.61
24:P:507:CLA:HMA2	24:P:507:CLA:H2	1.81	0.61
2:0:52:ARG:NH1	2:0:69:GLY:HA3	2.15	0.61
3:AB:239:MET:HE1	27:AB:613:XAT:C13	2.31	0.61
24:AB:610:CLA:HED3	24:AB:611:CLA:HBC1	1.81	0.61
5:O:9:HIS:HB2	24:O:611:CLA:HBA1	1.83	0.61
17:AS:229:GLY:O	17:AS:233:MET:HG3	1.99	0.61
21:x:101:ILE:O	21:x:105:VAL:HG22	2.00	0.61
2:AD:183:GLU:OE1	2:AD:183:GLU:N	2.31	0.61
3:AF:256:LEU:HD11	25:AF:611:LUT:H172	1.82	0.61
7:Q:193:THR:HG23	24:Q:403:CLA:HBC2	1.82	0.61
11:j:24:LYS:HE2	11:j:24:LYS:HA	1.82	0.61
10:AH:107:MET:HE1	24:AH:609:CLA:HHC	1.82	0.61
9:f:27:PHE:HE2	29:f:101:BCR:H12C	1.65	0.61
3:AF:161:TRP:CD1	23:AF:608:CHL:HBA2	2.35	0.61
16:q:59:TYR:O	16:q:61:GLY:N	2.34	0.61
17:v:266:LEU:O	17:v:270:ILE:HG22	2.01	0.61
23:V:606:CHL:C20	23:p:601:CHL:H91	2.28	0.61
24:p:603:CLA:H152	23:p:609:CHL:H91	1.81	0.61
10:AQ:182:PRO:HB2	23:AQ:608:CHL:HBB2	1.82	0.61
6:P:240:LEU:HD21	24:P:501:CLA:CAB	2.30	0.60
24:AL:505:CLA:H72	35:AL:518:DGD:HBF2	1.83	0.60
23:AR:605:CHL:HBA1	26:AR:615:NEX:H403	1.83	0.60
24:AN:603:CLA:H193	23:AN:608:CHL:H91	1.83	0.60
12:I:4:LEU:O	12:I:8:VAL:HG23	2.01	0.60
24:AJ:404:CLA:H2A	24:AJ:404:CLA:O1D	2.01	0.60
10:AN:247:HIS:HB2	24:AN:612:CLA:HAA2	1.83	0.60
10:p:215:GLU:HG3	24:p:610:CLA:C1B	2.31	0.60
10:AQ:76:GLY:HA3	10:AQ:216:LEU:HD23	1.83	0.60
17:AS:196:PHE:HB2	23:AS:308:CHL:HBC3	1.82	0.60
3:AB:106:GLY:HA3	3:AB:232:SER:HB2	1.83	0.60
23:AD:301:CHL:H91	23:AD:301:CHL:C12	2.27	0.60
7:AM:344:GLU:H	7:AM:344:GLU:CD	2.09	0.60
23:9:607:CHL:H162	23:9:609:CHL:C9	2.31	0.60
24:O:608:CLA:HMB2	7:Q:127:MET:HE2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AL:240:LEU:HD21	24:AL:502:CLA:CAB	2.32	0.60
1:AC:103:SER:HB2	1:AC:219:GLY:HA3	1.84	0.60
5:AK:285:TYR:HE2	19:u:88:TYR:HA	1.66	0.60
23:AQ:608:CHL:H152	26:AQ:617:NEX:H402	1.84	0.60
32:AJ:407:PHO:H41	34:AJ:411:SQD:H223	1.83	0.60
7:AM:85:SER:HB2	19:u:102:ARG:HH22	1.66	0.60
7:AM:193:THR:HG23	24:AM:403:CLA:HBC2	1.84	0.60
28:AS:301:LHG:H101	24:AS:311:CLA:HAB	1.83	0.60
1:AC:226:MET:HG3	25:AC:615:LUT:H12	1.84	0.60
24:O:604:CLA:H161	24:O:616:CLA:H201	1.84	0.60
16:q:282:THR:HG23	16:q:284:ILE:H	1.66	0.60
3:AF:106:GLY:O	3:AF:110:MET:HB2	2.02	0.60
22:AI:19:LEU:O	22:AI:23:VAL:HG23	2.01	0.60
23:AE:616:CHL:HHD	23:AE:617:CHL:OBD	2.03	0.59
10:V:160:ALA:O	10:V:164:THR:HG22	2.01	0.59
16:q:188:ILE:O	16:q:192:ILE:HG13	2.02	0.59
24:AK:611:CLA:HAA1	11:AO:43:MET:HE1	1.82	0.59
23:AN:606:CHL:HHC	23:AN:606:CHL:HBB1	1.84	0.59
10:AU:107:MET:HE1	24:AU:609:CLA:HHC	1.83	0.59
23:AA:605:CHL:HMC	23:AA:606:CHL:C1C	2.32	0.59
1:AA:182:PRO:HB2	23:AA:607:CHL:HBB2	1.82	0.59
10:AU:196:PHE:HA	23:AU:608:CHL:H51	1.84	0.59
23:AH:601:CHL:C5	23:AH:601:CHL:H93	2.24	0.59
16:AR:226:LEU:HD12	25:AR:614:LUT:H222	1.84	0.59
23:0:601:CHL:C9	23:0:601:CHL:H143	2.30	0.59
24:AH:609:CLA:CHB	24:AH:609:CLA:H2	2.33	0.59
24:AU:609:CLA:H2	24:AU:609:CLA:CHB	2.32	0.59
16:q:137:ARG:NH1	16:q:140:GLU:OE2	2.31	0.59
10:AN:160:ALA:O	10:AN:164:THR:HG22	2.02	0.59
18:AG:13:THR:O	18:AG:16:ILE:HG22	2.03	0.59
1:AC:154:HIS:O	1:AC:156:GLN:NE2	2.26	0.59
24:AC:613:CLA:HBD	24:AC:613:CLA:HBA1	1.83	0.59
5:O:256:MET:HG2	5:O:451:PHE:CD1	2.38	0.59
16:q:76:TYR:HB2	24:q:602:CLA:OBD	2.03	0.59
24:AA:612:CLA:HBD	24:AA:612:CLA:HBA1	1.83	0.59
24:J:407:CLA:H2	12:I:12:VAL:HG11	1.85	0.59
24:O:601:CLA:HAC1	29:j:101:BCR:H383	1.84	0.58
10:AQ:141:ASP:OD1	10:AQ:141:ASP:N	2.36	0.58
24:9:604:CLA:H2	26:9:617:NEX:H241	1.83	0.58
2:AD:217:GLY:O	2:AD:221:MET:HG3	2.03	0.58
7:Q:49:TRP:O	7:Q:53:THR:HG23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:x:97:LEU:O	21:x:101:ILE:HG22	2.03	0.58
2:0:66:TYR:OH	2:0:78:ASP:OD2	2.16	0.58
2:AD:142:LEU:HD21	24:AD:305:CLA:HAA2	1.84	0.58
9:F:13:ARG:O	9:F:17:VAL:HG22	2.03	0.58
24:AL:513:CLA:H102	24:AL:514:CLA:H202	1.84	0.58
23:AQ:606:CHL:HMC	23:AQ:607:CHL:C4C	2.33	0.58
17:AS:175:VAL:HG22	23:AS:307:CHL:HBC1	1.85	0.58
26:9:617:NEX:H192	26:9:617:NEX:H183	1.86	0.58
23:AC:608:CHL:HBB1	23:AD:302:CHL:H51	1.84	0.58
2:AD:112:THR:HG21	24:AD:305:CLA:HAC2	1.85	0.58
25:AE:613:LUT:C8	25:AE:613:LUT:H181	2.34	0.58
24:O:612:CLA:HBB1	24:O:614:CLA:HMB2	1.83	0.58
16:q:135:ARG:NH1	24:q:618:CLA:O2D	2.36	0.58
24:O:616:CLA:H172	29:O:619:BCR:H331	1.86	0.58
28:AK:623:LHG:O4	7:AM:142:TYR:OH	2.21	0.58
7:Q:194:LEU:O	14:o:35:TYR:OH	2.20	0.58
6:AL:119:LEU:HD21	13:k:40:MET:HE1	1.85	0.58
24:AR:608:CLA:HMA2	24:AR:617:CLA:HHD	1.85	0.58
3:AF:170:GLN:HG3	23:AF:607:CHL:HMC	1.86	0.58
4:J:234:ASN:HA	7:Q:266:ARG:HD2	1.86	0.58
5:O:23:HIS:ND1	24:O:615:CLA:OBD	2.36	0.58
10:V:110:ALA:O	10:V:114:VAL:HG12	2.04	0.58
17:v:69:ILE:HG22	17:v:71:LEU:H	1.68	0.58
10:AH:252:VAL:O	10:AH:255:ASN:ND2	2.37	0.58
28:w:201:LHG:H191	24:AU:611:CLA:H13	1.85	0.58
28:O:622:LHG:O4	7:Q:142:TYR:OH	2.20	0.58
4:AJ:245:THR:OG1	7:AM:266:ARG:NH2	2.35	0.58
3:AB:70:PRO:HG2	3:AB:73:LEU:HG	1.86	0.58
1:AC:128:GLU:O	1:AC:137:GLN:NE2	2.37	0.58
4:J:223:LEU:HD21	7:Q:266:ARG:HD3	1.86	0.58
5:AK:42:LEU:HD11	5:AK:93:TYR:HB2	1.85	0.58
23:0:601:CHL:H93	23:0:601:CHL:H143	1.85	0.57
3:AF:236:MET:HE2	24:AF:602:CLA:CMC	2.34	0.57
10:AH:196:PHE:HA	23:AH:608:CHL:H51	1.86	0.57
24:AU:609:CLA:H92	24:AU:609:CLA:H41	1.85	0.57
5:O:126:GLU:OE2	5:O:126:GLU:N	2.38	0.57
1:AA:103:SER:O	1:AA:107:MET:HG3	2.04	0.57
25:AN:615:LUT:H181	25:AN:615:LUT:C8	2.33	0.57
26:AS:317:NEX:H181	26:AS:317:NEX:H10	1.87	0.57
1:9:103:SER:HB3	1:9:219:GLY:HA3	1.86	0.57
1:9:106:ALA:CB	1:9:223:MET:HG3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:85:LEU:HB2	24:AA:602:CLA:H11	1.85	0.57
17:v:178:GLU:OE1	23:v:307:CHL:HMC	2.05	0.57
10:AN:230:PHE:O	10:AN:234:ILE:HG22	2.05	0.57
16:AR:205:GLN:HB3	23:AR:607:CHL:CMC	2.33	0.57
23:AR:605:CHL:H101	23:AR:607:CHL:H52	1.86	0.57
23:AN:601:CHL:H18	23:AU:607:CHL:H121	1.86	0.57
23:AQ:607:CHL:HMB2	23:AQ:607:CHL:H91	1.87	0.57
10:V:107:MET:HE1	24:V:609:CLA:HAB	1.86	0.57
28:v:301:LHG:H101	24:v:311:CLA:HAB	1.86	0.57
24:P:511:CLA:H102	24:P:512:CLA:H202	1.87	0.57
10:AQ:65:GLU:OE1	10:AQ:65:GLU:N	2.35	0.57
23:AR:605:CHL:H122	23:AR:607:CHL:H61	1.87	0.57
17:AS:197:GLU:OE2	17:AS:197:GLU:N	2.26	0.57
10:AU:252:VAL:O	10:AU:255:ASN:ND2	2.37	0.57
9:F:18:HIS:O	9:F:22:VAL:HG23	2.05	0.57
23:V:601:CHL:H18	23:AH:607:CHL:H121	1.87	0.57
25:V:614:LUT:H181	25:V:614:LUT:C8	2.34	0.57
24:q:604:CLA:HBA1	24:q:604:CLA:HBD	1.84	0.57
23:AN:607:CHL:HBB1	23:AN:607:CHL:HHC	1.85	0.57
23:AU:608:CHL:H93	23:AU:608:CHL:H122	1.83	0.57
24:AB:603:CLA:HBC3	27:AB:613:XAT:C12	2.35	0.56
4:J:153:ALA:O	4:J:157:VAL:HG22	2.05	0.56
24:O:604:CLA:H203	28:O:621:LHG:H321	1.86	0.56
7:Q:22:TRP:HB2	21:X:110:PHE:HZ	1.69	0.56
23:V:601:CHL:HED1	28:V:615:LHG:H141	1.86	0.56
16:q:147:ALA:O	16:q:151:THR:HG23	2.05	0.56
24:q:602:CLA:HMC2	27:q:617:XAT:H391	1.86	0.56
17:v:238:GLY:O	17:v:242:GLN:HG3	2.05	0.56
28:W:201:LHG:H191	24:AH:611:CLA:H13	1.86	0.56
15:m:3:VAL:HG11	18:AT:1:MET:SD	2.45	0.56
16:AR:163:VAL:HG11	16:AR:171:VAL:HG11	1.87	0.56
10:AU:121:ARG:HH12	10:AU:245:ALA:HB2	1.70	0.56
2:AD:61:VAL:HG13	2:AD:62:GLN:HG3	1.87	0.56
4:J:64:ARG:HH22	6:P:337:LEU:HD21	1.70	0.56
23:V:607:CHL:C9	23:V:607:CHL:C4	2.83	0.56
21:X:97:LEU:O	21:X:101:ILE:HG22	2.05	0.56
23:AN:606:CHL:H91	23:AN:606:CHL:CMB	2.35	0.56
3:AF:83:PHE:CE1	27:AF:613:XAT:H383	2.39	0.56
4:J:185:VAL:O	4:J:189:GLU:HG2	2.05	0.56
5:O:383:PHE:CE2	7:Q:353:LEU:HD21	2.40	0.56
7:Q:37:LEU:HD12	24:Q:404:CLA:HBB1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:337:HIS:HE1	7:Q:338:GLU:OE2	1.87	0.56
34:o:101:SQD:H131	34:m:101:SQD:H142	1.87	0.56
23:p:608:CHL:H92	23:p:608:CHL:C3	2.36	0.56
5:AK:462:PHE:CE2	24:AK:606:CLA:HAC2	2.40	0.56
10:AN:169:MET:HA	10:AN:172:VAL:HG22	1.88	0.56
3:AB:109:ALA:O	3:AB:113:VAL:HG13	2.05	0.56
3:AB:173:GLU:OE1	3:AB:173:GLU:N	2.29	0.56
1:AE:103:SER:HB3	1:AE:219:GLY:HA3	1.88	0.56
5:AK:8:VAL:O	24:AK:616:CLA:HED1	2.06	0.56
2:0:209:LEU:HD21	3:AB:198:ARG:HH22	1.71	0.56
2:AD:167:MET:HA	2:AD:170:VAL:HG22	1.87	0.56
11:j:37:TRP:O	11:j:40:THR:HG23	2.05	0.56
23:p:608:CHL:H152	26:p:616:NEX:H402	1.88	0.56
6:AL:255:LYS:HD3	6:AL:255:LYS:N	2.19	0.56
23:AN:607:CHL:C9	23:AN:607:CHL:C4	2.84	0.56
23:9:605:CHL:HAA1	23:9:605:CHL:CGD	2.36	0.56
3:AB:170:GLN:HG3	23:AB:607:CHL:HMC	1.86	0.56
1:AC:161:ILE:HD11	23:AC:606:CHL:C3D	2.35	0.56
25:AE:613:LUT:H181	25:AE:613:LUT:H8	1.88	0.56
10:V:107:MET:HG3	10:V:219:GLY:HA2	1.87	0.56
23:q:605:CHL:HBA2	26:q:615:NEX:H28	1.87	0.56
4:AJ:185:VAL:O	4:AJ:189:GLU:HG2	2.05	0.56
17:AS:69:ILE:HG22	17:AS:71:LEU:H	1.69	0.56
2:0:167:MET:CE	23:0:608:CHL:HAC2	2.36	0.56
23:0:608:CHL:C4B	1:AA:82:THR:HG21	2.35	0.56
24:J:403:CLA:O1D	24:J:403:CLA:H2A	2.05	0.56
10:V:187:GLU:OE2	10:V:187:GLU:N	2.25	0.56
16:q:244:LYS:NZ	28:q:616:LHG:O5	2.38	0.56
17:AS:185:ALA:HB1	23:AS:308:CHL:HMA3	1.87	0.56
24:V:602:CLA:HAB	25:V:614:LUT:H32	1.87	0.56
16:q:223:PHE:O	25:q:614:LUT:H24	2.06	0.56
10:AN:117:GLU:HB3	10:AN:241:ILE:HD12	1.87	0.56
10:AN:144:LEU:HB2	10:AN:155:ALA:HB3	1.88	0.56
10:AN:163:ALA:O	10:AN:167:ILE:HG12	2.06	0.56
16:AR:59:TYR:O	16:AR:61:GLY:N	2.38	0.56
17:AS:118:ALA:HB1	17:AS:229:GLY:HA3	1.88	0.56
10:V:106:ALA:HB3	10:V:223:MET:HG2	1.88	0.56
23:AA:601:CHL:HBB1	23:AA:601:CHL:HHC	1.88	0.55
24:q:609:CLA:H2	25:q:614:LUT:H373	1.89	0.55
5:AK:247:PHE:HB2	24:AK:610:CLA:HBC1	1.88	0.55
9:f:18:HIS:O	9:f:22:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AC:605:CHL:HAA1	23:AC:605:CHL:CGD	2.36	0.55
10:AN:110:ALA:O	10:AN:114:VAL:HG12	2.06	0.55
3:AB:221:LEU:O	3:AB:225:LYS:HG3	2.06	0.55
8:E:80:SER:OG	8:E:81:ARG:NH1	2.40	0.55
23:V:607:CHL:H92	23:V:607:CHL:C4	2.35	0.55
17:AS:168:PRO:C	17:AS:169:ILE:HD13	2.31	0.55
21:x:80:SER:OG	21:x:81:PRO:HD3	2.06	0.55
16:q:217:TYR:HB3	24:q:609:CLA:CGD	2.36	0.55
17:AS:169:ILE:HG13	23:AS:306:CHL:HMD1	1.88	0.55
23:AE:601:CHL:HHC	23:AE:601:CHL:HBB1	1.87	0.55
5:O:18:ARG:NH1	14:o:5:ASN:HD22	2.05	0.55
10:p:211:LEU:HD13	24:p:610:CLA:H12	1.89	0.55
17:v:214:ASP:OD2	17:v:217:GLN:NE2	2.39	0.55
16:AR:55:ARG:NH1	16:AR:55:ARG:HB2	2.21	0.55
16:AR:125:GLN:HG3	24:AR:617:CLA:O1D	2.06	0.55
24:AC:602:CLA:H12	24:AC:602:CLA:H3A	1.87	0.55
11:j:19:VAL:HA	11:j:22:LEU:HG	1.88	0.55
3:AF:256:LEU:HD21	25:AF:611:LUT:H163	1.87	0.55
34:M:101:SQD:H142	34:AP:101:SQD:H131	1.87	0.55
6:AL:443:TRP:HE1	24:AL:509:CLA:HED3	1.72	0.55
9:f:21:ALA:O	9:f:25:VAL:HG22	2.07	0.55
23:AE:605:CHL:C9	23:AE:605:CHL:CMB	2.84	0.55
5:AK:285:TYR:CE2	19:u:88:TYR:HA	2.41	0.55
1:AE:206:GLU:OE1	1:AE:206:GLU:N	2.23	0.55
11:j:59:GLU:HG3	11:j:64:SER:HB2	1.89	0.55
10:p:141:ASP:OD1	10:p:142:GLY:N	2.40	0.55
24:AB:602:CLA:O2A	27:AB:613:XAT:H241	2.06	0.55
1:AE:197:ASP:OD1	1:AE:197:ASP:N	2.38	0.55
21:X:80:SER:OG	21:X:81:PRO:HD3	2.06	0.55
5:AK:468:TRP:NE1	5:AK:472:ARG:HH21	2.04	0.55
1:AA:226:MET:CE	25:AA:615:LUT:H12	2.36	0.54
3:AB:219:GLU:OE1	3:AB:219:GLU:N	2.23	0.54
1:AC:173:GLU:O	1:AC:177:VAL:HG12	2.07	0.54
17:v:118:ALA:HB1	17:v:229:GLY:HA3	1.88	0.54
23:AH:608:CHL:H93	23:AH:608:CHL:H122	1.85	0.54
17:v:122:MET:HE3	17:v:229:GLY:CA	2.37	0.54
1:9:226:MET:HG3	25:9:616:LUT:H12	1.89	0.54
5:O:328:GLY:N	24:O:607:CLA:O1A	2.29	0.54
24:O:610:CLA:HHC	24:O:610:CLA:HBB1	1.89	0.54
23:V:607:CHL:H93	23:V:607:CHL:H43	1.88	0.54
5:AK:383:PHE:CE2	7:AM:353:LEU:HD21	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AL:86:LEU:HD13	6:AL:89:LEU:HD12	1.90	0.54
23:AC:606:CHL:HAA2	23:AC:606:CHL:HBD	1.89	0.54
9:F:21:ALA:O	9:F:25:VAL:HG22	2.08	0.54
25:AN:614:LUT:H181	25:AN:614:LUT:C8	2.37	0.54
23:p:608:CHL:HHC	23:p:608:CHL:HBB1	1.88	0.54
17:v:241:ILE:HG21	24:v:313:CLA:HAC2	1.89	0.54
5:O:285:TYR:CE2	19:U:88:TYR:HA	2.41	0.54
24:AK:608:CLA:HHC	24:AK:608:CLA:HBB1	1.88	0.54
10:AQ:152:LEU:O	10:AQ:154:HIS:N	2.41	0.54
4:AJ:201:GLY:HA3	4:AJ:286:THR:OG1	2.08	0.54
5:AK:18:ARG:NH1	14:AP:5:ASN:HD22	2.05	0.54
34:AP:101:SQD:H262	15:m:24:ILE:HG21	1.90	0.54
10:AU:180:ASN:OD1	10:AU:185:GLU:HG2	2.08	0.54
1:AA:110:ALA:N	1:AA:226:MET:SD	2.81	0.54
4:J:63:ILE:HG13	4:J:65:GLU:HG2	1.90	0.54
23:V:606:CHL:HHC	23:V:606:CHL:HBB1	1.89	0.54
34:o:101:SQD:H262	15:M:24:ILE:HG21	1.89	0.54
10:p:231:VAL:CG1	24:p:613:CLA:HAC2	2.37	0.54
5:O:89:GLY:HA3	28:O:621:LHG:HC12	1.89	0.54
11:AO:37:TRP:O	11:AO:40:THR:HG23	2.07	0.54
1:AA:183:LEU:HG	23:AA:607:CHL:HBB1	1.89	0.54
26:AC:616:NEX:H192	26:AC:616:NEX:H183	1.89	0.54
24:P:506:CLA:H72	29:P:514:BCR:H10C	1.90	0.54
28:AK:624:LHG:H192	14:AP:27:VAL:HG21	1.89	0.54
24:AU:602:CLA:H61	25:AU:615:LUT:H28	1.89	0.54
1:AC:170:GLY:HA2	23:AC:608:CHL:HAB	1.90	0.53
5:O:472:ARG:HH22	24:O:611:CLA:HED3	1.73	0.53
16:q:225:PRO:HD2	25:q:614:LUT:H23	1.90	0.53
16:q:226:LEU:HD12	25:q:614:LUT:H222	1.89	0.53
23:AQ:608:CHL:C9	23:AQ:608:CHL:C12	2.66	0.53
17:AS:199:LYS:HA	23:AS:308:CHL:HBC1	1.90	0.53
23:AU:606:CHL:HBB1	25:AU:615:LUT:H161	1.90	0.53
1:AA:165:GLN:NE2	23:AA:606:CHL:HMC	2.23	0.53
3:AB:120:GLN:HE22	3:AB:126:ALA:HA	1.72	0.53
24:AC:602:CLA:HAB	25:AC:615:LUT:H32	1.91	0.53
14:o:11:VAL:HG11	15:M:25:ILE:HD11	1.89	0.53
8:e:68:GLY:C	19:u:102:ARG:HH21	2.16	0.53
3:AB:125:VAL:HG11	3:AB:133:GLN:HE21	1.73	0.53
5:O:438:LYS:HD3	5:O:438:LYS:N	2.24	0.53
23:V:607:CHL:HAA1	23:V:607:CHL:CGD	2.39	0.53
25:V:613:LUT:H181	25:V:613:LUT:C8	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:v:189:ARG:HG3	23:v:308:CHL:CHD	2.37	0.53
24:AH:602:CLA:H61	25:AH:615:LUT:H28	1.89	0.53
17:AS:266:LEU:O	17:AS:270:ILE:HG22	2.08	0.53
1:9:121:ARG:NH1	1:9:121:ARG:HB2	2.23	0.53
3:AF:161:TRP:HD1	23:AF:608:CHL:HBA2	1.73	0.53
24:q:609:CLA:H172	25:q:614:LUT:H391	1.90	0.53
23:AN:607:CHL:H92	23:AN:607:CHL:C4	2.36	0.53
10:AQ:103:SER:O	10:AQ:107:MET:HG3	2.09	0.53
24:9:610:CLA:H11	25:9:615:LUT:H221	1.89	0.53
23:p:607:CHL:HMB2	23:p:607:CHL:H91	1.91	0.53
23:p:608:CHL:C12	23:p:608:CHL:H93	2.25	0.53
19:U:80:GLY:HA3	19:U:103:TYR:HA	1.90	0.53
8:E:23:HIS:NE2	38:F:102:HEM:NA	2.57	0.53
10:p:103:SER:O	10:p:107:MET:HG3	2.09	0.53
24:AA:602:CLA:H2A	24:AA:602:CLA:HED2	1.90	0.53
3:AB:241:ILE:O	3:AB:245:GLU:HG2	2.09	0.53
5:O:462:PHE:CE2	24:O:604:CLA:HAC2	2.43	0.53
16:q:142:ILE:HG22	24:q:608:CLA:HMD2	1.91	0.53
1:9:93:ALA:O	1:9:97:GLU:HG3	2.08	0.53
1:9:113:CYS:HG	1:9:131:TRP:CG	2.26	0.53
24:O:609:CLA:OBD	11:j:39:THR:OG1	2.26	0.53
23:q:605:CHL:HBB2	23:q:606:CHL:CAB	2.38	0.53
17:v:83:GLU:H	17:v:83:GLU:CD	2.15	0.53
26:v:317:NEX:H10	26:v:317:NEX:H181	1.90	0.53
10:AQ:191:TYR:HD1	24:AQ:610:CLA:O1D	1.92	0.53
1:AA:188:ASP:OD1	1:AA:191:TYR:N	2.41	0.53
5:O:150:CYS:HB2	24:O:603:CLA:HMC2	1.91	0.53
23:V:606:CHL:H91	23:V:606:CHL:CMB	2.39	0.53
5:AK:277:GLN:OE1	35:AO:102:DGD:O5E	2.24	0.53
38:f:102:HEM:HMB2	38:f:102:HEM:HBB2	1.91	0.53
16:AR:164:THR:OG1	16:AR:167:ASP:HB2	2.09	0.53
15:M:12:ALA:O	15:M:16:LEU:HD22	2.09	0.53
6:AL:36:TRP:O	24:AL:509:CLA:H42	2.09	0.53
9:f:30:SER:O	9:f:34:MET:HG3	2.09	0.53
11:AO:18:THR:HA	11:AO:21:LYS:HD2	1.91	0.53
24:AR:612:CLA:HMB2	25:AR:614:LUT:H162	1.90	0.53
23:AS:307:CHL:HBA1	23:AS:307:CHL:H92	1.91	0.53
23:AU:607:CHL:HMB2	23:AU:607:CHL:C9	2.32	0.53
23:0:601:CHL:C9	23:0:601:CHL:C12	2.87	0.52
24:AB:603:CLA:HAB	27:AB:613:XAT:H403	1.91	0.52
16:q:282:THR:HG22	16:q:285:ASP:CG	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AK:121:GLU:OE1	5:AK:121:GLU:N	2.39	0.52
23:AN:607:CHL:H93	23:AN:607:CHL:H43	1.90	0.52
23:AN:608:CHL:HBB1	23:AQ:601:CHL:C2	2.18	0.52
24:AD:309:CLA:H51	24:AD:311:CLA:HBA2	1.92	0.52
24:V:603:CLA:H193	23:V:608:CHL:H91	1.91	0.52
16:q:207:ASN:ND2	24:q:618:CLA:HHD	2.23	0.52
5:AK:256:MET:HG2	5:AK:451:PHE:CD1	2.44	0.52
7:AM:96:PRO:HA	7:AM:99:GLN:NE2	2.24	0.52
24:AN:602:CLA:HAB	25:AN:615:LUT:H32	1.92	0.52
25:AC:615:LUT:H181	25:AC:615:LUT:C8	2.39	0.52
1:AE:186:ALA:HB2	23:AE:606:CHL:HBC1	1.92	0.52
3:AF:105:HIS:HB3	3:AF:236:MET:SD	2.49	0.52
12:I:16:VAL:O	12:I:20:ILE:HG13	2.09	0.52
16:q:202:ILE:HD12	23:q:607:CHL:HMA3	1.91	0.52
23:AH:607:CHL:H91	23:AH:607:CHL:CMB	2.30	0.52
24:AK:611:CLA:OBD	11:AO:39:THR:OG1	2.21	0.52
23:9:609:CHL:H51	23:9:609:CHL:H92	1.91	0.52
3:AF:144:SER:O	3:AF:148:THR:HG22	2.09	0.52
7:Q:282:MET:HE2	7:Q:282:MET:HA	1.91	0.52
10:AH:187:GLU:H	10:AH:187:GLU:CD	2.17	0.52
22:AI:9:VAL:O	22:AI:13:ILE:HG12	2.08	0.52
24:AK:611:CLA:CHA	11:AO:43:MET:HE3	2.40	0.52
8:e:77:ASP:O	8:e:81:ARG:HG2	2.10	0.52
17:AS:98:PHE:HD2	25:AS:316:LUT:H222	1.75	0.52
2:0:217:GLY:O	2:0:221:MET:HG3	2.10	0.52
3:AB:192:GLN:OE1	3:AB:192:GLN:N	2.43	0.52
5:O:215:PHE:CZ	24:O:609:CLA:HMD2	2.44	0.52
8:E:77:ASP:O	8:E:81:ARG:HG2	2.10	0.52
23:AN:606:CHL:H121	23:AQ:601:CHL:H201	1.90	0.52
16:AR:271:TRP:CE3	25:AR:614:LUT:H172	2.44	0.52
24:AD:309:CLA:H61	25:AD:314:LUT:H373	1.90	0.52
6:P:70:PHE:HE1	24:P:504:CLA:HED2	1.74	0.52
7:AM:194:LEU:O	14:AP:35:TYR:OH	2.25	0.52
12:i:16:VAL:O	12:i:20:ILE:HG13	2.10	0.52
16:AR:198:VAL:O	16:AR:202:ILE:HG22	2.08	0.52
24:AR:604:CLA:HAA2	23:AR:605:CHL:CHD	2.39	0.52
24:9:604:CLA:HMB2	25:9:616:LUT:H162	1.91	0.52
1:AC:160:ALA:O	1:AC:164:THR:HG23	2.10	0.52
33:O:624:LMG:H122	35:AJ:401:DGD:HA32	1.92	0.52
6:P:36:TRP:O	24:P:508:CLA:H42	2.09	0.52
23:p:608:CHL:C9	23:p:608:CHL:C2	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AN:605:CHL:OBD	23:AN:617:CHL:HHD	2.09	0.52
23:AQ:608:CHL:H93	23:AQ:608:CHL:C2	2.39	0.52
10:AU:125:LYS:HA	10:AU:125:LYS:HE3	1.90	0.52
5:O:122:ILE:HA	11:j:24:LYS:HZ3	1.74	0.52
10:AH:158:ILE:O	10:AH:161:ILE:HG22	2.10	0.52
5:AK:7:ARG:HG2	24:AK:613:CLA:HED2	1.91	0.52
1:9:107:MET:HE1	24:9:610:CLA:HAB	1.91	0.52
3:AF:110:MET:HE2	24:AF:609:CLA:HHC	1.91	0.52
3:AF:256:LEU:HD21	25:AF:611:LUT:H22	1.91	0.52
24:V:609:CLA:H72	25:V:613:LUT:H28	1.92	0.52
23:p:607:CHL:HBB1	25:p:615:LUT:H171	1.92	0.52
18:AT:12:SER:O	18:AT:16:ILE:HG13	2.10	0.52
2:AD:253:ASN:HB2	24:AD:313:CLA:CED	2.38	0.52
3:AF:153:MET:HA	3:AF:156:VAL:HG12	1.92	0.52
38:F:102:HEM:HMC2	38:F:102:HEM:HBC2	1.91	0.52
16:q:148:MET:HE1	24:q:609:CLA:HHC	1.92	0.52
24:AL:507:CLA:H72	29:AL:516:BCR:H10C	1.92	0.52
24:AU:611:CLA:HMC3	25:AU:614:LUT:H191	1.91	0.52
8:E:42:LEU:O	8:E:46:VAL:HG22	2.10	0.51
9:F:30:SER:O	9:F:34:MET:HG3	2.11	0.51
15:M:22:LEU:HA	15:M:25:ILE:HG22	1.91	0.51
23:p:606:CHL:HAA1	23:p:606:CHL:CGD	2.40	0.51
24:q:609:CLA:H2	25:q:614:LUT:H26	1.92	0.51
24:AH:602:CLA:H12	24:AH:602:CLA:H3A	1.92	0.51
2:0:118:LYS:HD2	2:0:118:LYS:C	2.35	0.51
1:AE:107:MET:HE1	24:AE:608:CLA:HAB	1.92	0.51
10:AN:248:LEU:HD21	24:AN:613:CLA:HMC2	1.91	0.51
25:AN:614:LUT:H181	25:AN:614:LUT:H8	1.92	0.51
14:AP:13:LEU:N	15:m:29:THR:OG1	2.44	0.51
17:AS:167:ILE:HB	17:AS:168:PRO:HD3	1.92	0.51
10:AU:182:PRO:HB2	23:AU:608:CHL:HBB2	1.91	0.51
24:AU:602:CLA:HAB	25:AU:615:LUT:H32	1.91	0.51
25:9:616:LUT:H181	25:9:616:LUT:C8	2.40	0.51
1:AC:106:ALA:CB	1:AC:223:MET:HG3	2.41	0.51
1:AE:162:TRP:O	1:AE:166:VAL:HG12	2.10	0.51
23:AF:605:CHL:H3A	29:AF:612:BCR:H21C	1.91	0.51
11:j:19:VAL:O	11:j:23:LEU:HD12	2.10	0.51
24:AH:611:CLA:HMC3	25:AH:614:LUT:H191	1.91	0.51
6:AL:452:ALA:HB1	20:w:131:LEU:HD22	1.92	0.51
1:AA:86:SER:OG	24:AA:602:CLA:O1A	2.22	0.51
23:AA:601:CHL:HAA1	23:AA:601:CHL:CGD	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AH:609:CLA:H92	24:AH:609:CLA:H41	1.92	0.51
23:AR:605:CHL:HBB2	23:AR:606:CHL:CAB	2.40	0.51
23:AU:608:CHL:H93	23:AU:608:CHL:H43	1.93	0.51
6:P:223:TRP:HZ3	6:P:285:ILE:HD12	1.76	0.51
1:AA:106:ALA:HA	1:AA:226:MET:HE1	1.92	0.51
25:AA:614:LUT:H181	25:AA:614:LUT:C8	2.41	0.51
4:J:179:THR:O	4:J:183:MET:HG3	2.11	0.51
5:O:71:ILE:HD11	24:O:606:CLA:HAA2	1.92	0.51
23:V:607:CHL:HBA2	23:V:607:CHL:H192	1.92	0.51
16:q:158:GLU:OE1	16:q:164:THR:HA	2.11	0.51
6:AL:42:LEU:HD21	24:AL:512:CLA:H2A	1.92	0.51
6:AL:223:TRP:CE3	6:AL:224:ILE:HG12	2.46	0.51
10:AU:69:TYR:OH	10:AU:81:ASP:OD2	2.21	0.51
2:0:52:ARG:NH2	2:0:67:LEU:O	2.44	0.51
3:AB:156:VAL:HG21	23:AB:607:CHL:HMA3	1.91	0.51
23:AD:302:CHL:C14	23:AD:302:CHL:H93	2.39	0.51
3:AF:173:GLU:OE1	3:AF:173:GLU:N	2.32	0.51
5:O:143:LEU:HB2	24:O:610:CLA:HED1	1.92	0.51
6:P:223:TRP:CE3	6:P:224:ILE:HG12	2.46	0.51
23:AH:608:CHL:C9	23:AH:608:CHL:C4	2.88	0.51
5:AK:215:PHE:CZ	24:AK:611:CLA:HMD2	2.46	0.51
2:0:126:GLU:OE2	2:0:131:LYS:HB3	2.11	0.51
3:AB:163:ASP:OD1	3:AB:167:PRO:HA	2.10	0.51
5:O:260:SER:N	5:O:263:THR:OG1	2.44	0.51
16:q:135:ARG:NH2	24:q:603:CLA:O1A	2.44	0.51
20:W:120:THR:HA	20:W:123:LEU:HD23	1.92	0.51
23:AH:608:CHL:H93	23:AH:608:CHL:H43	1.91	0.51
6:AL:29:GLU:N	6:AL:29:GLU:OE1	2.43	0.51
16:AR:218:PRO:HG2	16:AR:223:PHE:HD2	1.76	0.51
1:9:228:GLY:O	1:9:232:GLN:HG3	2.11	0.51
24:AC:604:CLA:H2	26:AC:616:NEX:H241	1.92	0.51
10:p:169:MET:HA	10:p:169:MET:HE3	1.93	0.51
10:AH:180:ASN:OD1	10:AH:185:GLU:HG2	2.10	0.51
5:AK:9:HIS:HB2	24:AK:613:CLA:HBA1	1.93	0.51
8:e:71:ASP:HB2	8:e:74:GLU:OE1	2.11	0.51
23:AN:605:CHL:HAA1	23:AN:605:CHL:CGD	2.41	0.51
16:AR:283:ILE:HG13	24:AR:612:CLA:H42	1.93	0.51
24:O:610:CLA:H102	24:O:615:CLA:HAA1	1.91	0.51
24:p:602:CLA:H12	24:p:602:CLA:H3A	1.91	0.51
23:AR:605:CHL:HBB2	23:AR:606:CHL:HAB	1.92	0.51
2:0:160:LEU:O	2:0:164:VAL:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AC:604:CLA:H12	23:AC:606:CHL:C3D	2.42	0.50
35:J:413:DGD:HA32	33:AK:601:LMG:H122	1.93	0.50
5:O:256:MET:HA	5:O:256:MET:HE2	1.92	0.50
7:Q:108:LEU:HD21	8:E:72:SER:HB2	1.92	0.50
7:AM:320:ILE:O	7:AM:324:GLU:HG3	2.11	0.50
1:9:83:ALA:HA	23:AA:608:CHL:HBA2	1.93	0.50
1:AC:136:SER:HB3	23:AD:301:CHL:HED3	1.93	0.50
9:F:13:ARG:NH1	9:F:13:ARG:HB3	2.27	0.50
24:q:604:CLA:HAA2	23:q:605:CHL:CHD	2.40	0.50
22:AI:30:PRO:C	22:AI:32:GLY:H	2.20	0.50
23:AN:607:CHL:CBD	23:AN:607:CHL:HAA1	2.42	0.50
23:AN:607:CHL:HAA1	23:AN:607:CHL:HBD	1.93	0.50
14:AP:10:SER:OG	14:AP:11:VAL:N	2.45	0.50
24:AQ:602:CLA:H12	24:AQ:602:CLA:H3A	1.94	0.50
16:AR:250:MET:HE2	24:AR:602:CLA:HMC2	1.92	0.50
1:9:223:MET:HG2	25:9:616:LUT:C15	2.41	0.50
2:0:120:VAL:HA	2:0:121:ARG:HH21	1.76	0.50
6:P:223:TRP:CG	6:P:224:ILE:H	2.29	0.50
10:p:152:LEU:O	10:p:154:HIS:N	2.45	0.50
22:AV:19:LEU:O	22:AV:23:VAL:HG23	2.11	0.50
25:9:615:LUT:H181	25:9:615:LUT:C8	2.42	0.50
29:AB:612:BCR:H371	29:AB:612:BCR:H403	1.93	0.50
3:AF:185:PHE:CE1	23:AF:607:CHL:HBB1	2.46	0.50
4:J:20:TRP:NE1	34:J:410:SQD:O3	2.30	0.50
4:J:201:GLY:HA3	4:J:286:THR:OG1	2.11	0.50
10:AN:103:SER:O	10:AN:107:MET:HG3	2.10	0.50
1:AE:128:GLU:OE2	1:AE:130:VAL:HG12	2.12	0.50
8:E:22:ILE:O	8:E:25:ILE:HG22	2.11	0.50
4:AJ:133:LEU:HD23	7:AM:257:ILE:HG12	1.93	0.50
5:AK:438:LYS:HD3	5:AK:438:LYS:N	2.27	0.50
7:AM:162:PRO:HB3	7:AM:171:ALA:HB2	1.93	0.50
9:f:17:VAL:HG23	9:f:18:HIS:ND1	2.26	0.50
38:f:102:HEM:HBC2	38:f:102:HEM:HMC2	1.94	0.50
16:AR:134:GLN:H	16:AR:134:GLN:CD	2.16	0.50
23:0:601:CHL:H93	23:0:601:CHL:C12	2.42	0.50
23:AE:607:CHL:H92	23:AE:607:CHL:H51	1.92	0.50
3:AF:113:VAL:HG21	25:AF:611:LUT:H12	1.92	0.50
4:J:61:ASP:OD1	4:J:63:ILE:HG12	2.10	0.50
5:O:121:GLU:OE1	5:O:121:GLU:N	2.40	0.50
5:O:399:VAL:HG12	5:O:417:VAL:HG22	1.94	0.50
24:p:603:CLA:C15	23:p:609:CHL:H91	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AK:611:CLA:HMD3	11:AO:42:LEU:HD11	1.92	0.50
8:E:35:TRP:CD2	9:F:33:ALA:HB2	2.46	0.50
10:AH:161:ILE:HD11	23:AH:606:CHL:C1D	2.41	0.50
4:AJ:91:LEU:HD11	4:AJ:166:GLY:HA2	1.93	0.50
6:AL:71:GLU:OE2	6:AL:88:LEU:HB2	2.12	0.50
10:AQ:169:MET:HE3	10:AQ:169:MET:HA	1.94	0.50
23:AU:608:CHL:C9	23:AU:608:CHL:C4	2.90	0.50
24:9:610:CLA:C2B	24:9:610:CLA:H51	2.42	0.50
7:Q:320:ILE:O	7:Q:324:GLU:HG3	2.12	0.50
23:p:606:CHL:HBB2	23:p:607:CHL:CBB	2.42	0.50
24:AN:611:CLA:HMC2	25:AN:614:LUT:H11	1.92	0.50
10:AQ:107:MET:HE1	24:AQ:610:CLA:CAB	2.27	0.50
24:AS:310:CLA:H52	25:AS:315:LUT:H28	1.94	0.50
2:AD:209:LEU:HD21	3:AF:198:ARG:NH2	2.26	0.50
4:J:91:LEU:HD11	4:J:166:GLY:HA2	1.93	0.50
10:p:240:PRO:HG2	10:p:241:ILE:HD12	1.93	0.50
24:q:609:CLA:CBB	25:q:614:LUT:H32	2.42	0.50
16:AR:192:ILE:HD12	16:AR:192:ILE:H	1.77	0.50
20:w:84:ARG:NH1	20:w:86:SER:OG	2.45	0.50
23:9:609:CHL:HBB1	23:0:601:CHL:H51	1.93	0.49
1:AC:153:VAL:N	23:AC:605:CHL:O1D	2.28	0.49
2:AD:125:LYS:HE2	2:AD:125:LYS:HA	1.94	0.49
4:J:133:LEU:HD23	7:Q:257:ILE:HG12	1.94	0.49
5:O:207:THR:O	5:O:211:LEU:HD13	2.11	0.49
24:O:614:CLA:H11	24:O:614:CLA:C1A	2.42	0.49
10:AH:191:TYR:HD1	24:AH:609:CLA:O1D	1.95	0.49
24:AK:616:CLA:C1A	24:AK:616:CLA:H11	2.41	0.49
11:AO:59:GLU:HG2	11:AO:64:SER:HB2	1.94	0.49
16:AR:243:ILE:O	16:AR:247:ARG:HG3	2.12	0.49
24:AS:313:CLA:NC	24:AS:313:CLA:H51	2.27	0.49
28:O:623:LHG:H311	15:M:18:PRO:HB3	1.94	0.49
24:V:609:CLA:H72	25:V:613:LUT:H30	1.94	0.49
14:o:21:GLY:O	14:o:25:ILE:HG12	2.12	0.49
17:v:270:ILE:HD11	22:AI:60:LEU:HD21	1.93	0.49
20:w:110:GLY:HA3	28:w:201:LHG:H181	1.94	0.49
1:AA:230:PHE:O	1:AA:234:ILE:HG13	2.12	0.49
24:AD:304:CLA:CMA	24:AD:304:CLA:H2	2.42	0.49
28:O:623:LHG:H192	14:o:27:VAL:HG21	1.94	0.49
6:AL:55:ALA:HB1	29:k:101:BCR:H373	1.93	0.49
8:e:73:LEU:HD12	8:e:74:GLU:N	2.27	0.49
2:0:208:GLU:OE1	2:0:208:GLU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:608:CHL:HAA1	23:0:608:CHL:CGD	2.43	0.49
23:AD:301:CHL:C9	23:AD:301:CHL:C12	2.88	0.49
6:P:452:ALA:HB1	20:W:131:LEU:HD22	1.94	0.49
23:V:605:CHL:HAA1	23:V:605:CHL:CBD	2.42	0.49
11:j:43:MET:HE1	29:j:101:BCR:HC42	1.93	0.49
11:j:52:VAL:O	11:j:56:ILE:HG12	2.12	0.49
5:AK:237:VAL:HG21	24:AK:612:CLA:C1D	2.42	0.49
10:AN:105:TRP:CD1	23:AN:608:CHL:HMD2	2.47	0.49
23:0:601:CHL:HBC3	23:0:601:CHL:HMC	1.94	0.49
5:O:30:VAL:HG11	24:O:612:CLA:H112	1.95	0.49
24:AK:612:CLA:H13	24:AK:614:CLA:H12	1.94	0.49
16:AR:142:ILE:HG23	24:AR:608:CLA:HMD1	1.94	0.49
2:0:209:LEU:HD21	3:AB:198:ARG:NH2	2.28	0.49
1:AA:186:ALA:HB2	23:AA:607:CHL:HBC1	1.94	0.49
1:AE:166:VAL:HG23	23:AE:607:CHL:HBB2	1.93	0.49
3:AF:110:MET:HE1	25:AF:611:LUT:C33	2.42	0.49
7:Q:181:ARG:NH2	7:Q:334:ASP:OD1	2.32	0.49
4:AJ:179:THR:O	4:AJ:183:MET:HG3	2.12	0.49
5:AK:468:TRP:HE1	5:AK:472:ARG:NH2	2.09	0.49
7:AM:181:ARG:NH2	7:AM:334:ASP:OD1	2.39	0.49
20:w:128:GLU:OE1	20:w:128:GLU:N	2.45	0.49
2:AD:131:LYS:O	2:AD:131:LYS:HD3	2.12	0.49
6:P:443:TRP:HE1	24:P:508:CLA:HED3	1.78	0.49
28:P:517:LHG:HC5	24:AH:610:CLA:O1A	2.12	0.49
10:p:215:GLU:HG3	24:p:610:CLA:NB	2.28	0.49
24:AK:608:CLA:H2A	24:AK:608:CLA:O1D	2.13	0.49
6:AL:223:TRP:HZ3	6:AL:285:ILE:HD12	1.78	0.49
16:AR:55:ARG:HB2	16:AR:55:ARG:CZ	2.43	0.49
16:AR:223:PHE:O	25:AR:614:LUT:H24	2.12	0.49
10:V:103:SER:HB2	10:V:219:GLY:HA3	1.94	0.49
25:V:613:LUT:H181	25:V:613:LUT:H8	1.94	0.49
3:AB:210:ARG:HH11	3:AB:214:TYR:HB2	1.77	0.49
5:O:25:MET:HE2	29:O:617:BCR:H23C	1.95	0.49
10:V:231:VAL:HG11	24:V:611:CLA:HAC2	1.95	0.49
24:V:603:CLA:HBC1	23:V:608:CHL:HAC2	1.93	0.49
11:AO:29:GLU:CD	11:AO:29:GLU:H	2.21	0.49
24:AD:304:CLA:H2	24:AD:304:CLA:HMA3	1.95	0.49
4:AJ:30:ILE:HD11	34:AJ:411:SQD:H101	1.95	0.49
5:AK:66:MET:HE3	24:AK:607:CLA:HED3	1.94	0.49
10:AN:201:LEU:HD12	24:AN:609:CLA:H12	1.94	0.49
11:AO:17:THR:O	11:AO:21:LYS:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:617:CHL:HAA1	23:0:617:CHL:CGD	2.43	0.48
1:AA:107:MET:HE1	24:AA:609:CLA:HAB	1.94	0.48
23:p:601:CHL:H3A	23:p:601:CHL:HBA1	1.46	0.48
5:AK:25:MET:HE2	29:AK:619:BCR:H23C	1.95	0.48
24:AK:616:CLA:H3A	24:AK:616:CLA:HBA2	1.53	0.48
23:AQ:601:CHL:HHC	23:AQ:601:CHL:HBB1	1.93	0.48
24:9:604:CLA:C1C	26:9:617:NEX:H222	2.42	0.48
2:0:52:ARG:HG3	2:0:54:LYS:HE3	1.93	0.48
1:AA:103:SER:HB3	1:AA:219:GLY:HA3	1.95	0.48
23:AD:317:CHL:HAA1	23:AD:317:CHL:CGD	2.42	0.48
4:J:188:ALA:HB2	4:J:328:MET:HB3	1.94	0.48
32:J:405:PHO:H61	32:J:405:PHO:H2	1.64	0.48
24:V:602:CLA:H161	24:V:602:CLA:H141	1.65	0.48
23:q:606:CHL:H11	23:q:606:CHL:HED2	1.94	0.48
17:v:214:ASP:CG	17:v:217:GLN:HE21	2.21	0.48
6:AL:39:ASN:ND2	24:AL:511:CLA:O1A	2.40	0.48
17:AS:162:TYR:O	17:AS:162:TYR:HD1	1.95	0.48
1:AC:191:TYR:HA	24:AC:609:CLA:CGD	2.43	0.48
23:AC:608:CHL:C9	23:AD:301:CHL:H162	2.43	0.48
4:J:30:ILE:HD11	34:J:410:SQD:H101	1.95	0.48
5:O:384:ARG:NH1	7:Q:353:LEU:O	2.46	0.48
6:P:221:GLU:OE1	20:W:89:GLY:HA2	2.13	0.48
12:I:6:LEU:O	12:I:10:THR:HG22	2.13	0.48
17:v:214:ASP:HB3	17:v:217:GLN:HG2	1.94	0.48
23:AH:601:CHL:H93	23:AH:601:CHL:H41	1.95	0.48
4:AJ:20:TRP:HE1	34:AJ:411:SQD:HO3	1.57	0.48
24:AN:612:CLA:HMB1	25:AN:614:LUT:H162	1.94	0.48
1:9:165:GLN:OE1	23:9:607:CHL:HMC	2.13	0.48
1:AC:182:PRO:CB	23:AC:607:CHL:HBB2	2.43	0.48
1:AC:232:GLN:HE21	1:AC:232:GLN:H	1.60	0.48
6:P:86:LEU:HD13	6:P:89:LEU:HD12	1.94	0.48
23:V:616:CHL:O1D	23:V:616:CHL:HAA1	2.13	0.48
10:p:107:MET:HE3	25:p:614:LUT:C34	2.42	0.48
20:W:128:GLU:OE1	20:W:128:GLU:N	2.41	0.48
10:AH:202:ALA:HB2	24:AH:609:CLA:HAA2	1.94	0.48
6:AL:223:TRP:CG	6:AL:224:ILE:H	2.30	0.48
14:AP:21:GLY:O	14:AP:25:ILE:HG12	2.13	0.48
24:AR:609:CLA:H172	25:AR:614:LUT:H391	1.95	0.48
24:AU:610:CLA:H51	24:AU:611:CLA:O2D	2.13	0.48
1:AA:168:LEU:HB3	26:AA:616:NEX:H15	1.96	0.48
1:AE:169:MET:HA	1:AE:172:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AE:601:CHL:HAA1	23:AE:601:CHL:HBD	1.95	0.48
24:P:508:CLA:H161	24:P:508:CLA:H141	1.66	0.48
19:U:79:ARG:HA	19:U:100:ILE:HG13	1.94	0.48
23:AN:601:CHL:H3A	23:AN:601:CHL:HBA1	1.55	0.48
10:AQ:103:SER:HB3	10:AQ:219:GLY:HA3	1.94	0.48
25:AS:316:LUT:H171	25:AS:316:LUT:C8	2.42	0.48
5:O:366:PHE:HB3	5:O:425:GLN:NE2	2.28	0.48
24:O:606:CLA:HBA1	24:O:606:CLA:C4A	2.43	0.48
23:AH:606:CHL:HBB1	25:AH:615:LUT:H161	1.94	0.48
7:AM:135:ARG:O	7:AM:135:ARG:HD3	2.14	0.48
10:AN:183:LEU:HG	23:AN:607:CHL:CBB	2.43	0.48
10:AQ:105:TRP:CD1	23:AQ:609:CHL:HMD2	2.49	0.48
10:AQ:223:MET:HG2	25:AQ:616:LUT:C15	2.44	0.48
24:AQ:603:CLA:C15	23:AQ:609:CHL:H91	2.43	0.48
16:AR:281:THR:O	16:AR:281:THR:OG1	2.29	0.48
10:AU:208:PHE:O	10:AU:212:LYS:HG3	2.13	0.48
2:0:214:ILE:O	2:0:218:ARG:HG3	2.13	0.48
24:O:608:CLA:H3A	24:O:608:CLA:HBA2	1.71	0.48
8:E:69:ARG:H	19:U:102:ARG:NH1	2.12	0.48
23:p:607:CHL:H191	23:AH:601:CHL:H91	1.96	0.48
16:q:140:GLU:OE2	16:q:243:ILE:HD11	2.12	0.48
23:q:605:CHL:HBA1	26:q:615:NEX:H403	1.95	0.48
24:AK:616:CLA:H62	24:AK:616:CLA:H41	1.58	0.48
23:AQ:609:CHL:H62	23:AQ:609:CHL:H92	1.60	0.48
24:AQ:610:CLA:HBB1	24:AQ:610:CLA:HMB3	1.96	0.48
23:AU:608:CHL:H41	23:AU:608:CHL:H62	1.66	0.48
1:AA:161:ILE:CD1	23:AA:617:CHL:HAC1	2.43	0.48
24:AC:604:CLA:C1C	26:AC:616:NEX:H222	2.44	0.48
23:AC:608:CHL:H92	23:AC:608:CHL:H51	1.96	0.48
3:AF:219:GLU:O	3:AF:222:GLU:HG3	2.14	0.48
7:Q:337:HIS:C	7:Q:337:HIS:ND1	2.71	0.48
10:V:99:GLU:HG3	24:V:602:CLA:C1B	2.44	0.48
24:AQ:610:CLA:H42	25:AQ:615:LUT:H26	1.96	0.48
10:AU:202:ALA:HB2	24:AU:609:CLA:HAA2	1.96	0.48
23:9:609:CHL:HBD	23:9:609:CHL:HBA1	1.95	0.48
3:AF:154:GLY:O	3:AF:158:SER:OG	2.26	0.48
5:O:7:ARG:O	5:O:10:THR:HG22	2.14	0.48
5:AK:150:CYS:HB2	24:AK:605:CLA:HMC2	1.96	0.48
24:AL:509:CLA:H3A	24:AL:509:CLA:HBA2	1.53	0.48
24:AL:509:CLA:HBC3	24:AL:511:CLA:H92	1.95	0.48
10:AN:141:ASP:OD1	10:AN:141:ASP:N	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AQ:605:CHL:HBA2	23:AQ:605:CHL:H3A	1.40	0.48
17:AS:178:GLU:OE2	23:AS:307:CHL:HMC	2.13	0.48
1:9:191:TYR:HA	24:9:610:CLA:CGD	2.43	0.48
2:0:167:MET:HA	2:0:170:VAL:HG22	1.95	0.48
23:AE:601:CHL:H3A	23:AE:601:CHL:HBA1	1.51	0.48
4:J:245:THR:OG1	7:Q:266:ARG:NH2	2.47	0.48
6:P:39:ASN:HB2	24:P:508:CLA:HBA1	1.95	0.48
13:K:46:PHE:HA	13:K:49:LEU:HD12	1.96	0.48
25:q:614:LUT:H181	25:q:614:LUT:C8	2.44	0.48
17:v:109:LYS:HG2	17:v:113:PHE:CE2	2.49	0.48
23:AH:601:CHL:H93	23:AH:601:CHL:C4	2.44	0.48
15:m:12:ALA:O	15:m:16:LEU:HD22	2.13	0.48
24:AF:614:CLA:HBA2	24:AF:614:CLA:H3A	1.51	0.47
5:O:155:ALA:O	5:O:159:THR:OG1	2.24	0.47
24:P:508:CLA:HBC3	24:P:510:CLA:H92	1.94	0.47
28:AL:519:LHG:HC5	24:AU:610:CLA:O1A	2.13	0.47
21:x:94:GLY:HA2	21:x:97:LEU:CD2	2.44	0.47
23:V:605:CHL:HMC	23:V:606:CHL:C1C	2.43	0.47
24:v:310:CLA:H12	24:v:310:CLA:H3A	1.96	0.47
4:AJ:193:LEU:HD11	24:AJ:404:CLA:HMC1	1.96	0.47
5:AK:132:SER:HB2	11:AO:30:TYR:CD2	2.49	0.47
8:e:35:TRP:CD2	9:f:33:ALA:HB2	2.49	0.47
24:AR:612:CLA:H12	23:AR:613:CHL:CAD	2.44	0.47
1:9:182:PRO:CB	23:9:608:CHL:HBB2	2.44	0.47
2:0:45:ASP:OD1	2:0:46:LEU:N	2.47	0.47
24:0:602:CLA:HBA2	24:0:602:CLA:H3A	1.44	0.47
23:V:606:CHL:HAA1	23:V:606:CHL:CGD	2.44	0.47
5:AK:399:VAL:HG12	5:AK:417:VAL:HG22	1.96	0.47
24:AQ:610:CLA:H62	24:AQ:612:CLA:HBA1	1.95	0.47
17:AS:109:LYS:HG2	17:AS:113:PHE:CE2	2.49	0.47
24:AA:604:CLA:HMB2	25:AA:615:LUT:H162	1.96	0.47
24:AB:604:CLA:HBA2	24:AB:604:CLA:H3A	1.48	0.47
1:AC:158:ILE:O	1:AC:161:ILE:HG22	2.14	0.47
24:O:605:CLA:HBA2	24:O:605:CLA:H3A	1.54	0.47
24:O:609:CLA:C4D	11:j:43:MET:SD	3.03	0.47
8:E:70:PHE:HB2	19:U:103:TYR:CE2	2.46	0.47
23:V:601:CHL:H91	23:AH:607:CHL:H201	1.95	0.47
24:V:610:CLA:HMC1	25:V:613:LUT:H203	1.96	0.47
15:M:24:ILE:CD1	15:m:24:ILE:HD13	2.40	0.47
16:q:270:ASN:CG	24:q:612:CLA:HED1	2.40	0.47
23:q:607:CHL:HBA2	23:q:607:CHL:H3A	1.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:v:242:GLN:HG2	24:v:313:CLA:ND	2.29	0.47
5:AK:198:ILE:HD11	5:AK:262:THR:HG22	1.96	0.47
23:AQ:601:CHL:H3A	23:AQ:601:CHL:HBA1	1.48	0.47
17:AS:135:ASN:HA	17:AS:139:ALA:O	2.14	0.47
3:AB:210:ARG:HA	3:AB:213:VAL:O	2.14	0.47
1:AC:197:ASP:HB2	24:AC:609:CLA:HBA2	1.95	0.47
5:O:121:GLU:O	11:j:24:LYS:NZ	2.40	0.47
24:AH:602:CLA:HAB	25:AH:615:LUT:H32	1.96	0.47
24:AH:604:CLA:H3A	24:AH:604:CLA:HBA2	1.63	0.47
5:AK:260:SER:N	5:AK:263:THR:OG1	2.47	0.47
5:AK:366:PHE:HB3	5:AK:425:GLN:NE2	2.30	0.47
10:AU:191:TYR:HD1	24:AU:609:CLA:O1D	1.97	0.47
23:AA:606:CHL:H121	23:AA:606:CHL:H91	1.95	0.47
24:AC:612:CLA:CAB	25:AC:614:LUT:H183	2.44	0.47
24:P:512:CLA:H51	23:v:302:CHL:C3B	2.45	0.47
14:o:10:SER:OG	14:o:11:VAL:N	2.46	0.47
34:o:101:SQD:H251	34:o:101:SQD:H92	1.96	0.47
4:AJ:93:PHE:HZ	24:AJ:409:CLA:HAA1	1.79	0.47
24:AN:613:CLA:HED2	24:AN:613:CLA:H2A	1.95	0.47
16:AR:214:LYS:HE2	16:AR:214:LYS:HA	1.95	0.47
10:AU:187:GLU:H	10:AU:187:GLU:CD	2.17	0.47
2:0:120:VAL:C	2:0:121:ARG:HE	2.23	0.47
24:AA:604:CLA:HBA2	24:AA:604:CLA:H3A	1.34	0.47
24:AF:602:CLA:CMC	27:AF:613:XAT:H31	2.45	0.47
8:E:57:THR:HG21	8:E:82:SER:HB2	1.96	0.47
23:V:605:CHL:HMC	23:V:606:CHL:C2C	2.45	0.47
14:o:11:VAL:CG1	15:M:25:ILE:HD11	2.45	0.47
10:AH:125:LYS:HE2	10:AH:125:LYS:HA	1.96	0.47
10:AH:208:PHE:O	10:AH:212:LYS:HG3	2.14	0.47
10:AH:251:PRO:HB2	24:AH:613:CLA:CMA	2.45	0.47
23:AH:606:CHL:HMC	25:AH:615:LUT:H163	1.97	0.47
22:AI:56:ILE:O	22:AI:60:LEU:HD23	2.14	0.47
5:AK:243:ALA:HA	5:AK:246:PHE:CD2	2.49	0.47
5:AK:256:MET:HE2	5:AK:256:MET:HA	1.97	0.47
24:AL:514:CLA:H51	23:AS:302:CHL:C3B	2.45	0.47
23:AR:605:CHL:HBA2	26:AR:615:NEX:H28	1.96	0.47
24:AU:602:CLA:H12	24:AU:602:CLA:H3A	1.96	0.47
23:AU:608:CHL:H92	23:AU:608:CHL:H62	1.60	0.47
2:0:121:ARG:HE	2:0:121:ARG:N	2.13	0.47
4:J:324:ALA:HB2	7:Q:330:MET:HE3	1.97	0.47
5:O:237:VAL:HG21	24:O:610:CLA:C1D	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:O:615:CLA:H91	24:O:615:CLA:H111	1.71	0.47
7:Q:121:PHE:O	7:Q:124:ILE:HB	2.14	0.47
24:p:610:CLA:H12	24:p:610:CLA:HBA2	1.63	0.47
16:q:207:ASN:OD1	16:q:207:ASN:C	2.57	0.47
10:AH:69:TYR:OH	10:AH:81:ASP:OD2	2.22	0.47
34:AJ:411:SQD:H291	34:AJ:411:SQD:H321	1.54	0.47
24:AK:614:CLA:H3A	24:AK:614:CLA:HBA2	1.40	0.47
34:m:101:SQD:H342	34:m:101:SQD:H312	1.69	0.47
17:AS:168:PRO:O	17:AS:169:ILE:HD13	2.15	0.47
5:O:63:ILE:N	5:O:64:PRO:HD2	2.29	0.47
6:P:343:ARG:HE	6:P:347:GLY:HA2	1.80	0.47
24:P:512:CLA:HBA1	24:P:512:CLA:CBD	2.43	0.47
10:V:94:ARG:HH21	10:V:97:GLU:CD	2.23	0.47
16:q:282:THR:OG1	23:q:613:CHL:HED3	2.15	0.47
24:AK:616:CLA:HBB1	24:AK:616:CLA:HMB1	1.97	0.47
10:AQ:170:GLY:CA	23:AQ:609:CHL:HAB	2.45	0.47
1:9:196:PHE:O	25:9:615:LUT:H24	2.14	0.47
1:AC:240:PRO:HA	1:AC:243:ASN:HD22	1.79	0.47
5:O:359:MET:HE3	5:O:363:PHE:O	2.16	0.47
24:P:507:CLA:H2	24:P:507:CLA:CMA	2.45	0.47
7:Q:176:VAL:HG11	24:Q:401:CLA:HED1	1.97	0.47
23:q:605:CHL:HBB2	23:q:606:CHL:HAB	1.97	0.47
34:AM:401:SQD:H142	34:AM:401:SQD:H111	1.60	0.47
10:AQ:170:GLY:HA2	23:AQ:609:CHL:HAB	1.98	0.47
23:AR:607:CHL:HAA1	23:AR:607:CHL:CBD	2.45	0.47
24:AR:610:CLA:HBA2	24:AR:610:CLA:H3A	1.45	0.47
10:AU:161:ILE:HD11	23:AU:606:CHL:C1D	2.45	0.47
24:9:602:CLA:HAB	25:9:616:LUT:H32	1.96	0.46
2:0:131:LYS:NZ	23:0:606:CHL:HED3	2.30	0.46
2:0:229:VAL:HG21	24:0:612:CLA:HAC2	1.97	0.46
2:AD:103:ALA:HB3	2:AD:221:MET:HG2	1.97	0.46
4:J:259:ILE:HG22	4:J:260:PHE:CD2	2.51	0.46
32:J:406:PHO:H3A	24:Q:403:CLA:H142	1.98	0.46
28:O:621:LHG:H142	28:O:621:LHG:H332	1.96	0.46
10:V:214:LYS:HD3	24:V:610:CLA:HAA2	1.97	0.46
17:v:242:GLN:HG2	24:v:313:CLA:C1D	2.45	0.46
10:AH:211:LEU:HD13	24:AH:609:CLA:H12	1.97	0.46
23:AH:607:CHL:H91	23:AH:607:CHL:H112	1.81	0.46
5:AK:359:MET:HE3	5:AK:363:PHE:O	2.15	0.46
24:AN:609:CLA:H72	25:AN:614:LUT:H30	1.97	0.46
24:AR:617:CLA:HBA2	24:AR:617:CLA:H3A	1.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AU:107:MET:CE	24:AU:609:CLA:HHC	2.45	0.46
1:9:211:LEU:HD22	24:9:610:CLA:H41	1.97	0.46
1:AE:236:THR:HG21	1:AE:243:ASN:OD1	2.15	0.46
25:AE:614:LUT:H163	23:AE:617:CHL:CMC	2.44	0.46
3:AF:170:GLN:HG3	23:AF:607:CHL:CMC	2.44	0.46
4:J:131:TRP:CZ3	24:P:505:CLA:HBA1	2.51	0.46
24:V:611:CLA:HMB3	25:V:613:LUT:H162	1.96	0.46
11:j:40:THR:O	11:j:43:MET:HB2	2.15	0.46
24:AH:610:CLA:H91	24:AH:610:CLA:H111	1.67	0.46
24:AR:612:CLA:HBA2	24:AR:612:CLA:H3A	1.30	0.46
24:AB:611:CLA:HAA1	24:AB:611:CLA:CGD	2.45	0.46
23:AD:308:CHL:H92	23:AD:308:CHL:H62	1.58	0.46
1:AE:106:ALA:HA	1:AE:226:MET:HE1	1.97	0.46
23:AE:606:CHL:H3A	23:AE:606:CHL:HBA2	1.69	0.46
38:F:102:HEM:HBB2	38:F:102:HEM:HMB1	1.98	0.46
23:AH:601:CHL:H202	23:AH:601:CHL:H161	1.64	0.46
23:AH:608:CHL:H92	23:AH:608:CHL:C4	2.44	0.46
5:AK:464:PHE:HD2	24:AK:613:CLA:HAC2	1.80	0.46
24:AK:617:CLA:H51	24:AK:618:CLA:H192	1.98	0.46
10:AN:69:TYR:OH	10:AN:81:ASP:OD2	2.23	0.46
14:AP:11:VAL:HG11	15:m:25:ILE:HD11	1.97	0.46
10:AQ:201:LEU:HD12	24:AQ:610:CLA:H11	1.98	0.46
23:AB:605:CHL:CBD	29:AB:612:BCR:H21C	2.45	0.46
23:AD:307:CHL:O1A	24:AD:309:CLA:HHD	2.16	0.46
23:AE:605:CHL:H91	23:AE:605:CHL:H121	1.97	0.46
6:P:281:VAL:O	6:P:285:ILE:HG12	2.15	0.46
24:Q:403:CLA:H41	24:Q:403:CLA:H62	1.52	0.46
10:V:180:ASN:OD1	10:V:181:GLY:N	2.48	0.46
16:q:134:GLN:H	16:q:134:GLN:CD	2.21	0.46
17:v:98:PHE:HD2	25:v:316:LUT:H222	1.81	0.46
20:W:84:ARG:NH1	20:W:86:SER:OG	2.49	0.46
32:AJ:407:PHO:H141	32:AJ:407:PHO:H161	1.64	0.46
11:AO:18:THR:O	11:AO:22:LEU:HG	2.15	0.46
10:AQ:106:ALA:HB3	10:AQ:223:MET:HG3	1.98	0.46
10:AU:141:ASP:N	10:AU:141:ASP:OD1	2.47	0.46
3:AB:207:GLY:O	3:AB:208:LYS:HD2	2.16	0.46
24:AD:303:CLA:HBA2	24:AD:303:CLA:H3A	1.56	0.46
5:O:8:VAL:O	24:O:614:CLA:HED1	2.14	0.46
24:O:615:CLA:H2	24:O:615:CLA:H61	1.71	0.46
7:Q:22:TRP:HD1	21:X:110:PHE:HE1	1.64	0.46
7:Q:162:PRO:HB3	7:Q:171:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:q:616:LHG:H161	28:q:616:LHG:H132	1.73	0.46
24:AK:609:CLA:HBA2	24:AK:609:CLA:H3A	1.70	0.46
24:AK:616:CLA:H112	24:AK:616:CLA:H91	1.70	0.46
24:AN:602:CLA:HBA2	24:AN:602:CLA:H12	1.55	0.46
24:AN:609:CLA:H72	25:AN:614:LUT:H28	1.97	0.46
12:i:6:LEU:O	12:i:10:THR:HG22	2.16	0.46
10:AQ:106:ALA:CB	10:AQ:223:MET:HG3	2.45	0.46
1:9:152:LEU:O	1:9:154:HIS:N	2.48	0.46
24:AC:609:CLA:H11	25:AC:614:LUT:H221	1.98	0.46
32:J:406:PHO:H71	32:J:406:PHO:H112	1.66	0.46
6:P:135:LEU:HD21	22:AI:33:TRP:HB2	1.98	0.46
23:V:607:CHL:HAA1	23:V:607:CHL:O1D	2.15	0.46
10:p:170:GLY:HA2	23:p:609:CHL:HAB	1.97	0.46
10:p:170:GLY:CA	23:p:609:CHL:HAB	2.45	0.46
23:v:302:CHL:HMA2	23:v:302:CHL:HBA1	1.97	0.46
5:AK:277:GLN:HG2	19:u:99:LYS:HE2	1.98	0.46
24:AK:604:CLA:H93	24:AK:604:CLA:H61	1.75	0.46
6:AL:221:GLU:OE1	20:w:89:GLY:HA2	2.15	0.46
6:AL:376:ASP:O	6:AL:380:LEU:HG	2.16	0.46
34:AP:101:SQD:H92	34:AP:101:SQD:H251	1.97	0.46
16:AR:158:GLU:OE1	16:AR:164:THR:HA	2.15	0.46
17:AS:189:ARG:HG3	23:AS:308:CHL:CHD	2.44	0.46
24:9:613:CLA:H2	24:9:613:CLA:H61	1.53	0.46
2:0:108:PHE:CE2	24:0:604:CLA:HAC1	2.50	0.46
1:AA:144:LEU:HD21	24:AA:604:CLA:HAA2	1.97	0.46
24:O:608:CLA:H91	24:O:608:CLA:H111	1.64	0.46
8:E:36:LEU:HA	8:E:39:SER:OG	2.15	0.46
11:j:62:ASN:O	11:j:63:SER:OG	2.30	0.46
34:M:101:SQD:H312	34:M:101:SQD:H342	1.69	0.46
24:p:604:CLA:HBA1	23:p:606:CHL:CHD	2.45	0.46
10:AH:121:ARG:HH12	10:AH:245:ALA:HB2	1.81	0.46
10:AH:206:GLU:HG3	10:AH:207:ALA:N	2.29	0.46
5:AK:384:ARG:NH1	7:AM:353:LEU:O	2.48	0.46
23:AN:601:CHL:C5	23:AN:601:CHL:C9	2.93	0.46
24:AQ:611:CLA:H61	24:AQ:611:CLA:H41	1.73	0.46
1:9:78:TYR:HB2	24:9:602:CLA:OBD	2.15	0.46
23:0:605:CHL:HBA2	23:0:605:CHL:H3A	1.52	0.46
1:AE:152:LEU:O	1:AE:154:HIS:N	2.49	0.46
23:AE:605:CHL:CMB	23:AE:605:CHL:H91	2.45	0.46
3:AF:83:PHE:HB3	24:AF:602:CLA:CAD	2.46	0.46
5:O:42:LEU:HD23	5:O:42:LEU:HA	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:128:THR:OG1	5:O:130:LYS:HG2	2.16	0.46
8:E:66:ILE:HD11	8:E:68:GLY:O	2.16	0.46
23:V:607:CHL:H92	23:V:607:CHL:H62	1.67	0.46
24:K:101:CLA:H202	22:AI:20:LEU:HD13	1.98	0.46
23:p:605:CHL:HBA2	23:p:605:CHL:H3A	1.38	0.46
23:AH:601:CHL:C9	23:AH:601:CHL:C3	2.89	0.46
23:AH:601:CHL:H41	23:AH:601:CHL:H61	1.51	0.46
5:AK:30:VAL:HG11	24:AK:614:CLA:H112	1.97	0.46
5:AK:218:SER:OG	5:AK:219:VAL:HG23	2.16	0.46
5:AK:472:ARG:HH12	24:AK:613:CLA:CED	2.29	0.46
24:AL:509:CLA:H41	24:AL:509:CLA:H62	1.59	0.46
7:AM:78:ALA:HB2	7:AM:175:GLY:HA3	1.96	0.46
23:AQ:606:CHL:HBB2	23:AQ:607:CHL:CBB	2.46	0.46
17:AS:84:TYR:OH	17:AS:96:ASP:OD2	2.15	0.46
2:0:167:MET:HE2	2:0:167:MET:HB3	1.66	0.46
5:O:243:ALA:HA	5:O:246:PHE:CD2	2.50	0.46
24:P:504:CLA:H3A	24:P:504:CLA:HBA2	1.63	0.46
7:Q:60:TYR:O	8:E:66:ILE:HG22	2.16	0.46
10:AH:107:MET:CE	24:AH:609:CLA:HHC	2.44	0.46
24:AK:603:CLA:H151	29:AO:101:BCR:H21C	1.98	0.46
24:AK:609:CLA:H61	24:AK:609:CLA:H41	1.67	0.46
24:AQ:612:CLA:HMC2	25:AQ:615:LUT:H11	1.96	0.46
24:AC:611:CLA:HAB	25:AC:614:LUT:C35	2.46	0.46
25:AC:615:LUT:H181	25:AC:615:LUT:H8	1.98	0.46
23:AD:308:CHL:HHC	23:AD:308:CHL:HBB1	1.97	0.46
34:J:410:SQD:H202	34:J:410:SQD:H172	1.76	0.46
23:p:608:CHL:H142	23:p:608:CHL:H112	1.73	0.46
4:AJ:43:THR:HG23	29:AJ:410:BCR:H362	1.98	0.46
5:AK:328:GLY:N	24:AK:609:CLA:O1A	2.29	0.46
5:AK:458:PHE:HB3	24:AK:606:CLA:HBC2	1.97	0.46
24:AL:508:CLA:H202	24:AL:508:CLA:H161	1.73	0.46
23:AN:601:CHL:H91	23:AU:607:CHL:H201	1.97	0.46
2:0:141:GLY:HA3	2:0:154:GLN:HE22	1.81	0.45
23:0:601:CHL:O1D	28:0:616:LHG:H122	2.15	0.45
23:AA:606:CHL:H92	23:AA:606:CHL:H61	1.54	0.45
1:AC:239:GLY:O	1:AC:243:ASN:ND2	2.49	0.45
23:AC:607:CHL:HBA2	23:AC:607:CHL:H3A	1.46	0.45
25:AC:614:LUT:H181	25:AC:614:LUT:C8	2.46	0.45
23:AE:607:CHL:HBD	23:AE:607:CHL:HBA1	1.98	0.45
3:AF:156:VAL:HG21	23:AF:607:CHL:HMA3	1.98	0.45
5:O:458:PHE:HB3	24:O:604:CLA:HBC2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:605:CHL:HED3	23:V:605:CHL:HAA2	1.98	0.45
16:q:192:ILE:O	16:q:196:VAL:HG12	2.16	0.45
17:v:211:LEU:HB2	24:v:310:CLA:O1A	2.16	0.45
5:AK:352:ARG:HH11	5:AK:352:ARG:HG3	1.79	0.45
6:AL:254:THR:C	6:AL:255:LYS:HD3	2.40	0.45
24:AL:505:CLA:HBA2	24:AL:505:CLA:H3A	1.62	0.45
8:e:23:HIS:HA	8:e:26:THR:OG1	2.16	0.45
23:AN:601:CHL:H41	28:AN:616:LHG:H192	1.98	0.45
10:AU:206:GLU:O	10:AU:210:GLU:HG2	2.16	0.45
2:0:118:LYS:HD2	2:0:118:LYS:O	2.16	0.45
23:0:607:CHL:H3A	23:0:607:CHL:HBA2	1.50	0.45
1:AA:146:TYR:HB2	1:AA:153:VAL:CG2	2.46	0.45
24:AE:604:CLA:HMB2	25:AE:614:LUT:H162	1.97	0.45
24:O:612:CLA:H3A	24:O:612:CLA:HBA2	1.39	0.45
6:P:39:ASN:ND2	24:P:510:CLA:O1A	2.42	0.45
16:q:205:GLN:OE1	16:q:205:GLN:HA	2.15	0.45
5:AK:256:MET:HG2	5:AK:451:PHE:HD1	1.80	0.45
7:AM:282:MET:HE2	7:AM:282:MET:HA	1.97	0.45
11:AO:32:LYS:HD2	11:AO:32:LYS:HA	1.77	0.45
16:AR:202:ILE:HD11	23:AR:607:CHL:C4A	2.46	0.45
21:x:94:GLY:HA2	21:x:97:LEU:HD23	1.96	0.45
23:AU:606:CHL:HMC	25:AU:615:LUT:H163	1.98	0.45
23:9:601:CHL:HED1	24:9:602:CLA:HAC2	1.98	0.45
23:9:607:CHL:H3A	23:9:607:CHL:HBA1	1.67	0.45
24:0:603:CLA:H2	24:0:603:CLA:HMA2	1.99	0.45
1:AE:226:MET:SD	25:AE:614:LUT:H10	2.56	0.45
3:AF:181:THR:OG1	3:AF:184:ASN:OD1	2.26	0.45
4:J:331:MET:HE2	4:J:331:MET:HA	1.96	0.45
5:O:233:ASN:OD1	5:O:235:GLU:N	2.44	0.45
24:O:603:CLA:H3A	24:O:603:CLA:CGA	2.45	0.45
6:P:376:ASP:O	6:P:380:LEU:HG	2.17	0.45
23:V:607:CHL:H93	23:V:607:CHL:C4	2.46	0.45
4:AJ:187:GLN:HB2	24:AJ:404:CLA:HAC2	1.99	0.45
24:AK:607:CLA:H62	24:AK:607:CLA:H41	1.45	0.45
6:AL:39:ASN:HB2	24:AL:509:CLA:HBA1	1.97	0.45
6:AL:281:VAL:O	6:AL:285:ILE:HG12	2.16	0.45
24:AS:309:CLA:HBA2	24:AS:309:CLA:H3A	1.42	0.45
20:w:110:GLY:O	20:w:114:THR:HG23	2.15	0.45
1:9:169:MET:HE2	1:9:169:MET:HA	1.97	0.45
24:0:613:CLA:HBA2	24:0:613:CLA:H3A	1.64	0.45
24:AE:603:CLA:HMD2	23:AE:607:CHL:H2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AF:224:LEU:HB3	24:AF:609:CLA:HMA1	1.98	0.45
23:AF:607:CHL:HAA1	23:AF:607:CHL:HBD	1.98	0.45
24:O:603:CLA:H152	11:j:50:PHE:HE2	1.81	0.45
24:O:614:CLA:H91	24:O:614:CLA:H112	1.70	0.45
6:P:361:LEU:HD12	35:P:516:DGD:O3E	2.17	0.45
24:V:602:CLA:HBA2	24:V:602:CLA:H12	1.52	0.45
23:AH:608:CHL:H193	23:AH:608:CHL:H161	1.79	0.45
24:AK:617:CLA:H91	24:AK:617:CLA:H111	1.66	0.45
24:AL:509:CLA:H141	24:AL:509:CLA:H161	1.66	0.45
24:AL:512:CLA:H141	24:AL:512:CLA:H162	1.80	0.45
10:AQ:231:VAL:CG1	24:AQ:613:CLA:HAC2	2.44	0.45
23:AA:606:CHL:H91	23:AA:606:CHL:C12	2.46	0.45
3:AB:239:MET:HE1	27:AB:613:XAT:C12	2.47	0.45
24:AC:604:CLA:HBA2	24:AC:604:CLA:H3A	1.62	0.45
23:AE:616:CHL:HAA1	23:AE:616:CHL:CGD	2.47	0.45
4:J:192:ILE:HG13	4:J:293:MET:HE1	1.99	0.45
10:V:108:LEU:HB3	24:V:604:CLA:HBB2	1.99	0.45
24:V:602:CLA:HBA2	24:V:602:CLA:H3A	1.78	0.45
10:p:188:ASP:OD2	10:p:189:LEU:N	2.50	0.45
23:AH:605:CHL:HBA2	23:AH:605:CHL:H3A	1.46	0.45
24:AH:609:CLA:H52	25:AH:614:LUT:H28	1.98	0.45
4:AJ:192:ILE:HG13	4:AJ:293:MET:HE1	1.99	0.45
4:AJ:225:ARG:N	4:AJ:225:ARG:HD2	2.31	0.45
6:AL:437:LEU:HA	24:AL:509:CLA:HMC2	1.98	0.45
10:AQ:226:MET:O	10:AQ:226:MET:HE3	2.16	0.45
24:AU:609:CLA:H52	25:AU:614:LUT:H28	1.99	0.45
23:AD:302:CHL:H93	23:AD:302:CHL:H143	1.96	0.45
24:AD:304:CLA:HBC1	23:AD:308:CHL:HAC2	1.99	0.45
23:AE:605:CHL:H92	23:AE:605:CHL:H61	1.56	0.45
6:P:324:LEU:O	6:P:324:LEU:HD23	2.15	0.45
24:q:609:CLA:H141	24:q:609:CLA:H162	1.72	0.45
17:v:146:VAL:O	17:v:150:THR:HG23	2.17	0.45
17:v:236:MET:HG2	25:v:316:LUT:H12	1.98	0.45
4:AJ:131:TRP:CZ3	24:AL:506:CLA:HBA1	2.52	0.45
4:AJ:259:ILE:HG22	4:AJ:260:PHE:CD2	2.51	0.45
24:AL:508:CLA:H2	24:AL:508:CLA:CMA	2.45	0.45
19:u:102:ARG:HG3	19:u:103:TYR:N	2.32	0.45
23:9:607:CHL:H61	23:9:607:CHL:H92	1.66	0.45
3:AB:99:ARG:O	3:AB:103:LEU:HD22	2.17	0.45
3:AB:206:ALA:HB3	24:AB:609:CLA:HED1	1.98	0.45
3:AF:233:ARG:HB3	24:AF:602:CLA:HAC2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:P:514:BCR:H24C	29:P:514:BCR:H371	1.84	0.45
23:AN:606:CHL:HAA1	23:AN:606:CHL:CGD	2.47	0.45
16:AR:271:TRP:CD1	16:AR:271:TRP:C	2.94	0.45
2:0:118:LYS:HG3	2:0:119:TRP:CD1	2.46	0.45
2:0:197:LEU:HD13	3:AB:203:LEU:HD22	1.99	0.45
24:AC:612:CLA:H3A	24:AC:613:CLA:CGD	2.47	0.45
1:AE:176:ARG:NH2	23:AE:607:CHL:O2D	2.50	0.45
3:AF:236:MET:HE3	27:AF:613:XAT:C33	2.46	0.45
24:O:601:CLA:H151	29:j:101:BCR:H21C	1.98	0.45
24:O:612:CLA:H162	24:O:612:CLA:H193	1.82	0.45
6:P:55:ALA:HB1	29:P:515:BCR:H373	1.97	0.45
6:P:70:PHE:CE1	24:P:504:CLA:HED2	2.50	0.45
24:P:501:CLA:H3A	24:P:501:CLA:HBA2	1.29	0.45
23:V:606:CHL:H121	23:p:601:CHL:H201	1.98	0.45
24:p:610:CLA:H42	25:p:614:LUT:H26	1.97	0.45
17:v:236:MET:HG2	25:v:316:LUT:H14	1.99	0.45
23:AH:607:CHL:HMB2	23:AH:607:CHL:C9	2.32	0.45
24:AK:611:CLA:HMA3	24:AK:612:CLA:C1C	2.47	0.45
6:AL:343:ARG:HG3	6:AL:344:SER:O	2.17	0.45
7:AM:68:TYR:C	9:f:34:MET:HE1	2.42	0.45
16:AR:179:TYR:OH	26:AR:615:NEX:O23	2.20	0.45
24:9:613:CLA:CAB	25:9:615:LUT:H183	2.47	0.45
2:0:226:GLY:O	2:0:230:GLN:HG3	2.17	0.45
2:AD:227:PHE:CE1	25:AD:314:LUT:H182	2.52	0.45
35:J:411:DGD:HAE2	35:J:411:DGD:HA82	1.84	0.45
24:p:610:CLA:HAA1	24:p:610:CLA:CGD	2.47	0.45
24:q:618:CLA:H3A	24:q:618:CLA:HBA2	1.40	0.45
24:v:312:CLA:HMC3	25:v:315:LUT:H191	1.99	0.45
5:AK:69:LEU:HD12	24:AK:607:CLA:HBA1	1.99	0.45
7:AM:240:GLN:HG3	7:AM:242:GLU:H	1.82	0.45
24:AN:602:CLA:HBA2	24:AN:602:CLA:H3A	1.75	0.45
24:AN:611:CLA:HHC	24:AN:611:CLA:HBB1	1.99	0.45
29:k:101:BCR:H24C	29:k:101:BCR:H371	1.84	0.45
10:AQ:162:TRP:O	10:AQ:166:VAL:HG12	2.17	0.45
2:AD:168:GLY:HA2	23:AD:308:CHL:HAB	1.99	0.45
25:AE:614:LUT:C8	25:AE:614:LUT:H181	2.47	0.45
4:J:43:THR:HG23	29:J:408:BCR:H362	1.99	0.45
4:J:193:LEU:HD11	24:J:403:CLA:HMC1	1.98	0.45
24:O:606:CLA:H142	24:O:606:CLA:H111	1.72	0.45
6:P:382:LYS:HG3	6:P:383:ASP:OD1	2.17	0.45
14:o:22:LEU:CD1	15:M:22:LEU:HD12	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:q:610:CLA:HBA2	24:q:610:CLA:H3A	1.43	0.45
2:0:112:THR:HG21	24:0:604:CLA:HAC2	1.99	0.44
23:AB:605:CHL:O1A	29:AB:612:BCR:H24C	2.17	0.44
5:O:226:TYR:HA	5:O:231:MET:CG	2.37	0.44
24:O:609:CLA:HBA2	24:O:609:CLA:H3A	1.50	0.44
29:P:515:BCR:H332	22:AI:12:LEU:HD23	1.99	0.44
10:V:201:LEU:HD12	24:V:609:CLA:H12	1.98	0.44
24:V:603:CLA:H92	24:V:603:CLA:H61	1.77	0.44
11:j:41:PRO:O	11:j:45:VAL:HG23	2.17	0.44
24:AH:610:CLA:H51	24:AH:611:CLA:O2D	2.17	0.44
4:AJ:303:ASN:H	4:AJ:303:ASN:HD22	1.65	0.44
24:AK:609:CLA:H92	24:AK:609:CLA:H62	1.65	0.44
11:AO:40:THR:O	11:AO:43:MET:HB2	2.17	0.44
11:AO:73:ASN:C	19:u:79:ARG:HH21	2.25	0.44
10:AQ:223:MET:HE1	24:AQ:602:CLA:HAB	1.99	0.44
17:AS:169:ILE:HG21	23:AS:306:CHL:HMD3	1.99	0.44
23:AA:617:CHL:HBA2	23:AA:617:CHL:H3A	1.67	0.44
3:AB:83:PHE:CE2	27:AB:613:XAT:H242	2.52	0.44
24:AC:604:CLA:HBA1	23:AC:606:CHL:CHD	2.47	0.44
24:O:614:CLA:H62	24:O:614:CLA:H41	1.60	0.44
6:P:437:LEU:HA	24:P:508:CLA:HMC2	1.99	0.44
23:V:607:CHL:H41	23:V:607:CHL:H62	1.65	0.44
23:p:601:CHL:H61	23:p:601:CHL:H93	1.33	0.44
24:p:618:CLA:HHC	24:p:618:CLA:CBB	2.39	0.44
24:q:602:CLA:H93	24:q:602:CLA:H111	1.79	0.44
10:AH:158:ILE:HA	10:AH:161:ILE:HG22	1.97	0.44
5:AK:472:ARG:NH2	24:AK:613:CLA:CGD	2.77	0.44
24:AK:605:CLA:H152	11:AO:50:PHE:HE2	1.82	0.44
23:AN:605:CHL:HMC	23:AN:606:CHL:C2C	2.47	0.44
24:AN:612:CLA:CMB	25:AN:614:LUT:H162	2.48	0.44
23:AR:605:CHL:HMC	23:AR:606:CHL:C3C	2.47	0.44
1:9:106:ALA:HB2	1:9:223:MET:HG3	1.98	0.44
2:0:102:TRP:NE1	23:0:608:CHL:CGD	2.80	0.44
28:0:616:LHG:H341	28:0:616:LHG:H372	1.81	0.44
1:AC:137:GLN:HE22	24:AC:604:CLA:HED2	1.81	0.44
1:AE:170:GLY:CA	23:AE:607:CHL:HAB	2.47	0.44
3:AF:83:PHE:HD1	24:AF:602:CLA:C2D	2.30	0.44
23:AF:605:CHL:H3A	29:AF:612:BCR:H23C	1.98	0.44
24:O:614:CLA:H3A	24:O:614:CLA:HBA2	1.56	0.44
29:O:619:BCR:H371	29:O:619:BCR:H24C	1.81	0.44
29:P:514:BCR:H15C	29:P:514:BCR:H351	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:15:LEU:HD12	7:Q:19:MET:HE3	1.99	0.44
10:p:191:TYR:HD1	24:p:610:CLA:O1D	1.99	0.44
23:p:601:CHL:HHC	23:p:601:CHL:HBB1	2.00	0.44
24:AH:610:CLA:HAA2	24:AH:610:CLA:HED3	1.98	0.44
34:AJ:411:SQD:H202	34:AJ:411:SQD:H172	1.65	0.44
24:AK:605:CLA:H3A	24:AK:605:CLA:CGA	2.47	0.44
24:AN:609:CLA:H3A	24:AN:609:CLA:HBA2	1.40	0.44
17:AS:129:ILE:HD11	17:AS:239:PHE:CZ	2.53	0.44
17:AS:211:LEU:HB2	24:AS:310:CLA:O1A	2.18	0.44
24:AS:312:CLA:HMC3	25:AS:315:LUT:H191	1.98	0.44
25:AU:614:LUT:H181	25:AU:614:LUT:C8	2.47	0.44
23:AD:307:CHL:HBA2	23:AD:307:CHL:H3A	1.52	0.44
24:AE:604:CLA:HBA2	24:AE:604:CLA:H3A	1.30	0.44
29:O:617:BCR:H15C	29:O:617:BCR:H351	1.81	0.44
24:P:507:CLA:H202	24:P:507:CLA:H161	1.73	0.44
29:P:515:BCR:H20C	29:P:515:BCR:H361	1.85	0.44
7:Q:68:TYR:C	9:F:34:MET:HE1	2.42	0.44
21:X:87:LEU:HD23	21:X:87:LEU:HA	1.63	0.44
5:AK:63:ILE:N	5:AK:64:PRO:HD2	2.32	0.44
5:AK:128:THR:OG1	5:AK:130:LYS:HG2	2.17	0.44
24:AN:602:CLA:H161	24:AN:602:CLA:H141	1.65	0.44
23:AN:605:CHL:HAA1	23:AN:605:CHL:CBD	2.47	0.44
24:AN:611:CLA:HMC2	25:AN:614:LUT:H203	1.98	0.44
23:AQ:608:CHL:H12	23:AQ:608:CHL:H51	1.65	0.44
24:AR:610:CLA:HBA2	24:AR:610:CLA:H12	1.54	0.44
23:AS:302:CHL:HMA2	23:AS:302:CHL:HBA1	1.99	0.44
25:AA:615:LUT:H181	25:AA:615:LUT:C8	2.48	0.44
23:AB:607:CHL:H3A	23:AB:607:CHL:HBA2	1.38	0.44
23:AC:605:CHL:HAA1	23:AC:605:CHL:CBD	2.48	0.44
24:Q:404:CLA:H112	24:Q:404:CLA:H91	1.74	0.44
8:E:73:LEU:HD12	8:E:74:GLU:CD	2.42	0.44
9:F:18:HIS:NE2	38:F:102:HEM:NA	2.66	0.44
17:v:83:GLU:OE1	17:v:83:GLU:N	2.33	0.44
5:AK:71:ILE:HD11	24:AK:608:CLA:HAA2	2.00	0.44
8:e:66:ILE:HD11	8:e:68:GLY:O	2.17	0.44
23:AQ:608:CHL:O1A	23:AQ:608:CHL:H172	2.16	0.44
17:AS:257:HIS:CE1	24:AS:313:CLA:HBA1	2.52	0.44
23:AU:608:CHL:H93	23:AU:608:CHL:C4	2.48	0.44
23:AB:605:CHL:H3A	23:AB:605:CHL:HBA2	1.60	0.44
2:AD:91:LYS:HD2	2:AD:91:LYS:HA	1.73	0.44
24:J:404:CLA:H111	24:J:404:CLA:H152	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:O:601:CLA:H142	24:O:601:CLA:H112	1.70	0.44
25:p:614:LUT:H181	25:p:614:LUT:C8	2.47	0.44
4:AJ:324:ALA:HB2	7:AM:330:MET:HE3	2.00	0.44
24:AK:604:CLA:HBD	24:AK:604:CLA:H2	2.00	0.44
24:AK:611:CLA:HAA1	11:AO:43:MET:CE	2.47	0.44
24:AK:615:CLA:H111	24:AK:615:CLA:H91	1.70	0.44
6:AL:361:LEU:HD12	35:AL:517:DGD:O3E	2.17	0.44
23:AQ:606:CHL:CBD	23:AQ:606:CHL:HAA1	2.47	0.44
16:AR:270:ASN:CG	24:AR:612:CLA:HED1	2.42	0.44
16:AR:282:THR:O	16:AR:286:THR:HG23	2.18	0.44
20:w:112:ILE:HD13	20:w:112:ILE:HA	1.84	0.44
10:AU:196:PHE:O	25:AU:614:LUT:H24	2.17	0.44
25:AA:614:LUT:H181	25:AA:614:LUT:H8	2.00	0.44
1:AE:206:GLU:O	1:AE:210:GLU:HG3	2.18	0.44
23:AE:617:CHL:H3A	23:AE:617:CHL:HBA2	1.63	0.44
23:p:608:CHL:H172	23:p:608:CHL:O1A	2.18	0.44
23:v:306:CHL:HMC	23:v:307:CHL:C3C	2.47	0.44
24:v:311:CLA:HAA2	24:v:311:CLA:HED2	2.00	0.44
15:m:8:PHE:CD1	15:m:8:PHE:C	2.96	0.44
17:AS:214:ASP:HB3	17:AS:217:GLN:HG2	2.00	0.44
1:AA:85:LEU:HD12	24:AA:602:CLA:H11	2.00	0.44
23:AA:606:CHL:HMB1	23:AA:606:CHL:C9	2.47	0.44
24:AE:603:CLA:CMD	23:AE:607:CHL:H2	2.48	0.44
24:O:605:CLA:H91	24:O:605:CLA:H111	1.74	0.44
7:Q:22:TRP:HD1	21:X:110:PHE:CE1	2.36	0.44
23:p:607:CHL:H43	23:p:607:CHL:HMA2	2.00	0.44
23:p:608:CHL:H93	23:p:608:CHL:C1	2.43	0.44
20:W:112:ILE:HD13	20:W:112:ILE:HA	1.85	0.44
24:AQ:602:CLA:H93	24:AQ:602:CLA:H111	1.72	0.44
25:AQ:615:LUT:H181	25:AQ:615:LUT:C8	2.47	0.44
24:9:604:CLA:H12	23:9:606:CHL:CAD	2.48	0.44
2:0:163:GLN:O	2:0:167:MET:HB3	2.18	0.44
24:0:603:CLA:H2	24:0:603:CLA:CMA	2.47	0.44
24:AC:604:CLA:C1B	26:AC:616:NEX:H383	2.47	0.44
24:AC:613:CLA:HBA1	24:AC:613:CLA:CBD	2.47	0.44
2:AD:103:ALA:CB	2:AD:221:MET:HG2	2.48	0.44
23:AE:616:CHL:HHC	23:AE:616:CHL:HBB1	1.99	0.44
5:O:18:ARG:O	5:O:22:VAL:HG22	2.18	0.44
5:O:122:ILE:HA	11:j:24:LYS:NZ	2.33	0.44
16:q:145:ARG:HD2	24:q:609:CLA:C4C	2.48	0.44
24:AH:603:CLA:H3A	24:AH:603:CLA:HBA1	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AK:610:CLA:H111	24:AK:610:CLA:H91	1.64	0.44
23:AN:601:CHL:H93	23:AN:601:CHL:H61	1.49	0.44
16:AR:171:VAL:HA	16:AR:174:VAL:HG22	2.00	0.44
24:AU:612:CLA:H3A	24:AU:612:CLA:HBA2	1.70	0.44
29:AV:101:BCR:H15C	29:AV:101:BCR:H351	1.87	0.44
23:AD:317:CHL:HHC	23:AD:317:CHL:HBB1	2.00	0.43
1:AE:223:MET:HE3	24:AE:602:CLA:CMC	2.45	0.43
29:J:408:BCR:H371	29:J:408:BCR:H24C	1.81	0.43
23:V:601:CHL:C5	23:V:601:CHL:C9	2.92	0.43
23:V:601:CHL:H61	23:V:601:CHL:H93	1.49	0.43
24:V:602:CLA:HMB1	24:V:602:CLA:H51	2.00	0.43
24:v:314:CLA:H3A	24:v:314:CLA:HBA2	1.79	0.43
23:AH:607:CHL:H92	23:AH:607:CHL:H61	1.44	0.43
24:AK:618:CLA:H11	24:AK:618:CLA:H51	1.78	0.43
24:AL:512:CLA:H202	22:AV:20:LEU:HD13	2.00	0.43
23:AN:607:CHL:H143	23:AN:607:CHL:H162	1.80	0.43
24:AU:613:CLA:HED2	24:AU:613:CLA:HBD	1.65	0.43
22:AV:48:ILE:HA	22:AV:51:VAL:HG12	1.99	0.43
23:9:607:CHL:H162	23:9:609:CHL:H91	2.00	0.43
1:AE:107:MET:HE3	25:AE:613:LUT:C34	2.48	0.43
4:J:96:ILE:HG12	12:I:1:MET:CE	2.45	0.43
5:O:363:PHE:CD2	5:O:366:PHE:HD2	2.36	0.43
23:V:601:CHL:H52	23:V:601:CHL:C9	2.47	0.43
23:p:606:CHL:HAA1	23:p:606:CHL:CBD	2.48	0.43
23:p:609:CHL:H62	23:p:609:CHL:H92	1.59	0.43
24:v:309:CLA:HBA2	24:v:309:CLA:H3A	1.42	0.43
24:v:311:CLA:HBA2	24:v:311:CLA:H3A	1.30	0.43
23:AH:607:CHL:H143	23:AH:607:CHL:H111	1.82	0.43
5:AK:227:LYS:O	5:AK:230:ARG:HD3	2.18	0.43
24:AL:507:CLA:H61	24:AL:507:CLA:H92	1.78	0.43
24:AM:403:CLA:H41	24:AM:403:CLA:H62	1.52	0.43
9:f:38:GLN:OE1	9:f:38:GLN:HA	2.18	0.43
23:AQ:607:CHL:HMA1	23:AQ:607:CHL:HHB	1.89	0.43
24:AS:303:CLA:H3A	24:AS:303:CLA:HBA2	1.62	0.43
24:AS:305:CLA:HBD	24:AS:305:CLA:HBA1	2.00	0.43
24:AS:313:CLA:H3A	24:AS:313:CLA:HBA2	1.69	0.43
1:9:118:LEU:O	1:9:122:ASN:ND2	2.48	0.43
23:9:609:CHL:H92	23:9:609:CHL:C5	2.46	0.43
23:0:601:CHL:H3A	23:0:601:CHL:HBA1	1.41	0.43
3:AF:236:MET:HE3	27:AF:613:XAT:C34	2.47	0.43
23:AF:607:CHL:H3A	23:AF:607:CHL:HBA2	1.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:212:SER:HB2	7:Q:212:CYS:HB2	2.00	0.43
9:F:27:PHE:CD2	29:F:101:BCR:H14C	2.53	0.43
23:V:601:CHL:H202	23:V:601:CHL:H161	1.76	0.43
12:I:6:LEU:HD12	20:W:101:LEU:HD21	2.00	0.43
16:q:282:THR:HG23	16:q:284:ILE:N	2.33	0.43
23:q:605:CHL:HMC	23:q:606:CHL:C3C	2.47	0.43
24:v:303:CLA:HBA2	24:v:303:CLA:H3A	1.57	0.43
24:AS:310:CLA:H12	24:AS:310:CLA:H3A	2.00	0.43
23:9:605:CHL:HAA1	23:9:605:CHL:CBD	2.48	0.43
24:AD:304:CLA:CMD	23:AD:308:CHL:H2	2.48	0.43
1:AE:236:THR:HG23	1:AE:238:LYS:H	1.82	0.43
5:O:138:ILE:HD13	5:O:138:ILE:HA	1.81	0.43
7:Q:196:PRO:O	7:Q:200:MET:HG3	2.18	0.43
24:v:313:CLA:H3A	24:v:313:CLA:HBA2	1.61	0.43
24:AJ:404:CLA:C2	32:AJ:407:PHO:HBB1	2.49	0.43
5:AK:363:PHE:CD2	5:AK:366:PHE:HD2	2.36	0.43
24:AK:603:CLA:H142	24:AK:603:CLA:H112	1.72	0.43
15:m:22:LEU:HA	15:m:25:ILE:HG22	2.00	0.43
23:AU:607:CHL:H143	23:AU:607:CHL:H111	1.82	0.43
24:AA:612:CLA:HBA2	24:AA:613:CLA:O1D	2.18	0.43
23:AE:601:CHL:HAA1	23:AE:601:CHL:CBD	2.48	0.43
3:AF:240:LEU:HB2	27:AF:613:XAT:C40	2.48	0.43
6:P:381:LYS:HD3	6:P:381:LYS:HA	1.81	0.43
34:Q:402:SQD:H142	34:Q:402:SQD:H111	1.61	0.43
8:E:32:ILE:O	8:E:36:LEU:HD13	2.19	0.43
10:V:152:LEU:O	10:V:154:HIS:N	2.51	0.43
10:p:110:ALA:N	10:p:226:MET:HE1	2.33	0.43
16:q:134:GLN:OE1	16:q:134:GLN:N	2.32	0.43
17:v:135:ASN:HA	17:v:139:ALA:O	2.17	0.43
21:X:110:PHE:CD1	21:X:110:PHE:N	2.85	0.43
23:AH:608:CHL:H93	23:AH:608:CHL:C4	2.47	0.43
4:AJ:120:LEU:HB3	24:AL:506:CLA:H191	2.00	0.43
4:AJ:272:HIS:CD2	7:AM:219:VAL:HG11	2.54	0.43
35:AJ:401:DGD:HBH1	34:AJ:411:SQD:H341	2.01	0.43
24:AJ:405:CLA:H91	24:AJ:405:CLA:H112	1.88	0.43
35:AJ:412:DGD:HAE2	35:AJ:412:DGD:HA82	1.85	0.43
24:AK:603:CLA:H72	24:AK:603:CLA:H111	1.83	0.43
7:AM:181:ARG:C	7:AM:181:ARG:HD3	2.43	0.43
10:AQ:107:MET:HE3	10:AQ:107:MET:HB3	1.65	0.43
23:AQ:607:CHL:HBA1	23:AQ:607:CHL:H3A	1.74	0.43
24:AQ:611:CLA:H2A	24:AQ:611:CLA:O1D	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AS:189:ARG:HG3	23:AS:308:CHL:C1D	2.47	0.43
19:u:87:LYS:HD2	19:u:88:TYR:CZ	2.54	0.43
23:AU:608:CHL:H161	23:AU:608:CHL:H193	1.78	0.43
22:AV:31:ASP:O	22:AV:31:ASP:OD2	2.35	0.43
24:AC:609:CLA:H72	24:AC:609:CLA:HBB1	2.00	0.43
1:AE:183:LEU:HG	23:AE:606:CHL:HBB1	1.99	0.43
3:AF:251:THR:HG23	3:AF:254:GLY:H	1.84	0.43
5:O:19:LEU:HD11	5:O:23:HIS:CE1	2.54	0.43
5:O:371:VAL:HG12	5:O:377:VAL:HA	2.01	0.43
24:O:607:CLA:H41	24:O:607:CLA:H61	1.67	0.43
29:O:618:BCR:HC42	33:O:620:LMG:H362	2.01	0.43
24:P:508:CLA:H3A	24:P:508:CLA:HBA2	1.53	0.43
24:AH:602:CLA:H141	24:AH:602:CLA:H161	1.73	0.43
24:AH:611:CLA:H61	24:AH:611:CLA:H102	1.78	0.43
24:AK:607:CLA:H91	24:AK:607:CLA:H111	1.71	0.43
7:AM:90:LEU:H	7:AM:90:LEU:HD12	1.84	0.43
8:e:71:ASP:CG	19:u:103:TYR:HD2	2.26	0.43
23:AU:601:CHL:H41	23:AU:601:CHL:H61	1.50	0.43
2:0:141:GLY:HA3	2:0:154:GLN:NE2	2.34	0.43
3:AB:234:LEU:HD11	24:AB:610:CLA:HMD1	2.00	0.43
1:AC:169:MET:HA	1:AC:172:VAL:HG22	1.99	0.43
25:AD:315:LUT:H31	25:AD:315:LUT:H391	1.91	0.43
24:AE:603:CLA:H2	24:AE:603:CLA:H62	1.81	0.43
4:J:120:LEU:HB3	24:P:505:CLA:H191	2.00	0.43
34:J:410:SQD:H321	34:J:410:SQD:H291	1.59	0.43
29:O:619:BCR:H20C	29:O:619:BCR:H361	1.81	0.43
10:V:105:TRP:CD1	23:V:608:CHL:HMD3	2.53	0.43
23:p:607:CHL:H191	23:AH:601:CHL:C9	2.49	0.43
16:q:270:ASN:OD1	24:q:612:CLA:HED1	2.18	0.43
24:v:313:CLA:NC	24:v:313:CLA:H51	2.34	0.43
29:AI:101:BCR:H15C	29:AI:101:BCR:H351	1.87	0.43
32:AJ:407:PHO:H2	32:AJ:407:PHO:H61	1.64	0.43
29:AJ:410:BCR:H371	29:AJ:410:BCR:H24C	1.82	0.43
29:AL:515:BCR:H20C	29:AL:515:BCR:H361	1.83	0.43
28:AM:406:LHG:O1	14:AP:14:ASN:ND2	2.52	0.43
23:AN:607:CHL:H41	23:AN:607:CHL:H62	1.63	0.43
10:AQ:247:HIS:CG	24:AQ:613:CLA:HAA2	2.54	0.43
24:AQ:610:CLA:H12	24:AQ:610:CLA:HBA2	1.54	0.43
23:AS:302:CHL:HMA1	23:AS:302:CHL:HHB	1.84	0.43
23:AS:307:CHL:H3A	23:AS:307:CHL:C9	2.48	0.43
27:9:618:XAT:H382	23:0:601:CHL:C4B	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:206:GLU:O	1:AA:210:GLU:HG3	2.19	0.43
23:AA:605:CHL:HBA2	23:AA:605:CHL:H3A	1.71	0.43
3:AB:208:LYS:O	3:AB:210:ARG:N	2.52	0.43
2:AD:104:MET:HE1	24:AD:309:CLA:HHC	2.01	0.43
3:AF:153:MET:HA	3:AF:153:MET:HE2	1.99	0.43
24:J:403:CLA:C2	32:J:405:PHO:HBB1	2.48	0.43
24:O:607:CLA:HBB1	24:O:607:CLA:HMB1	2.00	0.43
24:O:614:CLA:HMD2	34:o:101:SQD:H241	2.01	0.43
28:P:517:LHG:H112	28:P:517:LHG:HC81	1.58	0.43
9:F:14:TRP:CD2	9:F:18:HIS:CE1	3.07	0.43
23:p:601:CHL:H61	23:p:601:CHL:H41	1.67	0.43
17:v:84:TYR:OH	17:v:96:ASP:OD2	2.17	0.43
17:v:188:TYR:HD1	23:v:308:CHL:CAB	2.32	0.43
24:v:303:CLA:H61	25:v:316:LUT:H373	2.01	0.43
24:AH:610:CLA:HBA2	24:AH:610:CLA:H3A	1.80	0.43
25:AH:614:LUT:C8	25:AH:614:LUT:H181	2.48	0.43
28:AK:624:LHG:H311	15:m:18:PRO:HB3	2.00	0.43
23:AS:308:CHL:HBA2	23:AS:308:CHL:H3A	1.32	0.43
10:AU:251:PRO:HB2	24:AU:613:CLA:HMA3	2.01	0.43
23:9:607:CHL:H91	23:9:607:CHL:C12	2.41	0.43
29:J:408:BCR:H15C	29:J:408:BCR:H351	1.86	0.43
5:O:62:VAL:O	5:O:66:MET:HG3	2.18	0.43
5:O:144:PHE:CE1	5:O:210:ILE:HG23	2.54	0.43
5:O:218:SER:OG	5:O:219:VAL:HG23	2.18	0.43
7:Q:181:ARG:C	7:Q:181:ARG:HD3	2.44	0.43
14:o:29:ALA:O	14:o:33:SER:HB3	2.19	0.43
23:p:607:CHL:H203	23:p:607:CHL:H161	1.71	0.43
16:q:213:GLU:OE1	16:q:213:GLU:HA	2.19	0.43
17:v:242:GLN:HE22	25:v:315:LUT:H42	1.83	0.43
23:AH:605:CHL:HBD	23:AH:605:CHL:HAA1	2.01	0.43
23:AH:608:CHL:H92	23:AH:608:CHL:H62	1.60	0.43
5:AK:371:VAL:HG12	5:AK:377:VAL:HA	1.99	0.43
29:AL:516:BCR:H15C	29:AL:516:BCR:H351	1.82	0.43
7:AM:121:PHE:O	7:AM:124:ILE:HB	2.18	0.43
24:AM:404:CLA:H91	24:AM:404:CLA:H112	1.73	0.43
24:AS:304:CLA:HBA1	24:AS:304:CLA:H3A	1.80	0.43
23:AU:607:CHL:H91	23:AU:607:CHL:CMB	2.33	0.43
24:AU:610:CLA:H91	24:AU:610:CLA:H111	1.68	0.43
23:AA:601:CHL:HBA1	23:AA:601:CHL:H3A	1.57	0.43
3:AB:77:LEU:HD11	3:AB:95:LEU:HD21	2.01	0.43
2:AD:174:ARG:HH22	23:AD:308:CHL:CGD	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:321:ILE:HD11	7:Q:180:PHE:HB2	2.01	0.43
24:O:601:CLA:H93	29:j:101:BCR:H282	2.01	0.43
23:V:616:CHL:HAA1	23:V:616:CHL:CGD	2.49	0.43
18:AG:18:PHE:HB2	29:AK:602:BCR:HC7	1.99	0.43
19:U:79:ARG:HD2	19:U:103:TYR:OXT	2.19	0.43
29:AJ:410:BCR:H20C	29:AJ:410:BCR:H361	1.86	0.43
24:AK:610:CLA:H3A	24:AK:610:CLA:HBA2	1.79	0.43
6:AL:342:MET:HE3	6:AL:352:GLY:HA2	1.99	0.43
10:AQ:169:MET:HG3	23:AQ:609:CHL:CMC	2.48	0.43
24:AQ:604:CLA:HBA2	24:AQ:604:CLA:H3A	1.78	0.43
23:AQ:608:CHL:C9	23:AQ:608:CHL:C3	2.95	0.43
2:0:142:LEU:HD21	24:0:604:CLA:HAA2	2.00	0.42
23:AD:306:CHL:HBA1	23:AD:306:CHL:H3A	1.63	0.42
3:AF:242:PHE:HE1	25:AF:611:LUT:H41	1.82	0.42
5:O:132:SER:HB2	11:j:30:TYR:CD2	2.53	0.42
5:O:256:MET:HG2	5:O:451:PHE:HD1	1.80	0.42
7:Q:37:LEU:CD1	24:Q:404:CLA:HBB1	2.49	0.42
7:Q:133:LEU:O	7:Q:137:VAL:HG22	2.19	0.42
10:V:94:ARG:NE	10:V:94:ARG:HA	2.35	0.42
23:p:607:CHL:H143	23:p:607:CHL:H111	1.83	0.42
24:q:610:CLA:HBA2	24:q:610:CLA:H12	1.57	0.42
17:v:201:HIS:HB3	24:v:310:CLA:CGD	2.49	0.42
24:AH:604:CLA:HMB2	25:AH:615:LUT:H162	2.00	0.42
22:AI:31:ASP:O	22:AI:31:ASP:OD2	2.37	0.42
32:AJ:408:PHO:H3A	24:AM:403:CLA:H142	2.00	0.42
5:AK:207:THR:O	5:AK:211:LEU:HD13	2.19	0.42
24:AK:617:CLA:H2	24:AK:617:CLA:H61	1.70	0.42
23:AN:607:CHL:C9	23:AN:607:CHL:H41	2.41	0.42
29:k:101:BCR:H20C	29:k:101:BCR:H361	1.84	0.42
23:AU:605:CHL:HBA2	23:AU:605:CHL:H3A	1.46	0.42
24:9:604:CLA:C1B	26:9:617:NEX:H383	2.49	0.42
23:9:608:CHL:HBA2	23:9:608:CHL:H3A	1.51	0.42
2:0:178:LEU:HD12	2:0:179:ASP:H	1.84	0.42
1:AA:105:TRP:NE1	23:AA:607:CHL:HED3	2.34	0.42
3:AB:125:VAL:HG11	3:AB:133:GLN:NE2	2.34	0.42
1:AC:211:LEU:HD22	24:AC:609:CLA:H41	2.00	0.42
25:AC:615:LUT:H11	25:AC:615:LUT:H191	1.92	0.42
3:AF:188:TYR:HE2	3:AF:214:TYR:H	1.66	0.42
24:O:605:CLA:H62	24:O:605:CLA:H41	1.45	0.42
24:O:609:CLA:HMA3	24:O:610:CLA:C1C	2.49	0.42
6:P:59:LEU:HD21	29:P:515:BCR:H372	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:13:ILE:HD13	12:I:13:ILE:HA	1.87	0.42
17:v:144:GLU:HG3	17:v:144:GLU:O	2.19	0.42
24:v:313:CLA:HMB2	25:v:315:LUT:H162	2.01	0.42
4:AJ:321:ILE:HD11	7:AM:180:PHE:HB2	2.02	0.42
24:AK:611:CLA:CMD	11:AO:42:LEU:HD11	2.49	0.42
25:AN:614:LUT:H15	25:AN:614:LUT:H201	1.90	0.42
24:AQ:613:CLA:HBD	24:AQ:613:CLA:HED2	1.74	0.42
17:AS:224:LYS:HG2	24:AS:311:CLA:CED	2.49	0.42
24:AS:311:CLA:HED2	24:AS:311:CLA:HBD	1.70	0.42
23:AU:601:CHL:H3A	23:AU:601:CHL:HBA1	1.50	0.42
24:AU:604:CLA:H3A	24:AU:604:CLA:HBA2	1.60	0.42
2:AD:168:GLY:CA	23:AD:308:CHL:HAB	2.50	0.42
23:AD:306:CHL:HAA1	23:AD:306:CHL:HBD	2.01	0.42
5:O:113:TRP:HD1	29:O:619:BCR:H403	1.84	0.42
5:O:285:TYR:CD2	19:U:88:TYR:HD1	2.37	0.42
24:O:611:CLA:H2A	24:O:611:CLA:O2D	2.20	0.42
7:Q:234:ARG:CZ	34:Q:402:SQD:H61	2.49	0.42
23:p:606:CHL:CBB	25:p:615:LUT:H161	2.49	0.42
17:v:224:LYS:HG2	24:v:311:CLA:CED	2.49	0.42
23:v:302:CHL:HMA1	23:v:302:CHL:HHB	1.84	0.42
4:AJ:186:PHE:HE1	4:AJ:293:MET:SD	2.42	0.42
24:AL:503:CLA:HBA2	24:AL:503:CLA:H3A	1.82	0.42
23:AN:617:CHL:CGA	23:AN:617:CHL:H3A	2.49	0.42
10:AQ:228:GLY:O	10:AQ:232:GLN:HG3	2.18	0.42
24:AR:601:CLA:HHC	24:AR:601:CLA:HBB1	2.00	0.42
25:AA:614:LUT:H161	25:AA:614:LUT:H7	1.79	0.42
3:AB:73:LEU:HD12	3:AB:82:GLY:HA2	2.01	0.42
24:AD:304:CLA:OBD	23:AD:308:CHL:HBA2	2.19	0.42
5:O:363:PHE:HD2	5:O:366:PHE:HD2	1.66	0.42
5:O:419:LYS:HE2	5:O:423:ARG:NH2	2.29	0.42
10:p:107:MET:HE2	24:p:610:CLA:HHC	2.01	0.42
17:v:122:MET:HE3	17:v:229:GLY:N	2.33	0.42
23:v:307:CHL:HAA1	23:v:307:CHL:HBD	2.01	0.42
24:AK:606:CLA:H3A	24:AK:606:CLA:HBA2	1.33	0.42
24:AK:607:CLA:H193	24:AK:611:CLA:HBB2	2.01	0.42
24:AK:609:CLA:HBB1	24:AK:609:CLA:HMB1	2.00	0.42
29:AK:621:BCR:H20C	29:AK:621:BCR:H361	1.80	0.42
8:e:36:LEU:HA	8:e:39:SER:OG	2.20	0.42
24:AS:311:CLA:H92	24:AS:311:CLA:H62	1.88	0.42
10:AU:54:ASP:OD1	10:AU:54:ASP:O	2.36	0.42
2:0:49:GLY:O	2:0:52:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:605:CHL:HAA1	23:0:605:CHL:HBD	2.01	0.42
23:AC:601:CHL:HBA1	23:AC:601:CHL:H3A	1.50	0.42
1:AE:105:TRP:NE1	23:AE:606:CHL:HED3	2.33	0.42
24:AE:609:CLA:HBA2	24:AE:609:CLA:H3A	1.28	0.42
3:AF:149:GLN:NE2	23:AF:606:CHL:OMC	2.42	0.42
3:AF:238:ALA:HA	25:AF:611:LUT:H182	2.00	0.42
5:O:243:ALA:HA	5:O:246:PHE:CE2	2.54	0.42
5:O:281:GLN:HG2	19:U:91:VAL:HG22	2.01	0.42
6:P:42:LEU:HD21	24:K:101:CLA:H2A	2.01	0.42
24:AK:603:CLA:H141	24:AK:603:CLA:H193	2.02	0.42
7:AM:234:ARG:NH1	34:AM:401:SQD:H61	2.35	0.42
23:AN:617:CHL:OMC	23:AN:617:CHL:HHC	2.20	0.42
24:AQ:610:CLA:HBA2	24:AQ:610:CLA:H3A	1.46	0.42
19:u:79:ARG:HB3	19:u:102:ARG:O	2.19	0.42
24:AU:610:CLA:H61	24:AU:610:CLA:H41	1.92	0.42
2:0:126:GLU:OE2	2:0:128:VAL:HB	2.20	0.42
1:AA:115:PHE:CD2	24:AA:604:CLA:HAC2	2.55	0.42
32:J:406:PHO:H92	32:J:406:PHO:H61	1.80	0.42
24:p:603:CLA:H61	24:p:603:CLA:H92	1.69	0.42
10:AH:102:HIS:HB3	10:AH:223:MET:SD	2.60	0.42
10:AH:204:ASP:C	10:AH:204:ASP:OD2	2.62	0.42
24:AH:612:CLA:HBA2	24:AH:612:CLA:H3A	1.71	0.42
4:AJ:242:GLU:HB3	7:AM:242:GLU:OE1	2.20	0.42
24:AK:605:CLA:H193	24:AK:605:CLA:H162	1.87	0.42
24:AL:508:CLA:H142	29:AL:516:BCR:H362	2.02	0.42
10:AQ:121:ARG:HG2	10:AQ:121:ARG:HH11	1.84	0.42
24:AR:604:CLA:C1C	26:AR:615:NEX:H222	2.50	0.42
24:AR:617:CLA:HHC	24:AR:617:CLA:CBB	2.50	0.42
24:AU:603:CLA:H3A	24:AU:603:CLA:HBA1	1.78	0.42
23:AB:606:CHL:HBD	23:AB:606:CHL:HAA1	2.01	0.42
1:AE:183:LEU:HG	23:AE:606:CHL:CBB	2.50	0.42
1:AE:238:LYS:HD2	1:AE:242:GLU:OE2	2.19	0.42
3:AF:224:LEU:HB3	24:AF:609:CLA:CMA	2.50	0.42
24:AF:604:CLA:H3A	24:AF:604:CLA:HBA2	1.30	0.42
34:J:410:SQD:H222	29:AK:602:BCR:HC21	2.01	0.42
24:O:614:CLA:H52	29:O:617:BCR:H372	2.01	0.42
10:V:107:MET:CG	10:V:219:GLY:HA2	2.48	0.42
23:V:605:CHL:HAA1	23:V:605:CHL:HBD	2.00	0.42
10:p:88:ASP:OD2	10:p:90:GLU:N	2.50	0.42
24:p:602:CLA:H93	24:p:602:CLA:H111	1.73	0.42
23:q:605:CHL:H101	23:q:607:CHL:H52	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AJ:30:ILE:HD13	4:AJ:30:ILE:HA	1.90	0.42
24:AK:603:CLA:H141	24:AK:603:CLA:H161	1.73	0.42
24:AK:611:CLA:HBA2	24:AK:611:CLA:H3A	1.57	0.42
24:AK:616:CLA:HMD2	34:AP:101:SQD:H241	2.02	0.42
29:AK:620:BCR:HC42	33:AK:622:LMG:H362	2.01	0.42
10:AN:106:ALA:HB3	10:AN:223:MET:HG3	2.01	0.42
13:k:45:LEU:O	13:k:49:LEU:HD23	2.19	0.42
29:k:101:BCR:H15C	29:k:101:BCR:H351	1.83	0.42
17:AS:236:MET:HG3	17:AS:240:PHE:CZ	2.55	0.42
23:AU:607:CHL:H203	23:AU:607:CHL:H161	1.76	0.42
23:9:601:CHL:HAA1	23:9:601:CHL:CGD	2.49	0.42
23:AC:601:CHL:HBD	23:AC:601:CHL:HAA1	2.01	0.42
24:AC:602:CLA:H93	24:AC:602:CLA:H111	1.72	0.42
24:AC:609:CLA:H51	24:AC:609:CLA:C2B	2.50	0.42
24:AD:309:CLA:HBB1	24:AD:311:CLA:H3A	2.01	0.42
5:O:69:LEU:HD12	24:O:605:CLA:HBA1	2.00	0.42
5:O:153:PHE:HB2	24:O:606:CLA:HBB1	2.02	0.42
24:O:610:CLA:H13	24:O:612:CLA:H12	2.00	0.42
7:Q:22:TRP:CD1	21:X:110:PHE:HE1	2.38	0.42
8:E:66:ILE:HD11	8:E:72:SER:HA	2.02	0.42
10:V:117:GLU:HB3	10:V:241:ILE:HD12	2.00	0.42
35:j:102:DGD:O4D	35:j:102:DGD:O5D	2.29	0.42
16:q:241:ALA:O	16:q:245:HIS:ND1	2.52	0.42
23:v:306:CHL:HMC	23:v:307:CHL:C4C	2.49	0.42
25:AH:614:LUT:H15	25:AH:614:LUT:H201	1.93	0.42
24:AK:603:CLA:H92	24:AK:603:CLA:H61	1.83	0.42
24:AK:610:CLA:HMB1	24:AK:610:CLA:HBB1	2.01	0.42
10:AN:169:MET:HE2	10:AN:169:MET:HB3	1.83	0.42
35:AO:102:DGD:HB62	35:AO:102:DGD:HB91	1.71	0.42
23:9:607:CHL:CHC	23:0:601:CHL:H141	2.50	0.42
25:9:615:LUT:H15	25:9:615:LUT:H201	1.90	0.42
1:AC:214:LYS:HE3	24:AC:610:CLA:CGD	2.49	0.42
2:AD:83:SER:HB3	2:AD:89:PHE:HB2	2.02	0.42
25:AE:613:LUT:H31	25:AE:613:LUT:H391	1.96	0.42
23:AE:616:CHL:HHC	23:AE:616:CHL:OMC	2.19	0.42
4:J:219:VAL:HG11	7:Q:269:HIS:CD2	2.54	0.42
24:O:609:CLA:C3D	11:j:43:MET:SD	3.08	0.42
24:O:612:CLA:H102	24:O:612:CLA:H61	1.62	0.42
7:Q:316:TYR:O	7:Q:320:ILE:HG12	2.19	0.42
10:p:169:MET:HG3	23:p:609:CHL:CMC	2.50	0.42
10:p:204:ASP:OD1	10:p:204:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:X:94:GLY:O	21:X:97:LEU:HG	2.20	0.42
5:AK:138:ILE:HA	5:AK:138:ILE:HD13	1.83	0.42
5:AK:144:PHE:CE1	5:AK:210:ILE:HG23	2.55	0.42
5:AK:233:ASN:OD1	5:AK:235:GLU:N	2.43	0.42
25:AN:615:LUT:H161	25:AN:615:LUT:H7	1.82	0.42
16:AR:274:HIS:CE1	24:AR:612:CLA:HBA1	2.55	0.42
17:AS:188:TYR:HD1	23:AS:308:CHL:CAB	2.33	0.42
24:9:613:CLA:HBB1	24:9:613:CLA:HMB3	2.02	0.42
24:0:610:CLA:H2	24:0:611:CLA:HMD2	2.01	0.42
24:AD:305:CLA:HBA2	24:AD:305:CLA:H3A	1.28	0.42
1:AE:107:MET:HE2	24:AE:608:CLA:HHC	2.00	0.42
5:O:133:LEU:H	11:j:30:TYR:HE2	1.68	0.42
24:O:601:CLA:H141	24:O:601:CLA:H161	1.73	0.42
7:Q:89:SER:HB2	8:E:69:ARG:CZ	2.50	0.42
28:Q:406:LHG:O1	14:o:14:ASN:ND2	2.53	0.42
23:V:607:CHL:C9	23:V:607:CHL:H43	2.48	0.42
13:K:43:ILE:HA	13:K:46:PHE:HD1	1.83	0.42
23:q:607:CHL:CBD	23:q:607:CHL:HAA1	2.50	0.42
10:AH:211:LEU:HD23	10:AH:214:LYS:HD2	2.02	0.42
24:AJ:405:CLA:H152	24:AJ:405:CLA:H111	1.77	0.42
35:AO:102:DGD:HO4D	35:AO:102:DGD:HE3	1.85	0.42
12:i:25:SER:O	12:i:25:SER:OG	2.34	0.42
14:AP:13:LEU:HD23	14:AP:14:ASN:O	2.20	0.42
10:AQ:69:TYR:OH	10:AQ:81:ASP:OD2	2.22	0.42
10:AQ:102:HIS:HB3	10:AQ:223:MET:SD	2.59	0.42
23:AQ:607:CHL:H91	23:AQ:607:CHL:H112	1.59	0.42
24:AQ:612:CLA:HMB1	24:AQ:612:CLA:HBB1	2.02	0.42
24:AR:609:CLA:CBB	25:AR:614:LUT:H32	2.50	0.42
17:AS:115:LEU:HD21	17:AS:119:ARG:CZ	2.50	0.42
24:AU:609:CLA:H102	24:AU:609:CLA:H13	1.46	0.42
25:AU:615:LUT:C8	25:AU:615:LUT:H181	2.50	0.42
24:9:604:CLA:H12	23:9:606:CHL:C3D	2.50	0.41
2:0:164:VAL:HA	2:0:167:MET:HE2	2.01	0.41
2:0:227:PHE:CE1	25:0:614:LUT:H182	2.54	0.41
23:AB:606:CHL:H3A	23:AB:606:CHL:HBA2	1.53	0.41
23:AC:608:CHL:H92	23:AC:608:CHL:C5	2.50	0.41
2:AD:237:GLY:N	2:AD:240:GLU:OE1	2.44	0.41
25:AD:315:LUT:H11	25:AD:315:LUT:H191	1.92	0.41
23:AD:317:CHL:HHC	23:AD:317:CHL:OMC	2.19	0.41
24:J:403:CLA:C3	32:J:405:PHO:HBB1	2.50	0.41
5:O:8:VAL:HG23	5:O:9:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:241:SER:O	5:O:245:VAL:HG23	2.20	0.41
5:O:464:PHE:HD2	24:O:611:CLA:HAC2	1.84	0.41
24:O:601:CLA:H141	24:O:601:CLA:H193	2.02	0.41
24:O:604:CLA:H3A	24:O:604:CLA:HBA2	1.34	0.41
6:P:342:MET:SD	6:P:352:GLY:HA2	2.60	0.41
24:P:511:CLA:H112	24:P:511:CLA:H91	1.79	0.41
17:v:178:GLU:HG2	23:v:306:CHL:C1B	2.50	0.41
18:AG:18:PHE:C	18:AG:18:PHE:CD1	2.98	0.41
24:AH:611:CLA:HBA1	24:AH:611:CLA:H3A	1.83	0.41
24:AJ:404:CLA:H72	24:AJ:404:CLA:H111	1.78	0.41
32:AJ:408:PHO:H92	32:AJ:408:PHO:H61	1.80	0.41
5:AK:8:VAL:HG23	5:AK:9:HIS:ND1	2.35	0.41
5:AK:10:THR:CG2	24:AK:613:CLA:HED1	2.49	0.41
7:AM:196:PRO:O	7:AM:200:MET:HG3	2.20	0.41
10:AN:110:ALA:HA	10:AN:226:MET:HE1	2.02	0.41
24:AN:603:CLA:H92	24:AN:603:CLA:H61	1.76	0.41
16:AR:271:TRP:HD1	16:AR:271:TRP:O	2.03	0.41
17:AS:128:PHE:HE1	25:AS:316:LUT:C6	2.33	0.41
23:AU:601:CHL:H93	23:AU:601:CHL:C4	2.50	0.41
23:AU:605:CHL:HBD	23:AU:605:CHL:HAA1	2.01	0.41
24:0:609:CLA:H52	25:0:614:LUT:H28	2.01	0.41
1:AA:176:ARG:HH22	23:AA:608:CHL:CED	2.33	0.41
23:AA:605:CHL:HMC	23:AA:606:CHL:NC	2.34	0.41
23:AB:608:CHL:H3A	23:AB:608:CHL:HBA2	1.28	0.41
1:AC:204:ASP:OD1	1:AC:204:ASP:C	2.63	0.41
4:J:187:GLN:HB2	24:J:403:CLA:HAC2	2.01	0.41
24:J:403:CLA:H111	24:J:403:CLA:H72	1.78	0.41
29:O:618:BCR:H371	29:O:618:BCR:H24C	1.88	0.41
7:Q:14:ASP:OD1	7:Q:15:LEU:N	2.53	0.41
7:Q:30:PHE:CD2	7:Q:133:LEU:HD21	2.54	0.41
7:Q:226:ASP:OD1	7:Q:226:ASP:O	2.38	0.41
10:V:144:LEU:HD12	23:V:605:CHL:HMD1	2.02	0.41
23:AH:607:CHL:H203	23:AH:607:CHL:H161	1.77	0.41
22:AI:15:THR:HA	22:AI:18:ILE:HG22	2.01	0.41
24:AJ:404:CLA:H192	24:AJ:404:CLA:H161	1.89	0.41
5:AK:358:ARG:CZ	5:AK:427:GLY:HA2	2.49	0.41
14:AP:29:ALA:O	14:AP:33:SER:HB3	2.20	0.41
25:AQ:616:LUT:H15	25:AQ:616:LUT:H201	1.91	0.41
10:AU:169:MET:HA	10:AU:172:VAL:HG22	2.01	0.41
25:AU:615:LUT:H11	25:AU:615:LUT:H191	1.93	0.41
23:9:601:CHL:HMA1	23:9:601:CHL:HHB	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:9:615:LUT:H11	25:9:615:LUT:H191	1.84	0.41
2:AD:75:TYR:HB2	24:AD:303:CLA:OBD	2.20	0.41
24:AD:303:CLA:H142	25:AD:315:LUT:H393	2.01	0.41
4:J:93:PHE:HZ	24:J:407:CLA:HAA1	1.85	0.41
24:O:608:CLA:H141	24:O:608:CLA:H161	1.84	0.41
23:p:607:CHL:H91	23:p:607:CHL:H112	1.59	0.41
24:q:612:CLA:H3A	24:q:612:CLA:HBA2	1.75	0.41
25:q:614:LUT:H161	25:q:614:LUT:H7	1.87	0.41
17:v:220:LEU:O	17:v:224:LYS:HG3	2.20	0.41
23:v:307:CHL:HBA1	23:v:307:CHL:H3A	1.59	0.41
22:AI:20:LEU:HD21	29:AI:101:BCR:H343	2.01	0.41
4:AJ:64:ARG:HG2	4:AJ:64:ARG:HH11	1.85	0.41
24:AJ:404:CLA:H142	24:AJ:404:CLA:H112	1.89	0.41
5:AK:326:ARG:HH21	7:AM:298:ASP:CG	2.29	0.41
5:AK:363:PHE:CE1	7:AM:189:PHE:HE2	2.38	0.41
5:AK:431:GLU:C	5:AK:432:LEU:HD23	2.45	0.41
24:AK:610:CLA:H141	24:AK:610:CLA:H161	1.84	0.41
7:AM:316:TYR:O	7:AM:320:ILE:HG12	2.20	0.41
10:AQ:121:ARG:NH1	10:AQ:121:ARG:O	2.53	0.41
10:AQ:186:ALA:HB2	23:AQ:608:CHL:HBC1	2.02	0.41
10:AQ:226:MET:HG3	25:AQ:616:LUT:H12	2.02	0.41
23:AQ:606:CHL:HMC	23:AQ:607:CHL:NC	2.36	0.41
25:AR:614:LUT:H15	25:AR:614:LUT:H201	1.90	0.41
29:AB:612:BCR:H333	24:q:601:CLA:HBB1	2.02	0.41
1:AC:232:GLN:NE2	1:AC:232:GLN:N	2.69	0.41
2:AD:141:GLY:HA3	2:AD:154:GLN:HE22	1.85	0.41
23:AE:617:CHL:HMA1	23:AE:617:CHL:HHB	1.87	0.41
24:O:603:CLA:H62	24:O:603:CLA:H41	1.71	0.41
29:O:625:BCR:HC7	18:AT:18:PHE:HB2	2.02	0.41
24:P:503:CLA:H41	24:P:503:CLA:H62	1.55	0.41
29:P:515:BCR:H24C	29:P:515:BCR:H371	1.84	0.41
23:V:606:CHL:H143	23:V:606:CHL:H111	1.92	0.41
24:V:609:CLA:C2	25:V:613:LUT:H26	2.51	0.41
25:V:614:LUT:H31	25:V:614:LUT:H391	1.94	0.41
35:j:102:DGD:HB91	35:j:102:DGD:HB62	1.74	0.41
23:q:607:CHL:HAA1	23:q:607:CHL:HBD	2.03	0.41
25:AH:615:LUT:C8	25:AH:615:LUT:H181	2.50	0.41
4:AJ:131:TRP:CZ2	6:AL:449:ARG:HD2	2.47	0.41
29:AJ:410:BCR:H11C	29:AJ:410:BCR:H341	1.94	0.41
5:AK:330:MET:HA	5:AK:444:ARG:HB2	2.03	0.41
24:AK:610:CLA:H92	24:AK:610:CLA:H62	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AK:615:CLA:H61	24:AK:615:CLA:H41	1.67	0.41
6:AL:381:LYS:HD3	6:AL:381:LYS:HA	1.69	0.41
7:AM:81:THR:OG1	7:AM:169:PHE:HA	2.21	0.41
7:AM:133:LEU:O	7:AM:137:VAL:HG22	2.21	0.41
7:AM:258:PHE:CZ	28:AM:406:LHG:H312	2.56	0.41
29:f:101:BCR:H20C	29:f:101:BCR:H361	1.85	0.41
17:AS:152:ALA:HB2	23:AS:307:CHL:HED3	2.01	0.41
17:AS:207:ASP:OD1	25:AS:315:LUT:O23	2.38	0.41
17:AS:220:LEU:O	17:AS:224:LYS:HG3	2.21	0.41
10:AU:207:ALA:O	10:AU:211:LEU:HD23	2.20	0.41
1:AC:152:LEU:O	1:AC:154:HIS:N	2.52	0.41
2:AD:102:TRP:CD1	23:AD:308:CHL:HMD3	2.56	0.41
25:AE:613:LUT:H161	25:AE:613:LUT:H7	1.76	0.41
34:J:410:SQD:H341	35:J:413:DGD:HBH1	2.02	0.41
5:O:231:MET:HE2	24:O:610:CLA:HAC1	2.02	0.41
24:O:610:CLA:H151	24:O:615:CLA:CAD	2.50	0.41
28:O:623:LHG:H171	28:O:623:LHG:H202	1.89	0.41
7:Q:25:ARG:HB2	7:Q:27:ARG:HH21	1.85	0.41
23:V:607:CHL:O1A	23:V:607:CHL:H3A	2.20	0.41
16:q:85:LYS:HD2	16:q:86:PRO:N	2.35	0.41
24:AJ:404:CLA:C3	32:AJ:407:PHO:HBB1	2.51	0.41
24:AL:509:CLA:H92	24:AL:509:CLA:H61	1.81	0.41
9:f:27:PHE:CD2	29:f:101:BCR:H14C	2.55	0.41
23:AN:606:CHL:HHC	23:AN:606:CHL:CBB	2.49	0.41
16:AR:167:ASP:O	16:AR:171:VAL:HG12	2.20	0.41
23:AR:607:CHL:HAA1	23:AR:607:CHL:HBD	2.02	0.41
19:u:99:LYS:HA	19:u:102:ARG:HB3	2.03	0.41
10:AU:153:VAL:N	23:AU:605:CHL:O1D	2.28	0.41
1:9:223:MET:HG2	25:9:616:LUT:C35	2.51	0.41
24:9:602:CLA:H111	24:9:602:CLA:H93	1.73	0.41
23:0:617:CHL:HHC	23:0:617:CHL:OMC	2.21	0.41
3:AB:149:GLN:OE1	23:AB:606:CHL:HMC	2.21	0.41
3:AB:157:GLU:HB3	23:AB:608:CHL:HMA3	2.02	0.41
3:AB:224:LEU:HB3	24:AB:609:CLA:HMA1	2.01	0.41
1:AC:69:TYR:OH	1:AC:81:ASP:OD2	2.34	0.41
1:AC:196:PHE:O	25:AC:614:LUT:H24	2.20	0.41
24:AD:310:CLA:CHA	24:AD:310:CLA:HBA1	2.51	0.41
1:AE:226:MET:CE	25:AE:614:LUT:H12	2.50	0.41
5:O:472:ARG:NH1	24:O:611:CLA:CGD	2.79	0.41
29:O:617:BCR:H11C	29:O:617:BCR:H341	1.89	0.41
29:O:618:BCR:H15C	29:O:618:BCR:H351	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:p:208:PHE:CE2	10:p:212:LYS:HE3	2.55	0.41
10:AH:199:LEU:HD12	25:AH:614:LUT:H222	2.02	0.41
23:AN:607:CHL:H92	23:AN:607:CHL:H62	1.66	0.41
23:AQ:607:CHL:HAA1	23:AQ:607:CHL:HBD	2.02	0.41
24:AQ:612:CLA:H143	24:AQ:612:CLA:H111	1.91	0.41
25:AR:614:LUT:H35	25:AR:614:LUT:H401	1.91	0.41
24:AS:311:CLA:H3A	24:AS:311:CLA:HBA2	1.30	0.41
23:AU:601:CHL:H93	23:AU:601:CHL:H41	2.02	0.41
1:AA:54:ASP:O	1:AA:54:ASP:OD1	2.38	0.41
3:AB:170:GLN:HG3	23:AB:607:CHL:CMC	2.49	0.41
2:AD:118:LYS:HD2	2:AD:118:LYS:C	2.45	0.41
1:AE:182:PRO:HB2	23:AE:606:CHL:CBB	2.48	0.41
24:AF:610:CLA:HBA2	24:AF:610:CLA:CGD	2.50	0.41
4:J:313:VAL:C	4:J:314:ILE:HD13	2.45	0.41
29:P:513:BCR:H361	29:P:513:BCR:H20C	1.83	0.41
8:E:36:LEU:O	8:E:40:THR:HG23	2.20	0.41
10:V:202:ALA:HB2	24:V:609:CLA:HBA1	2.02	0.41
23:V:601:CHL:H41	28:V:615:LHG:H192	2.03	0.41
14:o:26:PHE:HE2	18:AG:12:SER:HB2	1.85	0.41
24:q:612:CLA:H91	24:q:612:CLA:H112	1.83	0.41
10:AH:188:ASP:OD1	10:AH:188:ASP:C	2.64	0.41
5:AK:363:PHE:HD2	5:AK:366:PHE:HD2	1.68	0.41
10:AN:105:TRP:HD1	23:AN:608:CHL:HMD2	1.84	0.41
23:AN:608:CHL:H62	23:AN:608:CHL:H92	1.76	0.41
10:AQ:234:ILE:HD13	10:AQ:234:ILE:HA	1.82	0.41
23:AQ:606:CHL:HAA1	23:AQ:606:CHL:CGD	2.50	0.41
24:AQ:613:CLA:H61	24:AQ:613:CLA:H2	1.83	0.41
16:AR:243:ILE:HG12	16:AR:247:ARG:HE	1.86	0.41
10:AU:187:GLU:OE1	10:AU:187:GLU:N	2.30	0.41
23:9:607:CHL:HHC	23:9:607:CHL:HBB1	2.02	0.41
24:0:602:CLA:H142	25:0:615:LUT:H393	2.02	0.41
24:0:609:CLA:H62	24:0:609:CLA:H41	1.77	0.41
24:AA:611:CLA:HMC2	25:AA:614:LUT:H11	2.03	0.41
23:AD:301:CHL:H2	23:AD:301:CHL:H62	1.92	0.41
1:AE:54:ASP:OD1	1:AE:54:ASP:O	2.39	0.41
13:K:37:VAL:HA	13:K:40:MET:HG3	2.03	0.41
16:q:164:THR:OG1	16:q:166:GLN:HG2	2.21	0.41
16:q:217:TYR:HB3	24:q:609:CLA:O1D	2.21	0.41
23:v:307:CHL:HAA1	23:v:307:CHL:CBD	2.51	0.41
7:AM:21:ASP:OD1	7:AM:21:ASP:C	2.64	0.41
13:k:53:VAL:CG2	29:AV:101:BCR:H21C	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AQ:603:CLA:H92	24:AQ:603:CLA:H61	1.68	0.41
24:AR:609:CLA:H2	25:AR:614:LUT:H26	2.03	0.41
23:9:607:CHL:H162	23:9:609:CHL:H93	2.02	0.41
2:0:167:MET:HE3	23:0:608:CHL:HHD	2.03	0.41
2:0:200:ALA:HB2	24:0:609:CLA:HAA2	2.02	0.41
23:0:607:CHL:HMA1	23:0:607:CHL:HHB	1.93	0.41
1:AA:208:PHE:O	1:AA:212:LYS:HG3	2.21	0.41
25:AA:614:LUT:H35	25:AA:614:LUT:H401	1.96	0.41
1:AC:240:PRO:HA	1:AC:243:ASN:ND2	2.35	0.41
2:AD:235:GLY:C	2:AD:236:LYS:HD2	2.46	0.41
23:AD:302:CHL:H143	23:AD:302:CHL:H161	1.73	0.41
23:AE:616:CHL:HBA2	23:AE:616:CHL:H3A	1.66	0.41
4:J:138:GLY:HA2	6:P:455:PHE:CZ	2.56	0.41
24:O:601:CLA:H12	24:O:601:CLA:H52	1.83	0.41
24:O:613:CLA:H111	24:O:613:CLA:H91	1.71	0.41
29:O:618:BCR:H11C	29:O:618:BCR:H341	1.94	0.41
6:P:152:LYS:HE2	6:P:152:LYS:HB2	1.78	0.41
24:P:502:CLA:HBA2	24:P:502:CLA:H3A	1.84	0.41
29:P:513:BCR:H11C	29:P:513:BCR:H341	1.97	0.41
7:Q:25:ARG:NH2	21:X:110:PHE:HD1	2.19	0.41
7:Q:44:PHE:HE2	24:Q:404:CLA:C2C	2.34	0.41
23:p:601:CHL:O1D	28:p:617:LHG:H122	2.21	0.41
17:v:115:LEU:HD21	17:v:119:ARG:CZ	2.50	0.41
17:v:128:PHE:HE1	25:v:316:LUT:C5	2.34	0.41
25:v:316:LUT:H31	25:v:316:LUT:H391	1.97	0.41
10:AH:223:MET:HE3	24:AH:602:CLA:HMC2	2.03	0.41
32:AJ:408:PHO:HBC3	7:AM:280:LEU:HG	2.03	0.41
5:AK:246:PHE:CD1	5:AK:246:PHE:C	2.98	0.41
5:AK:315:ILE:HG22	5:AK:426:LEU:HB3	2.03	0.41
24:AK:605:CLA:HAB	24:AK:607:CLA:H18	2.03	0.41
24:AL:502:CLA:HBA2	24:AL:502:CLA:H3A	1.26	0.41
29:AL:515:BCR:H11C	29:AL:515:BCR:H341	1.96	0.41
7:AM:226:ASP:OD1	7:AM:226:ASP:O	2.39	0.41
10:AN:107:MET:HE2	10:AN:107:MET:HB3	1.90	0.41
23:AN:607:CHL:H93	23:AN:607:CHL:C4	2.47	0.41
23:AQ:607:CHL:H191	23:AU:601:CHL:H91	2.03	0.41
20:w:123:LEU:HD23	20:w:123:LEU:HA	1.91	0.41
10:AU:144:LEU:HD11	24:AU:604:CLA:HAA2	2.02	0.41
10:AU:152:LEU:O	10:AU:154:HIS:N	2.53	0.41
23:AU:601:CHL:H162	23:AU:601:CHL:H141	1.79	0.41
22:AV:23:VAL:HB	22:AV:24:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:9:606:CHL:HMB1	23:9:609:CHL:HMC	2.03	0.41
24:0:610:CLA:CHA	24:0:610:CLA:HBA1	2.50	0.41
24:AC:604:CLA:CMB	25:AC:615:LUT:H162	2.49	0.41
2:AD:139:GLU:OE2	2:AD:140:GLY:N	2.54	0.41
23:AD:302:CHL:HBA1	23:AD:302:CHL:H3A	1.35	0.41
3:AF:251:THR:CG2	3:AF:254:GLY:H	2.34	0.41
23:AF:607:CHL:HAA1	23:AF:607:CHL:CBD	2.51	0.41
24:J:407:CLA:H111	24:J:407:CLA:H91	1.86	0.41
5:O:144:PHE:O	5:O:148:VAL:HG12	2.21	0.41
5:O:187:VAL:HG12	11:j:70:ILE:HG13	2.03	0.41
29:O:619:BCR:H15C	29:O:619:BCR:H351	1.89	0.41
33:P:518:LMG:HC91	33:P:518:LMG:H291	1.85	0.41
23:p:607:CHL:HBD	23:p:607:CHL:HAA1	2.02	0.41
4:AJ:127:MET:HE3	4:AJ:127:MET:HB2	1.89	0.41
24:AK:605:CLA:HAB	24:AK:607:CLA:H152	2.02	0.41
24:AL:514:CLA:HBA1	24:AL:514:CLA:CBD	2.43	0.41
7:AM:127:MET:HE2	7:AM:151:ILE:HD12	2.01	0.41
8:e:27:ILE:HB	8:e:28:PRO:HD3	2.02	0.41
10:AN:152:LEU:O	10:AN:154:HIS:N	2.53	0.41
24:AN:603:CLA:OBD	23:AN:608:CHL:HBA2	2.20	0.41
24:AN:612:CLA:HMB1	24:AN:612:CLA:HBB1	2.03	0.41
25:AR:614:LUT:H11	25:AR:614:LUT:H191	1.94	0.41
19:u:95:MET:HE2	19:u:95:MET:HB2	1.87	0.41
10:AU:255:ASN:OD1	10:AU:257:TRP:HD1	2.03	0.41
23:9:601:CHL:HBC2	23:9:601:CHL:HHD	2.02	0.40
2:0:103:ALA:CB	2:0:221:MET:HG2	2.51	0.40
2:AD:250:VAL:O	2:AD:253:ASN:ND2	2.54	0.40
1:AE:59:LEU:HB2	1:AE:63:SER:HA	2.03	0.40
25:AE:613:LUT:H35	25:AE:613:LUT:H401	1.96	0.40
26:AE:615:NEX:H35	26:AE:615:NEX:H401	1.96	0.40
3:AF:103:LEU:HD13	3:AF:103:LEU:HA	1.90	0.40
5:O:187:VAL:O	11:j:70:ILE:HD11	2.21	0.40
24:O:605:CLA:H193	24:O:609:CLA:HBB2	2.03	0.40
24:O:614:CLA:H111	24:O:614:CLA:H142	1.86	0.40
23:V:607:CHL:HAA1	23:V:607:CHL:CBD	2.51	0.40
10:p:138:ILE:HG21	10:p:158:ILE:HD13	2.02	0.40
24:p:604:CLA:H3A	24:p:604:CLA:HBA2	1.77	0.40
23:p:606:CHL:HMC	23:p:607:CHL:NC	2.36	0.40
16:q:166:GLN:CD	16:q:166:GLN:H	2.29	0.40
17:v:168:PRO:O	17:v:169:ILE:HD13	2.20	0.40
5:AK:243:ALA:HA	5:AK:246:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AK:614:CLA:H61	24:AK:614:CLA:H102	1.62	0.40
33:AL:501:LMG:H372	33:AL:501:LMG:H341	1.81	0.40
33:AL:520:LMG:H152	17:AS:262:PHE:CE1	2.57	0.40
25:AN:615:LUT:H31	25:AN:615:LUT:H391	1.95	0.40
14:AP:8:GLU:HB3	34:AP:101:SQD:O8	2.20	0.40
24:AU:611:CLA:H61	24:AU:611:CLA:H102	1.81	0.40
23:AD:306:CHL:HAB	25:AD:315:LUT:H171	2.04	0.40
5:O:246:PHE:CD1	5:O:246:PHE:C	2.99	0.40
24:O:601:CLA:H61	24:O:601:CLA:H92	1.82	0.40
6:P:361:LEU:O	6:P:362:ARG:HD3	2.21	0.40
7:Q:72:CYS:HB3	7:Q:76:THR:OG1	2.21	0.40
10:V:169:MET:HA	10:V:172:VAL:HG22	2.03	0.40
10:p:223:MET:HE3	25:p:615:LUT:C34	2.52	0.40
24:q:618:CLA:HED3	24:q:618:CLA:CAA	2.51	0.40
19:U:84:ALA:HB1	19:U:100:ILE:HD11	2.03	0.40
10:AH:107:MET:HE1	24:AH:609:CLA:HAB	2.03	0.40
10:AH:187:GLU:OE1	10:AH:187:GLU:N	2.30	0.40
4:AJ:223:LEU:HD12	4:AJ:245:THR:O	2.21	0.40
24:AK:618:CLA:OBD	11:AO:17:THR:HG21	2.21	0.40
29:AK:619:BCR:H11C	29:AK:619:BCR:H341	1.89	0.40
29:AK:621:BCR:H11C	29:AK:621:BCR:H341	1.96	0.40
24:AL:513:CLA:H112	24:AL:513:CLA:H91	1.78	0.40
23:AN:605:CHL:HAB	23:AN:606:CHL:OMC	2.21	0.40
23:AN:606:CHL:HMA1	23:AN:606:CHL:HHB	1.93	0.40
25:AN:614:LUT:H35	25:AN:614:LUT:H401	1.92	0.40
16:AR:170:LYS:O	16:AR:174:VAL:HG22	2.20	0.40
16:AR:205:GLN:HB3	23:AR:607:CHL:OMC	2.21	0.40
24:AR:609:CLA:H141	24:AR:609:CLA:H162	1.72	0.40
10:AU:247:HIS:CE1	24:AU:612:CLA:HBA1	2.55	0.40
23:AU:601:CHL:H202	23:AU:601:CHL:H161	1.63	0.40
24:AU:604:CLA:HMB2	25:AU:615:LUT:H162	2.03	0.40
29:AV:101:BCR:H11C	29:AV:101:BCR:H341	1.96	0.40
3:AB:151:LEU:HD23	3:AB:151:LEU:HA	1.84	0.40
3:AB:176:THR:H	24:q:601:CLA:HBB2	1.85	0.40
1:AC:103:SER:O	1:AC:107:MET:HG3	2.21	0.40
23:AC:606:CHL:HMA1	23:AC:606:CHL:HHB	1.96	0.40
25:AE:613:LUT:H15	25:AE:613:LUT:H201	1.94	0.40
25:AE:614:LUT:H35	25:AE:614:LUT:H401	1.91	0.40
3:AF:145:LEU:HD21	23:AF:605:CHL:C1D	2.52	0.40
29:J:408:BCR:H11C	29:J:408:BCR:H341	1.94	0.40
6:P:223:TRP:CG	6:P:224:ILE:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:508:CLA:H92	24:P:508:CLA:H61	1.81	0.40
7:Q:343:PRO:O	7:Q:346:VAL:HG22	2.22	0.40
9:F:14:TRP:CG	9:F:18:HIS:CE1	3.10	0.40
10:V:136:SER:HB3	23:V:606:CHL:O1D	2.22	0.40
24:V:610:CLA:HHC	24:V:610:CLA:CBB	2.48	0.40
14:o:8:GLU:HB3	34:o:101:SQD:O8	2.21	0.40
16:q:202:ILE:CD1	23:q:607:CHL:HMA3	2.51	0.40
16:q:235:THR:O	16:q:239:GLN:HG3	2.22	0.40
24:q:609:CLA:C4A	24:q:609:CLA:H11	2.52	0.40
10:AH:152:LEU:O	10:AH:154:HIS:N	2.53	0.40
4:AJ:225:ARG:N	4:AJ:225:ARG:CD	2.85	0.40
5:AK:208:LEU:HD12	5:AK:208:LEU:HA	1.85	0.40
5:AK:467:ILE:HD13	5:AK:467:ILE:HA	1.92	0.40
24:AK:608:CLA:HHC	24:AK:608:CLA:CBB	2.52	0.40
29:AK:620:BCR:H15C	29:AK:620:BCR:H351	1.85	0.40
6:AL:324:LEU:HD23	6:AL:324:LEU:O	2.22	0.40
28:AL:519:LHG:HC81	28:AL:519:LHG:H112	1.56	0.40
10:AN:97:GLU:HG3	10:AN:190:LEU:HD21	2.03	0.40
10:AN:167:ILE:HD13	10:AN:167:ILE:N	2.36	0.40
23:AQ:601:CHL:O1D	28:AQ:618:LHG:H122	2.21	0.40
23:AQ:607:CHL:H143	23:AQ:607:CHL:H111	1.82	0.40
24:AQ:610:CLA:H92	24:AQ:610:CLA:H61	1.80	0.40
25:AR:614:LUT:H181	25:AR:614:LUT:C8	2.51	0.40
25:AU:615:LUT:H35	25:AU:615:LUT:H401	1.93	0.40
28:0:616:LHG:H251	28:0:616:LHG:H282	1.79	0.40
24:AA:603:CLA:HBC1	23:AA:608:CHL:HBC2	2.02	0.40
24:AA:610:CLA:H3A	24:AA:610:CLA:HBA2	1.23	0.40
3:AB:185:PHE:CE1	23:AB:607:CHL:HBB1	2.56	0.40
3:AB:251:THR:OG1	3:AB:252:PRO:HD2	2.21	0.40
25:AC:614:LUT:H15	25:AC:614:LUT:H201	1.90	0.40
24:AE:611:CLA:C3B	25:AE:613:LUT:H183	2.52	0.40
24:O:610:CLA:HHC	24:O:610:CLA:CBB	2.51	0.40
33:P:518:LMG:H292	33:P:518:LMG:H322	1.97	0.40
7:Q:258:PHE:CZ	28:Q:406:LHG:H312	2.56	0.40
23:V:601:CHL:H141	23:V:601:CHL:H162	1.92	0.40
25:V:614:LUT:H161	25:V:614:LUT:H7	1.85	0.40
16:q:127:TYR:CD2	16:q:135:ARG:HG3	2.56	0.40
20:W:110:GLY:HA3	28:W:201:LHG:H181	2.02	0.40
5:AK:42:LEU:HD23	5:AK:42:LEU:HA	1.82	0.40
5:AK:217:LEU:HD23	24:AR:617:CLA:CBA	2.45	0.40
24:AL:506:CLA:H161	24:AL:506:CLA:H192	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:f:18:HIS:NE2	38:f:102:HEM:NA	2.67	0.40
24:AN:602:CLA:H51	24:AN:602:CLA:HMB1	2.03	0.40
23:AN:607:CHL:C9	23:AN:607:CHL:H43	2.51	0.40
11:AO:41:PRO:O	11:AO:45:VAL:HG23	2.21	0.40
11:AO:67:LEU:HD23	11:AO:67:LEU:HA	1.80	0.40
10:AU:231:VAL:O	10:AU:234:ILE:HG22	2.22	0.40
24:AU:610:CLA:H3A	24:AU:610:CLA:HBA2	1.79	0.40
25:0:615:LUT:H181	25:0:615:LUT:C8	2.51	0.40
1:AA:223:MET:HG3	1:AA:223:MET:H	1.74	0.40
24:AA:603:CLA:H3A	24:AA:603:CLA:HBA1	1.84	0.40
23:AA:617:CHL:HAA1	23:AA:617:CHL:CGD	2.51	0.40
3:AB:116:ILE:HG13	3:AB:116:ILE:H	1.69	0.40
1:AC:78:TYR:HB2	24:AC:602:CLA:OBD	2.22	0.40
24:AE:603:CLA:H61	24:AE:603:CLA:H92	1.91	0.40
23:V:605:CHL:HAA1	23:V:605:CHL:CGD	2.51	0.40
24:V:609:CLA:H3A	24:V:609:CLA:HBA2	1.45	0.40
25:V:614:LUT:H15	25:V:614:LUT:H201	1.92	0.40
10:p:121:ARG:HB2	10:p:121:ARG:NH1	2.36	0.40
24:AH:609:CLA:H13	24:AH:609:CLA:H102	1.47	0.40
22:AI:52:PHE:O	22:AI:56:ILE:HG12	2.21	0.40
4:AJ:212:SER:HB2	7:AM:212:CYS:HB2	2.02	0.40
5:AK:423:ARG:HD2	5:AK:429:ILE:HG23	2.03	0.40
24:AK:616:CLA:H52	29:AK:619:BCR:H372	2.04	0.40
29:AK:619:BCR:H351	29:AK:619:BCR:H15C	1.81	0.40
17:AS:161:ASN:C	17:AS:163:PHE:H	2.29	0.40
10:AU:251:PRO:HB2	24:AU:613:CLA:CMA	2.51	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	9	200/266 (75%)	198 (99%)	2 (1%)	0	100	100
1	AA	200/266 (75%)	196 (98%)	3 (2%)	1 (0%)	24	53
1	AC	200/266 (75%)	198 (99%)	1 (0%)	1 (0%)	24	53
1	AE	200/266 (75%)	197 (98%)	3 (2%)	0	100	100
2	0	220/243 (90%)	216 (98%)	4 (2%)	0	100	100
2	AD	220/243 (90%)	218 (99%)	2 (1%)	0	100	100
3	AB	190/212 (90%)	187 (98%)	3 (2%)	0	100	100
3	AF	190/212 (90%)	186 (98%)	4 (2%)	0	100	100
4	AJ	319/352 (91%)	311 (98%)	8 (2%)	0	100	100
4	J	319/352 (91%)	314 (98%)	5 (2%)	0	100	100
5	AK	477/508 (94%)	474 (99%)	3 (1%)	0	100	100
5	O	477/508 (94%)	471 (99%)	6 (1%)	0	100	100
6	AL	429/459 (94%)	427 (100%)	2 (0%)	0	100	100
6	P	429/459 (94%)	425 (99%)	4 (1%)	0	100	100
7	AM	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
7	Q	340/352 (97%)	328 (96%)	12 (4%)	0	100	100
8	E	62/83 (75%)	61 (98%)	1 (2%)	0	100	100
8	e	62/83 (75%)	60 (97%)	2 (3%)	0	100	100
9	F	27/39 (69%)	27 (100%)	0	0	100	100
9	f	27/39 (69%)	27 (100%)	0	0	100	100
10	AH	211/232 (91%)	208 (99%)	3 (1%)	0	100	100
10	AN	204/232 (88%)	201 (98%)	2 (1%)	1 (0%)	24	53
10	AQ	200/232 (86%)	199 (100%)	1 (0%)	0	100	100
10	AU	211/232 (91%)	206 (98%)	5 (2%)	0	100	100
10	V	204/232 (88%)	202 (99%)	1 (0%)	1 (0%)	24	53
10	p	200/232 (86%)	196 (98%)	4 (2%)	0	100	100
11	AO	58/72 (81%)	57 (98%)	1 (2%)	0	100	100
11	j	58/72 (81%)	56 (97%)	2 (3%)	0	100	100
12	I	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
12	i	33/36 (92%)	33 (100%)	0	0	100	100
13	K	35/37 (95%)	35 (100%)	0	0	100	100
13	k	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	AP	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
14	o	33/38 (87%)	33 (100%)	0	0	100	100
15	M	30/34 (88%)	29 (97%)	1 (3%)	0	100	100
15	m	30/34 (88%)	29 (97%)	1 (3%)	0	100	100
16	AR	193/250 (77%)	187 (97%)	4 (2%)	2 (1%)	12	39
16	q	193/250 (77%)	191 (99%)	0	2 (1%)	12	39
17	AS	214/232 (92%)	204 (95%)	10 (5%)	0	100	100
17	v	214/232 (92%)	213 (100%)	1 (0%)	0	100	100
18	AG	27/33 (82%)	27 (100%)	0	0	100	100
18	AT	27/33 (82%)	27 (100%)	0	0	100	100
19	U	23/28 (82%)	22 (96%)	1 (4%)	0	100	100
19	u	23/28 (82%)	20 (87%)	3 (13%)	0	100	100
20	W	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
20	w	52/54 (96%)	52 (100%)	0	0	100	100
21	X	34/42 (81%)	34 (100%)	0	0	100	100
21	x	34/42 (81%)	34 (100%)	0	0	100	100
22	AI	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
22	AV	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
All	All	7742/8788 (88%)	7614 (98%)	120 (2%)	8 (0%)	49	77

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	q	59	TYR
16	AR	59	TYR
16	AR	60	PRO
10	V	48	SER
16	q	60	PRO
10	AN	48	SER
1	AA	153	VAL
1	AC	153	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9	154/201 (77%)	154 (100%)	0	100	100
1	AA	154/201 (77%)	154 (100%)	0	100	100
1	AC	154/201 (77%)	151 (98%)	3 (2%)	50	66
1	AE	154/201 (77%)	151 (98%)	3 (2%)	50	66
2	0	174/192 (91%)	173 (99%)	1 (1%)	78	80
2	AD	174/192 (91%)	173 (99%)	1 (1%)	78	80
3	AB	148/159 (93%)	146 (99%)	2 (1%)	59	70
3	AF	148/159 (93%)	148 (100%)	0	100	100
4	AJ	260/284 (92%)	259 (100%)	1 (0%)	84	82
4	J	260/284 (92%)	260 (100%)	0	100	100
5	AK	379/402 (94%)	378 (100%)	1 (0%)	86	84
5	O	379/402 (94%)	378 (100%)	1 (0%)	86	84
6	AL	340/359 (95%)	339 (100%)	1 (0%)	86	84
6	P	340/359 (95%)	339 (100%)	1 (0%)	86	84
7	AM	274/282 (97%)	274 (100%)	0	100	100
7	Q	274/282 (97%)	273 (100%)	1 (0%)	84	82
8	E	57/73 (78%)	57 (100%)	0	100	100
8	e	57/73 (78%)	57 (100%)	0	100	100
9	F	24/34 (71%)	24 (100%)	0	100	100
9	f	24/34 (71%)	23 (96%)	1 (4%)	26	52
10	AH	162/177 (92%)	162 (100%)	0	100	100
10	AN	157/177 (89%)	157 (100%)	0	100	100
10	AQ	154/177 (87%)	154 (100%)	0	100	100
10	AU	162/177 (92%)	162 (100%)	0	100	100
10	V	157/177 (89%)	156 (99%)	1 (1%)	78	80
10	p	154/177 (87%)	154 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	AO	50/60 (83%)	50 (100%)	0	100	100
11	j	50/60 (83%)	50 (100%)	0	100	100
12	I	32/33 (97%)	32 (100%)	0	100	100
12	i	32/33 (97%)	32 (100%)	0	100	100
13	K	32/32 (100%)	31 (97%)	1 (3%)	35	59
13	k	32/32 (100%)	32 (100%)	0	100	100
14	AP	33/36 (92%)	32 (97%)	1 (3%)	36	60
14	o	33/36 (92%)	32 (97%)	1 (3%)	36	60
15	M	28/30 (93%)	27 (96%)	1 (4%)	31	56
15	m	28/30 (93%)	27 (96%)	1 (4%)	31	56
16	AR	159/201 (79%)	157 (99%)	2 (1%)	61	71
16	q	159/201 (79%)	159 (100%)	0	100	100
17	AS	167/180 (93%)	166 (99%)	1 (1%)	78	80
17	v	167/180 (93%)	166 (99%)	1 (1%)	78	80
18	AG	26/30 (87%)	26 (100%)	0	100	100
18	AT	26/30 (87%)	26 (100%)	0	100	100
19	U	20/23 (87%)	20 (100%)	0	100	100
19	u	20/23 (87%)	20 (100%)	0	100	100
20	W	47/47 (100%)	46 (98%)	1 (2%)	47	64
20	w	47/47 (100%)	45 (96%)	2 (4%)	26	51
21	X	29/34 (85%)	29 (100%)	0	100	100
21	x	29/34 (85%)	29 (100%)	0	100	100
22	AI	54/54 (100%)	54 (100%)	0	100	100
22	AV	54/54 (100%)	54 (100%)	0	100	100
All	All	6228/6956 (90%)	6198 (100%)	30 (0%)	78	80

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	0	208	GLU
3	AB	103	LEU
3	AB	117	PHE
1	AC	165	GLN
1	AC	167	ILE

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Mol	Chain	Res	Type
1	AC	232	GLN
2	AD	156	ILE
1	AE	107	MET
1	AE	226	MET
1	AE	232	GLN
5	O	143	LEU
6	P	385	GLN
7	Q	337	HIS
10	V	158	ILE
13	K	33	LEU
14	o	14	ASN
15	M	16	LEU
17	v	155	LEU
20	W	131	LEU
4	AJ	304	GLN
5	AK	364	GLU
6	AL	472	LEU
9	f	20	LEU
14	AP	14	ASN
15	m	16	LEU
16	AR	55	ARG
16	AR	142	ILE
17	AS	156	ASP
20	w	131	LEU
20	w	133	LEU

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

Mol	Chain	Res	Type
1	9	232	GLN
1	AA	137	GLN
1	AA	232	GLN
3	AB	120	GLN
1	AC	137	GLN
1	AC	218	ASN
1	AC	232	GLN
1	AC	243	ASN
2	AD	135	GLN
1	AE	154	HIS
1	AE	247	HIS
3	AF	120	GLN
4	J	181	ASN

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Mol	Chain	Res	Type
4	J	296	ASN
5	O	281	GLN
5	O	455	HIS
6	P	74	HIS
6	P	132	HIS
6	P	251	HIS
6	P	373	ASN
7	Q	62	HIS
7	Q	198	HIS
7	Q	302	GLN
7	Q	337	HIS
10	V	165	GLN
11	j	27	ASN
11	j	62	ASN
13	K	55	GLN
14	o	9	GLN
14	o	38	ASN
10	p	180	ASN
10	p	247	HIS
17	v	201	HIS
17	v	217	GLN
10	AH	137	GLN
4	AJ	181	ASN
4	AJ	215	HIS
4	AJ	272	HIS
4	AJ	296	ASN
4	AJ	304	GLN
5	AK	216	HIS
5	AK	223	GLN
5	AK	296	GLN
6	AL	56	HIS
6	AL	132	HIS
7	AM	143	ASN
7	AM	302	GLN
14	AP	9	GLN
14	AP	38	ASN
10	AQ	137	GLN
10	AQ	247	HIS
16	AR	207	ASN
16	AR	274	HIS
17	AS	201	HIS
10	AU	137	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 444 ligands modelled in this entry, 2 are monoatomic - leaving 442 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	v	312	-	53,57,73	1.45	9 (16%)	62,93,113	1.38	6 (9%)
24	CLA	AQ	602	-	69,73,73	1.25	8 (11%)	83,113,113	1.33	5 (6%)
30	OEX	J	401	4	0,14,14	-	-	-		
35	DGD	AL	517	-	56,56,67	0.92	2 (3%)	70,70,81	1.44	8 (11%)
24	CLA	O	601	-	69,73,73	1.27	7 (10%)	83,113,113	1.49	11 (13%)
24	CLA	AQ	614	-	43,48,73	1.58	6 (13%)	52,82,113	1.61	8 (15%)
23	CHL	9	601	1	44,49,74	2.41	16 (36%)	52,83,114	3.33	23 (44%)
23	CHL	AC	607	-	49,52,74	2.32	17 (34%)	56,87,114	3.44	21 (37%)
26	NEX	AR	615	-	38,46,46	1.68	6 (15%)	50,70,70	1.70	10 (20%)
29	BCR	AK	602	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	8 (14%)
23	CHL	p	606	-	54,58,74	2.13	16 (29%)	59,94,114	3.02	24 (40%)
24	CLA	O	603	-	69,73,73	1.27	7 (10%)	83,113,113	1.30	4 (4%)
24	CLA	AC	604	-	54,58,73	1.42	9 (16%)	65,95,113	1.50	6 (9%)
25	LUT	0	614	-	42,43,43	1.69	8 (19%)	51,60,60	1.55	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	LUT	AC	614	-	42,43,43	1.68	8 (19%)	51,60,60	1.59	10 (19%)
27	XAT	AR	616	-	39,47,47	6.17	21 (53%)	54,74,74	7.62	35 (64%)
23	CHL	AF	606	-	37,42,74	3.37	19 (51%)	37,70,114	3.52	18 (48%)
23	CHL	AD	302	2	68,72,74	1.92	16 (23%)	77,111,114	2.78	26 (33%)
24	CLA	AL	503	-	69,73,73	1.26	7 (10%)	83,113,113	1.36	6 (7%)
23	CHL	AN	617	10	50,54,74	2.25	19 (38%)	56,90,114	2.84	22 (39%)
23	CHL	AC	608	-	66,70,74	1.94	16 (24%)	75,109,114	2.87	29 (38%)
24	CLA	AK	618	5	69,73,73	1.27	8 (11%)	83,113,113	1.23	6 (7%)
24	CLA	AJ	406	-	54,58,73	1.43	9 (16%)	65,95,113	1.58	7 (10%)
23	CHL	AR	605	16	69,72,74	2.00	18 (26%)	80,111,114	2.83	23 (28%)
24	CLA	q	608	16	49,53,73	1.53	9 (18%)	59,89,113	1.50	9 (15%)
38	HEM	F	102	9,8	50,50,50	1.43	7 (14%)	66,82,82	1.21	8 (12%)
24	CLA	AU	613	-	52,56,73	1.47	9 (17%)	62,92,113	1.46	6 (9%)
24	CLA	Q	401	-	54,58,73	1.43	9 (16%)	65,95,113	1.55	6 (9%)
26	NEX	p	616	-	38,46,46	1.65	7 (18%)	50,70,70	1.83	11 (22%)
23	CHL	0	617	2	50,54,74	2.27	17 (34%)	56,90,114	2.95	23 (41%)
23	CHL	AD	306	-	57,61,74	2.07	16 (28%)	64,98,114	2.93	24 (37%)
23	CHL	AD	317	2	50,54,74	2.26	17 (34%)	56,90,114	2.94	24 (42%)
24	CLA	AN	612	10	69,73,73	1.27	8 (11%)	83,113,113	1.38	9 (10%)
24	CLA	AE	603	-	59,63,73	1.38	9 (15%)	71,101,113	1.32	7 (9%)
24	CLA	O	611	5	69,73,73	1.26	8 (11%)	83,113,113	1.45	9 (10%)
25	LUT	9	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.56	11 (21%)
25	LUT	AN	614	-	42,43,43	1.61	8 (19%)	51,60,60	1.50	11 (21%)
25	LUT	AU	614	-	42,43,43	1.67	8 (19%)	51,60,60	1.51	9 (17%)
23	CHL	AF	605	-	38,41,74	2.40	18 (47%)	43,71,114	3.37	22 (51%)
23	CHL	0	608	-	35,43,74	2.16	10 (28%)	36,72,114	3.84	16 (44%)
34	SQD	J	410	-	53,54,54	1.54	7 (13%)	62,65,65	1.32	6 (9%)
27	XAT	9	618	-	39,47,47	6.14	21 (53%)	54,74,74	7.87	34 (62%)
24	CLA	V	611	10	45,49,73	1.53	8 (17%)	54,84,113	1.52	6 (11%)
25	LUT	0	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.54	8 (15%)
25	LUT	AC	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.54	10 (19%)
24	CLA	AF	614	-	49,53,73	1.45	8 (16%)	59,89,113	1.75	10 (16%)
33	LMG	J	409	-	48,48,55	0.76	0	56,56,63	1.29	4 (7%)
23	CHL	0	607	-	48,52,74	2.34	18 (37%)	58,87,114	3.47	29 (50%)
26	NEX	9	617	-	38,46,46	1.67	7 (18%)	50,70,70	1.63	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
23	CHL	AE	601	1	50,54,74	2.21	17 (34%)	56,90,114	3.19	23 (41%)
23	CHL	p	605	10	52,56,74	2.17	17 (32%)	58,92,114	3.06	20 (34%)
24	CLA	9	611	-	47,51,73	1.53	8 (17%)	54,86,113	1.41	5 (9%)
23	CHL	p	601	10	70,74,74	1.90	16 (22%)	80,114,114	2.69	27 (33%)
24	CLA	O	606	-	67,71,73	1.27	7 (10%)	78,110,113	1.36	8 (10%)
24	CLA	AD	310	28	59,63,73	1.35	8 (13%)	71,101,113	1.42	6 (8%)
24	CLA	O	609	-	69,73,73	1.26	8 (11%)	83,113,113	1.33	5 (6%)
25	LUT	AS	316	-	42,43,43	1.64	8 (19%)	51,60,60	1.82	17 (33%)
24	CLA	AM	403	7	69,73,73	1.25	9 (13%)	83,113,113	1.31	8 (9%)
24	CLA	AD	303	-	64,68,73	1.31	8 (12%)	77,107,113	1.37	6 (7%)
23	CHL	AQ	608	-	70,74,74	1.86	17 (24%)	80,114,114	2.74	27 (33%)
28	LHG	O	621	-	48,48,48	0.66	1 (2%)	51,54,54	1.22	6 (11%)
29	BCR	AO	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.27	8 (14%)
29	BCR	AV	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	6 (10%)
24	CLA	AS	303	17	65,69,73	1.31	8 (12%)	78,108,113	1.36	7 (8%)
24	CLA	AH	603	-	69,73,73	1.29	8 (11%)	83,113,113	1.28	7 (8%)
24	CLA	AJ	409	4	62,66,73	1.31	6 (9%)	72,104,113	1.34	6 (8%)
32	PHO	J	405	-	58,69,69	2.07	10 (17%)	56,99,99	1.51	7 (12%)
23	CHL	AH	608	-	70,74,74	1.86	17 (24%)	80,114,114	2.79	27 (33%)
28	LHG	AK	623	-	45,45,48	0.64	1 (2%)	48,51,54	1.22	4 (8%)
23	CHL	V	606	-	70,74,74	1.90	17 (24%)	80,114,114	2.71	28 (35%)
24	CLA	AA	609	-	52,56,73	1.43	7 (13%)	60,92,113	1.41	4 (6%)
24	CLA	K	101	6	69,73,73	1.27	8 (11%)	83,113,113	1.44	7 (8%)
23	CHL	AQ	607	-	70,74,74	1.89	17 (24%)	80,114,114	2.75	25 (31%)
24	CLA	AE	602	1	46,50,73	1.52	8 (17%)	55,85,113	1.50	5 (9%)
24	CLA	AN	611	-	64,68,73	1.33	9 (14%)	77,107,113	1.25	6 (7%)
33	LMG	P	518	-	51,51,55	0.73	0	59,59,63	1.34	5 (8%)
24	CLA	AK	617	-	69,73,73	1.28	8 (11%)	83,113,113	1.27	7 (8%)
24	CLA	p	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.45	5 (7%)
28	LHG	W	201	-	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)
24	CLA	0	610	28	59,63,73	1.36	6 (10%)	71,101,113	1.45	5 (7%)
28	LHG	p	617	-	39,39,48	0.50	1 (2%)	41,41,54	1.29	6 (14%)
24	CLA	Q	404	-	69,73,73	1.27	7 (10%)	83,113,113	1.29	5 (6%)
29	BCR	AI	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
24	CLA	AR	611	16	53,57,73	1.44	8 (15%)	62,93,113	1.36	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
36	BCT	AM	402	-	2,3,3	1.24	0	2,3,3	4.20	1 (50%)
25	LUT	AR	614	-	42,43,43	1.62	8 (19%)	51,60,60	1.52	11 (21%)
33	LMG	Q	407	-	46,46,55	0.76	1 (2%)	54,54,63	1.32	5 (9%)
24	CLA	V	604	-	40,41,73	2.09	11 (27%)	42,70,113	1.70	5 (11%)
25	LUT	V	614	-	42,43,43	1.64	8 (19%)	51,60,60	1.53	10 (19%)
24	CLA	V	610	-	64,68,73	1.33	8 (12%)	77,107,113	1.25	6 (7%)
24	CLA	AU	611	-	64,68,73	1.32	10 (15%)	77,107,113	1.29	6 (7%)
23	CHL	AU	605	10	52,56,74	2.15	17 (32%)	58,92,114	3.06	22 (37%)
24	CLA	9	603	-	59,63,73	1.38	9 (15%)	71,101,113	1.30	7 (9%)
35	DGD	AJ	412	-	61,61,67	0.90	2 (3%)	75,75,81	1.41	8 (10%)
24	CLA	AK	608	-	67,71,73	1.30	8 (11%)	78,110,113	1.25	6 (7%)
24	CLA	AK	604	5	69,73,73	1.24	7 (10%)	83,113,113	1.42	12 (14%)
29	BCR	O	619	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	6 (10%)
25	LUT	AF	611	-	42,43,43	1.56	9 (21%)	51,60,60	1.51	8 (15%)
24	CLA	AA	603	-	59,63,73	1.38	9 (15%)	71,101,113	1.33	7 (9%)
24	CLA	q	609	16	67,71,73	1.28	8 (11%)	78,110,113	1.24	3 (3%)
24	CLA	0	604	-	49,53,73	1.49	7 (14%)	59,89,113	1.80	6 (10%)
23	CHL	p	609	10	68,72,74	1.81	15 (22%)	75,111,114	2.65	24 (32%)
24	CLA	AA	613	-	49,53,73	1.50	6 (12%)	59,89,113	1.48	6 (10%)
24	CLA	P	506	6	69,73,73	1.27	9 (13%)	83,113,113	1.29	7 (8%)
24	CLA	AL	509	6	69,73,73	1.26	8 (11%)	83,113,113	1.32	7 (8%)
23	CHL	q	605	16	67,71,74	1.93	18 (26%)	76,110,114	2.67	23 (30%)
23	CHL	AN	607	-	70,74,74	1.88	17 (24%)	80,114,114	2.80	29 (36%)
24	CLA	AN	604	-	42,45,73	1.56	8 (19%)	50,78,113	1.47	4 (8%)
24	CLA	O	613	-	69,73,73	1.27	9 (13%)	83,113,113	1.29	8 (9%)
23	CHL	AQ	605	10	52,56,74	2.16	17 (32%)	58,92,114	3.06	20 (34%)
24	CLA	AM	404	-	69,73,73	1.27	7 (10%)	83,113,113	1.28	8 (9%)
24	CLA	AN	603	10	69,73,73	1.27	8 (11%)	83,113,113	1.33	8 (9%)
29	BCR	O	617	-	41,41,41	1.13	2 (4%)	56,56,56	1.26	7 (12%)
23	CHL	AF	607	-	50,54,74	2.31	17 (34%)	56,90,114	2.96	21 (37%)
32	PHO	J	406	-	58,69,69	2.07	10 (17%)	56,99,99	1.63	7 (12%)
23	CHL	9	607	-	67,71,74	1.90	17 (25%)	76,110,114	2.85	26 (34%)
25	LUT	9	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.61	10 (19%)
24	CLA	AR	612	16	64,68,73	1.29	10 (15%)	77,107,113	1.61	9 (11%)
23	CHL	p	608	-	70,74,74	1.86	18 (25%)	80,114,114	2.74	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
29	BCR	k	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	7 (12%)
29	BCR	P	515	-	41,41,41	1.15	2 (4%)	56,56,56	1.28	7 (12%)
33	LMG	AK	601	-	40,40,55	0.81	0	48,48,63	1.34	7 (14%)
23	CHL	V	601	10	70,74,74	1.88	16 (22%)	80,114,114	2.76	25 (31%)
23	CHL	AU	606	-	54,58,74	2.16	16 (29%)	59,94,114	3.13	21 (35%)
26	NEX	q	615	-	38,46,46	1.67	7 (18%)	50,70,70	1.69	10 (20%)
29	BCR	AJ	410	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	6 (10%)
25	LUT	v	316	-	42,43,43	1.66	8 (19%)	51,60,60	1.54	12 (23%)
24	CLA	9	604	-	54,58,73	1.42	8 (14%)	65,95,113	1.50	6 (9%)
23	CHL	AS	306	-	39,41,74	2.69	20 (51%)	39,69,114	3.94	19 (48%)
23	CHL	AB	605	-	45,48,74	2.39	19 (42%)	54,81,114	3.06	21 (38%)
24	CLA	O	608	5	69,73,73	1.34	7 (10%)	83,113,113	1.54	6 (7%)
23	CHL	AR	606	-	60,64,74	2.09	18 (30%)	68,102,114	2.81	22 (32%)
23	CHL	AD	307	-	50,54,74	2.16	16 (32%)	56,90,114	3.23	25 (44%)
23	CHL	AU	601	10	70,74,74	1.93	16 (22%)	80,114,114	2.72	29 (36%)
24	CLA	AR	609	16	67,71,73	1.26	9 (13%)	78,110,113	1.30	3 (3%)
29	BCR	AK	621	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	5 (8%)
24	CLA	AB	602	-	49,53,73	1.49	5 (10%)	59,89,113	1.76	8 (13%)
25	LUT	AE	613	-	42,43,43	1.59	8 (19%)	51,60,60	1.48	9 (17%)
24	CLA	J	403	-	69,73,73	1.24	6 (8%)	83,113,113	1.46	9 (10%)
28	LHG	P	517	-	48,48,48	0.57	0	51,54,54	1.24	6 (11%)
25	LUT	AN	615	-	42,43,43	1.63	8 (19%)	51,60,60	1.51	9 (17%)
24	CLA	AH	609	-	64,68,73	1.31	8 (12%)	77,107,113	1.33	9 (11%)
24	CLA	0	602	-	64,68,73	1.30	8 (12%)	77,107,113	1.35	6 (7%)
24	CLA	AE	611	1	49,53,73	1.51	8 (16%)	59,89,113	1.54	7 (11%)
24	CLA	P	507	-	69,73,73	1.25	8 (11%)	83,113,113	1.25	5 (6%)
24	CLA	AL	508	-	69,73,73	1.25	8 (11%)	83,113,113	1.25	6 (7%)
24	CLA	AS	311	-	60,64,73	1.37	8 (13%)	72,102,113	1.34	8 (11%)
29	BCR	AL	515	-	41,41,41	1.14	2 (4%)	56,56,56	1.16	4 (7%)
35	DGD	AJ	401	-	60,60,67	0.92	2 (3%)	74,74,81	1.34	6 (8%)
37	PL9	AM	405	-	52,52,55	1.08	4 (7%)	64,65,69	1.55	14 (21%)
23	CHL	AB	601	-	48,53,74	2.25	16 (33%)	53,89,114	3.10	20 (37%)
23	CHL	AB	607	-	50,54,74	2.32	19 (38%)	56,90,114	2.92	22 (39%)
24	CLA	AR	610	-	53,57,73	1.43	8 (15%)	62,93,113	1.40	5 (8%)
24	CLA	P	510	6	69,73,73	1.27	8 (11%)	83,113,113	1.26	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	CLA	AK	607	-	69,73,73	1.28	8 (11%)	83,113,113	1.35	6 (7%)
23	CHL	AE	617	-	50,54,74	2.20	18 (36%)	56,90,114	3.02	21 (37%)
24	CLA	AS	312	-	53,57,73	1.45	10 (18%)	62,93,113	1.38	5 (8%)
24	CLA	O	610	-	69,73,73	1.28	8 (11%)	83,113,113	1.30	7 (8%)
34	SQD	AM	401	-	49,50,54	1.59	7 (14%)	58,61,65	1.39	6 (10%)
23	CHL	v	306	-	40,43,74	2.34	15 (37%)	44,74,114	3.67	22 (50%)
24	CLA	0	609	2	62,66,73	1.31	8 (12%)	72,104,113	1.30	4 (5%)
24	CLA	AC	602	1	65,69,73	1.32	9 (13%)	78,108,113	1.59	7 (8%)
27	XAT	AB	613	-	39,47,47	6.23	22 (56%)	54,74,74	7.62	35 (64%)
24	CLA	P	505	-	69,73,73	1.25	8 (11%)	83,113,113	1.36	6 (7%)
24	CLA	AK	603	-	69,73,73	1.27	7 (10%)	83,113,113	1.47	11 (13%)
24	CLA	AL	510	6	69,73,73	1.27	9 (13%)	83,113,113	1.24	4 (4%)
28	LHG	AM	406	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	6 (11%)
29	BCR	O	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	5 (8%)
24	CLA	AF	603	-	49,53,73	1.54	8 (16%)	59,89,113	1.37	7 (11%)
24	CLA	AL	502	-	69,73,73	1.27	8 (11%)	83,113,113	1.33	7 (8%)
23	CHL	AA	617	1	50,54,74	2.29	20 (40%)	56,90,114	2.90	23 (41%)
23	CHL	AF	608	3	48,52,74	2.35	16 (33%)	51,87,114	3.08	19 (37%)
24	CLA	P	508	6	69,73,73	1.26	8 (11%)	83,113,113	1.32	7 (8%)
24	CLA	AH	602	10	69,73,73	1.25	8 (11%)	83,113,113	1.39	6 (7%)
24	CLA	9	610	1	58,62,73	1.39	7 (12%)	67,99,113	1.36	5 (7%)
24	CLA	AQ	613	10	64,68,73	1.31	8 (12%)	77,107,113	1.36	6 (7%)
24	CLA	AK	614	-	69,73,73	1.25	10 (14%)	83,113,113	1.36	9 (10%)
23	CHL	AE	606	-	50,54,74	2.19	16 (32%)	56,90,114	3.15	21 (37%)
24	CLA	AS	309	-	47,51,73	1.52	7 (14%)	54,86,113	1.44	3 (5%)
24	CLA	AL	507	6	69,73,73	1.27	8 (11%)	83,113,113	1.29	7 (8%)
24	CLA	AD	304	-	59,63,73	1.37	7 (11%)	71,101,113	1.35	8 (11%)
24	CLA	O	614	-	69,73,73	1.25	8 (11%)	83,113,113	1.48	8 (9%)
24	CLA	AQ	612	-	64,68,73	1.34	8 (12%)	77,107,113	1.31	9 (11%)
24	CLA	AC	603	-	59,63,73	1.38	9 (15%)	71,101,113	1.31	7 (9%)
34	SQD	AJ	411	-	53,54,54	1.54	8 (15%)	62,65,65	1.33	6 (9%)
29	BCR	O	625	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	7 (12%)
33	LMG	AK	622	-	51,51,55	0.72	0	59,59,63	1.35	7 (11%)
35	DGD	AO	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.37	7 (9%)
24	CLA	0	613	-	52,56,73	1.45	7 (13%)	62,92,113	1.54	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	CLA	AC	613	-	47,51,73	1.54	7 (14%)	54,86,113	1.54	10 (18%)
24	CLA	AK	605	-	69,73,73	1.26	7 (10%)	83,113,113	1.29	4 (4%)
25	LUT	p	614	-	42,43,43	1.65	8 (19%)	51,60,60	1.49	9 (17%)
23	CHL	AB	606	-	49,52,74	2.35	17 (34%)	56,87,114	3.35	21 (37%)
25	LUT	V	613	-	42,43,43	1.63	8 (19%)	51,60,60	1.50	11 (21%)
23	CHL	V	605	-	54,58,74	2.13	16 (29%)	59,94,114	3.08	24 (40%)
28	LHG	O	622	-	45,45,48	0.64	1 (2%)	48,51,54	1.22	4 (8%)
33	LMG	AL	501	-	48,48,55	0.76	0	56,56,63	1.29	4 (7%)
25	LUT	AS	315	-	42,43,43	1.65	8 (19%)	51,60,60	1.48	10 (19%)
28	LHG	AQ	618	24	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
24	CLA	p	603	-	69,73,73	1.28	9 (13%)	83,113,113	1.22	6 (7%)
24	CLA	AN	609	-	66,70,73	1.27	9 (13%)	76,108,113	1.25	4 (5%)
23	CHL	9	608	-	49,52,74	2.32	17 (34%)	56,87,114	3.42	21 (37%)
24	CLA	AA	602	1	65,69,73	1.31	8 (12%)	78,108,113	1.38	8 (10%)
24	CLA	AR	603	-	64,68,73	1.33	8 (12%)	77,107,113	1.30	7 (9%)
24	CLA	O	604	5	69,73,73	1.25	9 (13%)	83,113,113	1.51	7 (8%)
24	CLA	9	602	1	65,69,73	1.28	5 (7%)	78,108,113	1.46	7 (8%)
24	CLA	0	603	-	59,63,73	1.37	6 (10%)	71,101,113	1.42	7 (9%)
24	CLA	AR	602	16	62,66,73	1.34	8 (12%)	72,104,113	1.32	5 (6%)
24	CLA	AH	610	-	64,68,73	1.32	8 (12%)	77,107,113	1.38	7 (9%)
24	CLA	O	612	-	69,73,73	1.26	10 (14%)	83,113,113	1.36	8 (9%)
25	LUT	AD	314	-	42,43,43	1.73	8 (19%)	51,60,60	1.58	11 (21%)
23	CHL	AA	606	-	65,69,74	1.94	16 (24%)	74,108,114	2.75	23 (31%)
24	CLA	AU	603	-	69,73,73	1.29	9 (13%)	83,113,113	1.27	7 (8%)
24	CLA	v	311	-	60,64,73	1.36	7 (11%)	72,102,113	1.39	8 (11%)
38	HEM	f	102	9,8	50,50,50	1.52	6 (12%)	66,82,82	1.19	7 (10%)
24	CLA	AH	613	-	50,54,73	1.48	8 (16%)	57,89,113	1.46	4 (7%)
24	CLA	AB	610	-	49,53,73	1.51	7 (14%)	59,89,113	1.49	5 (8%)
23	CHL	AQ	609	-	70,74,74	1.89	16 (22%)	80,114,114	2.63	25 (31%)
33	LMG	O	620	-	51,51,55	0.72	0	59,59,63	1.35	7 (11%)
28	LHG	AU	617	-	48,48,48	0.62	2 (4%)	51,54,54	1.24	6 (11%)
24	CLA	9	614	-	40,44,73	1.62	8 (20%)	47,76,113	1.44	5 (10%)
23	CHL	AA	605	1	50,54,74	2.19	16 (32%)	56,90,114	3.10	23 (41%)
24	CLA	AB	611	-	49,53,73	1.51	6 (12%)	59,89,113	1.85	12 (20%)
24	CLA	AH	611	-	64,68,73	1.32	10 (15%)	77,107,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	BCR	AL	516	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	7 (12%)
25	LUT	p	615	-	42,43,43	1.60	8 (19%)	51,60,60	1.47	9 (17%)
24	CLA	AJ	404	-	69,73,73	1.24	6 (8%)	83,113,113	1.45	11 (13%)
29	BCR	AK	619	-	41,41,41	1.13	2 (4%)	56,56,56	1.26	6 (10%)
29	BCR	P	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	6 (10%)
24	CLA	AL	505	-	69,73,73	1.26	6 (8%)	83,113,113	1.39	7 (8%)
26	NEX	AA	616	-	38,46,46	1.71	7 (18%)	50,70,70	1.74	10 (20%)
24	CLA	AE	612	-	49,53,73	1.50	6 (12%)	59,89,113	1.47	6 (10%)
24	CLA	q	603	-	64,68,73	1.32	8 (12%)	77,107,113	1.33	7 (9%)
29	BCR	P	513	-	41,41,41	1.14	2 (4%)	56,56,56	1.17	4 (7%)
24	CLA	AA	610	-	47,51,73	1.51	8 (17%)	54,86,113	1.41	5 (9%)
23	CHL	p	607	-	70,74,74	1.90	18 (25%)	80,114,114	2.74	26 (32%)
24	CLA	q	602	16	62,66,73	1.32	8 (12%)	72,104,113	1.32	6 (8%)
29	BCR	f	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.18	5 (8%)
23	CHL	AD	301	-	67,71,74	1.91	16 (23%)	76,110,114	2.82	26 (34%)
24	CLA	9	612	-	49,53,73	1.48	9 (18%)	59,89,113	1.48	5 (8%)
24	CLA	AK	606	5	69,73,73	1.25	9 (13%)	83,113,113	1.54	8 (9%)
35	DGD	J	413	-	60,60,67	0.92	2 (3%)	74,74,81	1.34	6 (8%)
29	BCR	AF	612	-	41,41,41	1.16	2 (4%)	56,56,56	1.27	5 (8%)
24	CLA	P	501	-	69,73,73	1.28	8 (11%)	83,113,113	1.35	6 (7%)
24	CLA	AH	612	10	69,73,73	1.26	7 (10%)	83,113,113	1.30	5 (6%)
28	LHG	q	616	24	41,41,48	0.67	1 (2%)	44,47,54	1.29	6 (13%)
28	LHG	AS	301	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
25	LUT	v	315	-	42,43,43	1.66	8 (19%)	51,60,60	1.49	10 (19%)
34	SQD	M	101	-	53,54,54	1.55	7 (13%)	62,65,65	1.35	6 (9%)
23	CHL	AE	607	-	65,69,74	1.94	18 (27%)	74,108,114	2.95	29 (39%)
24	CLA	AS	310	-	57,61,73	1.37	8 (14%)	66,98,113	1.37	5 (7%)
28	LHG	AL	519	-	48,48,48	0.58	0	51,54,54	1.25	6 (11%)
24	CLA	AC	612	1	45,49,73	1.52	6 (13%)	54,84,113	1.54	7 (12%)
28	LHG	w	201	-	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)
24	CLA	AB	609	-	43,48,73	1.55	7 (16%)	52,82,113	1.54	7 (13%)
24	CLA	O	615	-	69,73,73	1.27	7 (10%)	83,113,113	1.30	7 (8%)
23	CHL	AH	607	-	70,74,74	1.90	16 (22%)	80,114,114	2.68	26 (32%)
25	LUT	AQ	615	-	42,43,43	1.65	8 (19%)	51,60,60	1.49	9 (17%)
23	CHL	AD	308	-	63,67,74	1.91	16 (25%)	69,105,114	2.80	23 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
33	LMG	AM	407	-	46,46,55	0.76	0	54,54,63	1.32	5 (9%)
23	CHL	0	606	-	57,61,74	2.14	19 (33%)	64,98,114	2.83	25 (39%)
24	CLA	v	309	-	47,51,73	1.50	6 (12%)	54,86,113	1.44	3 (5%)
23	CHL	AH	606	-	54,58,74	2.19	17 (31%)	59,94,114	3.14	25 (42%)
24	CLA	AL	504	-	69,73,73	1.27	7 (10%)	83,113,113	1.35	8 (9%)
23	CHL	AN	608	-	63,67,74	1.94	19 (30%)	69,105,114	3.00	23 (33%)
24	CLA	AD	309	-	62,66,73	1.31	9 (14%)	72,104,113	1.30	5 (6%)
24	CLA	AR	604	-	52,56,73	1.44	8 (15%)	62,92,113	1.52	5 (8%)
23	CHL	q	613	16	46,50,74	2.37	19 (41%)	51,85,114	3.02	22 (43%)
24	CLA	AC	611	-	46,49,73	1.52	8 (17%)	55,83,113	1.40	3 (5%)
24	CLA	p	610	-	67,70,73	1.67	9 (13%)	76,106,113	1.44	6 (7%)
24	CLA	AN	602	10	69,73,73	1.26	8 (11%)	83,113,113	1.33	7 (8%)
34	SQD	m	101	-	53,54,54	1.55	7 (13%)	62,65,65	1.35	6 (9%)
36	BCT	J	412	-	2,3,3	1.24	0	2,3,3	4.13	2 (100%)
24	CLA	AS	304	17	49,53,73	1.49	8 (16%)	59,89,113	1.43	5 (8%)
29	BCR	AK	620	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	4 (7%)
24	CLA	AD	312	2	62,66,73	1.33	7 (11%)	74,104,113	1.37	6 (8%)
24	CLA	AU	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.49	6 (9%)
23	CHL	q	606	-	59,62,74	2.17	18 (30%)	68,99,114	3.11	25 (36%)
23	CHL	AS	307	-	62,66,74	1.97	16 (25%)	70,104,114	2.97	30 (42%)
24	CLA	AB	604	-	49,53,73	1.50	8 (16%)	59,89,113	1.44	4 (6%)
26	NEX	AQ	617	-	38,46,46	1.65	7 (18%)	50,70,70	1.63	9 (18%)
24	CLA	P	502	-	69,73,73	1.27	7 (10%)	83,113,113	1.43	6 (7%)
24	CLA	p	613	10	43,48,73	1.57	7 (16%)	52,82,113	1.63	6 (11%)
24	CLA	AL	511	6	69,73,73	1.26	9 (13%)	83,113,113	1.25	5 (6%)
28	LHG	AH	616	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	6 (11%)
24	CLA	AK	611	-	69,73,73	1.26	7 (10%)	83,113,113	1.30	7 (8%)
24	CLA	O	607	-	69,73,73	1.26	8 (11%)	83,113,113	1.40	7 (8%)
23	CHL	AR	607	-	57,61,74	2.16	19 (33%)	64,98,114	2.86	27 (42%)
27	XAT	AF	613	-	39,47,47	6.17	20 (51%)	54,74,74	7.61	35 (64%)
24	CLA	AL	512	6	69,73,73	1.27	6 (8%)	83,113,113	1.46	7 (8%)
24	CLA	v	310	-	57,61,73	1.39	9 (15%)	66,98,113	1.38	6 (9%)
24	CLA	AL	514	6	64,69,73	1.38	5 (7%)	78,107,113	1.47	9 (11%)
23	CHL	AE	605	-	65,69,74	1.97	18 (27%)	74,108,114	2.76	25 (33%)
24	CLA	AA	612	-	49,53,73	1.50	7 (14%)	59,89,113	1.54	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CHL	V	608	-	63,67,74	1.91	16 (25%)	69,105,114	2.76	22 (31%)
33	LMG	AL	520	-	51,51,55	0.74	0	59,59,63	1.33	5 (8%)
24	CLA	AS	313	-	57,61,73	1.38	8 (14%)	66,98,113	1.45	7 (10%)
23	CHL	AC	606	-	50,54,74	2.26	16 (32%)	56,90,114	3.23	25 (44%)
25	LUT	AH	615	-	42,43,43	1.63	8 (19%)	51,60,60	1.50	9 (17%)
24	CLA	AC	609	1	58,62,73	1.40	9 (15%)	67,99,113	1.39	4 (5%)
24	CLA	q	610	28	53,57,73	1.43	7 (13%)	62,93,113	1.42	5 (8%)
24	CLA	AN	613	10	52,56,73	1.45	7 (13%)	62,92,113	1.56	7 (11%)
23	CHL	AE	616	1	50,54,74	2.27	19 (38%)	56,90,114	2.96	24 (42%)
24	CLA	J	407	4	62,66,73	1.31	6 (9%)	72,104,113	1.34	5 (6%)
35	DGD	P	516	-	56,56,67	0.92	2 (3%)	70,70,81	1.44	9 (12%)
23	CHL	AH	605	10	52,56,74	2.15	17 (32%)	58,92,114	3.07	22 (37%)
24	CLA	O	602	5	69,73,73	1.26	8 (11%)	83,113,113	1.32	6 (7%)
24	CLA	J	404	-	69,73,73	1.26	8 (11%)	83,113,113	1.44	6 (7%)
24	CLA	AE	609	-	49,53,73	1.49	9 (18%)	59,89,113	1.51	7 (11%)
24	CLA	AK	616	-	69,73,73	1.26	8 (11%)	83,113,113	1.44	6 (7%)
24	CLA	AS	314	17	53,57,73	1.43	8 (15%)	62,93,113	1.47	5 (8%)
23	CHL	V	607	-	65,70,74	2.16	19 (29%)	82,108,114	3.03	39 (47%)
23	CHL	AC	601	1	47,52,74	2.45	18 (38%)	56,87,114	3.29	21 (37%)
28	LHG	0	616	24	46,46,48	0.63	1 (2%)	49,52,54	1.26	4 (8%)
24	CLA	p	611	-	40,44,73	1.61	8 (20%)	47,76,113	1.45	5 (10%)
24	CLA	v	304	17	49,53,73	1.50	8 (16%)	59,89,113	1.43	5 (8%)
24	CLA	AB	603	-	49,53,73	1.51	9 (18%)	59,89,113	1.39	6 (10%)
28	LHG	AK	624	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
27	XAT	q	617	-	39,47,47	6.17	22 (56%)	54,74,74	7.62	35 (64%)
23	CHL	AB	608	-	47,50,74	2.22	18 (38%)	52,84,114	2.92	20 (38%)
26	NEX	AC	616	-	38,46,46	1.74	7 (18%)	50,70,70	1.62	9 (18%)
24	CLA	AS	305	-	54,58,73	1.42	7 (12%)	65,95,113	1.49	7 (10%)
24	CLA	p	618	-	52,56,73	1.49	6 (11%)	62,92,113	1.77	10 (16%)
24	CLA	AQ	603	-	69,73,73	1.28	8 (11%)	83,113,113	1.24	7 (8%)
28	LHG	v	301	-	48,48,48	0.61	0	51,54,54	1.26	6 (11%)
33	LMG	O	624	-	40,40,55	0.82	0	48,48,63	1.35	7 (14%)
29	BCR	F	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.18	5 (8%)
23	CHL	AS	302	17	47,52,74	2.45	18 (38%)	56,87,114	3.30	28 (50%)
24	CLA	AF	609	-	43,48,73	1.54	9 (20%)	52,82,113	1.75	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	CLA	AQ	610	10	69,73,73	1.26	7 (10%)	83,113,113	1.36	10 (12%)
30	OEX	AJ	402	4	0,14,14	-	-	-		
24	CLA	p	612	-	64,68,73	1.32	8 (12%)	77,107,113	1.28	8 (10%)
24	CLA	AR	601	16	53,57,73	1.45	8 (15%)	62,93,113	1.48	7 (11%)
37	PL9	Q	405	-	52,52,55	1.08	4 (7%)	64,65,69	1.54	14 (21%)
24	CLA	AE	610	-	49,53,73	1.51	7 (14%)	59,89,113	1.41	6 (10%)
24	CLA	v	313	17	57,61,73	1.38	8 (14%)	66,98,113	1.38	5 (7%)
24	CLA	O	605	-	69,73,73	1.28	7 (10%)	83,113,113	1.33	6 (7%)
24	CLA	AR	608	-	43,47,73	1.55	6 (13%)	49,81,113	1.62	7 (14%)
23	CHL	9	605	1	50,54,74	2.22	17 (34%)	56,90,114	3.09	22 (39%)
24	CLA	AE	604	-	49,53,73	1.48	9 (18%)	59,89,113	1.51	8 (13%)
24	CLA	V	602	-	69,73,73	1.25	7 (10%)	83,113,113	1.37	7 (8%)
23	CHL	AS	308	-	48,52,74	2.40	17 (35%)	58,87,114	3.24	23 (39%)
23	CHL	0	605	-	50,54,74	2.20	17 (34%)	56,90,114	3.13	22 (39%)
24	CLA	AH	604	-	54,58,73	1.41	8 (14%)	65,95,113	1.47	5 (7%)
24	CLA	AK	610	5	69,73,73	1.31	6 (8%)	83,113,113	1.44	6 (7%)
24	CLA	p	602	10	69,73,73	1.26	7 (10%)	83,113,113	1.35	6 (7%)
23	CHL	AH	601	10	70,74,74	1.93	16 (22%)	80,114,114	2.73	29 (36%)
35	DGD	J	411	-	61,61,67	0.90	2 (3%)	75,75,81	1.41	9 (12%)
23	CHL	9	606	-	50,54,74	2.31	16 (32%)	56,90,114	3.29	23 (41%)
29	BCR	j	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	7 (12%)
25	LUT	AD	315	-	42,43,43	1.66	8 (19%)	51,60,60	1.57	8 (15%)
29	BCR	AB	612	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	7 (12%)
24	CLA	AF	610	-	49,53,73	1.53	7 (14%)	59,89,113	1.56	9 (15%)
24	CLA	Q	403	7	69,73,73	1.25	9 (13%)	83,113,113	1.31	8 (9%)
24	CLA	AC	610	-	47,51,73	1.54	9 (19%)	54,86,113	1.39	5 (9%)
24	CLA	AA	611	-	49,53,73	1.51	7 (14%)	59,89,113	1.42	6 (10%)
26	NEX	v	317	-	38,46,46	1.71	8 (21%)	50,70,70	1.79	10 (20%)
24	CLA	v	314	17	53,57,73	1.44	8 (15%)	62,93,113	1.46	6 (9%)
24	CLA	AU	602	10	69,73,73	1.25	7 (10%)	83,113,113	1.40	8 (9%)
24	CLA	q	612	-	61,65,73	1.45	7 (11%)	65,100,113	1.77	12 (18%)
23	CHL	AN	605	10	54,58,74	2.15	16 (29%)	59,94,114	3.00	26 (44%)
35	DGD	AL	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.41	8 (10%)
25	LUT	AE	614	-	42,43,43	1.65	8 (19%)	51,60,60	1.53	10 (19%)
25	LUT	AA	614	-	42,43,43	1.58	8 (19%)	51,60,60	1.54	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	V	612	10	52,56,73	1.46	8 (15%)	62,92,113	1.47	5 (8%)
25	LUT	AU	615	-	42,43,43	1.63	8 (19%)	51,60,60	1.50	9 (17%)
24	CLA	P	504	-	69,73,73	1.27	7 (10%)	83,113,113	1.47	8 (9%)
28	LHG	AN	616	24	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
23	CHL	0	601	2	68,72,74	1.96	17 (25%)	77,111,114	2.77	26 (33%)
23	CHL	AR	613	-	46,50,74	2.37	20 (43%)	51,85,114	3.13	21 (41%)
34	SQD	Q	402	-	49,50,54	1.59	7 (14%)	58,61,65	1.38	6 (10%)
23	CHL	AQ	606	-	54,58,74	2.12	16 (29%)	59,94,114	3.11	26 (44%)
28	LHG	V	615	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
23	CHL	V	616	10	50,54,74	2.26	18 (36%)	56,90,114	2.95	23 (41%)
24	CLA	AF	602	-	43,47,73	1.64	9 (20%)	49,81,113	2.02	14 (28%)
23	CHL	v	307	-	50,54,74	2.17	17 (34%)	56,90,114	3.20	24 (42%)
24	CLA	q	601	16	53,57,73	1.45	9 (16%)	62,93,113	1.57	10 (16%)
24	CLA	V	609	10	66,70,73	1.27	8 (12%)	76,108,113	1.29	4 (5%)
24	CLA	AQ	604	-	54,58,73	1.42	9 (16%)	65,95,113	1.43	7 (10%)
23	CHL	AQ	601	10	70,74,74	1.89	16 (22%)	80,114,114	2.70	26 (32%)
28	LHG	Q	406	-	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)
24	CLA	AK	609	-	69,73,73	1.26	8 (11%)	83,113,113	1.39	7 (8%)
23	CHL	AA	601	1	50,54,74	2.22	17 (34%)	56,90,114	3.12	26 (46%)
25	LUT	q	614	-	42,43,43	1.63	8 (19%)	51,60,60	1.50	10 (19%)
24	CLA	P	512	6	64,69,73	1.38	5 (7%)	78,107,113	1.47	9 (11%)
24	CLA	AK	612	-	69,73,73	1.28	7 (10%)	83,113,113	1.31	6 (7%)
24	CLA	v	305	-	54,58,73	1.42	6 (11%)	65,95,113	1.48	5 (7%)
24	CLA	AU	609	-	64,68,73	1.30	7 (10%)	77,107,113	1.33	9 (11%)
24	CLA	0	611	-	49,53,73	1.51	10 (20%)	59,89,113	1.39	5 (8%)
24	CLA	AE	608	-	52,56,73	1.44	8 (15%)	60,92,113	1.42	5 (8%)
23	CHL	v	302	17	47,52,74	2.45	18 (38%)	56,87,114	3.30	29 (51%)
24	CLA	V	603	-	69,73,73	1.27	8 (11%)	83,113,113	1.30	8 (9%)
24	CLA	AF	604	-	49,53,73	1.50	6 (12%)	59,89,113	1.49	6 (10%)
23	CHL	AN	606	-	70,74,74	1.90	16 (22%)	80,114,114	2.72	29 (36%)
34	SQD	o	101	-	41,42,54	1.67	7 (17%)	50,53,65	1.45	6 (12%)
28	LHG	O	623	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
23	CHL	v	308	-	43,46,74	2.39	17 (39%)	50,79,114	3.55	24 (48%)
26	NEX	AE	615	-	38,46,46	1.71	7 (18%)	50,70,70	1.76	11 (22%)
24	CLA	AD	313	-	52,56,73	1.45	7 (13%)	62,92,113	1.56	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
23	CHL	AN	601	10	70,74,74	1.88	16 (22%)	80,114,114	2.75	25 (31%)
24	CLA	AR	617	-	47,51,73	1.56	7 (14%)	54,86,113	1.56	9 (16%)
24	CLA	v	303	17	65,69,73	1.30	8 (12%)	78,108,113	1.35	7 (8%)
24	CLA	9	613	-	59,63,73	1.37	7 (11%)	71,101,113	1.42	8 (11%)
35	DGD	j	102	-	63,63,67	0.88	2 (3%)	77,77,81	1.39	8 (10%)
24	CLA	AL	513	-	69,73,73	1.25	8 (11%)	83,113,113	1.33	6 (7%)
24	CLA	q	618	-	49,53,73	1.51	8 (16%)	59,89,113	1.66	6 (10%)
28	LHG	AD	316	24	46,46,48	0.62	1 (2%)	49,52,54	1.25	5 (10%)
24	CLA	AJ	405	-	69,73,73	1.26	8 (11%)	83,113,113	1.46	6 (7%)
23	CHL	9	609	-	66,70,74	1.96	17 (25%)	75,109,114	2.84	28 (37%)
24	CLA	q	604	-	52,56,73	1.45	9 (17%)	62,92,113	1.53	5 (8%)
24	CLA	AN	610	28	43,47,73	1.56	8 (18%)	49,81,113	1.49	4 (8%)
23	CHL	AU	607	-	70,74,74	1.91	16 (22%)	80,114,114	2.68	27 (33%)
25	LUT	AH	614	-	42,43,43	1.67	8 (19%)	51,60,60	1.50	9 (17%)
29	BCR	J	408	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	6 (10%)
25	LUT	AA	615	-	42,43,43	1.68	8 (19%)	51,60,60	1.53	11 (21%)
24	CLA	AL	506	-	69,73,73	1.26	9 (13%)	83,113,113	1.35	6 (7%)
26	NEX	AS	317	-	38,46,46	1.59	6 (15%)	50,70,70	1.70	11 (22%)
23	CHL	AF	601	-	48,53,74	2.25	17 (35%)	53,89,114	3.09	20 (37%)
24	CLA	AQ	611	28	64,68,73	1.32	7 (10%)	77,107,113	1.34	7 (9%)
32	PHO	AJ	407	-	58,69,69	2.06	10 (17%)	56,99,99	1.50	8 (14%)
24	CLA	AD	305	-	49,53,73	1.48	9 (18%)	59,89,113	1.54	5 (8%)
24	CLA	0	612	-	62,66,73	1.33	8 (12%)	74,104,113	1.38	7 (9%)
23	CHL	AA	607	-	50,54,74	2.19	16 (32%)	56,90,114	3.15	21 (37%)
24	CLA	AU	612	-	69,73,73	1.26	9 (13%)	83,113,113	1.31	4 (4%)
24	CLA	AK	615	-	69,73,73	1.27	9 (13%)	83,113,113	1.28	8 (9%)
34	SQD	AP	101	-	41,42,54	1.66	7 (17%)	50,53,65	1.45	6 (12%)
23	CHL	AC	605	1	50,54,74	2.22	17 (34%)	56,90,114	3.12	24 (42%)
24	CLA	AD	311	-	49,53,73	1.50	10 (20%)	59,89,113	1.40	4 (6%)
26	NEX	AU	616	-	38,46,46	1.68	7 (18%)	50,70,70	1.64	9 (18%)
24	CLA	P	509	6	69,73,73	1.26	8 (11%)	83,113,113	1.24	4 (4%)
24	CLA	O	616	5	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
24	CLA	P	511	-	69,73,73	1.25	8 (11%)	83,113,113	1.33	7 (8%)
23	CHL	AU	608	-	70,74,74	1.85	17 (24%)	80,114,114	2.78	27 (33%)
24	CLA	AA	604	-	49,53,73	1.48	9 (18%)	59,89,113	1.50	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	AK	613	5	69,73,73	1.27	8 (11%)	83,113,113	1.50	8 (9%)
32	PHO	AJ	408	-	58,69,69	2.07	9 (15%)	56,99,99	1.63	7 (12%)
24	CLA	AU	610	-	64,68,73	1.34	8 (12%)	77,107,113	1.41	9 (11%)
23	CHL	q	607	-	56,60,74	2.16	19 (33%)	63,97,114	2.90	26 (41%)
25	LUT	AQ	616	-	42,43,43	1.60	8 (19%)	51,60,60	1.51	11 (21%)
24	CLA	q	611	16	53,57,73	1.44	8 (15%)	62,93,113	1.36	6 (9%)
23	CHL	AA	608	-	63,66,74	2.36	20 (31%)	67,101,114	2.80	28 (41%)
24	CLA	P	503	-	69,73,73	1.27	7 (10%)	83,113,113	1.48	8 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	v	312	-	-	7/20/96/115	-
24	CLA	AQ	602	-	-	17/39/115/115	-
35	DGD	AL	517	-	-	11/44/84/95	0/2/2/2
24	CLA	O	601	-	-	17/39/115/115	-
24	CLA	AQ	614	-	-	2/10/82/115	-
23	CHL	9	601	1	-	5/12/88/117	-
23	CHL	AC	607	-	-	9/15/91/117	-
26	NEX	AR	615	-	-	16/27/83/83	0/3/3/3
29	BCR	AK	602	-	-	15/29/63/63	0/2/2/2
23	CHL	p	606	-	-	11/22/98/117	-
24	CLA	O	603	-	-	9/39/115/115	-
24	CLA	AC	604	-	-	6/21/97/115	-
25	LUT	0	614	-	-	0/29/67/67	0/2/2/2
25	LUT	AC	614	-	-	3/29/67/67	0/2/2/2
27	XAT	AR	616	-	-	19/31/93/93	0/4/4/4
23	CHL	AF	606	-	-	2/8/77/117	-
23	CHL	AD	302	2	-	18/39/115/117	-
24	CLA	AL	503	-	-	17/39/115/115	-
23	CHL	AN	617	10	-	7/17/93/117	-
23	CHL	AC	608	-	-	18/37/113/117	-
24	CLA	AK	618	5	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AJ	406	-	-	6/21/97/115	-
23	CHL	AR	605	16	-	23/39/115/117	-
24	CLA	q	608	16	-	6/15/91/115	-
38	HEM	F	102	9,8	-	5/14/54/54	-
24	CLA	AU	613	-	-	7/19/95/115	-
24	CLA	Q	401	-	-	6/21/97/115	-
26	NEX	p	616	-	-	14/27/83/83	0/3/3/3
23	CHL	0	617	2	-	3/17/93/117	-
23	CHL	AD	306	-	-	10/26/102/117	-
23	CHL	AD	317	2	-	3/17/93/117	-
24	CLA	AN	612	10	-	15/39/115/115	-
24	CLA	AE	603	-	-	11/27/103/115	-
24	CLA	O	611	5	-	11/39/115/115	-
25	LUT	9	616	-	-	3/29/67/67	0/2/2/2
25	LUT	AN	614	-	-	3/29/67/67	0/2/2/2
25	LUT	AU	614	-	-	2/29/67/67	0/2/2/2
23	CHL	AF	605	-	-	0/2/70/117	-
23	CHL	0	608	-	-	0/6/82/117	-
34	SQD	J	410	-	-	27/49/69/69	0/1/1/1
27	XAT	9	618	-	-	16/31/93/93	0/4/4/4
24	CLA	V	611	10	-	0/10/86/115	-
25	LUT	0	615	-	-	1/29/67/67	0/2/2/2
25	LUT	AC	615	-	-	2/29/67/67	0/2/2/2
24	CLA	AF	614	-	-	10/15/91/115	-
33	LMG	J	409	-	-	17/43/63/70	0/1/1/1
23	CHL	0	607	-	-	9/15/91/117	-
26	NEX	9	617	-	-	13/27/83/83	0/3/3/3
23	CHL	AE	601	1	-	5/17/93/117	-
23	CHL	p	605	10	-	9/20/96/117	-
24	CLA	9	611	-	-	5/9/87/115	-
23	CHL	p	601	10	-	25/41/117/117	-
24	CLA	O	606	-	-	11/33/111/115	-
24	CLA	AD	310	28	-	12/27/103/115	-
24	CLA	O	609	-	-	13/39/115/115	-
25	LUT	AS	316	-	-	3/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AM	403	7	-	17/39/115/115	-
24	CLA	AD	303	-	-	16/33/109/115	-
23	CHL	AQ	608	-	-	15/41/117/117	-
28	LHG	O	621	-	-	27/53/53/53	-
29	BCR	AO	101	-	-	5/29/63/63	0/2/2/2
29	BCR	AV	101	-	-	9/29/63/63	0/2/2/2
24	CLA	AS	303	17	-	17/35/111/115	-
24	CLA	AH	603	-	-	9/39/115/115	-
24	CLA	AJ	409	4	-	7/27/105/115	-
32	PHO	J	405	-	-	6/37/103/103	0/5/6/6
23	CHL	AH	608	-	-	20/41/117/117	-
28	LHG	AK	623	-	-	15/50/50/53	-
23	CHL	V	606	-	-	18/41/117/117	-
24	CLA	AA	609	-	-	6/15/93/115	-
24	CLA	K	101	6	-	11/39/115/115	-
23	CHL	AQ	607	-	-	22/41/117/117	-
24	CLA	AE	602	1	-	5/12/88/115	-
24	CLA	AN	611	-	-	8/33/109/115	-
33	LMG	P	518	-	-	19/46/66/70	0/1/1/1
24	CLA	AK	617	-	-	14/39/115/115	-
24	CLA	p	604	-	-	10/21/97/115	-
28	LHG	W	201	-	-	14/53/53/53	-
24	CLA	0	610	28	-	11/27/103/115	-
28	LHG	p	617	-	-	15/41/41/53	-
24	CLA	Q	404	-	-	15/39/115/115	-
29	BCR	AI	101	-	-	10/29/63/63	0/2/2/2
24	CLA	AR	611	16	-	8/20/96/115	-
25	LUT	AR	614	-	-	1/29/67/67	0/2/2/2
33	LMG	Q	407	-	-	16/41/61/70	0/1/1/1
24	CLA	V	604	-	-	0/4/61/115	-
25	LUT	V	614	-	-	2/29/67/67	0/2/2/2
24	CLA	V	610	-	-	8/33/109/115	-
24	CLA	AU	611	-	-	11/33/109/115	-
23	CHL	AU	605	10	-	9/20/96/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	9	603	-	-	9/27/103/115	-
35	DGD	AJ	412	-	-	26/49/89/95	0/2/2/2
24	CLA	AK	608	-	-	11/33/111/115	-
24	CLA	AK	604	5	-	13/39/115/115	-
29	BCR	O	619	-	-	4/29/63/63	0/2/2/2
25	LUT	AF	611	-	-	2/29/67/67	0/2/2/2
24	CLA	AA	603	-	-	10/27/103/115	-
24	CLA	q	609	16	-	13/33/111/115	-
24	CLA	0	604	-	-	7/15/91/115	-
23	CHL	p	609	10	-	18/35/113/117	-
24	CLA	AA	613	-	-	5/15/91/115	-
24	CLA	P	506	6	-	15/39/115/115	-
24	CLA	AL	509	6	-	18/39/115/115	-
23	CHL	q	605	16	-	22/38/114/117	-
23	CHL	AN	607	-	-	26/41/117/117	-
24	CLA	AN	604	-	-	0/4/76/115	-
24	CLA	O	613	-	-	12/39/115/115	-
23	CHL	AQ	605	10	-	7/20/96/117	-
24	CLA	AM	404	-	-	15/39/115/115	-
24	CLA	AN	603	10	-	16/39/115/115	-
29	BCR	O	617	-	-	5/29/63/63	0/2/2/2
23	CHL	AF	607	-	-	6/17/93/117	-
32	PHO	J	406	-	-	18/37/103/103	0/5/6/6
23	CHL	9	607	-	-	17/38/114/117	-
25	LUT	9	615	-	-	3/29/67/67	0/2/2/2
24	CLA	AR	612	16	-	12/33/109/115	-
23	CHL	p	608	-	-	11/41/117/117	-
29	BCR	k	101	-	-	6/29/63/63	0/2/2/2
29	BCR	P	515	-	-	7/29/63/63	0/2/2/2
33	LMG	AK	601	-	-	14/35/55/70	0/1/1/1
23	CHL	V	601	10	-	25/41/117/117	-
23	CHL	AU	606	-	-	8/22/98/117	-
26	NEX	q	615	-	-	20/27/83/83	0/3/3/3
29	BCR	AJ	410	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LUT	v	316	-	-	2/29/67/67	0/2/2/2
24	CLA	9	604	-	-	5/21/97/115	-
23	CHL	AS	306	-	-	2/6/62/117	-
23	CHL	AB	605	-	-	5/9/81/117	-
24	CLA	O	608	5	-	12/39/115/115	-
23	CHL	AR	606	-	-	9/29/105/117	-
23	CHL	AD	307	-	-	8/17/93/117	-
23	CHL	AU	601	10	-	24/41/117/117	-
24	CLA	AR	609	16	-	13/33/111/115	-
29	BCR	AK	621	-	-	4/29/63/63	0/2/2/2
24	CLA	AB	602	-	-	2/15/91/115	-
25	LUT	AE	613	-	-	2/29/67/67	0/2/2/2
24	CLA	J	403	-	-	12/39/115/115	-
28	LHG	P	517	-	-	24/53/53/53	-
25	LUT	AN	615	-	-	2/29/67/67	0/2/2/2
24	CLA	AH	609	-	-	14/33/109/115	-
24	CLA	0	602	-	-	18/33/109/115	-
24	CLA	AE	611	1	-	7/15/91/115	-
24	CLA	P	507	-	-	17/39/115/115	-
24	CLA	AL	508	-	-	17/39/115/115	-
24	CLA	AS	311	-	-	13/29/105/115	-
29	BCR	AL	515	-	-	3/29/63/63	0/2/2/2
35	DGD	AJ	401	-	-	18/48/88/95	0/2/2/2
37	PL9	AM	405	-	-	3/50/70/73	0/1/1/1
23	CHL	AB	601	-	-	0/15/91/117	-
23	CHL	AB	607	-	-	7/17/93/117	-
24	CLA	AR	610	-	-	11/20/96/115	-
24	CLA	P	510	6	-	17/39/115/115	-
24	CLA	AK	607	-	-	18/39/115/115	-
23	CHL	AE	617	-	-	7/17/93/117	-
24	CLA	AS	312	-	-	8/20/96/115	-
24	CLA	O	610	-	-	12/39/115/115	-
34	SQD	AM	401	-	-	20/45/65/69	0/1/1/1
23	CHL	v	306	-	-	2/4/72/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	0	609	2	-	11/27/105/115	-
24	CLA	AC	602	1	-	20/35/111/115	-
27	XAT	AB	613	-	-	19/31/93/93	0/4/4/4
24	CLA	P	505	-	-	22/39/115/115	-
24	CLA	AK	603	-	-	16/39/115/115	-
24	CLA	AL	510	6	-	10/39/115/115	-
28	LHG	AM	406	-	-	17/53/53/53	-
29	BCR	O	618	-	-	6/29/63/63	0/2/2/2
24	CLA	AF	603	-	-	5/15/91/115	-
24	CLA	AL	502	-	-	17/39/115/115	-
23	CHL	AA	617	1	-	7/17/93/117	-
23	CHL	AF	608	3	-	4/11/89/117	-
24	CLA	P	508	6	-	18/39/115/115	-
24	CLA	AH	602	10	-	18/39/115/115	-
24	CLA	9	610	1	-	8/23/101/115	-
24	CLA	AQ	613	10	-	8/33/109/115	-
24	CLA	AK	614	-	-	15/39/115/115	-
23	CHL	AE	606	-	-	12/17/93/117	-
24	CLA	AS	309	-	-	2/9/87/115	-
24	CLA	AL	507	6	-	15/39/115/115	-
24	CLA	AD	304	-	-	11/27/103/115	-
24	CLA	O	614	-	-	18/39/115/115	-
24	CLA	AQ	612	-	-	2/33/109/115	-
24	CLA	AC	603	-	-	9/27/103/115	-
34	SQD	AJ	411	-	-	27/49/69/69	0/1/1/1
29	BCR	O	625	-	-	17/29/63/63	0/2/2/2
33	LMG	AK	622	-	-	18/46/66/70	0/1/1/1
35	DGD	AO	102	-	-	19/51/91/95	0/2/2/2
24	CLA	0	613	-	-	12/19/95/115	-
24	CLA	AC	613	-	-	5/9/87/115	-
24	CLA	AK	605	-	-	8/39/115/115	-
25	LUT	p	614	-	-	1/29/67/67	0/2/2/2
23	CHL	AB	606	-	-	7/15/91/117	-
25	LUT	V	613	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	V	605	-	-	12/22/98/117	-
28	LHG	O	622	-	-	15/50/50/53	-
33	LMG	AL	501	-	-	17/43/63/70	0/1/1/1
25	LUT	AS	315	-	-	2/29/67/67	0/2/2/2
28	LHG	AQ	618	24	-	16/53/53/53	-
24	CLA	p	603	-	-	16/39/115/115	-
24	CLA	AN	609	-	-	18/32/110/115	-
23	CHL	9	608	-	-	9/15/91/117	-
24	CLA	AA	602	1	-	9/35/111/115	-
24	CLA	AR	603	-	-	7/33/109/115	-
24	CLA	O	604	5	-	15/39/115/115	-
24	CLA	9	602	1	-	17/35/111/115	-
24	CLA	0	603	-	-	13/27/103/115	-
24	CLA	AR	602	16	-	11/27/105/115	-
24	CLA	AH	610	-	-	12/33/109/115	-
24	CLA	O	612	-	-	14/39/115/115	-
25	LUT	AD	314	-	-	0/29/67/67	0/2/2/2
23	CHL	AA	606	-	-	16/35/111/117	-
24	CLA	AU	603	-	-	10/39/115/115	-
24	CLA	v	311	-	-	10/29/105/115	-
38	HEM	f	102	9,8	-	5/14/54/54	-
24	CLA	AH	613	-	-	6/13/91/115	-
24	CLA	AB	610	-	-	7/15/91/115	-
23	CHL	AQ	609	-	-	21/41/117/117	-
33	LMG	O	620	-	-	18/46/66/70	0/1/1/1
28	LHG	AU	617	-	-	12/53/53/53	-
24	CLA	9	614	-	-	0/4/72/115	-
23	CHL	AA	605	1	-	9/17/93/117	-
24	CLA	AB	611	-	-	7/15/91/115	-
24	CLA	AH	611	-	-	11/33/109/115	-
29	BCR	AL	516	-	-	6/29/63/63	0/2/2/2
25	LUT	p	615	-	-	1/29/67/67	0/2/2/2
24	CLA	AJ	404	-	-	13/39/115/115	-
29	BCR	AK	619	-	-	5/29/63/63	0/2/2/2
29	BCR	P	514	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AL	505	-	-	16/39/115/115	-
26	NEX	AA	616	-	-	18/27/83/83	0/3/3/3
24	CLA	AE	612	-	-	5/15/91/115	-
24	CLA	q	603	-	-	6/33/109/115	-
29	BCR	P	513	-	-	3/29/63/63	0/2/2/2
24	CLA	AA	610	-	-	6/9/87/115	-
23	CHL	p	607	-	-	22/41/117/117	-
24	CLA	q	602	16	-	11/27/105/115	-
29	BCR	f	101	-	-	11/29/63/63	0/2/2/2
23	CHL	AD	301	-	-	13/38/114/117	-
24	CLA	9	612	-	-	6/15/91/115	-
24	CLA	AK	606	5	-	17/39/115/115	-
35	DGD	J	413	-	-	18/48/88/95	0/2/2/2
29	BCR	AF	612	-	-	13/29/63/63	0/2/2/2
24	CLA	P	501	-	-	16/39/115/115	-
24	CLA	AH	612	10	-	15/39/115/115	-
28	LHG	q	616	24	-	14/46/46/53	-
28	LHG	AS	301	-	-	22/53/53/53	-
25	LUT	v	315	-	-	2/29/67/67	0/2/2/2
34	SQD	M	101	-	-	19/49/69/69	0/1/1/1
23	CHL	AE	607	-	-	13/35/111/117	-
24	CLA	AS	310	-	-	5/21/99/115	-
28	LHG	AL	519	-	-	25/53/53/53	-
24	CLA	AC	612	1	-	3/10/86/115	-
28	LHG	w	201	-	-	14/53/53/53	-
24	CLA	AB	609	-	-	4/10/82/115	-
24	CLA	O	615	-	-	12/39/115/115	-
23	CHL	AH	607	-	-	18/41/117/117	-
25	LUT	AQ	615	-	-	1/29/67/67	0/2/2/2
23	CHL	AD	308	-	-	12/29/107/117	-
33	LMG	AM	407	-	-	16/41/61/70	0/1/1/1
23	CHL	0	606	-	-	10/26/102/117	-
24	CLA	v	309	-	-	2/9/87/115	-
23	CHL	AH	606	-	-	8/22/98/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AL	504	-	-	21/39/115/115	-
23	CHL	AN	608	-	-	15/29/107/117	-
24	CLA	AD	309	-	-	9/27/105/115	-
24	CLA	AR	604	-	-	5/19/95/115	-
23	CHL	q	613	16	-	4/12/88/117	-
24	CLA	AC	611	-	-	5/9/81/115	-
24	CLA	p	610	-	-	21/40/101/115	-
24	CLA	AN	602	10	-	15/39/115/115	-
34	SQD	m	101	-	-	18/49/69/69	0/1/1/1
24	CLA	AS	304	17	-	2/15/91/115	-
29	BCR	AK	620	-	-	6/29/63/63	0/2/2/2
24	CLA	AD	312	2	-	8/31/107/115	-
24	CLA	AU	604	-	-	7/21/97/115	-
23	CHL	q	606	-	-	9/27/103/117	-
23	CHL	AS	307	-	-	10/32/108/117	-
24	CLA	AB	604	-	-	5/15/91/115	-
26	NEX	AQ	617	-	-	17/27/83/83	0/3/3/3
24	CLA	P	502	-	-	17/39/115/115	-
24	CLA	p	613	10	-	2/10/82/115	-
24	CLA	AL	511	6	-	17/39/115/115	-
28	LHG	AH	616	-	-	12/53/53/53	-
24	CLA	AK	611	-	-	13/39/115/115	-
24	CLA	O	607	-	-	17/39/115/115	-
23	CHL	AR	607	-	-	11/26/102/117	-
27	XAT	AF	613	-	-	19/31/93/93	0/4/4/4
24	CLA	AL	512	6	-	13/39/115/115	-
24	CLA	v	310	-	-	5/21/99/115	-
24	CLA	AL	514	6	-	14/31/109/115	-
23	CHL	AE	605	-	-	16/35/111/117	-
24	CLA	AA	612	-	-	9/15/91/115	-
23	CHL	V	608	-	-	13/29/107/117	-
33	LMG	AL	520	-	-	20/46/66/70	0/1/1/1
24	CLA	AS	313	-	-	12/21/99/115	-
23	CHL	AC	606	-	-	5/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LUT	AH	615	-	-	1/29/67/67	0/2/2/2
24	CLA	AC	609	1	-	6/23/101/115	-
24	CLA	q	610	28	-	11/20/96/115	-
24	CLA	AN	613	10	-	12/19/95/115	-
23	CHL	AE	616	1	-	9/17/93/117	-
24	CLA	J	407	4	-	7/27/105/115	-
35	DGD	P	516	-	-	11/44/84/95	0/2/2/2
23	CHL	AH	605	10	-	9/20/96/117	-
24	CLA	O	602	5	-	12/39/115/115	-
24	CLA	J	404	-	-	7/39/115/115	-
24	CLA	AE	609	-	-	9/15/91/115	-
24	CLA	AK	616	-	-	18/39/115/115	-
24	CLA	AS	314	17	-	11/20/96/115	-
23	CHL	V	607	-	-	24/37/113/117	-
23	CHL	AC	601	1	-	9/15/91/117	-
28	LHG	0	616	24	-	8/51/51/53	-
24	CLA	p	611	-	-	2/4/72/115	-
24	CLA	v	304	17	-	2/15/91/115	-
24	CLA	AB	603	-	-	4/15/91/115	-
28	LHG	AK	624	-	-	21/53/53/53	-
27	XAT	q	617	-	-	20/31/93/93	0/4/4/4
23	CHL	AB	608	-	-	5/11/83/117	-
26	NEX	AC	616	-	-	15/27/83/83	0/3/3/3
24	CLA	AS	305	-	-	11/21/97/115	-
24	CLA	p	618	-	-	9/19/95/115	-
24	CLA	AQ	603	-	-	16/39/115/115	-
28	LHG	v	301	-	-	22/53/53/53	-
33	LMG	O	624	-	-	14/35/55/70	0/1/1/1
29	BCR	F	101	-	-	11/29/63/63	0/2/2/2
23	CHL	AS	302	17	-	3/15/91/117	-
24	CLA	AF	609	-	-	4/10/82/115	-
24	CLA	AQ	610	10	-	18/39/115/115	-
24	CLA	p	612	-	-	10/33/109/115	-
24	CLA	AR	601	16	-	10/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PL9	Q	405	-	-	3/50/70/73	0/1/1/1
24	CLA	AE	610	-	-	6/15/91/115	-
24	CLA	v	313	17	-	11/21/99/115	-
24	CLA	O	605	-	-	19/39/115/115	-
24	CLA	AR	608	-	-	0/4/82/115	-
23	CHL	9	605	1	-	8/17/93/117	-
24	CLA	AE	604	-	-	8/15/91/115	-
24	CLA	V	602	-	-	16/39/115/115	-
23	CHL	AS	308	-	-	5/15/91/117	-
23	CHL	0	605	-	-	5/17/93/117	-
24	CLA	AH	604	-	-	7/21/97/115	-
24	CLA	AK	610	5	-	13/39/115/115	-
24	CLA	p	602	10	-	15/39/115/115	-
23	CHL	AH	601	10	-	24/41/117/117	-
35	DGD	J	411	-	-	26/49/89/95	0/2/2/2
23	CHL	9	606	-	-	8/17/93/117	-
29	BCR	j	101	-	-	6/29/63/63	0/2/2/2
25	LUT	AD	315	-	-	1/29/67/67	0/2/2/2
29	BCR	AB	612	-	-	13/29/63/63	0/2/2/2
24	CLA	AF	610	-	-	5/15/91/115	-
24	CLA	Q	403	7	-	17/39/115/115	-
24	CLA	AC	610	-	-	5/9/87/115	-
24	CLA	AA	611	-	-	6/15/91/115	-
26	NEX	v	317	-	-	16/27/83/83	0/3/3/3
24	CLA	v	314	17	-	11/20/96/115	-
24	CLA	AU	602	10	-	18/39/115/115	-
24	CLA	q	612	-	-	12/33/106/115	-
23	CHL	AN	605	10	-	12/22/98/117	-
35	DGD	AL	518	-	-	21/51/91/95	0/2/2/2
25	LUT	AE	614	-	-	1/29/67/67	0/2/2/2
25	LUT	AA	614	-	-	2/29/67/67	0/2/2/2
24	CLA	V	612	10	-	11/19/95/115	-
25	LUT	AU	615	-	-	1/29/67/67	0/2/2/2
24	CLA	P	504	-	-	11/39/115/115	-
28	LHG	AN	616	24	-	16/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	0	601	2	-	19/39/115/117	-
23	CHL	AR	613	-	-	5/12/88/117	-
34	SQD	Q	402	-	-	19/45/65/69	0/1/1/1
23	CHL	AQ	606	-	-	11/22/98/117	-
28	LHG	V	615	-	-	18/53/53/53	-
23	CHL	V	616	10	-	9/17/93/117	-
24	CLA	AF	602	-	-	1/4/82/115	-
23	CHL	v	307	-	-	9/17/93/117	-
24	CLA	q	601	16	-	8/20/96/115	-
24	CLA	V	609	10	-	19/32/110/115	-
24	CLA	AQ	604	-	-	10/21/97/115	-
23	CHL	AQ	601	10	-	23/41/117/117	-
28	LHG	Q	406	-	-	17/53/53/53	-
24	CLA	AK	609	-	-	17/39/115/115	-
23	CHL	AA	601	1	-	6/17/93/117	-
25	LUT	q	614	-	-	1/29/67/67	0/2/2/2
24	CLA	P	512	6	-	13/31/109/115	-
24	CLA	AK	612	-	-	10/39/115/115	-
24	CLA	v	305	-	-	6/21/97/115	-
24	CLA	AU	609	-	-	12/33/109/115	-
24	CLA	0	611	-	-	8/15/91/115	-
24	CLA	AE	608	-	-	6/15/93/115	-
23	CHL	v	302	17	-	4/15/91/117	-
24	CLA	V	603	-	-	15/39/115/115	-
24	CLA	AF	604	-	-	3/15/91/115	-
23	CHL	AN	606	-	-	18/41/117/117	-
34	SQD	o	101	-	-	20/37/57/69	0/1/1/1
28	LHG	O	623	-	-	23/53/53/53	-
23	CHL	v	308	-	-	1/8/84/117	-
26	NEX	AE	615	-	-	17/27/83/83	0/3/3/3
24	CLA	AD	313	-	-	14/19/95/115	-
23	CHL	AN	601	10	-	24/41/117/117	-
24	CLA	AR	617	-	-	5/9/87/115	-
24	CLA	v	303	17	-	16/35/111/115	-
24	CLA	9	613	-	-	11/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	j	102	-	-	16/51/91/95	0/2/2/2
24	CLA	AL	513	-	-	13/39/115/115	-
24	CLA	q	618	-	-	7/15/91/115	-
28	LHG	AD	316	24	-	11/51/51/53	-
24	CLA	AJ	405	-	-	8/39/115/115	-
23	CHL	9	609	-	-	15/37/113/117	-
24	CLA	q	604	-	-	8/19/95/115	-
24	CLA	AN	610	28	-	2/4/82/115	-
23	CHL	AU	607	-	-	18/41/117/117	-
25	LUT	AH	614	-	-	2/29/67/67	0/2/2/2
29	BCR	J	408	-	-	4/29/63/63	0/2/2/2
25	LUT	AA	615	-	-	1/29/67/67	0/2/2/2
24	CLA	AL	506	-	-	23/39/115/115	-
26	NEX	AS	317	-	-	15/27/83/83	0/3/3/3
23	CHL	AF	601	-	-	1/15/91/117	-
24	CLA	AQ	611	28	-	18/33/109/115	-
32	PHO	AJ	407	-	-	6/37/103/103	0/5/6/6
24	CLA	AD	305	-	-	9/15/91/115	-
24	CLA	0	612	-	-	7/31/107/115	-
23	CHL	AA	607	-	-	12/17/93/117	-
24	CLA	AU	612	-	-	17/39/115/115	-
24	CLA	AK	615	-	-	12/39/115/115	-
34	SQD	AP	101	-	-	19/37/57/69	0/1/1/1
23	CHL	AC	605	1	-	9/17/93/117	-
24	CLA	AD	311	-	-	8/15/91/115	-
26	NEX	AU	616	-	-	14/27/83/83	0/3/3/3
24	CLA	P	509	6	-	9/39/115/115	-
24	CLA	O	616	5	-	16/39/115/115	-
24	CLA	P	511	-	-	12/39/115/115	-
23	CHL	AU	608	-	-	21/41/117/117	-
24	CLA	AA	604	-	-	9/15/91/115	-
24	CLA	AK	613	5	-	11/39/115/115	-
32	PHO	AJ	408	-	-	19/37/103/103	0/5/6/6
24	CLA	AU	610	-	-	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	q	607	-	-	13/25/101/117	-
25	LUT	AQ	616	-	-	1/29/67/67	0/2/2/2
24	CLA	q	611	16	-	8/20/96/115	-
23	CHL	AA	608	-	-	18/36/97/117	-
24	CLA	P	503	-	-	21/39/115/115	-

All (3944) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AF	613	XAT	C14-C13	15.14	1.55	1.35
27	AB	613	XAT	C34-C33	15.10	1.55	1.35
27	AB	613	XAT	C14-C13	15.03	1.55	1.35
27	AB	613	XAT	C30-C29	14.94	1.55	1.35
27	q	617	XAT	C30-C29	14.93	1.55	1.35
27	q	617	XAT	C10-C9	14.91	1.55	1.35
27	AR	616	XAT	C10-C9	14.90	1.55	1.35
27	AR	616	XAT	C14-C13	14.88	1.55	1.35
27	AR	616	XAT	C30-C29	14.87	1.55	1.35
27	9	618	XAT	C10-C9	14.87	1.55	1.35
27	q	617	XAT	C14-C13	14.82	1.55	1.35
27	AF	613	XAT	C10-C9	14.81	1.55	1.35
27	9	618	XAT	C14-C13	14.79	1.55	1.35
27	AB	613	XAT	C10-C9	14.79	1.55	1.35
27	9	618	XAT	C30-C29	14.71	1.55	1.35
27	AF	613	XAT	C30-C29	14.68	1.55	1.35
27	AR	616	XAT	C34-C33	14.57	1.55	1.35
27	q	617	XAT	C34-C33	14.52	1.55	1.35
27	9	618	XAT	C34-C33	14.50	1.55	1.35
27	AF	613	XAT	C34-C33	14.43	1.54	1.35
27	AF	613	XAT	C28-C27	11.04	1.56	1.32
27	q	617	XAT	C8-C7	10.98	1.56	1.32
27	AR	616	XAT	C8-C7	10.96	1.56	1.32
27	AB	613	XAT	C8-C7	10.91	1.56	1.32
27	AF	613	XAT	C8-C7	10.86	1.56	1.32
27	9	618	XAT	C8-C7	10.86	1.56	1.32
27	9	618	XAT	C28-C27	10.84	1.56	1.32
27	AB	613	XAT	C28-C27	10.77	1.56	1.32
27	q	617	XAT	C28-C27	10.70	1.55	1.32
27	AR	616	XAT	C28-C27	10.69	1.55	1.32
32	AJ	408	PHO	C1B-C2B	9.60	1.50	1.39
32	J	406	PHO	C1B-C2B	9.59	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	J	405	PHO	C1B-C2B	9.42	1.50	1.39
32	AJ	407	PHO	C1B-C2B	9.41	1.50	1.39
24	p	610	CLA	C1A-NA	8.60	1.41	1.33
27	AF	613	XAT	C11-C12	8.08	1.55	1.34
27	AB	613	XAT	C11-C12	8.07	1.55	1.34
27	q	617	XAT	C11-C12	8.01	1.55	1.34
27	AR	616	XAT	C11-C12	7.99	1.55	1.34
27	AB	613	XAT	C31-C32	7.98	1.55	1.34
27	9	618	XAT	C11-C12	7.98	1.55	1.34
27	q	617	XAT	C31-C32	7.98	1.55	1.34
23	AF	606	CHL	C3D-C4D	-7.96	1.39	1.51
27	AR	616	XAT	C31-C32	7.96	1.55	1.34
27	9	618	XAT	C31-C32	7.94	1.55	1.34
24	V	604	CLA	C1A-NA	7.87	1.40	1.33
27	AF	613	XAT	C31-C32	7.74	1.54	1.34
32	J	405	PHO	C3B-C4B	7.67	1.50	1.41
32	AJ	407	PHO	C3B-C4B	7.65	1.50	1.41
27	AB	613	XAT	C35-C15	7.54	1.55	1.36
32	AJ	408	PHO	C3B-C4B	7.48	1.50	1.41
32	J	406	PHO	C3B-C4B	7.42	1.50	1.41
27	AF	613	XAT	C35-C15	7.39	1.55	1.36
27	AR	616	XAT	C35-C15	7.35	1.55	1.36
27	q	617	XAT	C35-C15	7.34	1.55	1.36
27	9	618	XAT	C35-C15	7.29	1.54	1.36
23	AF	606	CHL	C4D-CHA	7.27	1.47	1.35
23	AA	608	CHL	C1A-NA	-6.03	1.27	1.33
23	AS	306	CHL	C3C-C4C	5.99	1.49	1.40
23	AR	605	CHL	C3C-C4C	5.93	1.49	1.40
23	q	606	CHL	C3C-C4C	5.90	1.49	1.40
23	v	306	CHL	C3C-C4C	5.89	1.49	1.40
23	AC	607	CHL	C3C-C4C	5.88	1.49	1.40
23	9	608	CHL	C3C-C4C	5.88	1.49	1.40
23	AF	606	CHL	C3C-C4C	5.88	1.49	1.40
23	AB	606	CHL	C3C-C4C	5.83	1.49	1.40
23	AB	605	CHL	C2C-C1C	5.70	1.49	1.40
23	AS	308	CHL	C2C-C1C	5.69	1.49	1.40
23	AF	605	CHL	C3C-C2C	5.68	1.47	1.35
23	V	607	CHL	C2C-C1C	5.64	1.49	1.40
23	0	607	CHL	C2C-C1C	5.61	1.48	1.40
23	0	617	CHL	O2D-CGD	5.54	1.46	1.33
23	AF	606	CHL	C1D-CHD	5.52	1.47	1.35
23	AA	617	CHL	O2D-CGD	5.50	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AS	306	CHL	C3D-C2D	5.47	1.48	1.37
24	q	612	CLA	C4D-CHA	5.44	1.44	1.35
23	AA	608	CHL	CHD-C1D	5.43	1.48	1.38
23	AE	616	CHL	O2D-CGD	5.43	1.46	1.33
23	v	308	CHL	C3C-C2C	5.39	1.47	1.35
23	0	606	CHL	O2D-CGD	5.36	1.46	1.33
23	AD	317	CHL	O2D-CGD	5.36	1.46	1.33
23	V	606	CHL	O2D-CGD	5.36	1.46	1.33
23	AN	606	CHL	O2D-CGD	5.35	1.46	1.33
23	AA	605	CHL	O2D-CGD	5.28	1.46	1.33
23	AD	306	CHL	O2D-CGD	5.28	1.46	1.33
23	AN	605	CHL	O2D-CGD	5.26	1.46	1.33
23	AQ	606	CHL	O2D-CGD	5.25	1.46	1.33
23	AC	605	CHL	O2D-CGD	5.25	1.46	1.33
23	AF	606	CHL	O2D-CGD	5.25	1.46	1.33
23	AU	607	CHL	O2D-CGD	5.25	1.46	1.33
23	AR	605	CHL	O2D-CGD	5.25	1.46	1.33
23	AH	601	CHL	O2D-CGD	5.24	1.46	1.33
23	AE	605	CHL	O2D-CGD	5.24	1.46	1.33
23	AQ	609	CHL	O2D-CGD	5.24	1.46	1.33
23	p	606	CHL	O2D-CGD	5.24	1.46	1.33
23	v	308	CHL	O2D-CGD	5.24	1.46	1.33
23	AC	606	CHL	O2D-CGD	5.24	1.46	1.33
23	AU	601	CHL	O2D-CGD	5.23	1.46	1.33
23	0	601	CHL	O2D-CGD	5.23	1.46	1.33
23	AH	607	CHL	O2D-CGD	5.22	1.45	1.33
23	p	607	CHL	O2D-CGD	5.22	1.45	1.33
23	9	605	CHL	O2D-CGD	5.22	1.45	1.33
23	AR	606	CHL	O2D-CGD	5.21	1.45	1.33
23	AU	606	CHL	O2D-CGD	5.21	1.45	1.33
23	AB	607	CHL	O2D-CGD	5.21	1.45	1.33
23	AE	617	CHL	O2D-CGD	5.21	1.45	1.33
23	0	605	CHL	O2D-CGD	5.20	1.45	1.33
23	AB	606	CHL	O2D-CGD	5.19	1.45	1.33
23	AA	606	CHL	O2D-CGD	5.19	1.45	1.33
23	q	606	CHL	O2D-CGD	5.19	1.45	1.33
23	q	605	CHL	O2D-CGD	5.19	1.45	1.33
38	f	102	HEM	FE-NA	5.18	2.12	1.95
23	9	606	CHL	O2D-CGD	5.18	1.45	1.33
23	AD	302	CHL	O2D-CGD	5.18	1.45	1.33
23	AQ	607	CHL	O2D-CGD	5.17	1.45	1.33
23	p	605	CHL	O2D-CGD	5.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AS	307	CHL	O2D-CGD	5.17	1.45	1.33
23	AS	308	CHL	O2D-CGD	5.16	1.45	1.33
23	AQ	605	CHL	O2D-CGD	5.16	1.45	1.33
23	AH	606	CHL	O2D-CGD	5.16	1.45	1.33
23	v	302	CHL	O2D-CGD	5.15	1.45	1.33
23	AH	605	CHL	O2D-CGD	5.15	1.45	1.33
23	AQ	601	CHL	O2D-CGD	5.14	1.45	1.33
23	AS	302	CHL	O2D-CGD	5.13	1.45	1.33
23	AF	607	CHL	O2D-CGD	5.12	1.45	1.33
23	p	608	CHL	O2D-CGD	5.12	1.45	1.33
23	AU	605	CHL	O2D-CGD	5.12	1.45	1.33
23	v	307	CHL	O2D-CGD	5.12	1.45	1.33
23	p	601	CHL	O2D-CGD	5.11	1.45	1.33
23	AC	607	CHL	O2D-CGD	5.11	1.45	1.33
23	AA	607	CHL	O2D-CGD	5.10	1.45	1.33
23	AC	601	CHL	O2D-CGD	5.09	1.45	1.33
23	AE	601	CHL	O2D-CGD	5.08	1.45	1.33
23	V	605	CHL	O2D-CGD	5.07	1.45	1.33
23	9	608	CHL	O2D-CGD	5.07	1.45	1.33
23	AE	606	CHL	O2D-CGD	5.06	1.45	1.33
23	AA	608	CHL	O2D-CGD	5.05	1.45	1.33
23	AU	601	CHL	O2A-CGA	5.05	1.48	1.33
23	AH	601	CHL	O2A-CGA	5.05	1.48	1.33
23	AQ	608	CHL	O2D-CGD	5.05	1.45	1.33
23	AH	608	CHL	O2D-CGD	5.04	1.45	1.33
23	AR	613	CHL	O2D-CGD	5.03	1.45	1.33
23	AU	608	CHL	O2D-CGD	5.02	1.45	1.33
23	AA	601	CHL	O2D-CGD	5.02	1.45	1.33
23	AF	608	CHL	CHC-C1C	5.01	1.48	1.38
23	V	616	CHL	O2D-CGD	5.00	1.45	1.33
23	AA	608	CHL	C2C-C3C	4.98	1.47	1.36
23	V	607	CHL	O2D-CGD	4.98	1.45	1.33
23	AE	607	CHL	O2D-CGD	4.97	1.45	1.33
23	q	607	CHL	O2D-CGD	4.97	1.45	1.33
23	9	609	CHL	O2D-CGD	4.97	1.45	1.33
23	V	601	CHL	O2D-CGD	4.97	1.45	1.33
23	AN	601	CHL	O2D-CGD	4.96	1.45	1.33
23	AA	608	CHL	CHC-C1C	4.95	1.48	1.38
23	AN	607	CHL	O2D-CGD	4.94	1.45	1.33
23	AN	617	CHL	CHD-C1D	4.94	1.48	1.38
23	9	601	CHL	O2D-CGD	4.92	1.45	1.33
23	AD	301	CHL	O2D-CGD	4.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AC	608	CHL	O2D-CGD	4.91	1.45	1.33
23	V	616	CHL	CHD-C1D	4.90	1.47	1.38
27	AF	613	XAT	C28-C29	4.89	1.56	1.45
23	AA	617	CHL	C2C-C3C	4.88	1.47	1.36
23	AN	608	CHL	C3D-C4D	-4.87	1.33	1.44
23	0	608	CHL	C3D-C4D	-4.85	1.33	1.44
23	AR	607	CHL	O2D-CGD	4.84	1.45	1.33
23	AE	616	CHL	CHD-C1D	4.83	1.47	1.38
23	9	607	CHL	O2D-CGD	4.83	1.45	1.33
23	q	613	CHL	O2D-CGD	4.82	1.45	1.33
23	AF	606	CHL	CHC-C1C	4.81	1.48	1.38
23	AB	607	CHL	C2C-C3C	4.81	1.47	1.36
23	9	606	CHL	C3D-C4D	-4.79	1.33	1.44
24	AL	514	CLA	C3B-C4B	4.79	1.49	1.39
23	0	601	CHL	C2C-C3C	4.79	1.47	1.36
23	AR	613	CHL	C2C-C3C	4.79	1.47	1.36
24	P	512	CLA	C3B-C4B	4.78	1.49	1.39
23	AB	607	CHL	CHC-C1C	4.78	1.48	1.38
23	0	607	CHL	O2D-CGD	4.77	1.44	1.33
23	AF	605	CHL	CHC-C1C	4.77	1.48	1.38
23	AH	606	CHL	C2C-C3C	4.77	1.47	1.36
23	AF	606	CHL	C3B-C4B	4.77	1.49	1.39
23	AN	617	CHL	O2D-CGD	4.76	1.44	1.33
23	AD	307	CHL	O2D-CGD	4.75	1.44	1.33
23	9	606	CHL	C2C-C3C	4.75	1.46	1.36
26	AA	616	NEX	C14-C13	4.75	1.42	1.35
23	AA	608	CHL	CHD-C4C	4.75	1.50	1.39
23	AF	607	CHL	C2C-C3C	4.75	1.46	1.36
23	AF	605	CHL	C3D-C4D	-4.74	1.33	1.44
27	AB	613	XAT	C8-C9	4.73	1.56	1.45
23	AS	306	CHL	CHA-C4D	4.72	1.47	1.38
23	0	617	CHL	C2C-C3C	4.72	1.46	1.36
24	AL	514	CLA	C1B-C2B	4.71	1.49	1.41
34	Q	402	SQD	O48-C23	4.71	1.47	1.33
27	q	617	XAT	C8-C9	4.71	1.56	1.45
23	AD	317	CHL	CHD-C1D	4.71	1.47	1.38
34	M	101	SQD	O48-C23	4.71	1.47	1.33
23	AF	608	CHL	O2A-CGA	4.70	1.46	1.30
23	v	306	CHL	C3D-C4D	-4.70	1.33	1.44
34	m	101	SQD	O48-C23	4.70	1.47	1.33
34	AM	401	SQD	O48-C23	4.70	1.47	1.33
24	P	512	CLA	C1B-C2B	4.70	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	p	601	CHL	O2A-CGA	4.70	1.47	1.33
23	AF	608	CHL	C3D-C4D	-4.69	1.33	1.44
26	AE	615	NEX	C14-C13	4.68	1.42	1.35
27	AR	616	XAT	C8-C9	4.68	1.56	1.45
23	AU	606	CHL	C2C-C3C	4.68	1.46	1.36
23	9	601	CHL	C3B-C4B	4.68	1.49	1.39
23	AS	302	CHL	O2A-CGA	4.67	1.46	1.30
23	v	302	CHL	O2A-CGA	4.67	1.46	1.30
23	9	606	CHL	CHC-C1C	4.67	1.48	1.38
34	AJ	411	SQD	O48-C23	4.67	1.47	1.33
23	AS	307	CHL	O2A-CGA	4.67	1.47	1.33
23	AF	607	CHL	CHD-C1D	4.67	1.47	1.38
23	AF	601	CHL	O2D-CGD	4.66	1.45	1.30
23	AB	601	CHL	O2D-CGD	4.66	1.45	1.30
23	AF	608	CHL	CHD-C1D	4.66	1.47	1.38
27	AB	613	XAT	C28-C29	4.66	1.55	1.45
23	AC	601	CHL	C3B-C4B	4.66	1.49	1.39
27	AF	613	XAT	C8-C9	4.65	1.55	1.45
23	q	613	CHL	C2C-C3C	4.65	1.46	1.36
34	AP	101	SQD	O48-C23	4.65	1.46	1.33
34	J	410	SQD	O48-C23	4.65	1.46	1.33
34	o	101	SQD	O48-C23	4.65	1.46	1.33
23	q	606	CHL	O2A-CGA	4.65	1.46	1.33
23	q	613	CHL	C3D-C4D	-4.64	1.33	1.44
23	AB	605	CHL	CHC-C1C	4.64	1.47	1.38
23	AA	608	CHL	C3D-C4D	-4.64	1.33	1.44
23	AC	606	CHL	C2C-C3C	4.64	1.46	1.36
23	0	606	CHL	C2C-C3C	4.64	1.46	1.36
23	AE	617	CHL	O2A-CGA	4.63	1.46	1.30
27	9	618	XAT	C28-C29	4.63	1.55	1.45
23	AS	302	CHL	C2C-C3C	4.63	1.46	1.36
23	AR	606	CHL	O2A-CGA	4.63	1.46	1.33
23	AA	617	CHL	CHD-C1D	4.63	1.47	1.38
23	q	613	CHL	CHD-C1D	4.63	1.47	1.38
23	AR	613	CHL	CHC-C1C	4.63	1.47	1.38
23	q	613	CHL	CHC-C1C	4.62	1.47	1.38
23	AR	607	CHL	CHC-C1C	4.62	1.47	1.38
23	V	607	CHL	C3B-C4B	4.61	1.49	1.39
23	AS	302	CHL	C3B-C4B	4.61	1.49	1.39
23	AB	608	CHL	CHC-C1C	4.61	1.47	1.38
27	9	618	XAT	C8-C9	4.61	1.55	1.45
23	AH	606	CHL	C3D-C4D	-4.61	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AH	607	CHL	O2A-CGA	4.61	1.46	1.33
23	v	302	CHL	C3B-C4B	4.61	1.49	1.39
23	v	302	CHL	C2C-C3C	4.60	1.46	1.36
23	AN	606	CHL	O2A-CGA	4.60	1.46	1.33
23	AD	308	CHL	C2C-C3C	4.60	1.46	1.36
23	AQ	607	CHL	CHC-C1C	4.59	1.47	1.38
23	V	606	CHL	O2A-CGA	4.59	1.46	1.33
23	AR	607	CHL	C2C-C3C	4.59	1.46	1.36
23	AN	608	CHL	CHD-C1D	4.58	1.47	1.38
23	AD	317	CHL	C2C-C3C	4.58	1.46	1.36
23	p	607	CHL	CHC-C1C	4.58	1.47	1.38
23	AC	606	CHL	C3D-C4D	-4.58	1.33	1.44
23	v	306	CHL	CHC-C1C	4.57	1.47	1.38
23	AU	607	CHL	O2A-CGA	4.57	1.46	1.33
23	AC	606	CHL	O2A-CGA	4.57	1.46	1.30
23	9	601	CHL	C2C-C3C	4.56	1.46	1.36
26	v	317	NEX	C14-C13	4.56	1.41	1.35
27	AB	613	XAT	C32-C33	4.56	1.55	1.45
23	AF	608	CHL	C2C-C3C	4.56	1.46	1.36
23	AQ	601	CHL	O2A-CGA	4.56	1.46	1.33
23	9	608	CHL	C3D-C4D	-4.56	1.33	1.44
23	9	606	CHL	CHD-C1D	4.56	1.47	1.38
23	AC	601	CHL	C2C-C3C	4.56	1.46	1.36
23	9	605	CHL	C2C-C3C	4.56	1.46	1.36
23	AR	613	CHL	C3D-C4D	-4.56	1.33	1.44
23	AS	306	CHL	CHC-C1C	4.55	1.47	1.38
23	AR	607	CHL	CHD-C1D	4.55	1.47	1.38
23	AD	308	CHL	C3D-C4D	-4.55	1.33	1.44
23	AQ	609	CHL	C3D-C4D	-4.55	1.33	1.44
27	AR	616	XAT	C28-C29	4.55	1.55	1.45
23	p	607	CHL	C2C-C3C	4.55	1.46	1.36
23	V	616	CHL	O2A-CGA	4.55	1.46	1.30
23	V	605	CHL	CHC-C1C	4.55	1.47	1.38
23	AB	608	CHL	C2C-C3C	4.55	1.46	1.36
23	AB	605	CHL	O2A-CGA	4.55	1.46	1.30
23	0	601	CHL	O2A-CGA	4.55	1.46	1.33
23	0	607	CHL	C3D-C4D	-4.55	1.33	1.44
23	AF	607	CHL	CHC-C1C	4.55	1.47	1.38
23	q	607	CHL	CHC-C1C	4.54	1.47	1.38
26	AE	615	NEX	C34-C33	4.54	1.41	1.35
23	AQ	607	CHL	C2C-C3C	4.54	1.46	1.36
23	AD	302	CHL	O2A-CGA	4.54	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AF	605	CHL	CHD-C1D	4.54	1.47	1.38
25	AD	314	LUT	C34-C33	4.53	1.41	1.35
23	AF	601	CHL	C2C-C3C	4.53	1.46	1.36
23	9	605	CHL	O2A-CGA	4.53	1.46	1.30
23	9	606	CHL	O2A-CGA	4.53	1.46	1.30
23	v	308	CHL	C3D-C4D	-4.53	1.33	1.44
23	q	607	CHL	C2C-C3C	4.53	1.46	1.36
23	V	616	CHL	C2C-C3C	4.53	1.46	1.36
23	AR	605	CHL	CHC-C1C	4.53	1.47	1.38
23	V	601	CHL	C3D-C4D	-4.53	1.34	1.44
23	AC	607	CHL	C3D-C4D	-4.53	1.34	1.44
23	AH	601	CHL	C3D-C4D	-4.53	1.34	1.44
23	AU	601	CHL	C3D-C4D	-4.53	1.34	1.44
23	AH	606	CHL	O2A-CGA	4.52	1.46	1.33
26	AA	616	NEX	C34-C33	4.52	1.41	1.35
23	V	605	CHL	C3D-C4D	-4.52	1.34	1.44
23	AA	617	CHL	O2A-CGA	4.52	1.45	1.30
23	AE	606	CHL	O2A-CGA	4.52	1.45	1.30
23	AB	601	CHL	O2A-CGA	4.52	1.45	1.30
23	AN	605	CHL	CHC-C1C	4.52	1.47	1.38
23	0	601	CHL	CHD-C1D	4.52	1.47	1.38
26	AC	616	NEX	C34-C33	4.51	1.41	1.35
23	AH	601	CHL	C2C-C3C	4.51	1.46	1.36
23	AN	617	CHL	O2A-CGA	4.51	1.45	1.30
23	AC	605	CHL	O2A-CGA	4.51	1.45	1.30
23	AA	607	CHL	O2A-CGA	4.51	1.45	1.30
23	AR	606	CHL	C2C-C3C	4.51	1.46	1.36
23	AN	605	CHL	C2C-C3C	4.51	1.46	1.36
23	AR	606	CHL	CHD-C1D	4.51	1.47	1.38
23	0	605	CHL	C3D-C4D	-4.51	1.34	1.44
23	AN	601	CHL	C3D-C4D	-4.51	1.34	1.44
23	AB	608	CHL	C3D-C4D	-4.51	1.34	1.44
23	q	606	CHL	C3D-C4D	-4.51	1.34	1.44
23	AN	605	CHL	C3D-C4D	-4.51	1.34	1.44
23	9	608	CHL	O2A-CGA	4.51	1.45	1.30
23	0	605	CHL	O2A-CGA	4.51	1.45	1.30
23	AE	616	CHL	C2C-C3C	4.51	1.46	1.36
23	AA	601	CHL	O2A-CGA	4.51	1.45	1.30
27	q	617	XAT	C28-C29	4.51	1.55	1.45
23	AU	606	CHL	C3D-C4D	-4.50	1.34	1.44
23	AF	601	CHL	O2A-CGA	4.50	1.45	1.30
23	AB	607	CHL	C3D-C4D	-4.50	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AC	605	CHL	C2C-C3C	4.50	1.46	1.36
23	q	607	CHL	C3D-C4D	-4.50	1.34	1.44
23	AB	601	CHL	C2C-C3C	4.50	1.46	1.36
23	AE	616	CHL	O2A-CGA	4.50	1.45	1.30
23	AC	601	CHL	O2A-CGA	4.50	1.45	1.30
23	AU	601	CHL	C2C-C3C	4.50	1.46	1.36
23	AS	302	CHL	C3D-C4D	-4.50	1.34	1.44
23	9	601	CHL	C3D-C4D	-4.49	1.34	1.44
23	p	609	CHL	C3D-C4D	-4.49	1.34	1.44
26	AE	615	NEX	C30-C29	4.49	1.41	1.35
23	V	608	CHL	C3D-C4D	-4.49	1.34	1.44
23	9	609	CHL	CHD-C1D	4.49	1.47	1.38
23	p	601	CHL	C3D-C4D	-4.49	1.34	1.44
23	0	617	CHL	CHD-C1D	4.49	1.47	1.38
23	AR	606	CHL	CHC-C1C	4.49	1.47	1.38
23	p	606	CHL	CHC-C1C	4.49	1.47	1.38
23	AQ	607	CHL	O2A-CGA	4.48	1.46	1.33
23	AC	607	CHL	O2A-CGA	4.48	1.45	1.30
23	AN	607	CHL	C3D-C4D	-4.48	1.34	1.44
23	AC	608	CHL	C2C-C3C	4.48	1.46	1.36
23	AQ	606	CHL	CHC-C1C	4.48	1.47	1.38
23	0	608	CHL	C2C-C3C	4.48	1.46	1.36
23	v	307	CHL	O2A-CGA	4.48	1.45	1.30
23	9	609	CHL	C2C-C3C	4.48	1.46	1.36
23	AE	606	CHL	C3D-C4D	-4.48	1.34	1.44
23	AN	605	CHL	O2A-CGA	4.48	1.46	1.33
23	AQ	601	CHL	C2C-C3C	4.48	1.46	1.36
23	AE	601	CHL	O2A-CGA	4.48	1.45	1.30
23	AD	307	CHL	C3D-C4D	-4.48	1.34	1.44
23	AN	601	CHL	O2A-CGA	4.48	1.46	1.33
23	AB	607	CHL	O2A-CGA	4.48	1.45	1.30
23	V	606	CHL	C2C-C3C	4.48	1.46	1.36
23	AQ	605	CHL	C2C-C3C	4.48	1.46	1.36
23	p	607	CHL	C3D-C4D	-4.48	1.34	1.44
23	AR	605	CHL	C3D-C4D	-4.47	1.34	1.44
23	V	608	CHL	C2C-C3C	4.47	1.46	1.36
26	v	317	NEX	C34-C33	4.47	1.41	1.35
23	v	302	CHL	C3D-C4D	-4.47	1.34	1.44
26	AR	615	NEX	C14-C13	4.47	1.41	1.35
23	9	605	CHL	C3D-C4D	-4.47	1.34	1.44
23	AU	607	CHL	C2C-C3C	4.47	1.46	1.36
23	V	601	CHL	O2A-CGA	4.47	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AB	606	CHL	O2A-CGA	4.47	1.45	1.30
23	AN	606	CHL	C2C-C3C	4.47	1.46	1.36
23	AQ	607	CHL	C3D-C4D	-4.47	1.34	1.44
23	p	605	CHL	C2C-C3C	4.47	1.46	1.36
23	AQ	606	CHL	O2A-CGA	4.47	1.46	1.33
23	AA	605	CHL	O2A-CGA	4.47	1.45	1.30
23	AB	606	CHL	C3D-C4D	-4.46	1.34	1.44
23	V	605	CHL	O2A-CGA	4.46	1.46	1.33
23	AE	601	CHL	C2C-C3C	4.46	1.46	1.36
23	AH	605	CHL	C2C-C3C	4.46	1.46	1.36
23	p	607	CHL	O2A-CGA	4.46	1.46	1.33
23	AH	607	CHL	C2C-C3C	4.46	1.46	1.36
23	9	609	CHL	C3D-C4D	-4.46	1.34	1.44
23	AB	605	CHL	CHD-C1D	4.46	1.47	1.38
23	AD	308	CHL	CHD-C1D	4.46	1.47	1.38
23	AS	306	CHL	CHD-C1D	4.46	1.47	1.38
24	AF	602	CLA	C1D-ND	4.46	1.43	1.37
23	V	607	CHL	C3D-C4D	-4.46	1.34	1.44
23	AB	608	CHL	O2A-CGA	4.45	1.45	1.30
23	p	606	CHL	O2A-CGA	4.45	1.46	1.33
23	AE	605	CHL	C2C-C3C	4.45	1.46	1.36
23	AQ	601	CHL	C3D-C4D	-4.45	1.34	1.44
23	AF	607	CHL	O2A-CGA	4.45	1.45	1.30
23	AA	607	CHL	C3D-C4D	-4.45	1.34	1.44
23	AC	605	CHL	C3D-C4D	-4.45	1.34	1.44
23	AS	308	CHL	C3D-C4D	-4.45	1.34	1.44
23	AD	302	CHL	C2C-C3C	4.45	1.46	1.36
23	AF	607	CHL	C3D-C4D	-4.45	1.34	1.44
23	AB	608	CHL	CHD-C1D	4.44	1.47	1.38
23	AS	307	CHL	C3D-C4D	-4.44	1.34	1.44
23	AC	601	CHL	C3D-C4D	-4.44	1.34	1.44
23	AR	607	CHL	C3D-C4D	-4.44	1.34	1.44
23	AU	607	CHL	C3D-C4D	-4.44	1.34	1.44
23	AB	601	CHL	C3D-C4D	-4.44	1.34	1.44
23	AQ	608	CHL	C3D-C4D	-4.44	1.34	1.44
23	AF	601	CHL	C3D-C4D	-4.43	1.34	1.44
27	AF	613	XAT	C12-C13	4.43	1.55	1.45
23	0	606	CHL	C3D-C4D	-4.43	1.34	1.44
23	q	605	CHL	C3D-C4D	-4.43	1.34	1.44
23	V	605	CHL	C2C-C3C	4.43	1.46	1.36
23	AD	307	CHL	O2A-CGA	4.43	1.45	1.30
23	AA	601	CHL	C3D-C4D	-4.43	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AN	607	CHL	O2A-CGA	4.43	1.46	1.33
23	V	608	CHL	CHD-C1D	4.43	1.47	1.38
23	AH	606	CHL	CHD-C1D	4.42	1.47	1.38
27	q	617	XAT	C32-C33	4.42	1.55	1.45
23	AU	605	CHL	C2C-C3C	4.42	1.46	1.36
23	AB	605	CHL	C3D-C4D	-4.42	1.34	1.44
23	AH	607	CHL	C3D-C4D	-4.42	1.34	1.44
23	AH	606	CHL	CHC-C1C	4.42	1.47	1.38
23	AE	607	CHL	C2C-C3C	4.42	1.46	1.36
23	AA	606	CHL	C3D-C4D	-4.42	1.34	1.44
23	AH	608	CHL	C3D-C4D	-4.42	1.34	1.44
23	AU	605	CHL	C3D-C4D	-4.42	1.34	1.44
23	0	606	CHL	CHC-C1C	4.42	1.47	1.38
23	AS	308	CHL	O2A-CGA	4.42	1.45	1.30
23	AE	607	CHL	C3D-C4D	-4.42	1.34	1.44
23	0	601	CHL	C3D-C4D	-4.42	1.34	1.44
23	AB	607	CHL	CHD-C1D	4.42	1.47	1.38
25	AD	314	LUT	C14-C13	4.42	1.41	1.35
23	AE	605	CHL	CHC-C1C	4.42	1.47	1.38
27	9	618	XAT	C32-C33	4.42	1.55	1.45
23	p	606	CHL	C3D-C4D	-4.42	1.34	1.44
23	0	607	CHL	O2A-CGA	4.42	1.45	1.30
23	0	617	CHL	O2A-CGA	4.41	1.45	1.30
23	q	605	CHL	CHC-C1C	4.41	1.47	1.38
23	AD	301	CHL	C2C-C3C	4.41	1.46	1.36
23	0	605	CHL	C2C-C3C	4.41	1.46	1.36
23	p	608	CHL	C3D-C4D	-4.41	1.34	1.44
23	AR	613	CHL	CHD-C1D	4.41	1.46	1.38
23	AU	608	CHL	C3D-C4D	-4.40	1.34	1.44
23	AA	601	CHL	C2C-C3C	4.40	1.46	1.36
23	AA	606	CHL	C2C-C3C	4.40	1.46	1.36
23	AD	306	CHL	C2C-C3C	4.40	1.46	1.36
23	AE	605	CHL	C3D-C4D	-4.40	1.34	1.44
26	AS	317	NEX	C34-C33	4.40	1.41	1.35
23	v	308	CHL	CHC-C1C	4.40	1.47	1.38
23	AN	617	CHL	C2C-C3C	4.40	1.46	1.36
23	q	607	CHL	CHD-C1D	4.40	1.46	1.38
23	9	607	CHL	C2C-C3C	4.39	1.46	1.36
23	v	307	CHL	C3D-C4D	-4.39	1.34	1.44
23	9	609	CHL	CHC-C1C	4.39	1.47	1.38
27	AR	616	XAT	C32-C33	4.39	1.55	1.45
25	AC	614	LUT	C34-C33	4.39	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	V	606	CHL	C3D-C4D	-4.39	1.34	1.44
23	AE	601	CHL	C3D-C4D	-4.39	1.34	1.44
23	AD	302	CHL	C3D-C4D	-4.39	1.34	1.44
23	q	605	CHL	C2C-C3C	4.39	1.46	1.36
23	AD	306	CHL	C3D-C4D	-4.39	1.34	1.44
23	p	601	CHL	C2C-C3C	4.39	1.46	1.36
23	AU	606	CHL	CHC-C1C	4.38	1.47	1.38
27	AR	616	XAT	C12-C13	4.38	1.55	1.45
23	AA	606	CHL	CHC-C1C	4.38	1.47	1.38
23	AN	606	CHL	C3D-C4D	-4.38	1.34	1.44
23	AH	605	CHL	C3D-C4D	-4.38	1.34	1.44
23	AQ	605	CHL	C3D-C4D	-4.38	1.34	1.44
23	AE	617	CHL	C2C-C3C	4.38	1.46	1.36
23	9	607	CHL	C3D-C4D	-4.38	1.34	1.44
26	AC	616	NEX	C10-C9	4.38	1.41	1.35
23	AE	617	CHL	C3D-C4D	-4.38	1.34	1.44
23	AQ	606	CHL	C3D-C4D	-4.38	1.34	1.44
23	AD	317	CHL	O2A-CGA	4.38	1.45	1.30
23	AC	608	CHL	CHC-C1C	4.38	1.47	1.38
23	V	601	CHL	C2C-C3C	4.37	1.46	1.36
23	AS	306	CHL	C3D-C4D	-4.37	1.38	1.46
23	0	605	CHL	CHC-C1C	4.37	1.47	1.38
23	AN	607	CHL	C2C-C3C	4.37	1.46	1.36
23	AQ	609	CHL	C2C-C3C	4.37	1.46	1.36
27	q	617	XAT	C12-C13	4.37	1.55	1.45
23	AA	607	CHL	CHC-C1C	4.37	1.47	1.38
23	AC	608	CHL	C3D-C4D	-4.37	1.34	1.44
23	p	605	CHL	C3D-C4D	-4.37	1.34	1.44
23	AA	605	CHL	C3D-C4D	-4.37	1.34	1.44
26	AC	616	NEX	C14-C13	4.36	1.41	1.35
23	AB	601	CHL	CHC-C1C	4.36	1.47	1.38
27	9	618	XAT	C12-C13	4.36	1.55	1.45
23	AE	605	CHL	O2A-CGA	4.36	1.46	1.33
23	AD	301	CHL	C3D-C4D	-4.36	1.34	1.44
23	AQ	606	CHL	C2C-C3C	4.36	1.46	1.36
23	AQ	608	CHL	C2C-C3C	4.36	1.46	1.36
23	AA	606	CHL	O2A-CGA	4.36	1.46	1.33
23	AA	608	CHL	O2A-CGA	4.36	1.46	1.33
26	AU	616	NEX	C34-C33	4.36	1.41	1.35
23	9	601	CHL	CHC-C1C	4.36	1.47	1.38
23	9	605	CHL	CHC-C1C	4.35	1.47	1.38
23	AE	605	CHL	CHD-C1D	4.35	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	V	607	CHL	CHD-C1D	4.35	1.46	1.38
23	V	607	CHL	CHC-C1C	4.35	1.47	1.38
23	V	607	CHL	O2A-CGA	4.35	1.46	1.33
23	AN	601	CHL	C2C-C3C	4.35	1.46	1.36
23	q	606	CHL	CHD-C1D	4.35	1.46	1.38
23	AD	301	CHL	O2A-CGA	4.35	1.46	1.33
23	0	608	CHL	CHD-C1D	4.35	1.46	1.38
23	AE	607	CHL	CHD-C1D	4.34	1.46	1.38
26	AR	615	NEX	C34-C33	4.34	1.41	1.35
23	AS	308	CHL	CHC-C1C	4.34	1.47	1.38
23	0	606	CHL	CHD-C1D	4.34	1.46	1.38
23	AN	607	CHL	CHD-C1D	4.34	1.46	1.38
25	AA	615	LUT	C14-C13	4.34	1.41	1.35
23	0	601	CHL	CHC-C1C	4.34	1.47	1.38
23	AU	607	CHL	CHC-C1C	4.34	1.47	1.38
23	p	606	CHL	C2C-C3C	4.34	1.46	1.36
23	V	608	CHL	CHC-C1C	4.33	1.47	1.38
23	AB	606	CHL	CHC-C1C	4.33	1.47	1.38
23	AU	608	CHL	CHC-C1C	4.33	1.47	1.38
23	AE	617	CHL	CHC-C1C	4.33	1.47	1.38
23	q	606	CHL	CHC-C1C	4.33	1.47	1.38
25	AD	314	LUT	C30-C29	4.33	1.41	1.35
27	AB	613	XAT	C12-C13	4.32	1.55	1.45
23	AC	607	CHL	CHC-C1C	4.32	1.47	1.38
23	p	608	CHL	C2C-C3C	4.32	1.46	1.36
23	9	608	CHL	CHC-C1C	4.32	1.47	1.38
23	AH	607	CHL	CHC-C1C	4.32	1.47	1.38
23	AU	606	CHL	O2A-CGA	4.32	1.46	1.33
26	AU	616	NEX	C14-C13	4.31	1.41	1.35
23	AQ	608	CHL	CHC-C1C	4.31	1.47	1.38
23	v	308	CHL	CHD-C1D	4.31	1.46	1.38
26	q	615	NEX	C14-C13	4.31	1.41	1.35
23	AC	606	CHL	CHD-C1D	4.31	1.46	1.38
23	AS	308	CHL	CHD-C1D	4.31	1.46	1.38
23	AC	605	CHL	CHC-C1C	4.31	1.47	1.38
23	p	609	CHL	C2C-C3C	4.31	1.46	1.36
23	AC	601	CHL	CHC-C1C	4.30	1.47	1.38
26	AA	616	NEX	C30-C29	4.30	1.41	1.35
23	v	306	CHL	CHD-C1D	4.30	1.46	1.38
23	AU	601	CHL	CHD-C1D	4.30	1.46	1.38
27	AF	613	XAT	C32-C33	4.29	1.55	1.45
26	AS	317	NEX	C14-C13	4.29	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AH	608	CHL	C2C-C3C	4.29	1.46	1.36
23	AS	302	CHL	CHD-C1D	4.29	1.46	1.38
23	AA	601	CHL	CHC-C1C	4.29	1.47	1.38
23	AQ	609	CHL	O2A-CGA	4.29	1.45	1.33
23	AF	601	CHL	CHC-C1C	4.29	1.47	1.38
26	p	616	NEX	C14-C13	4.29	1.41	1.35
23	p	609	CHL	O2A-CGA	4.29	1.45	1.33
23	AH	608	CHL	CHC-C1C	4.29	1.47	1.38
26	q	615	NEX	C34-C33	4.29	1.41	1.35
23	AR	606	CHL	C3D-C4D	-4.29	1.34	1.44
23	AA	607	CHL	C2C-C3C	4.29	1.45	1.36
23	AN	607	CHL	CHC-C1C	4.29	1.47	1.38
23	AQ	609	CHL	CHD-C1D	4.29	1.46	1.38
23	9	607	CHL	O2A-CGA	4.28	1.45	1.33
24	O	608	CLA	C1D-ND	4.28	1.43	1.37
23	AN	608	CHL	O2A-CGA	4.28	1.45	1.33
23	v	302	CHL	CHD-C1D	4.28	1.46	1.38
23	p	605	CHL	O2A-CGA	4.28	1.45	1.33
23	p	605	CHL	CHC-C1C	4.28	1.47	1.38
23	AU	608	CHL	C2C-C3C	4.28	1.45	1.36
23	AD	301	CHL	CHC-C1C	4.28	1.47	1.38
23	V	608	CHL	O2A-CGA	4.28	1.45	1.33
23	AD	307	CHL	C2C-C3C	4.27	1.45	1.36
23	AQ	605	CHL	CHC-C1C	4.27	1.47	1.38
23	0	606	CHL	O2A-CGA	4.27	1.45	1.33
23	AD	317	CHL	C3D-C4D	-4.27	1.34	1.44
23	p	609	CHL	CHD-C1D	4.27	1.46	1.38
23	AE	606	CHL	CHC-C1C	4.27	1.47	1.38
23	AQ	609	CHL	CHC-C1C	4.26	1.47	1.38
23	AU	606	CHL	CHD-C1D	4.26	1.46	1.38
23	p	608	CHL	CHC-C1C	4.26	1.47	1.38
23	AC	608	CHL	CHD-C1D	4.26	1.46	1.38
23	v	307	CHL	C2C-C3C	4.26	1.45	1.36
23	v	302	CHL	CHC-C1C	4.26	1.47	1.38
23	p	609	CHL	CHC-C1C	4.26	1.47	1.38
23	AR	605	CHL	CHD-C1D	4.25	1.46	1.38
23	AU	605	CHL	CHC-C1C	4.25	1.47	1.38
23	AA	601	CHL	CHD-C1D	4.25	1.46	1.38
23	AH	605	CHL	CHC-C1C	4.25	1.47	1.38
26	9	617	NEX	C14-C13	4.25	1.41	1.35
25	AA	615	LUT	C30-C29	4.25	1.41	1.35
23	AB	606	CHL	CHD-C1D	4.25	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AD	308	CHL	O2A-CGA	4.25	1.45	1.33
25	AD	314	LUT	C10-C9	4.25	1.41	1.35
26	AU	616	NEX	C30-C29	4.25	1.41	1.35
23	AC	605	CHL	CHD-C1D	4.25	1.46	1.38
23	AD	302	CHL	CHC-C1C	4.25	1.47	1.38
25	AA	615	LUT	C34-C33	4.25	1.41	1.35
23	AD	302	CHL	CHD-C1D	4.24	1.46	1.38
23	AD	306	CHL	O2A-CGA	4.24	1.45	1.33
23	AQ	605	CHL	O2A-CGA	4.24	1.45	1.33
23	AF	606	CHL	C2C-C1C	4.24	1.48	1.42
23	AH	601	CHL	CHD-C1D	4.24	1.46	1.38
23	AH	608	CHL	CHD-C1D	4.24	1.46	1.38
23	p	601	CHL	CHC-C1C	4.24	1.47	1.38
23	AU	607	CHL	CHD-C1D	4.24	1.46	1.38
23	AA	605	CHL	C2C-C3C	4.23	1.45	1.36
25	0	614	LUT	C14-C13	4.23	1.41	1.35
23	AS	302	CHL	CHC-C1C	4.23	1.47	1.38
23	AE	607	CHL	CHC-C1C	4.23	1.47	1.38
23	AE	606	CHL	C2C-C3C	4.23	1.45	1.36
25	0	614	LUT	C34-C33	4.23	1.41	1.35
23	AR	607	CHL	O2A-CGA	4.23	1.45	1.33
23	AA	605	CHL	CHC-C1C	4.23	1.47	1.38
26	9	617	NEX	C34-C33	4.23	1.41	1.35
23	AH	607	CHL	CHD-C1D	4.23	1.46	1.38
23	v	306	CHL	C2C-C1C	4.22	1.48	1.42
23	q	607	CHL	O2A-CGA	4.22	1.45	1.33
23	AH	605	CHL	O2A-CGA	4.22	1.45	1.33
23	AN	608	CHL	C2C-C3C	4.22	1.45	1.36
26	AC	616	NEX	C30-C29	4.22	1.41	1.35
23	AF	606	CHL	C1B-C2B	4.22	1.48	1.41
23	p	608	CHL	CHD-C1D	4.22	1.46	1.38
23	AD	308	CHL	CHC-C1C	4.21	1.47	1.38
23	AC	608	CHL	O2A-CGA	4.21	1.45	1.33
23	p	601	CHL	CHD-C1D	4.21	1.46	1.38
23	AN	606	CHL	CHC-C1C	4.21	1.47	1.38
23	AU	605	CHL	O2A-CGA	4.21	1.45	1.33
23	AB	601	CHL	CHD-C1D	4.21	1.46	1.38
23	AQ	601	CHL	CHD-C1D	4.21	1.46	1.38
23	AU	608	CHL	CHD-C1D	4.21	1.46	1.38
23	q	606	CHL	C2C-C1C	4.21	1.48	1.42
23	p	605	CHL	CHD-C1D	4.21	1.46	1.38
23	AS	306	CHL	C2C-C1C	4.20	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AF	601	CHL	CHD-C1D	4.20	1.46	1.38
23	AU	601	CHL	CHC-C1C	4.20	1.47	1.38
23	V	601	CHL	CHD-C1D	4.20	1.46	1.38
26	AR	615	NEX	C30-C29	4.20	1.41	1.35
23	AH	601	CHL	CHC-C1C	4.20	1.47	1.38
23	AQ	608	CHL	CHD-C1D	4.20	1.46	1.38
23	AQ	605	CHL	CHD-C1D	4.20	1.46	1.38
23	9	609	CHL	O2A-CGA	4.20	1.45	1.33
23	AE	606	CHL	CHD-C1D	4.20	1.46	1.38
23	AD	301	CHL	CHD-C1D	4.19	1.46	1.38
25	9	615	LUT	C34-C33	4.19	1.41	1.35
23	q	605	CHL	CHD-C1D	4.19	1.46	1.38
23	AC	606	CHL	CHC-C1C	4.19	1.47	1.38
25	AC	614	LUT	C14-C13	4.19	1.41	1.35
23	AQ	601	CHL	CHC-C1C	4.19	1.47	1.38
23	AQ	608	CHL	O2A-CGA	4.19	1.45	1.33
23	9	607	CHL	CHC-C1C	4.19	1.47	1.38
23	AN	601	CHL	CHD-C1D	4.19	1.46	1.38
23	0	607	CHL	CHC-C1C	4.19	1.46	1.38
23	AE	601	CHL	CHC-C1C	4.19	1.47	1.38
23	0	607	CHL	CHD-C1D	4.18	1.46	1.38
23	9	608	CHL	CHD-C1D	4.18	1.46	1.38
23	9	607	CHL	CHD-C1D	4.18	1.46	1.38
26	9	617	NEX	C30-C29	4.18	1.41	1.35
25	AD	315	LUT	C10-C9	4.18	1.41	1.35
23	AU	608	CHL	O2A-CGA	4.18	1.45	1.33
23	AE	607	CHL	O2A-CGA	4.18	1.45	1.33
23	p	607	CHL	CHD-C1D	4.17	1.46	1.38
23	AE	601	CHL	CHD-C1D	4.17	1.46	1.38
23	v	302	CHL	C1B-C2B	4.17	1.48	1.41
23	AC	607	CHL	CHD-C1D	4.17	1.46	1.38
26	AS	317	NEX	C30-C29	4.17	1.41	1.35
23	V	606	CHL	CHC-C1C	4.17	1.47	1.38
23	AC	601	CHL	C1B-C2B	4.17	1.48	1.41
24	O	608	CLA	C4B-NB	4.17	1.42	1.37
23	AA	607	CHL	CHD-C1D	4.16	1.46	1.38
23	q	605	CHL	O2A-CGA	4.16	1.45	1.33
23	p	608	CHL	O2A-CGA	4.16	1.45	1.33
23	AS	302	CHL	C1B-C2B	4.16	1.48	1.41
23	AD	306	CHL	CHC-C1C	4.16	1.47	1.38
23	0	617	CHL	C3D-C4D	-4.16	1.34	1.44
23	AH	608	CHL	O2A-CGA	4.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AR	605	CHL	C2C-C1C	4.16	1.48	1.42
23	V	616	CHL	C3D-C4D	-4.15	1.34	1.44
23	V	606	CHL	CHD-C1D	4.15	1.46	1.38
23	AD	307	CHL	CHC-C1C	4.15	1.47	1.38
23	p	606	CHL	CHD-C1D	4.15	1.46	1.38
23	AF	606	CHL	OBD-CAD	4.15	1.28	1.21
23	9	605	CHL	CHD-C1D	4.15	1.46	1.38
23	AQ	607	CHL	CHD-C1D	4.15	1.46	1.38
25	AC	614	LUT	C30-C29	4.15	1.41	1.35
32	J	405	PHO	C1D-C2D	4.14	1.44	1.39
26	v	317	NEX	C30-C29	4.14	1.41	1.35
25	0	614	LUT	C10-C9	4.13	1.41	1.35
23	AS	307	CHL	C2C-C3C	4.13	1.45	1.36
23	AD	306	CHL	CHD-C1D	4.13	1.46	1.38
23	AA	605	CHL	CHD-C1D	4.13	1.46	1.38
23	AQ	606	CHL	CHD-C1D	4.13	1.46	1.38
23	AN	601	CHL	CHC-C1C	4.13	1.46	1.38
23	AA	617	CHL	CHC-C1C	4.13	1.46	1.38
23	AS	307	CHL	CHC-C1C	4.12	1.46	1.38
23	v	307	CHL	CHC-C1C	4.12	1.46	1.38
23	V	601	CHL	CHC-C1C	4.12	1.46	1.38
25	AD	315	LUT	C14-C13	4.12	1.41	1.35
23	V	605	CHL	CHD-C1D	4.12	1.46	1.38
25	9	616	LUT	C14-C13	4.12	1.41	1.35
25	0	614	LUT	C30-C29	4.12	1.41	1.35
25	AH	614	LUT	C34-C33	4.12	1.41	1.35
23	AA	617	CHL	C3D-C4D	-4.12	1.34	1.44
23	AA	608	CHL	CHC-C4B	4.12	1.48	1.39
25	9	615	LUT	C14-C13	4.11	1.41	1.35
23	v	307	CHL	CHD-C1D	4.11	1.46	1.38
26	AQ	617	NEX	C34-C33	4.10	1.41	1.35
23	AN	606	CHL	CHD-C1D	4.10	1.46	1.38
23	V	607	CHL	C1B-C2B	4.10	1.48	1.41
23	AR	605	CHL	O2A-CGA	4.10	1.45	1.33
25	AC	615	LUT	C10-C9	4.10	1.41	1.35
25	v	315	LUT	C30-C29	4.09	1.41	1.35
23	AS	307	CHL	CHD-C1D	4.09	1.46	1.38
25	AU	614	LUT	C10-C9	4.09	1.41	1.35
26	AQ	617	NEX	C14-C13	4.09	1.41	1.35
26	q	615	NEX	C30-C29	4.09	1.41	1.35
23	AF	608	CHL	CHD-C4C	4.09	1.48	1.39
23	9	601	CHL	CHD-C1D	4.09	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	q	613	CHL	CHD-C4C	4.08	1.48	1.39
23	AN	605	CHL	CHD-C1D	4.08	1.46	1.38
25	AE	614	LUT	C14-C13	4.08	1.41	1.35
23	AE	616	CHL	C3D-C4D	-4.08	1.35	1.44
23	AA	617	CHL	CHD-C4C	4.08	1.48	1.39
23	AU	605	CHL	CHD-C1D	4.08	1.46	1.38
23	AB	606	CHL	C2C-C1C	4.07	1.48	1.42
23	AC	607	CHL	C2C-C1C	4.07	1.48	1.42
26	AQ	617	NEX	C30-C29	4.07	1.41	1.35
23	9	608	CHL	C2C-C1C	4.07	1.48	1.42
25	AS	315	LUT	C30-C29	4.07	1.41	1.35
32	AJ	407	PHO	C1D-C2D	4.07	1.44	1.39
25	AH	614	LUT	C10-C9	4.07	1.41	1.35
23	AA	608	CHL	CHB-C1B	4.06	1.49	1.41
23	AH	605	CHL	CHD-C1D	4.06	1.46	1.38
25	V	613	LUT	C34-C33	4.06	1.41	1.35
25	AD	315	LUT	C34-C33	4.06	1.41	1.35
26	p	616	NEX	C34-C33	4.05	1.41	1.35
24	AK	612	CLA	C1D-ND	4.05	1.42	1.37
23	9	606	CHL	CHD-C4C	4.05	1.48	1.39
25	v	316	LUT	C30-C29	4.05	1.41	1.35
23	0	605	CHL	CHD-C1D	4.05	1.46	1.38
25	AR	614	LUT	C10-C9	4.05	1.41	1.35
23	AN	617	CHL	C3D-C4D	-4.05	1.35	1.44
25	AU	614	LUT	C34-C33	4.05	1.41	1.35
25	AC	615	LUT	C14-C13	4.05	1.41	1.35
25	AU	614	LUT	C14-C13	4.04	1.41	1.35
25	9	616	LUT	C30-C29	4.04	1.41	1.35
24	O	605	CLA	C1D-ND	4.04	1.42	1.37
25	v	316	LUT	C10-C9	4.04	1.41	1.35
24	AR	617	CLA	C4B-NB	4.03	1.42	1.37
25	AD	315	LUT	C30-C29	4.03	1.41	1.35
23	9	601	CHL	C1B-C2B	4.03	1.48	1.41
25	9	616	LUT	C10-C9	4.02	1.41	1.35
24	AF	610	CLA	C1D-ND	4.02	1.42	1.37
25	9	615	LUT	C10-C9	4.02	1.41	1.35
25	AU	614	LUT	C30-C29	4.02	1.41	1.35
24	AB	602	CLA	C1D-ND	4.02	1.42	1.37
23	0	617	CHL	CHC-C1C	4.02	1.46	1.38
23	AF	607	CHL	CHD-C4C	4.02	1.48	1.39
24	0	603	CLA	C1D-ND	4.02	1.42	1.37
25	AE	614	LUT	C10-C9	4.02	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	v	316	LUT	C14-C13	4.02	1.41	1.35
23	AB	607	CHL	CHD-C4C	4.02	1.48	1.39
23	AA	606	CHL	CHD-C1D	4.02	1.46	1.38
25	AH	614	LUT	C30-C29	4.02	1.41	1.35
23	AC	601	CHL	CHD-C1D	4.01	1.46	1.38
32	J	406	PHO	C1D-C2D	4.01	1.44	1.39
24	p	610	CLA	C1D-ND	4.00	1.42	1.37
25	9	616	LUT	C34-C33	4.00	1.41	1.35
24	AB	611	CLA	C1D-ND	4.00	1.42	1.37
25	v	315	LUT	C10-C9	4.00	1.41	1.35
23	AD	317	CHL	CHC-C1C	4.00	1.46	1.38
25	AS	315	LUT	C10-C9	4.00	1.41	1.35
25	0	615	LUT	C14-C13	4.00	1.41	1.35
24	O	610	CLA	C1D-ND	3.99	1.42	1.37
25	AQ	615	LUT	C10-C9	3.99	1.41	1.35
23	AD	317	CHL	CHD-C4C	3.99	1.48	1.39
25	AE	614	LUT	C34-C33	3.99	1.41	1.35
25	p	614	LUT	C14-C13	3.99	1.41	1.35
23	AB	608	CHL	CHD-C4C	3.99	1.48	1.39
23	AB	605	CHL	CHD-C4C	3.99	1.48	1.39
24	AK	607	CLA	C1D-ND	3.99	1.42	1.37
24	AK	610	CLA	C1D-ND	3.98	1.42	1.37
24	AK	608	CLA	C1D-ND	3.98	1.42	1.37
25	0	615	LUT	C30-C29	3.98	1.41	1.35
25	9	615	LUT	C30-C29	3.98	1.41	1.35
25	AH	614	LUT	C14-C13	3.98	1.41	1.35
23	AR	607	CHL	CHD-C4C	3.98	1.48	1.39
25	v	316	LUT	C34-C33	3.98	1.41	1.35
25	v	315	LUT	C34-C33	3.97	1.41	1.35
25	AS	316	LUT	C10-C9	3.97	1.41	1.35
25	AC	615	LUT	C34-C33	3.97	1.41	1.35
24	AK	610	CLA	C4B-NB	3.97	1.42	1.37
25	AQ	615	LUT	C14-C13	3.97	1.41	1.35
24	p	618	CLA	C1D-ND	3.97	1.42	1.37
23	AE	616	CHL	CHD-C4C	3.97	1.48	1.39
23	AB	605	CHL	C2C-C3C	3.96	1.47	1.36
24	9	602	CLA	C1D-ND	3.96	1.42	1.37
23	AD	307	CHL	CHD-C1D	3.96	1.46	1.38
32	AJ	408	PHO	C1D-C2D	3.96	1.44	1.39
23	V	608	CHL	CHD-C4C	3.96	1.48	1.39
24	AK	617	CLA	C1D-ND	3.96	1.42	1.37
24	AC	610	CLA	C1D-ND	3.96	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AS	316	LUT	C30-C29	3.95	1.41	1.35
24	AC	602	CLA	C1D-ND	3.95	1.42	1.37
24	AC	609	CLA	C1D-ND	3.95	1.42	1.37
24	AQ	611	CLA	C1D-ND	3.95	1.42	1.37
23	V	616	CHL	CHD-C4C	3.94	1.48	1.39
25	p	614	LUT	C10-C9	3.94	1.41	1.35
24	9	613	CLA	C1D-ND	3.94	1.42	1.37
24	AK	603	CLA	C1D-ND	3.94	1.42	1.37
25	p	614	LUT	C34-C33	3.94	1.41	1.35
24	O	601	CLA	C1D-ND	3.94	1.42	1.37
25	p	614	LUT	C30-C29	3.94	1.41	1.35
25	0	615	LUT	C10-C9	3.94	1.41	1.35
25	AQ	615	LUT	C30-C29	3.94	1.41	1.35
24	0	613	CLA	C1D-ND	3.94	1.42	1.37
24	AU	610	CLA	C1D-ND	3.94	1.42	1.37
25	V	614	LUT	C34-C33	3.94	1.41	1.35
26	p	616	NEX	C30-C29	3.94	1.41	1.35
25	AC	614	LUT	C10-C9	3.93	1.41	1.35
27	AB	613	XAT	C35-C34	3.93	1.55	1.43
25	AH	615	LUT	C14-C13	3.93	1.41	1.35
25	v	315	LUT	C14-C13	3.93	1.41	1.35
23	AF	606	CHL	C4D-ND	3.92	1.39	1.34
23	AS	308	CHL	CHD-C4C	3.92	1.48	1.39
25	AA	615	LUT	C10-C9	3.92	1.41	1.35
25	V	614	LUT	C30-C29	3.92	1.41	1.35
23	q	607	CHL	CHD-C4C	3.92	1.48	1.39
24	Q	404	CLA	C1D-ND	3.92	1.42	1.37
24	q	601	CLA	C1D-ND	3.92	1.42	1.37
24	AA	613	CLA	C1D-ND	3.92	1.42	1.37
24	P	501	CLA	C1D-ND	3.92	1.42	1.37
23	AH	606	CHL	CHD-C4C	3.92	1.48	1.39
23	AD	308	CHL	CHD-C4C	3.92	1.48	1.39
24	O	615	CLA	C1D-ND	3.92	1.42	1.37
25	V	614	LUT	C14-C13	3.91	1.41	1.35
25	AN	615	LUT	C34-C33	3.91	1.41	1.35
25	AU	615	LUT	C14-C13	3.91	1.41	1.35
23	V	607	CHL	CHD-C4C	3.91	1.48	1.39
25	AQ	615	LUT	C34-C33	3.90	1.41	1.35
25	0	615	LUT	C34-C33	3.90	1.41	1.35
24	p	613	CLA	C1D-ND	3.90	1.42	1.37
24	AH	613	CLA	C1D-ND	3.90	1.42	1.37
23	0	617	CHL	CHD-C4C	3.90	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AH	615	LUT	C30-C29	3.90	1.41	1.35
25	AH	615	LUT	C10-C9	3.90	1.41	1.35
23	0	601	CHL	CHD-C4C	3.90	1.48	1.39
23	AF	608	CHL	CHC-C4B	3.90	1.48	1.39
25	AC	615	LUT	C30-C29	3.89	1.40	1.35
25	AU	615	LUT	C34-C33	3.89	1.40	1.35
24	AU	603	CLA	C1D-ND	3.89	1.42	1.37
24	K	101	CLA	C1D-ND	3.89	1.42	1.37
24	AH	610	CLA	C1D-ND	3.89	1.42	1.37
24	AA	612	CLA	C1D-ND	3.89	1.42	1.37
23	AR	613	CHL	CHD-C4C	3.89	1.48	1.39
24	AQ	614	CLA	C1D-ND	3.88	1.42	1.37
24	AR	601	CLA	C1D-ND	3.88	1.42	1.37
24	p	602	CLA	C1D-ND	3.88	1.42	1.37
25	AS	315	LUT	C14-C13	3.88	1.40	1.35
25	AH	615	LUT	C34-C33	3.88	1.40	1.35
23	v	308	CHL	C3A-C2A	-3.88	1.50	1.54
24	AM	404	CLA	C1D-ND	3.88	1.42	1.37
24	0	610	CLA	C1D-ND	3.88	1.42	1.37
24	AE	612	CLA	C1D-ND	3.88	1.42	1.37
24	AL	502	CLA	C1D-ND	3.88	1.42	1.37
27	AB	613	XAT	C31-C30	3.88	1.55	1.43
25	q	614	LUT	C10-C9	3.87	1.40	1.35
24	AL	513	CLA	C1D-ND	3.87	1.42	1.37
23	0	608	CHL	CHD-C4C	3.87	1.48	1.39
23	AF	605	CHL	CHC-C4B	3.87	1.48	1.39
24	AE	611	CLA	C1D-ND	3.87	1.42	1.37
24	AU	613	CLA	C1D-ND	3.87	1.42	1.37
23	AR	606	CHL	OBD-CAD	3.87	1.29	1.22
27	AB	613	XAT	C11-C10	3.87	1.55	1.43
24	AJ	406	CLA	C1D-ND	3.87	1.42	1.37
27	AF	613	XAT	C11-C10	3.87	1.55	1.43
24	V	610	CLA	C1D-ND	3.87	1.42	1.37
25	q	614	LUT	C30-C29	3.87	1.40	1.35
24	v	311	CLA	C1D-ND	3.87	1.42	1.37
24	AN	610	CLA	C1D-ND	3.87	1.42	1.37
24	AQ	612	CLA	C1D-ND	3.87	1.42	1.37
25	V	614	LUT	C10-C9	3.86	1.40	1.35
23	AB	607	CHL	CHC-C4B	3.86	1.48	1.39
24	q	612	CLA	C3D-CAD	-3.86	1.45	1.51
25	AS	315	LUT	C34-C33	3.86	1.40	1.35
25	AU	615	LUT	C10-C9	3.86	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	613	CLA	C1D-ND	3.86	1.42	1.37
24	9	610	CLA	C1D-ND	3.86	1.42	1.37
24	9	614	CLA	C1D-ND	3.86	1.42	1.37
24	AL	505	CLA	C1D-ND	3.86	1.42	1.37
24	AU	611	CLA	C1D-ND	3.86	1.42	1.37
24	AF	603	CLA	C1D-ND	3.86	1.42	1.37
24	AE	608	CLA	C1D-ND	3.86	1.42	1.37
23	AS	308	CHL	C2C-C3C	3.85	1.47	1.36
24	v	314	CLA	C1D-ND	3.85	1.42	1.37
25	AN	615	LUT	C14-C13	3.85	1.40	1.35
24	0	612	CLA	C1D-ND	3.85	1.42	1.37
23	AE	605	CHL	CHD-C4C	3.85	1.48	1.39
24	AL	514	CLA	C1D-ND	3.85	1.42	1.37
23	AH	601	CHL	CHD-C4C	3.85	1.48	1.39
24	P	504	CLA	C1D-ND	3.85	1.42	1.37
24	AH	611	CLA	C1D-ND	3.85	1.42	1.37
24	v	312	CLA	C1D-ND	3.85	1.42	1.37
24	AH	603	CLA	C1D-ND	3.85	1.42	1.37
24	AA	602	CLA	C1D-ND	3.85	1.42	1.37
24	O	611	CLA	C1D-ND	3.85	1.42	1.37
24	Q	401	CLA	C1D-ND	3.85	1.42	1.37
23	q	613	CHL	OBD-CAD	3.84	1.29	1.22
24	AN	612	CLA	C1D-ND	3.84	1.42	1.37
27	q	617	XAT	C11-C10	3.84	1.55	1.43
25	AU	615	LUT	C30-C29	3.84	1.40	1.35
24	AD	312	CLA	C1D-ND	3.84	1.42	1.37
24	P	511	CLA	C1D-ND	3.84	1.42	1.37
23	AE	616	CHL	CHC-C1C	3.84	1.46	1.38
24	AE	610	CLA	C1D-ND	3.84	1.42	1.37
24	AD	313	CLA	C1D-ND	3.84	1.42	1.37
24	v	303	CLA	C1D-ND	3.84	1.42	1.37
23	AU	601	CHL	CHD-C4C	3.84	1.48	1.39
24	P	512	CLA	C1D-ND	3.84	1.42	1.37
24	AF	604	CLA	C1D-ND	3.83	1.42	1.37
23	AR	606	CHL	CHD-C4C	3.83	1.48	1.39
24	AN	613	CLA	C1D-ND	3.83	1.42	1.37
25	AN	615	LUT	C30-C29	3.83	1.40	1.35
23	9	609	CHL	CHD-C4C	3.83	1.48	1.39
23	v	302	CHL	CHD-C4C	3.83	1.48	1.39
23	AE	606	CHL	CHD-C4C	3.83	1.48	1.39
27	AR	616	XAT	C11-C10	3.83	1.55	1.43
24	AS	303	CLA	C1D-ND	3.83	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AH	602	CLA	C1D-ND	3.83	1.42	1.37
24	AR	604	CLA	C1D-ND	3.83	1.42	1.37
23	AS	302	CHL	CHD-C4C	3.83	1.48	1.39
24	J	407	CLA	C1D-ND	3.83	1.42	1.37
24	P	510	CLA	C1D-ND	3.83	1.42	1.37
23	V	607	CHL	C2C-C3C	3.83	1.47	1.36
24	9	611	CLA	C1D-ND	3.83	1.42	1.37
24	AL	504	CLA	C1D-ND	3.82	1.42	1.37
27	9	618	XAT	C31-C30	3.82	1.55	1.43
24	AL	512	CLA	C1D-ND	3.82	1.42	1.37
25	AS	316	LUT	C34-C33	3.82	1.40	1.35
27	q	617	XAT	C35-C34	3.82	1.55	1.43
24	AA	611	CLA	C1D-ND	3.82	1.42	1.37
24	AF	603	CLA	C4B-NB	3.82	1.42	1.37
23	AQ	609	CHL	CHD-C4C	3.82	1.48	1.39
24	AN	603	CLA	C1D-ND	3.82	1.42	1.37
24	AQ	610	CLA	C1D-ND	3.82	1.42	1.37
23	AC	601	CHL	CHD-C4C	3.82	1.47	1.39
24	V	603	CLA	C1D-ND	3.82	1.42	1.37
27	AB	613	XAT	C15-C14	3.82	1.55	1.43
24	q	608	CLA	C1D-ND	3.82	1.42	1.37
25	p	615	LUT	C30-C29	3.82	1.40	1.35
23	AB	607	CHL	CHB-C1B	3.82	1.48	1.39
24	AD	310	CLA	C1D-ND	3.82	1.42	1.37
24	AE	602	CLA	C1D-ND	3.82	1.42	1.37
24	AS	309	CLA	C1D-ND	3.81	1.42	1.37
23	AA	601	CHL	CHD-C4C	3.81	1.47	1.39
27	AR	616	XAT	C31-C30	3.81	1.55	1.43
23	AD	302	CHL	CHD-C4C	3.81	1.47	1.39
27	9	618	XAT	C11-C10	3.81	1.55	1.43
24	AS	312	CLA	C1D-ND	3.81	1.42	1.37
23	AR	613	CHL	OBD-CAD	3.81	1.29	1.22
24	J	404	CLA	C1D-ND	3.81	1.42	1.37
24	O	603	CLA	C1D-ND	3.81	1.42	1.37
23	AN	617	CHL	CHD-C4C	3.81	1.47	1.39
24	J	403	CLA	C1D-ND	3.81	1.42	1.37
24	AJ	409	CLA	C1D-ND	3.81	1.42	1.37
24	AS	314	CLA	C1D-ND	3.81	1.42	1.37
24	q	610	CLA	C1D-ND	3.81	1.42	1.37
24	AH	612	CLA	C1D-ND	3.81	1.42	1.37
25	AS	316	LUT	C14-C13	3.81	1.40	1.35
24	v	305	CLA	C1D-ND	3.80	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AJ	405	CLA	C1D-ND	3.80	1.42	1.37
27	q	617	XAT	C31-C30	3.80	1.55	1.43
23	p	609	CHL	CHD-C4C	3.80	1.47	1.39
24	AN	611	CLA	C1D-ND	3.80	1.42	1.37
24	AR	602	CLA	C1D-ND	3.80	1.42	1.37
24	AA	609	CLA	C1D-ND	3.80	1.42	1.37
23	AN	617	CHL	CHC-C1C	3.80	1.46	1.38
23	AB	601	CHL	OBD-CAD	3.80	1.29	1.22
23	q	605	CHL	CHD-C4C	3.80	1.47	1.39
24	P	508	CLA	C1D-ND	3.80	1.42	1.37
24	AK	604	CLA	C1D-ND	3.80	1.42	1.37
23	AH	608	CHL	CHD-C4C	3.80	1.47	1.39
25	V	613	LUT	C10-C9	3.79	1.40	1.35
23	AB	601	CHL	CHD-C4C	3.79	1.47	1.39
24	AJ	404	CLA	C1D-ND	3.79	1.42	1.37
24	O	607	CLA	C1D-ND	3.79	1.42	1.37
24	v	304	CLA	C1D-ND	3.79	1.42	1.37
24	AR	610	CLA	C1D-ND	3.79	1.42	1.37
23	9	601	CHL	CHD-C4C	3.79	1.47	1.39
24	q	602	CLA	C1D-ND	3.79	1.42	1.37
23	p	607	CHL	CHD-C4C	3.79	1.47	1.39
27	AR	616	XAT	C35-C34	3.79	1.55	1.43
25	AR	614	LUT	C30-C29	3.79	1.40	1.35
23	AE	616	CHL	OBD-CAD	3.79	1.29	1.22
23	AF	601	CHL	CHD-C4C	3.79	1.47	1.39
24	AL	509	CLA	C1D-ND	3.79	1.42	1.37
24	AL	510	CLA	C1D-ND	3.78	1.42	1.37
25	AN	615	LUT	C10-C9	3.78	1.40	1.35
26	q	615	NEX	C10-C9	3.78	1.40	1.35
24	AE	609	CLA	C1D-ND	3.78	1.42	1.37
24	P	509	CLA	C1D-ND	3.78	1.42	1.37
23	AU	608	CHL	CHD-C4C	3.78	1.47	1.39
23	AN	601	CHL	CHD-C4C	3.78	1.47	1.39
24	P	506	CLA	C1D-ND	3.77	1.42	1.37
24	AL	506	CLA	C1D-ND	3.77	1.42	1.37
24	AL	507	CLA	C1D-ND	3.77	1.42	1.37
23	AE	617	CHL	CHD-C1D	3.77	1.45	1.38
23	9	605	CHL	CHD-C4C	3.77	1.47	1.39
24	AB	610	CLA	C1D-ND	3.77	1.42	1.37
24	AK	605	CLA	C1D-ND	3.77	1.42	1.37
23	AQ	601	CHL	CHD-C4C	3.77	1.47	1.39
24	V	611	CLA	C1D-ND	3.77	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AH	607	CHL	CHD-C4C	3.77	1.47	1.39
27	q	617	XAT	C15-C14	3.77	1.55	1.43
24	AQ	603	CLA	C1D-ND	3.77	1.42	1.37
24	AA	610	CLA	C1D-ND	3.77	1.42	1.37
23	V	601	CHL	CHD-C4C	3.77	1.47	1.39
23	AN	607	CHL	CHD-C4C	3.77	1.47	1.39
23	v	306	CHL	CHC-C4B	3.77	1.47	1.39
23	AS	306	CHL	CHC-C4B	3.77	1.47	1.39
24	0	611	CLA	C1D-ND	3.77	1.42	1.37
24	V	612	CLA	C1D-ND	3.77	1.42	1.37
23	V	608	CHL	OBD-CAD	3.76	1.29	1.22
25	AQ	616	LUT	C10-C9	3.76	1.40	1.35
23	p	601	CHL	CHD-C4C	3.76	1.47	1.39
23	AU	607	CHL	CHD-C4C	3.76	1.47	1.39
24	AK	609	CLA	C1D-ND	3.76	1.42	1.37
24	AQ	602	CLA	C1D-ND	3.76	1.42	1.37
23	AE	607	CHL	CHD-C4C	3.76	1.47	1.39
24	V	602	CLA	C1D-ND	3.76	1.42	1.37
24	AU	602	CLA	C1D-ND	3.76	1.42	1.37
24	p	612	CLA	C1D-ND	3.76	1.42	1.37
23	AF	605	CHL	CHB-C1B	3.76	1.47	1.39
23	AA	607	CHL	CHD-C4C	3.76	1.47	1.39
25	AR	614	LUT	C14-C13	3.76	1.40	1.35
24	AD	304	CLA	C1D-ND	3.76	1.42	1.37
24	AK	613	CLA	C1D-ND	3.76	1.42	1.37
24	P	505	CLA	C1D-ND	3.76	1.42	1.37
23	0	606	CHL	CHD-C4C	3.75	1.47	1.39
24	P	503	CLA	C1D-ND	3.75	1.42	1.37
23	AU	606	CHL	CHD-C4C	3.75	1.47	1.39
24	AC	603	CLA	C1D-ND	3.75	1.42	1.37
24	AU	612	CLA	C1D-ND	3.75	1.42	1.37
27	9	618	XAT	C15-C14	3.75	1.55	1.43
25	AQ	616	LUT	C14-C13	3.75	1.40	1.35
23	AR	613	CHL	CHC-C4B	3.75	1.47	1.39
24	0	609	CLA	C1D-ND	3.75	1.42	1.37
23	AB	608	CHL	CHC-C4B	3.75	1.47	1.39
24	AR	617	CLA	C1D-ND	3.75	1.42	1.37
23	AF	606	CHL	CHB-C1B	3.75	1.47	1.39
25	AE	614	LUT	C30-C29	3.75	1.40	1.35
23	AC	608	CHL	CHD-C4C	3.75	1.47	1.39
23	AQ	608	CHL	CHD-C4C	3.75	1.47	1.39
23	AC	606	CHL	CHD-C4C	3.75	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	604	CLA	C1D-ND	3.75	1.42	1.37
32	J	406	PHO	C4D-CHA	3.75	1.45	1.39
25	p	615	LUT	C10-C9	3.74	1.40	1.35
24	AS	311	CLA	C1D-ND	3.74	1.42	1.37
23	AD	308	CHL	OBD-CAD	3.74	1.28	1.22
27	AR	616	XAT	C15-C14	3.74	1.55	1.43
24	AR	608	CLA	C4B-NB	3.74	1.42	1.37
23	0	607	CHL	C2C-C3C	3.74	1.46	1.36
24	9	603	CLA	C1D-ND	3.74	1.42	1.37
25	q	614	LUT	C14-C13	3.74	1.40	1.35
24	AD	303	CLA	C1D-ND	3.74	1.42	1.37
24	v	309	CLA	C1D-ND	3.74	1.42	1.37
23	9	607	CHL	CHD-C4C	3.74	1.47	1.39
27	AF	613	XAT	C31-C30	3.74	1.55	1.43
23	AA	617	CHL	OBD-CAD	3.74	1.28	1.22
27	AF	613	XAT	C15-C14	3.73	1.55	1.43
27	9	618	XAT	C35-C34	3.73	1.55	1.43
24	O	602	CLA	C1D-ND	3.73	1.42	1.37
23	AF	607	CHL	OBD-CAD	3.73	1.28	1.22
23	AR	607	CHL	OBD-CAD	3.73	1.28	1.22
24	AK	618	CLA	C1D-ND	3.73	1.42	1.37
24	v	313	CLA	C1D-ND	3.73	1.42	1.37
23	p	608	CHL	CHD-C4C	3.73	1.47	1.39
23	AE	601	CHL	CHD-C4C	3.73	1.47	1.39
23	AE	605	CHL	OBD-CAD	3.73	1.28	1.22
23	0	607	CHL	CHD-C4C	3.73	1.47	1.39
23	AD	301	CHL	CHD-C4C	3.73	1.47	1.39
23	q	613	CHL	CHC-C4B	3.73	1.47	1.39
23	AR	605	CHL	OBD-CAD	3.73	1.28	1.22
24	AQ	613	CLA	C1D-ND	3.73	1.42	1.37
23	AN	605	CHL	CHD-C4C	3.73	1.47	1.39
24	P	507	CLA	C1D-ND	3.73	1.42	1.37
24	AN	604	CLA	C1D-ND	3.73	1.42	1.37
23	AC	605	CHL	CHD-C4C	3.73	1.47	1.39
23	AQ	605	CHL	OBD-CAD	3.73	1.28	1.22
25	AN	614	LUT	C34-C33	3.72	1.40	1.35
25	AQ	616	LUT	C30-C29	3.72	1.40	1.35
24	AE	603	CLA	C1D-ND	3.72	1.42	1.37
25	p	615	LUT	C14-C13	3.72	1.40	1.35
24	q	609	CLA	C1D-ND	3.72	1.42	1.37
24	AQ	604	CLA	C1D-ND	3.72	1.42	1.37
24	p	611	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AR	609	CLA	C1D-ND	3.72	1.42	1.37
23	p	605	CHL	OBD-CAD	3.72	1.28	1.22
23	9	606	CHL	CHC-C4B	3.72	1.47	1.39
24	9	604	CLA	C1D-ND	3.72	1.42	1.37
23	AF	601	CHL	OBD-CAD	3.72	1.28	1.22
24	AS	305	CLA	C1D-ND	3.72	1.42	1.37
23	V	605	CHL	CHD-C4C	3.72	1.47	1.39
24	O	614	CLA	C1D-ND	3.72	1.42	1.37
24	AD	309	CLA	C1D-ND	3.72	1.42	1.37
23	AH	607	CHL	OBD-CAD	3.72	1.28	1.22
24	V	604	CLA	C1D-ND	3.72	1.42	1.37
24	q	611	CLA	C1D-ND	3.72	1.42	1.37
23	AN	601	CHL	OBD-CAD	3.72	1.28	1.22
24	AB	603	CLA	C1D-ND	3.72	1.42	1.37
24	AS	304	CLA	C1D-ND	3.71	1.42	1.37
23	q	607	CHL	OBD-CAD	3.71	1.28	1.22
25	AN	614	LUT	C30-C29	3.71	1.40	1.35
27	AF	613	XAT	C35-C34	3.71	1.55	1.43
23	AQ	607	CHL	CHD-C4C	3.71	1.47	1.39
24	O	606	CLA	C1D-ND	3.71	1.42	1.37
23	AS	307	CHL	OBD-CAD	3.71	1.28	1.22
24	AB	604	CLA	C1D-ND	3.71	1.42	1.37
23	AC	608	CHL	OBD-CAD	3.71	1.28	1.22
24	P	502	CLA	C1D-ND	3.71	1.42	1.37
24	p	603	CLA	C1D-ND	3.71	1.42	1.37
23	V	601	CHL	OBD-CAD	3.71	1.28	1.22
23	V	606	CHL	OBD-CAD	3.71	1.28	1.22
23	AD	302	CHL	OBD-CAD	3.71	1.28	1.22
24	P	501	CLA	C4B-NB	3.71	1.42	1.37
23	AA	607	CHL	OBD-CAD	3.70	1.28	1.22
23	AS	308	CHL	OBD-CAD	3.70	1.28	1.22
24	AC	612	CLA	C1D-ND	3.70	1.42	1.37
23	v	308	CHL	OBD-CAD	3.70	1.28	1.22
24	AL	511	CLA	C1D-ND	3.70	1.42	1.37
24	AK	616	CLA	C1D-ND	3.70	1.42	1.37
23	q	605	CHL	OBD-CAD	3.70	1.28	1.22
24	V	609	CLA	C1D-ND	3.70	1.42	1.37
23	AN	606	CHL	OBD-CAD	3.70	1.28	1.22
23	AQ	608	CHL	OBD-CAD	3.70	1.28	1.22
23	AA	608	CHL	MG-NA	-3.70	1.97	2.06
23	AA	605	CHL	OBD-CAD	3.70	1.28	1.22
23	AU	606	CHL	OBD-CAD	3.70	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AR	607	CHL	CHC-C4B	3.69	1.47	1.39
24	AS	310	CLA	C1D-ND	3.69	1.42	1.37
23	AQ	605	CHL	CHD-C4C	3.69	1.47	1.39
23	q	606	CHL	OBD-CAD	3.69	1.28	1.22
24	0	602	CLA	C1D-ND	3.69	1.42	1.37
25	AQ	616	LUT	C34-C33	3.69	1.40	1.35
23	9	606	CHL	OBD-CAD	3.69	1.28	1.22
24	AR	612	CLA	C1D-ND	3.69	1.42	1.37
23	AB	607	CHL	OBD-CAD	3.69	1.28	1.22
24	AK	606	CLA	C1D-ND	3.68	1.42	1.37
23	AU	607	CHL	OBD-CAD	3.68	1.28	1.22
24	AF	609	CLA	C1D-ND	3.68	1.42	1.37
23	9	607	CHL	OBD-CAD	3.68	1.28	1.22
25	V	613	LUT	C14-C13	3.68	1.40	1.35
24	AA	603	CLA	C1D-ND	3.68	1.42	1.37
23	p	605	CHL	CHD-C4C	3.68	1.47	1.39
23	AU	605	CHL	OBD-CAD	3.68	1.28	1.22
23	AC	607	CHL	OBD-CAD	3.68	1.28	1.22
24	AC	604	CLA	C1D-ND	3.68	1.42	1.37
24	AR	603	CLA	C1D-ND	3.67	1.42	1.37
23	AC	606	CHL	OBD-CAD	3.67	1.28	1.22
23	AD	306	CHL	OBD-CAD	3.67	1.28	1.22
23	AN	606	CHL	CHD-C4C	3.67	1.47	1.39
23	0	607	CHL	OBD-CAD	3.67	1.28	1.22
23	p	607	CHL	OBD-CAD	3.67	1.28	1.22
24	AN	602	CLA	C1D-ND	3.67	1.42	1.37
23	AU	605	CHL	CHD-C4C	3.67	1.47	1.39
23	AD	301	CHL	OBD-CAD	3.67	1.28	1.22
23	AH	608	CHL	OBD-CAD	3.67	1.28	1.22
24	AC	611	CLA	C1D-ND	3.67	1.42	1.37
23	p	606	CHL	OBD-CAD	3.67	1.28	1.22
23	AH	605	CHL	CHD-C4C	3.67	1.47	1.39
23	AH	605	CHL	OBD-CAD	3.67	1.28	1.22
23	AQ	606	CHL	OBD-CAD	3.67	1.28	1.22
24	AL	508	CLA	C1D-ND	3.67	1.42	1.37
23	AE	617	CHL	CHC-C4B	3.67	1.47	1.39
23	p	608	CHL	OBD-CAD	3.67	1.28	1.22
24	AD	305	CLA	C1D-ND	3.67	1.42	1.37
24	AR	611	CLA	C1D-ND	3.67	1.42	1.37
23	AC	601	CHL	OBD-CAD	3.67	1.28	1.22
32	AJ	408	PHO	C4D-CHA	3.67	1.45	1.39
24	q	604	CLA	C1D-ND	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	v	307	CHL	CHD-C4C	3.66	1.47	1.39
23	V	605	CHL	CHC-C4B	3.66	1.47	1.39
23	AQ	606	CHL	CHD-C4C	3.66	1.47	1.39
24	AS	313	CLA	C1D-ND	3.66	1.42	1.37
23	AB	606	CHL	OBD-CAD	3.66	1.28	1.22
24	AB	609	CLA	C1D-ND	3.66	1.42	1.37
23	AU	601	CHL	OBD-CAD	3.66	1.28	1.22
24	q	608	CLA	C4B-NB	3.66	1.42	1.37
24	AH	609	CLA	C1D-ND	3.66	1.42	1.37
23	AD	306	CHL	CHD-C4C	3.66	1.47	1.39
23	0	606	CHL	CHC-C4B	3.66	1.47	1.39
23	p	606	CHL	CHD-C4C	3.66	1.47	1.39
25	AA	614	LUT	C10-C9	3.66	1.40	1.35
24	AK	615	CLA	C1D-ND	3.66	1.42	1.37
24	q	603	CLA	C1D-ND	3.66	1.42	1.37
25	AN	614	LUT	C14-C13	3.66	1.40	1.35
25	q	614	LUT	C34-C33	3.66	1.40	1.35
24	v	310	CLA	C1D-ND	3.65	1.42	1.37
23	9	608	CHL	OBD-CAD	3.65	1.28	1.22
25	p	615	LUT	C34-C33	3.65	1.40	1.35
24	AL	502	CLA	C4B-NB	3.65	1.42	1.37
24	9	612	CLA	C1D-ND	3.65	1.42	1.37
23	AU	608	CHL	OBD-CAD	3.65	1.28	1.22
23	AF	608	CHL	CHB-C1B	3.65	1.47	1.39
24	O	604	CLA	C1D-ND	3.65	1.42	1.37
23	AQ	609	CHL	OBD-CAD	3.65	1.28	1.22
23	AH	601	CHL	OBD-CAD	3.65	1.28	1.22
23	AA	608	CHL	OBD-CAD	3.65	1.28	1.22
23	AE	601	CHL	OBD-CAD	3.65	1.28	1.22
24	O	608	CLA	C1B-C2B	3.65	1.51	1.43
24	AU	609	CLA	C1D-ND	3.65	1.42	1.37
23	AR	607	CHL	CHB-C1B	3.64	1.47	1.39
24	AE	603	CLA	C4B-NB	3.64	1.42	1.37
23	AN	605	CHL	CHC-C4B	3.64	1.47	1.39
23	AE	606	CHL	OBD-CAD	3.64	1.28	1.22
23	9	601	CHL	OBD-CAD	3.64	1.28	1.22
24	AD	311	CLA	C1D-ND	3.64	1.42	1.37
24	O	613	CLA	C1D-ND	3.64	1.42	1.37
24	q	618	CLA	C4B-NB	3.64	1.42	1.37
24	q	601	CLA	C4B-NB	3.64	1.42	1.37
24	AQ	614	CLA	C4B-NB	3.64	1.42	1.37
23	V	606	CHL	CHD-C4C	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AA	605	CHL	CHD-C4C	3.63	1.47	1.39
23	AA	606	CHL	OBD-CAD	3.63	1.28	1.22
24	O	616	CLA	C1D-ND	3.63	1.42	1.37
24	AK	608	CLA	C4B-NB	3.63	1.42	1.37
23	AB	605	CHL	CHC-C4B	3.63	1.47	1.39
24	AU	604	CLA	C1D-ND	3.63	1.42	1.37
23	AN	608	CHL	CHD-C4C	3.63	1.47	1.39
23	AF	608	CHL	OBD-CAD	3.63	1.28	1.22
23	9	605	CHL	OBD-CAD	3.63	1.28	1.22
23	AD	307	CHL	OBD-CAD	3.63	1.28	1.22
23	V	607	CHL	OBD-CAD	3.63	1.28	1.22
24	AR	608	CLA	C1D-ND	3.63	1.42	1.37
23	AN	607	CHL	OBD-CAD	3.63	1.28	1.22
24	AF	614	CLA	C1D-ND	3.63	1.42	1.37
25	AR	614	LUT	C34-C33	3.62	1.40	1.35
23	9	609	CHL	OBD-CAD	3.62	1.28	1.22
23	AQ	601	CHL	OBD-CAD	3.62	1.28	1.22
29	P	513	BCR	C1-C6	-3.62	1.48	1.53
38	F	102	HEM	FE-ND	3.62	2.06	1.94
24	AH	603	CLA	C4B-NB	3.62	1.42	1.37
29	AL	515	BCR	C1-C6	-3.62	1.48	1.53
23	AC	605	CHL	OBD-CAD	3.62	1.28	1.22
23	p	609	CHL	OBD-CAD	3.62	1.28	1.22
23	0	601	CHL	OBD-CAD	3.61	1.28	1.22
23	AQ	607	CHL	OBD-CAD	3.61	1.28	1.22
23	p	607	CHL	CHC-C4B	3.61	1.47	1.39
23	AC	607	CHL	CHC-C4B	3.61	1.47	1.39
23	AQ	606	CHL	CHC-C4B	3.61	1.47	1.39
25	AE	613	LUT	C14-C13	3.61	1.40	1.35
29	AB	612	BCR	C1-C6	-3.61	1.48	1.53
24	O	609	CLA	C1D-ND	3.61	1.42	1.37
25	AN	614	LUT	C10-C9	3.61	1.40	1.35
23	AN	617	CHL	C3D-C2D	3.60	1.49	1.39
23	AE	607	CHL	OBD-CAD	3.60	1.28	1.22
26	AR	615	NEX	C10-C9	3.60	1.40	1.35
29	AF	612	BCR	C1-C6	-3.60	1.48	1.53
23	v	308	CHL	CHC-C4B	3.60	1.47	1.39
24	AK	611	CLA	C1D-ND	3.60	1.42	1.37
24	9	611	CLA	C4B-NB	3.60	1.42	1.37
24	AR	601	CLA	C4B-NB	3.60	1.42	1.37
23	AA	606	CHL	CHD-C4C	3.60	1.47	1.39
23	q	613	CHL	CHB-C1B	3.60	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AH	604	CLA	C1D-ND	3.60	1.42	1.37
23	0	606	CHL	OBD-CAD	3.60	1.28	1.22
23	AA	601	CHL	OBD-CAD	3.60	1.28	1.22
23	q	605	CHL	CHC-C4B	3.60	1.47	1.39
29	O	625	BCR	C1-C6	-3.60	1.48	1.53
24	AU	603	CLA	C4B-NB	3.60	1.42	1.37
26	AA	616	NEX	C10-C9	3.59	1.40	1.35
23	0	617	CHL	OBD-CAD	3.59	1.28	1.22
23	q	607	CHL	CHB-C1B	3.59	1.47	1.39
24	AB	603	CLA	C4B-NB	3.59	1.42	1.37
26	AQ	617	NEX	C10-C9	3.59	1.40	1.35
29	O	619	BCR	C1-C6	-3.59	1.48	1.53
29	AK	621	BCR	C1-C6	-3.59	1.48	1.53
24	p	604	CLA	C1D-ND	3.59	1.42	1.37
24	AA	603	CLA	C4B-NB	3.59	1.42	1.37
23	q	607	CHL	CHC-C4B	3.58	1.47	1.39
23	V	616	CHL	CHC-C1C	3.58	1.45	1.38
23	0	605	CHL	CHD-C4C	3.58	1.47	1.39
25	AE	613	LUT	C30-C29	3.58	1.40	1.35
24	p	603	CLA	C4B-NB	3.58	1.42	1.37
24	p	618	CLA	C4B-NB	3.58	1.42	1.37
23	AR	606	CHL	CHC-C4B	3.57	1.47	1.39
23	p	601	CHL	OBD-CAD	3.57	1.28	1.22
23	0	608	CHL	CBD-CGD	-3.57	1.48	1.51
24	AL	512	CLA	C4B-NB	3.57	1.42	1.37
23	AS	307	CHL	CHD-C4C	3.57	1.47	1.39
23	AF	607	CHL	CHC-C4B	3.57	1.47	1.39
24	AS	309	CLA	C4B-NB	3.57	1.42	1.37
24	Q	403	CLA	C1D-ND	3.57	1.42	1.37
24	AM	403	CLA	C1D-ND	3.57	1.42	1.37
29	AK	619	BCR	C1-C6	-3.57	1.48	1.53
23	AD	317	CHL	OBD-CAD	3.57	1.28	1.22
23	p	606	CHL	CHC-C4B	3.57	1.47	1.39
24	AL	503	CLA	C1D-ND	3.57	1.42	1.37
34	o	101	SQD	O47-C45	-3.57	1.37	1.46
24	AN	609	CLA	C1D-ND	3.56	1.42	1.37
23	AF	607	CHL	CHB-C1B	3.56	1.47	1.39
23	AE	616	CHL	C3D-C2D	3.56	1.48	1.39
23	AQ	607	CHL	CHC-C4B	3.56	1.47	1.39
23	AH	606	CHL	OBD-CAD	3.56	1.28	1.22
23	AA	606	CHL	CHC-C4B	3.56	1.47	1.39
26	p	616	NEX	C10-C9	3.56	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AD	307	CHL	CHD-C4C	3.56	1.47	1.39
23	AR	605	CHL	CHC-C4B	3.56	1.47	1.39
23	AB	608	CHL	CHB-C1B	3.55	1.47	1.39
24	AE	604	CLA	C1D-ND	3.55	1.42	1.37
24	O	615	CLA	C4B-NB	3.55	1.42	1.37
23	AA	605	CHL	CHC-C4B	3.55	1.47	1.39
23	AN	617	CHL	OBD-CAD	3.55	1.28	1.22
24	AK	617	CLA	C4B-NB	3.55	1.42	1.37
24	K	101	CLA	C4B-NB	3.55	1.42	1.37
24	v	309	CLA	C4B-NB	3.55	1.42	1.37
29	AK	602	BCR	C1-C6	-3.55	1.48	1.53
24	AU	610	CLA	C4B-NB	3.54	1.42	1.37
34	AP	101	SQD	O47-C45	-3.54	1.37	1.46
23	AS	308	CHL	CHC-C4B	3.54	1.47	1.39
24	v	312	CLA	C4B-NB	3.54	1.42	1.37
23	AN	608	CHL	CHC-C1C	3.54	1.45	1.38
24	AA	611	CLA	C4B-NB	3.54	1.42	1.37
24	AK	612	CLA	C4B-NB	3.54	1.42	1.37
26	9	617	NEX	C10-C9	3.53	1.40	1.35
24	AK	614	CLA	C1D-ND	3.53	1.42	1.37
25	V	613	LUT	C30-C29	3.53	1.40	1.35
23	AF	606	CHL	C3B-C2B	3.53	1.48	1.39
24	AN	611	CLA	C4B-NB	3.53	1.42	1.37
23	v	302	CHL	OBD-CAD	3.53	1.28	1.22
24	AC	610	CLA	C4B-NB	3.53	1.42	1.37
24	V	612	CLA	C4B-NB	3.53	1.42	1.37
23	p	606	CHL	CHB-C1B	3.53	1.47	1.39
24	V	610	CLA	C4B-NB	3.53	1.42	1.37
29	O	617	BCR	C1-C6	-3.53	1.48	1.53
23	AN	607	CHL	CHC-C4B	3.52	1.47	1.39
24	AN	603	CLA	C4B-NB	3.52	1.42	1.37
24	AR	611	CLA	C4B-NB	3.52	1.42	1.37
24	AF	610	CLA	C4B-NB	3.52	1.42	1.37
24	AQ	603	CLA	C4B-NB	3.52	1.42	1.37
23	AF	606	CHL	CBD-CAD	-3.52	1.48	1.53
26	AE	615	NEX	C10-C9	3.52	1.40	1.35
24	O	612	CLA	C1D-ND	3.52	1.42	1.37
23	AR	613	CHL	CHB-C1B	3.52	1.47	1.39
24	AU	613	CLA	C4B-NB	3.52	1.42	1.37
23	AA	601	CHL	CHC-C4B	3.52	1.47	1.39
34	J	410	SQD	O47-C45	-3.52	1.37	1.46
23	9	608	CHL	CHC-C4B	3.51	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AK	613	CLA	C4B-NB	3.51	1.42	1.37
23	AR	605	CHL	CHB-C1B	3.51	1.47	1.39
23	AF	601	CHL	CHC-C4B	3.51	1.47	1.39
23	AE	605	CHL	CHC-C4B	3.51	1.47	1.39
29	f	101	BCR	C1-C6	-3.51	1.48	1.53
24	AS	312	CLA	C4B-NB	3.51	1.42	1.37
29	F	101	BCR	C1-C6	-3.51	1.49	1.53
25	AA	614	LUT	C14-C13	3.50	1.40	1.35
24	AD	313	CLA	C4B-NB	3.50	1.42	1.37
24	O	609	CLA	C4B-NB	3.50	1.42	1.37
24	q	618	CLA	C1D-ND	3.50	1.42	1.37
38	f	102	HEM	FE-NB	3.50	2.05	1.94
24	O	606	CLA	C4B-NB	3.50	1.42	1.37
24	AR	603	CLA	C4B-NB	3.50	1.42	1.37
23	AU	608	CHL	CHC-C4B	3.50	1.47	1.39
25	AA	614	LUT	C30-C29	3.50	1.40	1.35
24	V	603	CLA	C4B-NB	3.50	1.42	1.37
23	0	605	CHL	CHC-C4B	3.50	1.47	1.39
24	q	611	CLA	C4B-NB	3.50	1.42	1.37
23	AU	601	CHL	CHC-C4B	3.50	1.47	1.39
24	O	613	CLA	C4B-NB	3.49	1.42	1.37
23	AB	601	CHL	CHC-C4B	3.49	1.47	1.39
24	AH	610	CLA	C4B-NB	3.49	1.42	1.37
29	AL	516	BCR	C1-C6	-3.49	1.49	1.53
24	AE	610	CLA	C4B-NB	3.49	1.42	1.37
24	O	605	CLA	C4B-NB	3.49	1.42	1.37
34	AM	401	SQD	O47-C45	-3.49	1.37	1.46
23	q	606	CHL	CHC-C4B	3.49	1.47	1.39
24	AD	311	CLA	C4B-NB	3.49	1.42	1.37
23	AH	601	CHL	CHC-C4B	3.49	1.47	1.39
24	q	603	CLA	C4B-NB	3.48	1.42	1.37
24	AJ	406	CLA	C4B-NB	3.48	1.42	1.37
29	P	514	BCR	C1-C6	-3.48	1.49	1.53
24	Q	401	CLA	C4B-NB	3.48	1.42	1.37
24	AN	613	CLA	C4B-NB	3.48	1.42	1.37
23	AQ	608	CHL	CHC-C4B	3.48	1.47	1.39
23	AU	607	CHL	CHC-C4B	3.48	1.47	1.39
34	AJ	411	SQD	O47-C45	-3.48	1.37	1.46
23	AS	308	CHL	C4C-C3C	3.48	1.49	1.45
23	AQ	601	CHL	CHC-C4B	3.48	1.47	1.39
24	AK	615	CLA	C4B-NB	3.48	1.42	1.37
23	p	608	CHL	CHC-C4B	3.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AB	605	CHL	CHB-C1B	3.47	1.47	1.39
24	9	603	CLA	C4B-NB	3.47	1.42	1.37
23	0	601	CHL	CHC-C4B	3.47	1.47	1.39
23	V	606	CHL	CHC-C4B	3.47	1.47	1.39
23	AA	617	CHL	C3D-C2D	3.47	1.48	1.39
23	AD	302	CHL	CHC-C4B	3.47	1.47	1.39
24	AK	603	CLA	C4B-NB	3.47	1.42	1.37
24	AC	603	CLA	C4B-NB	3.47	1.42	1.37
38	f	102	HEM	FE-ND	3.47	2.05	1.94
24	v	305	CLA	C4B-NB	3.47	1.42	1.37
23	AH	606	CHL	CHC-C4B	3.47	1.47	1.39
23	AH	608	CHL	CHC-C4B	3.47	1.47	1.39
24	AH	613	CLA	C4B-NB	3.47	1.42	1.37
23	AD	301	CHL	CHC-C4B	3.47	1.47	1.39
24	O	603	CLA	C4B-NB	3.47	1.42	1.37
24	O	610	CLA	C4B-NB	3.47	1.42	1.37
34	Q	402	SQD	O47-C45	-3.46	1.37	1.46
23	0	617	CHL	CHB-C1B	3.46	1.47	1.39
23	AA	608	CHL	C3D-C2D	3.46	1.48	1.39
24	AA	610	CLA	C4B-NB	3.46	1.42	1.37
24	9	604	CLA	C4B-NB	3.46	1.42	1.37
24	AK	611	CLA	C4B-NB	3.46	1.42	1.37
34	m	101	SQD	O47-C45	-3.46	1.37	1.46
34	m	101	SQD	O5-C1	3.46	1.50	1.41
23	V	616	CHL	C3D-C2D	3.46	1.48	1.39
24	AK	607	CLA	C4B-NB	3.46	1.42	1.37
23	q	605	CHL	CHB-C1B	3.45	1.47	1.39
23	AS	302	CHL	OBD-CAD	3.45	1.28	1.22
37	Q	405	PL9	C7-C3	-3.45	1.47	1.51
34	M	101	SQD	O47-C45	-3.45	1.38	1.46
23	V	605	CHL	OBD-CAD	3.45	1.28	1.22
23	9	609	CHL	CHC-C4B	3.45	1.47	1.39
23	AU	606	CHL	CHC-C4B	3.45	1.47	1.39
24	P	502	CLA	C4B-NB	3.45	1.42	1.37
38	F	102	HEM	FE-NA	3.45	2.06	1.95
23	V	608	CHL	CHC-C4B	3.45	1.47	1.39
24	AN	612	CLA	C4B-NB	3.45	1.42	1.37
23	9	605	CHL	CHC-C4B	3.44	1.47	1.39
23	AE	601	CHL	CHC-C4B	3.44	1.47	1.39
24	v	313	CLA	C4B-NB	3.44	1.42	1.37
23	AH	607	CHL	CHC-C4B	3.44	1.47	1.39
32	AJ	407	PHO	C4D-CHA	3.44	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AN	608	CHL	C4B-NB	-3.44	1.33	1.37
24	O	601	CLA	C4B-NB	3.44	1.42	1.37
23	V	616	CHL	OBD-CAD	3.44	1.28	1.22
23	AN	606	CHL	CHC-C4B	3.44	1.47	1.39
23	AF	608	CHL	C3D-C2D	3.43	1.48	1.39
24	AB	604	CLA	C4B-NB	3.43	1.42	1.37
29	J	408	BCR	C1-C6	-3.43	1.49	1.53
23	AC	608	CHL	CHC-C4B	3.43	1.47	1.39
29	k	101	BCR	C1-C6	-3.43	1.49	1.53
23	0	606	CHL	CHB-C1B	3.43	1.47	1.39
29	P	515	BCR	C1-C6	-3.43	1.49	1.53
24	0	610	CLA	C4B-NB	3.43	1.42	1.37
23	v	307	CHL	OBD-CAD	3.43	1.28	1.22
24	AA	604	CLA	C1D-ND	3.43	1.42	1.37
23	p	601	CHL	CHC-C4B	3.43	1.47	1.39
23	AA	607	CHL	CHC-C4B	3.43	1.47	1.39
23	AC	605	CHL	CHC-C4B	3.43	1.47	1.39
24	AC	604	CLA	C4B-NB	3.43	1.42	1.37
23	0	605	CHL	OBD-CAD	3.43	1.28	1.22
25	AF	611	LUT	C30-C29	3.42	1.40	1.35
24	AE	612	CLA	C4B-NB	3.42	1.42	1.37
24	AS	305	CLA	C4B-NB	3.42	1.42	1.37
25	AE	613	LUT	C34-C33	3.42	1.40	1.35
24	AL	503	CLA	C4B-NB	3.42	1.42	1.37
24	AJ	405	CLA	C4B-NB	3.42	1.42	1.37
24	AQ	604	CLA	C4B-NB	3.42	1.42	1.37
29	AJ	410	BCR	C1-C6	-3.42	1.49	1.53
24	AR	602	CLA	C4B-NB	3.42	1.42	1.37
23	AB	606	CHL	CHC-C4B	3.42	1.47	1.39
24	AL	510	CLA	C4B-NB	3.42	1.42	1.37
37	AM	405	PL9	C7-C3	-3.41	1.47	1.51
24	AS	313	CLA	C4B-NB	3.41	1.42	1.37
23	AE	617	CHL	CHD-C4C	3.41	1.47	1.39
23	AE	607	CHL	CHC-C4B	3.41	1.47	1.39
24	AB	609	CLA	C4B-NB	3.41	1.42	1.37
24	AQ	612	CLA	C4B-NB	3.41	1.42	1.37
32	J	405	PHO	C4D-CHA	3.41	1.45	1.39
24	P	506	CLA	C4B-NB	3.41	1.42	1.37
24	p	604	CLA	C4B-NB	3.41	1.42	1.37
23	V	607	CHL	CHB-C1B	3.40	1.47	1.39
24	P	503	CLA	C4B-NB	3.40	1.42	1.37
23	AC	606	CHL	CHC-C4B	3.40	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	p	605	CHL	CHC-C4B	3.40	1.47	1.39
23	0	608	CHL	C4C-C3C	3.40	1.50	1.45
24	AJ	409	CLA	C4B-NB	3.40	1.42	1.37
34	M	101	SQD	O5-C1	3.40	1.50	1.41
25	AE	613	LUT	C10-C9	3.40	1.40	1.35
24	p	612	CLA	C4B-NB	3.40	1.42	1.37
24	AA	613	CLA	C4B-NB	3.40	1.42	1.37
23	AA	601	CHL	CHB-C1B	3.40	1.47	1.39
24	AB	610	CLA	C4B-NB	3.40	1.42	1.37
24	O	611	CLA	C4B-NB	3.40	1.42	1.37
24	AQ	613	CLA	C4B-NB	3.40	1.42	1.37
24	AN	610	CLA	C4B-NB	3.40	1.42	1.37
24	AE	611	CLA	C4B-NB	3.39	1.42	1.37
29	AI	101	BCR	C1-C6	-3.39	1.49	1.53
23	p	609	CHL	CHC-C4B	3.39	1.47	1.39
34	AP	101	SQD	O5-C1	3.39	1.50	1.41
24	v	310	CLA	C4B-NB	3.39	1.42	1.37
24	P	510	CLA	C4B-NB	3.39	1.41	1.37
23	AQ	609	CHL	CHC-C4B	3.39	1.47	1.39
23	AH	605	CHL	CHC-C4B	3.39	1.47	1.39
24	AA	612	CLA	C4B-NB	3.39	1.41	1.37
24	J	404	CLA	C4B-NB	3.38	1.41	1.37
23	AA	617	CHL	CHC-C4B	3.38	1.47	1.39
24	p	611	CLA	C4B-NB	3.38	1.41	1.37
24	q	609	CLA	C4B-NB	3.38	1.41	1.37
25	AF	611	LUT	C8-C9	-3.38	1.38	1.45
23	AQ	605	CHL	CHC-C4B	3.38	1.47	1.39
24	q	610	CLA	C4B-NB	3.38	1.41	1.37
24	AH	604	CLA	C4B-NB	3.38	1.41	1.37
24	AB	611	CLA	C4B-NB	3.38	1.41	1.37
24	AK	606	CLA	C4B-NB	3.38	1.41	1.37
24	AL	511	CLA	C4B-NB	3.38	1.41	1.37
24	AL	505	CLA	C4B-NB	3.37	1.41	1.37
24	O	616	CLA	C4B-NB	3.37	1.41	1.37
23	AS	307	CHL	CHC-C4B	3.37	1.47	1.39
24	AE	609	CLA	C4B-NB	3.37	1.41	1.37
24	P	504	CLA	C4B-NB	3.37	1.41	1.37
23	AN	605	CHL	OBD-CAD	3.37	1.28	1.22
34	J	410	SQD	O5-C1	3.37	1.50	1.41
34	AJ	411	SQD	O5-C1	3.37	1.50	1.41
24	J	407	CLA	C4B-NB	3.37	1.41	1.37
23	9	607	CHL	CHC-C4B	3.37	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AK	605	CLA	C4B-NB	3.37	1.41	1.37
23	V	601	CHL	CHC-C4B	3.37	1.47	1.39
23	AU	605	CHL	CHC-C4B	3.37	1.47	1.39
23	AN	605	CHL	CHB-C1B	3.37	1.47	1.39
24	P	509	CLA	C4B-NB	3.37	1.41	1.37
24	v	311	CLA	C4B-NB	3.37	1.41	1.37
24	AL	506	CLA	C4B-NB	3.37	1.41	1.37
23	AE	606	CHL	CHC-C4B	3.36	1.47	1.39
24	AA	602	CLA	C4B-NB	3.36	1.41	1.37
24	O	607	CLA	C4B-NB	3.36	1.41	1.37
24	AM	404	CLA	C4B-NB	3.36	1.41	1.37
23	AD	317	CHL	CHB-C1B	3.36	1.46	1.39
25	AA	614	LUT	C34-C33	3.36	1.40	1.35
24	AR	610	CLA	C4B-NB	3.36	1.41	1.37
24	p	618	CLA	C1B-C2B	3.36	1.51	1.43
24	AU	604	CLA	C4B-NB	3.36	1.41	1.37
34	o	101	SQD	O5-C1	3.36	1.50	1.41
24	AC	613	CLA	C4D-ND	-3.36	1.33	1.37
26	AU	616	NEX	C10-C9	3.36	1.40	1.35
24	AK	616	CLA	C4B-NB	3.36	1.41	1.37
29	AK	620	BCR	C1-C6	-3.36	1.49	1.53
23	AB	606	CHL	CHB-C1B	3.36	1.46	1.39
38	F	102	HEM	CAB-C3B	3.36	1.56	1.47
24	v	314	CLA	C4B-NB	3.36	1.41	1.37
29	O	618	BCR	C1-C6	-3.35	1.49	1.53
34	Q	402	SQD	O5-C1	3.35	1.50	1.41
24	P	505	CLA	C4B-NB	3.35	1.41	1.37
24	9	614	CLA	C4B-NB	3.35	1.41	1.37
24	AH	611	CLA	C4B-NB	3.35	1.41	1.37
24	AD	305	CLA	C4B-NB	3.35	1.41	1.37
24	0	604	CLA	C4B-NB	3.35	1.41	1.37
24	AS	310	CLA	C4B-NB	3.35	1.41	1.37
24	0	613	CLA	C4B-NB	3.35	1.41	1.37
24	AF	614	CLA	C4B-NB	3.35	1.41	1.37
24	AK	609	CLA	C4B-NB	3.35	1.41	1.37
23	AD	306	CHL	CHC-C4B	3.34	1.46	1.39
24	AE	608	CLA	C4B-NB	3.34	1.41	1.37
24	AU	611	CLA	C4B-NB	3.34	1.41	1.37
23	AS	306	CHL	CHB-C1B	3.34	1.46	1.39
24	AS	311	CLA	C4B-NB	3.34	1.41	1.37
23	AN	601	CHL	CHC-C4B	3.34	1.46	1.39
34	AM	401	SQD	O5-C1	3.34	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AS	307	CHL	CHB-C1B	3.34	1.46	1.39
24	AA	609	CLA	C4B-NB	3.34	1.41	1.37
24	AC	609	CLA	C4B-NB	3.34	1.41	1.37
24	9	612	CLA	C4B-NB	3.34	1.41	1.37
24	AA	604	CLA	C4B-NB	3.34	1.41	1.37
24	AQ	611	CLA	C4B-NB	3.34	1.41	1.37
24	q	608	CLA	C3B-C4B	3.34	1.50	1.42
24	O	604	CLA	C4B-NB	3.34	1.41	1.37
24	0	611	CLA	C4B-NB	3.33	1.41	1.37
23	AU	601	CHL	CHB-C1B	3.33	1.46	1.39
24	v	304	CLA	C4B-NB	3.33	1.41	1.37
24	p	610	CLA	C4B-NB	3.33	1.41	1.37
23	AF	601	CHL	CHB-C1B	3.33	1.46	1.39
24	AK	618	CLA	C4B-NB	3.33	1.41	1.37
24	AL	507	CLA	C4B-NB	3.33	1.41	1.37
24	Q	404	CLA	C4B-NB	3.33	1.41	1.37
24	AC	612	CLA	C4B-NB	3.32	1.41	1.37
23	AE	617	CHL	OBD-CAD	3.32	1.28	1.22
24	AF	604	CLA	C4B-NB	3.32	1.41	1.37
24	AE	602	CLA	C4B-NB	3.32	1.41	1.37
23	v	307	CHL	CHC-C4B	3.32	1.46	1.39
23	AD	307	CHL	CHC-C4B	3.32	1.46	1.39
23	AA	608	CHL	C1D-C2D	3.32	1.51	1.45
23	AE	601	CHL	CHB-C1B	3.32	1.46	1.39
23	0	608	CHL	OBD-CAD	3.32	1.28	1.22
23	AH	601	CHL	CHB-C1B	3.32	1.46	1.39
24	AH	612	CLA	C4B-NB	3.32	1.41	1.37
24	AS	314	CLA	C4B-NB	3.32	1.41	1.37
24	AD	304	CLA	C4B-NB	3.32	1.41	1.37
24	AL	504	CLA	C4B-NB	3.32	1.41	1.37
24	V	604	CLA	C1A-CHA	-3.32	1.36	1.43
24	AR	608	CLA	C3B-C4B	3.31	1.50	1.42
24	AC	611	CLA	C4B-NB	3.31	1.41	1.37
23	0	607	CHL	CHC-C4B	3.31	1.46	1.39
24	AD	312	CLA	C4B-NB	3.31	1.41	1.37
24	AR	612	CLA	C4B-NB	3.31	1.41	1.37
24	P	508	CLA	C4B-NB	3.31	1.41	1.37
24	AS	303	CLA	C4B-NB	3.30	1.41	1.37
24	AR	609	CLA	C4B-NB	3.30	1.41	1.37
23	AN	608	CHL	C3D-C2D	3.30	1.48	1.39
23	0	617	CHL	CHC-C4B	3.30	1.46	1.39
24	AU	612	CLA	C4B-NB	3.30	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	AV	101	BCR	C1-C6	-3.30	1.49	1.53
23	V	605	CHL	CHB-C1B	3.29	1.46	1.39
24	AE	604	CLA	C4B-NB	3.29	1.41	1.37
24	V	610	CLA	C3B-C4B	3.29	1.50	1.42
23	AC	605	CHL	CHB-C1B	3.29	1.46	1.39
24	AF	614	CLA	C1B-C2B	3.29	1.51	1.43
24	V	611	CLA	C4B-NB	3.29	1.41	1.37
24	0	612	CLA	C4B-NB	3.29	1.41	1.37
23	AB	608	CHL	C3D-C2D	3.29	1.48	1.39
25	AF	611	LUT	C34-C33	3.28	1.40	1.35
24	q	604	CLA	C4B-NB	3.28	1.41	1.37
24	9	611	CLA	C3B-C4B	3.28	1.50	1.42
24	V	604	CLA	C4B-NB	3.28	1.41	1.37
24	AS	304	CLA	C4B-NB	3.28	1.41	1.37
34	M	101	SQD	O47-C7	3.28	1.43	1.34
23	AC	601	CHL	CHB-C1B	3.28	1.46	1.39
24	AR	617	CLA	C1B-C2B	3.28	1.51	1.43
24	AR	604	CLA	C4B-NB	3.28	1.41	1.37
29	k	101	BCR	C30-C25	-3.28	1.49	1.53
24	0	602	CLA	C4B-NB	3.28	1.41	1.37
23	AD	306	CHL	CHB-C1B	3.28	1.46	1.39
29	P	515	BCR	C30-C25	-3.28	1.49	1.53
24	O	614	CLA	C4B-NB	3.28	1.41	1.37
24	q	612	CLA	C4B-NB	3.28	1.41	1.37
34	AJ	411	SQD	O47-C7	3.28	1.43	1.34
23	AD	308	CHL	CHC-C4B	3.27	1.46	1.39
24	q	602	CLA	C4B-NB	3.27	1.41	1.37
23	AN	601	CHL	CHB-C1B	3.27	1.46	1.39
34	Q	402	SQD	O47-C7	3.27	1.43	1.34
24	AF	602	CLA	C4B-NB	3.27	1.41	1.37
24	AL	508	CLA	C4B-NB	3.26	1.41	1.37
23	AD	307	CHL	CHB-C1B	3.26	1.46	1.39
23	AF	606	CHL	MG-NA	-3.26	1.98	2.06
24	AL	509	CLA	C4B-NB	3.26	1.41	1.37
34	m	101	SQD	O47-C7	3.26	1.43	1.34
24	AD	303	CLA	C4B-NB	3.26	1.41	1.37
24	AF	609	CLA	C4D-ND	-3.26	1.33	1.37
23	AR	613	CHL	C3A-C2A	-3.26	1.51	1.54
23	AC	608	CHL	CHB-C1B	3.26	1.46	1.39
23	AQ	609	CHL	CHB-C1B	3.26	1.46	1.39
23	V	601	CHL	CHB-C1B	3.26	1.46	1.39
24	AL	502	CLA	C3B-C4B	3.25	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	V	616	CHL	CHB-C1B	3.25	1.46	1.39
23	AQ	601	CHL	CHB-C1B	3.25	1.46	1.39
24	AK	608	CLA	C3B-C4B	3.25	1.50	1.42
23	9	601	CHL	CHB-C1B	3.25	1.46	1.39
24	AF	603	CLA	C3B-C4B	3.25	1.50	1.42
34	AM	401	SQD	O47-C7	3.25	1.43	1.34
23	0	601	CHL	CHB-C1B	3.25	1.46	1.39
24	AJ	404	CLA	C4B-NB	3.25	1.41	1.37
24	AN	604	CLA	C4B-NB	3.25	1.41	1.37
23	AR	613	CHL	C3D-C2D	3.25	1.48	1.39
23	9	609	CHL	CHB-C1B	3.25	1.46	1.39
24	p	602	CLA	C4B-NB	3.25	1.41	1.37
24	AB	602	CLA	C4B-NB	3.25	1.41	1.37
24	AF	609	CLA	C4B-NB	3.24	1.41	1.37
23	v	302	CHL	CHB-C1B	3.24	1.46	1.39
24	AD	310	CLA	C4B-NB	3.24	1.41	1.37
24	P	501	CLA	C3B-C4B	3.24	1.50	1.42
24	9	613	CLA	C4B-NB	3.24	1.41	1.37
23	9	605	CHL	CHB-C1B	3.24	1.46	1.39
23	q	613	CHL	C3D-C2D	3.24	1.48	1.39
24	O	612	CLA	C4B-NB	3.24	1.41	1.37
24	AH	602	CLA	C4B-NB	3.24	1.41	1.37
23	AD	301	CHL	CHB-C1B	3.24	1.46	1.39
23	AA	605	CHL	CHB-C1B	3.24	1.46	1.39
24	q	618	CLA	C1B-C2B	3.23	1.50	1.43
24	P	507	CLA	C4B-NB	3.23	1.41	1.37
23	v	308	CHL	CHB-C1B	3.23	1.46	1.39
23	AB	601	CHL	CHB-C1B	3.23	1.46	1.39
24	AK	614	CLA	C4B-NB	3.23	1.41	1.37
24	v	303	CLA	C4B-NB	3.23	1.41	1.37
23	AB	605	CHL	C4C-C3C	3.23	1.48	1.45
23	AR	606	CHL	CHB-C1B	3.23	1.46	1.39
34	J	410	SQD	O47-C7	3.23	1.43	1.34
24	AR	601	CLA	C3B-C4B	3.23	1.50	1.42
23	AH	607	CHL	CHB-C1B	3.23	1.46	1.39
24	AC	610	CLA	C3B-C4B	3.23	1.50	1.42
24	AN	609	CLA	C4B-NB	3.23	1.41	1.37
23	AC	601	CHL	C4C-C3C	3.22	1.50	1.45
24	AC	613	CLA	C4B-NB	3.22	1.41	1.37
23	AU	606	CHL	CHB-C1B	3.22	1.46	1.39
23	AN	607	CHL	CHB-C1B	3.22	1.46	1.39
23	AS	302	CHL	CHB-C1B	3.22	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	V	607	CHL	C3B-C2B	3.22	1.47	1.39
23	AA	607	CHL	CHB-C1B	3.21	1.46	1.39
23	v	307	CHL	CHB-C1B	3.21	1.46	1.39
24	AU	602	CLA	C4B-NB	3.21	1.41	1.37
23	AS	308	CHL	CHB-C1B	3.21	1.46	1.39
24	AQ	610	CLA	C4B-NB	3.21	1.41	1.37
23	v	306	CHL	CHB-C1B	3.21	1.46	1.39
23	p	601	CHL	CHB-C1B	3.21	1.46	1.39
23	AU	607	CHL	CHB-C1B	3.21	1.46	1.39
23	0	607	CHL	CHB-C1B	3.21	1.46	1.39
24	AM	403	CLA	C4B-NB	3.21	1.41	1.37
23	AC	606	CHL	CHB-C1B	3.21	1.46	1.39
34	AP	101	SQD	O47-C7	3.20	1.43	1.34
24	J	403	CLA	C4B-NB	3.20	1.41	1.37
24	V	609	CLA	C4B-NB	3.20	1.41	1.37
24	9	610	CLA	C4B-NB	3.20	1.41	1.37
23	0	617	CHL	C3D-C2D	3.20	1.47	1.39
23	AF	606	CHL	C3C-C2C	3.20	1.47	1.39
23	9	606	CHL	C1D-C2D	3.19	1.51	1.45
34	o	101	SQD	O47-C7	3.19	1.43	1.34
23	AF	606	CHL	CHC-C4B	3.19	1.48	1.40
24	O	602	CLA	C4B-NB	3.19	1.41	1.37
24	AQ	610	CLA	C3B-C4B	3.19	1.50	1.42
23	q	606	CHL	CHB-C1B	3.19	1.46	1.39
23	AN	606	CHL	CHB-C1B	3.19	1.46	1.39
24	p	613	CLA	C4B-NB	3.19	1.41	1.37
23	V	606	CHL	CHB-C1B	3.18	1.46	1.39
29	AO	101	BCR	C1-C6	-3.18	1.49	1.53
26	v	317	NEX	C10-C9	3.18	1.40	1.35
29	AJ	410	BCR	C30-C25	-3.18	1.49	1.53
23	9	601	CHL	C3B-C2B	3.18	1.47	1.39
25	AE	613	LUT	C8-C9	-3.18	1.39	1.45
24	AN	611	CLA	C3B-C4B	3.18	1.50	1.42
24	Q	403	CLA	C4B-NB	3.17	1.41	1.37
24	AH	609	CLA	C4B-NB	3.17	1.41	1.37
23	V	616	CHL	C1B-NB	-3.17	1.33	1.37
24	p	610	CLA	C3B-C4B	3.17	1.50	1.42
24	AK	610	CLA	C3B-C4B	3.17	1.50	1.42
23	AD	302	CHL	CHB-C1B	3.17	1.46	1.39
23	AD	317	CHL	C3D-C2D	3.17	1.47	1.39
24	AK	612	CLA	C3B-C4B	3.17	1.50	1.42
23	9	606	CHL	CHB-C1B	3.16	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	608	CHL	CHB-C1B	3.16	1.46	1.39
23	AH	605	CHL	CHB-C1B	3.16	1.46	1.39
23	AQ	606	CHL	CHB-C1B	3.16	1.46	1.39
23	AU	605	CHL	CHB-C1B	3.16	1.46	1.39
24	O	608	CLA	C3B-C4B	3.16	1.50	1.42
23	V	607	CHL	C4C-C3C	3.16	1.48	1.45
24	O	610	CLA	C3B-C4B	3.15	1.50	1.42
23	AC	607	CHL	CHB-C1B	3.15	1.46	1.39
24	q	601	CLA	C3B-C4B	3.15	1.50	1.42
24	P	511	CLA	C4B-NB	3.15	1.41	1.37
23	p	609	CHL	CHB-C1B	3.15	1.46	1.39
23	AD	317	CHL	CHC-C4B	3.15	1.46	1.39
23	AE	606	CHL	CHB-C1B	3.14	1.46	1.39
23	AC	601	CHL	C3B-C2B	3.14	1.47	1.39
23	V	608	CHL	CHB-C1B	3.14	1.46	1.39
24	AQ	602	CLA	C4B-NB	3.14	1.41	1.37
23	AA	606	CHL	CHB-C1B	3.14	1.46	1.39
24	AK	610	CLA	C1B-C2B	3.14	1.50	1.43
24	AN	602	CLA	C4B-NB	3.14	1.41	1.37
24	AS	309	CLA	C3B-C4B	3.14	1.50	1.42
24	AQ	614	CLA	C3B-C4B	3.13	1.50	1.42
23	0	605	CHL	CHB-C1B	3.13	1.46	1.39
24	0	603	CLA	C4B-NB	3.13	1.41	1.37
24	p	618	CLA	C3B-C4B	3.13	1.50	1.42
24	AU	609	CLA	C4B-NB	3.13	1.41	1.37
23	AF	605	CHL	C3D-C2D	3.13	1.47	1.39
23	AN	617	CHL	CHB-C1B	3.13	1.46	1.39
23	v	302	CHL	C3B-C2B	3.13	1.47	1.39
24	AB	603	CLA	C3B-C4B	3.13	1.50	1.42
23	AQ	608	CHL	CHB-C1B	3.13	1.46	1.39
29	AL	516	BCR	C30-C25	-3.13	1.49	1.53
29	AO	101	BCR	C30-C25	-3.13	1.49	1.53
23	9	607	CHL	CHB-C1B	3.13	1.46	1.39
23	AE	617	CHL	C3D-C2D	3.13	1.47	1.39
24	AL	513	CLA	C4B-NB	3.13	1.41	1.37
24	V	602	CLA	C4B-NB	3.12	1.41	1.37
24	AE	603	CLA	C3B-C4B	3.12	1.50	1.42
23	AB	605	CHL	C3D-C2D	3.12	1.47	1.39
23	p	608	CHL	CHB-C1B	3.12	1.46	1.39
23	AN	608	CHL	OBD-CAD	3.12	1.27	1.22
29	F	101	BCR	C30-C25	-3.12	1.49	1.53
29	J	408	BCR	C30-C25	-3.11	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	O	606	CLA	C3B-C4B	3.11	1.50	1.42
23	AN	608	CHL	CHB-C1B	3.11	1.46	1.39
24	AK	603	CLA	C3B-C4B	3.11	1.50	1.42
24	9	610	CLA	C4D-ND	-3.11	1.33	1.37
29	P	514	BCR	C30-C25	-3.11	1.49	1.53
24	AC	602	CLA	C4B-NB	3.11	1.41	1.37
29	j	101	BCR	C30-C25	-3.10	1.49	1.53
23	V	607	CHL	C1B-NB	-3.10	1.34	1.37
23	AE	607	CHL	CHB-C1B	3.10	1.46	1.39
29	f	101	BCR	C30-C25	-3.10	1.49	1.53
38	f	102	HEM	CAB-C3B	3.10	1.55	1.47
29	AF	612	BCR	C30-C25	-3.10	1.49	1.53
24	O	601	CLA	C3B-C4B	3.09	1.50	1.42
24	AU	611	CLA	C3B-C4B	3.09	1.50	1.42
24	AA	603	CLA	C3B-C4B	3.09	1.50	1.42
24	O	611	CLA	C3B-C4B	3.08	1.50	1.42
23	AS	306	CHL	C3C-C2C	3.08	1.46	1.39
29	P	513	BCR	C30-C25	-3.08	1.49	1.53
23	p	605	CHL	CHB-C1B	3.08	1.46	1.39
23	AS	302	CHL	C3B-C2B	3.08	1.47	1.39
24	AC	609	CLA	C4D-ND	-3.08	1.33	1.37
29	O	617	BCR	C30-C25	-3.08	1.49	1.53
24	AE	610	CLA	C3B-C4B	3.07	1.49	1.42
24	0	609	CLA	C4B-NB	3.07	1.41	1.37
34	AM	401	SQD	C24-C23	3.07	1.59	1.50
24	AH	611	CLA	C3B-C4B	3.07	1.49	1.42
23	q	606	CHL	C3D-C2D	3.07	1.47	1.39
23	AH	608	CHL	CHB-C1B	3.07	1.46	1.39
23	0	607	CHL	C4C-C3C	3.07	1.48	1.45
34	Q	402	SQD	C24-C23	3.07	1.59	1.50
37	AM	405	PL9	C3-C4	-3.07	1.44	1.49
23	AN	617	CHL	C1B-NB	-3.06	1.34	1.37
24	v	311	CLA	C3B-C4B	3.06	1.49	1.42
24	AH	609	CLA	C4D-ND	-3.06	1.33	1.37
24	AS	311	CLA	C3B-C4B	3.06	1.49	1.42
24	p	613	CLA	C1B-C2B	3.06	1.50	1.43
24	AD	309	CLA	C4B-NB	3.06	1.41	1.37
24	AB	610	CLA	C3B-C4B	3.06	1.49	1.42
24	AU	603	CLA	C3B-C4B	3.06	1.49	1.42
23	0	606	CHL	C3D-C2D	3.05	1.47	1.39
24	AA	611	CLA	C3B-C4B	3.05	1.49	1.42
34	m	101	SQD	C24-C23	3.05	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	609	CLA	C4D-ND	-3.05	1.33	1.37
23	AD	308	CHL	CHB-C1B	3.05	1.46	1.39
23	V	616	CHL	CHC-C4B	3.05	1.46	1.39
23	AH	606	CHL	CHB-C1B	3.05	1.46	1.39
34	M	101	SQD	C24-C23	3.05	1.59	1.50
29	j	101	BCR	C1-C6	-3.05	1.49	1.53
24	v	310	CLA	C4D-ND	-3.05	1.33	1.37
23	AS	302	CHL	C3D-C2D	3.05	1.47	1.39
29	AL	515	BCR	C30-C25	-3.04	1.49	1.53
29	AK	619	BCR	C30-C25	-3.04	1.49	1.53
34	J	410	SQD	C24-C23	3.04	1.59	1.50
23	AR	606	CHL	C3D-C2D	3.04	1.47	1.39
24	AH	609	CLA	C3B-C4B	3.04	1.49	1.42
24	AU	609	CLA	C3B-C4B	3.04	1.49	1.42
23	AF	608	CHL	MG-NA	-3.04	1.99	2.06
24	AR	611	CLA	C3B-C4B	3.04	1.49	1.42
24	q	611	CLA	C3B-C4B	3.04	1.49	1.42
24	9	610	CLA	C3B-C4B	3.03	1.49	1.42
24	AH	603	CLA	C3B-C4B	3.03	1.49	1.42
23	AU	608	CHL	CHB-C1B	3.03	1.46	1.39
23	AN	617	CHL	C4C-C3C	3.03	1.50	1.45
23	AH	606	CHL	C1D-C2D	3.03	1.51	1.45
24	AD	309	CLA	C4D-ND	-3.03	1.33	1.37
25	AF	611	LUT	C14-C13	3.03	1.39	1.35
24	9	602	CLA	C4B-NB	3.03	1.41	1.37
24	AU	609	CLA	C4D-ND	-3.03	1.33	1.37
24	q	602	CLA	C3B-C4B	3.02	1.49	1.42
24	p	611	CLA	C4D-ND	-3.02	1.33	1.37
24	AQ	611	CLA	C3B-C4B	3.02	1.49	1.42
24	V	604	CLA	C4D-ND	-3.02	1.33	1.37
29	O	618	BCR	C30-C25	-3.02	1.49	1.53
23	AA	617	CHL	CHB-C1B	3.02	1.46	1.39
25	V	613	LUT	C8-C9	-3.02	1.39	1.45
24	q	609	CLA	C3B-C4B	3.02	1.49	1.42
23	v	302	CHL	C3D-C2D	3.02	1.47	1.39
24	v	309	CLA	C3B-C4B	3.01	1.49	1.42
24	AN	602	CLA	C4D-ND	-3.01	1.33	1.37
25	AF	611	LUT	C10-C9	3.01	1.39	1.35
29	AB	612	BCR	C30-C25	-3.01	1.49	1.53
38	F	102	HEM	FE-NB	3.01	2.04	1.94
34	AJ	411	SQD	C24-C23	3.01	1.59	1.50
24	AA	613	CLA	C3B-C4B	3.01	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	609	CHL	C3D-C2D	3.01	1.47	1.39
23	AE	616	CHL	C4C-C3C	3.01	1.50	1.45
23	AE	616	CHL	CHC-C4B	3.00	1.46	1.39
23	AN	617	CHL	CHC-C4B	3.00	1.46	1.39
24	AQ	612	CLA	C3B-C4B	3.00	1.49	1.42
24	O	616	CLA	C3B-C4B	3.00	1.49	1.42
29	AK	620	BCR	C30-C25	-3.00	1.49	1.53
24	AS	311	CLA	C4D-ND	-3.00	1.33	1.37
23	v	306	CHL	C3C-C2C	2.99	1.46	1.39
24	AK	613	CLA	C3B-C4B	2.99	1.49	1.42
23	AS	302	CHL	C1B-NB	-2.99	1.34	1.37
23	AQ	605	CHL	CHB-C1B	2.99	1.46	1.39
24	0	609	CLA	C4D-ND	-2.99	1.33	1.37
24	AQ	612	CLA	C4D-ND	-2.99	1.33	1.37
24	AH	610	CLA	C3B-C4B	2.99	1.49	1.42
24	AR	603	CLA	C3B-C4B	2.99	1.49	1.42
23	AR	607	CHL	C3D-C2D	2.99	1.47	1.39
24	q	603	CLA	C3B-C4B	2.99	1.49	1.42
23	v	306	CHL	C3D-C2D	2.99	1.47	1.39
24	O	609	CLA	C3B-C4B	2.99	1.49	1.42
23	0	601	CHL	C3D-C2D	2.99	1.47	1.39
23	q	606	CHL	C3C-C2C	2.98	1.46	1.39
24	AU	610	CLA	C3B-C4B	2.98	1.49	1.42
24	Q	403	CLA	C4D-ND	-2.98	1.33	1.37
24	V	609	CLA	C4D-ND	-2.98	1.33	1.37
24	V	603	CLA	C3B-C4B	2.98	1.49	1.42
24	p	603	CLA	C3B-C4B	2.98	1.49	1.42
23	p	609	CHL	C3D-C2D	2.98	1.47	1.39
24	AQ	602	CLA	C3B-C4B	2.98	1.49	1.42
24	AE	612	CLA	C3B-C4B	2.98	1.49	1.42
23	AB	601	CHL	C3D-C2D	2.98	1.47	1.39
24	AC	613	CLA	C3B-C4B	2.98	1.49	1.42
24	q	618	CLA	C3B-C4B	2.98	1.49	1.42
24	9	614	CLA	C3B-C4B	2.98	1.49	1.42
24	AN	610	CLA	C3B-C4B	2.97	1.49	1.42
24	O	613	CLA	C3B-C4B	2.97	1.49	1.42
24	v	312	CLA	C3B-C4B	2.97	1.49	1.42
23	AF	607	CHL	C3D-C2D	2.97	1.47	1.39
25	q	614	LUT	C8-C9	-2.97	1.39	1.45
24	AC	609	CLA	C3B-C4B	2.97	1.49	1.42
24	Q	401	CLA	C3B-C4B	2.97	1.49	1.42
24	AJ	409	CLA	C3B-C4B	2.97	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	611	CLA	C4D-ND	-2.97	1.33	1.37
23	v	302	CHL	C1B-NB	-2.97	1.34	1.37
23	AR	605	CHL	C3C-C2C	2.97	1.46	1.39
24	p	602	CLA	C3B-C4B	2.97	1.49	1.42
24	AC	610	CLA	C4D-ND	-2.96	1.33	1.37
24	AL	512	CLA	C3B-C4B	2.96	1.49	1.42
23	V	616	CHL	C4C-C3C	2.96	1.50	1.45
24	0	611	CLA	C4D-ND	-2.96	1.33	1.37
24	AK	615	CLA	C3B-C4B	2.96	1.49	1.42
23	AF	605	CHL	C1D-C2D	2.96	1.51	1.45
24	AN	612	CLA	C3B-C4B	2.96	1.49	1.42
23	AS	307	CHL	C3D-C2D	2.96	1.47	1.39
23	0	608	CHL	MG-NA	-2.96	1.99	2.06
24	J	407	CLA	C3B-C4B	2.96	1.49	1.42
37	Q	405	PL9	C3-C4	-2.96	1.44	1.49
24	p	612	CLA	C3B-C4B	2.96	1.49	1.42
24	Q	403	CLA	C3B-C4B	2.96	1.49	1.42
24	AK	617	CLA	C3B-C4B	2.96	1.49	1.42
24	AJ	406	CLA	C3B-C4B	2.95	1.49	1.42
24	V	604	CLA	C3B-C4B	2.95	1.49	1.42
23	p	601	CHL	C3D-C2D	2.95	1.47	1.39
24	AQ	603	CLA	C3B-C4B	2.95	1.49	1.42
24	AR	604	CLA	C3B-C4B	2.95	1.49	1.42
23	AD	302	CHL	C3D-C2D	2.95	1.47	1.39
24	AF	610	CLA	C1B-C2B	2.95	1.50	1.43
24	AD	303	CLA	C3B-C4B	2.95	1.49	1.42
24	AK	611	CLA	C3B-C4B	2.95	1.49	1.42
23	V	608	CHL	C3D-C2D	2.95	1.47	1.39
24	AF	603	CLA	C4D-ND	-2.95	1.33	1.37
24	AN	609	CLA	C4D-ND	-2.95	1.33	1.37
24	AS	312	CLA	C3B-C4B	2.95	1.49	1.42
24	AB	609	CLA	C3B-C4B	2.95	1.49	1.42
34	AP	101	SQD	C24-C23	2.95	1.59	1.50
23	p	607	CHL	CHB-C1B	2.95	1.46	1.39
23	AF	607	CHL	C1D-C2D	2.95	1.51	1.45
24	AM	403	CLA	C3B-C4B	2.95	1.49	1.42
23	AB	607	CHL	C3D-C2D	2.95	1.47	1.39
24	AK	604	CLA	C4B-NB	2.95	1.41	1.37
24	J	403	CLA	C3B-C4B	2.95	1.49	1.42
25	AN	614	LUT	C8-C9	-2.94	1.39	1.45
24	AC	603	CLA	C4D-ND	-2.94	1.33	1.37
23	AF	606	CHL	C1B-NB	-2.94	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	610	CLA	C3B-C4B	2.94	1.49	1.42
24	AU	611	CLA	C4D-ND	-2.94	1.33	1.37
24	O	615	CLA	C3B-C4B	2.94	1.49	1.42
24	AF	609	CLA	C3B-C4B	2.94	1.49	1.42
24	0	611	CLA	C3B-C4B	2.94	1.49	1.42
24	v	310	CLA	C3B-C4B	2.94	1.49	1.42
25	AH	614	LUT	C8-C9	-2.94	1.39	1.45
34	o	101	SQD	C24-C23	2.94	1.59	1.50
23	AB	606	CHL	C3C-C2C	2.94	1.46	1.39
24	AC	612	CLA	C1B-C2B	2.94	1.50	1.43
24	AM	403	CLA	C4D-ND	-2.94	1.33	1.37
24	AA	602	CLA	C3B-C4B	2.94	1.49	1.42
24	AL	509	CLA	C3B-C4B	2.94	1.49	1.42
23	AN	608	CHL	C1B-NB	-2.93	1.34	1.37
24	AN	613	CLA	C3B-C4B	2.93	1.49	1.42
23	AQ	607	CHL	CHB-C1B	2.93	1.46	1.39
24	AE	609	CLA	C3B-C4B	2.93	1.49	1.42
24	AN	609	CLA	C3B-C4B	2.93	1.49	1.42
23	AQ	601	CHL	C3D-C2D	2.93	1.47	1.39
24	V	602	CLA	C4D-ND	-2.93	1.33	1.37
24	AQ	603	CLA	C4D-ND	-2.93	1.33	1.37
24	AN	603	CLA	C3B-C4B	2.93	1.49	1.42
29	O	619	BCR	C30-C25	-2.93	1.49	1.53
25	AA	614	LUT	C8-C9	-2.93	1.39	1.45
24	AE	608	CLA	C4D-ND	-2.93	1.33	1.37
23	AE	616	CHL	CHB-C1B	2.93	1.46	1.39
24	AN	603	CLA	C4D-ND	-2.93	1.33	1.37
23	AE	605	CHL	C3D-C2D	2.93	1.47	1.39
23	AE	605	CHL	CHB-C1B	2.93	1.46	1.39
24	AK	618	CLA	C3B-C4B	2.92	1.49	1.42
23	AR	605	CHL	C3D-C2D	2.92	1.47	1.39
23	v	308	CHL	C3D-C2D	2.92	1.47	1.39
24	9	613	CLA	C3B-C4B	2.92	1.49	1.42
24	AR	602	CLA	C3B-C4B	2.92	1.49	1.42
23	AH	607	CHL	C3D-C2D	2.92	1.47	1.39
25	AS	315	LUT	C8-C9	-2.92	1.39	1.45
24	p	611	CLA	C3B-C4B	2.92	1.49	1.42
24	v	305	CLA	C3B-C4B	2.92	1.49	1.42
24	AM	404	CLA	C3B-C4B	2.92	1.49	1.42
23	AB	606	CHL	C3D-C2D	2.92	1.47	1.39
24	AD	311	CLA	C3B-C4B	2.92	1.49	1.42
24	AS	305	CLA	C3B-C4B	2.92	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AK	607	CLA	C3B-C4B	2.92	1.49	1.42
24	v	311	CLA	C4D-ND	-2.92	1.33	1.37
24	O	605	CLA	C3B-C4B	2.92	1.49	1.42
24	v	303	CLA	C3B-C4B	2.92	1.49	1.42
24	AR	602	CLA	C4D-ND	-2.91	1.33	1.37
23	AF	608	CHL	C1D-C2D	2.91	1.51	1.45
24	P	504	CLA	C3B-C4B	2.91	1.49	1.42
24	AL	510	CLA	C4D-ND	-2.91	1.33	1.37
23	q	613	CHL	C1D-C2D	2.91	1.51	1.45
23	AU	607	CHL	C3D-C2D	2.91	1.47	1.39
24	V	612	CLA	C3B-C4B	2.91	1.49	1.42
24	Q	404	CLA	C4D-ND	-2.91	1.33	1.37
24	K	101	CLA	C3B-C4B	2.91	1.49	1.42
24	AN	604	CLA	C4D-ND	-2.91	1.33	1.37
24	AJ	404	CLA	C3B-C4B	2.91	1.49	1.42
29	AV	101	BCR	C30-C25	-2.91	1.49	1.53
24	p	604	CLA	C3B-C4B	2.91	1.49	1.42
24	P	508	CLA	C3B-C4B	2.91	1.49	1.42
24	AL	513	CLA	C4D-ND	-2.91	1.33	1.37
24	0	613	CLA	C3B-C4B	2.91	1.49	1.42
24	AD	311	CLA	C4D-ND	-2.91	1.33	1.37
24	0	610	CLA	C3B-C4B	2.90	1.49	1.42
24	AH	611	CLA	C4D-ND	-2.90	1.33	1.37
23	AF	601	CHL	C3D-C2D	2.90	1.47	1.39
24	v	304	CLA	C3B-C4B	2.90	1.49	1.42
23	AU	601	CHL	C3D-C2D	2.90	1.47	1.39
24	0	602	CLA	C3B-C4B	2.90	1.49	1.42
24	AF	604	CLA	C3B-C4B	2.90	1.49	1.42
24	AH	602	CLA	C3B-C4B	2.90	1.49	1.42
24	AK	608	CLA	C4D-ND	-2.90	1.33	1.37
24	AE	602	CLA	C3B-C4B	2.90	1.49	1.42
24	q	610	CLA	C3B-C4B	2.90	1.49	1.42
24	AL	505	CLA	C3B-C4B	2.90	1.49	1.42
24	AB	603	CLA	C4D-ND	-2.90	1.33	1.37
24	p	603	CLA	C4D-ND	-2.90	1.33	1.37
23	AC	601	CHL	C1B-NB	-2.90	1.34	1.37
24	AF	602	CLA	C3B-C4B	2.90	1.49	1.42
24	AL	511	CLA	C3B-C4B	2.90	1.49	1.42
24	AU	602	CLA	C3B-C4B	2.90	1.49	1.42
24	AK	617	CLA	C4D-ND	-2.90	1.33	1.37
24	q	604	CLA	C3B-C4B	2.90	1.49	1.42
24	AU	613	CLA	C4D-ND	-2.90	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AS	313	CLA	C3B-C4B	2.90	1.49	1.42
24	AL	510	CLA	C3B-C4B	2.90	1.49	1.42
24	P	506	CLA	C4D-ND	-2.90	1.33	1.37
29	AK	621	BCR	C30-C25	-2.90	1.49	1.53
23	AB	605	CHL	OBD-CAD	2.90	1.28	1.23
24	AK	604	CLA	C3B-C4B	2.90	1.49	1.42
23	AH	601	CHL	C3D-C2D	2.90	1.47	1.39
24	AA	603	CLA	C4D-ND	-2.90	1.33	1.37
24	AL	504	CLA	C4D-ND	-2.90	1.33	1.37
23	p	605	CHL	C3D-C2D	2.90	1.47	1.39
23	AH	606	CHL	C3D-C2D	2.90	1.47	1.39
23	q	605	CHL	C3D-C2D	2.90	1.47	1.39
24	AD	310	CLA	C4D-ND	-2.90	1.33	1.37
25	AS	316	LUT	C8-C9	-2.90	1.39	1.45
24	AA	604	CLA	C3B-C4B	2.90	1.49	1.42
23	AA	606	CHL	C3D-C2D	2.89	1.47	1.39
23	AD	308	CHL	C1D-C2D	2.89	1.51	1.45
24	P	510	CLA	C3B-C4B	2.89	1.49	1.42
23	p	607	CHL	C3D-C2D	2.89	1.47	1.39
23	9	601	CHL	C1B-NB	-2.89	1.34	1.37
23	V	606	CHL	C3D-C2D	2.89	1.47	1.39
24	AS	304	CLA	C4D-ND	-2.89	1.33	1.37
24	AQ	604	CLA	C3B-C4B	2.89	1.49	1.42
23	AU	606	CHL	C1D-C2D	2.89	1.51	1.45
38	f	102	HEM	CAC-C3C	2.89	1.55	1.47
24	AJ	405	CLA	C4D-ND	-2.89	1.33	1.37
24	AS	303	CLA	C3B-C4B	2.89	1.49	1.42
24	P	511	CLA	C3B-C4B	2.89	1.49	1.42
24	O	612	CLA	C4D-ND	-2.89	1.33	1.37
25	AU	614	LUT	C8-C9	-2.89	1.39	1.45
24	AA	609	CLA	C4D-ND	-2.89	1.33	1.37
23	q	607	CHL	C3D-C2D	2.89	1.47	1.39
24	AE	608	CLA	C3B-C4B	2.89	1.49	1.42
24	P	511	CLA	C4D-ND	-2.88	1.33	1.37
29	O	625	BCR	C30-C25	-2.88	1.49	1.53
24	AD	313	CLA	C3B-C4B	2.88	1.49	1.42
25	v	315	LUT	C8-C9	-2.88	1.39	1.45
24	AC	603	CLA	C3B-C4B	2.88	1.49	1.42
24	P	509	CLA	C3B-C4B	2.88	1.49	1.42
23	AD	301	CHL	C3D-C2D	2.88	1.47	1.39
23	AS	306	CHL	MG-NA	-2.88	1.99	2.06
23	9	607	CHL	C3D-C2D	2.88	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	602	CLA	C4D-ND	-2.88	1.33	1.37
24	P	503	CLA	C4D-ND	-2.88	1.33	1.37
24	V	610	CLA	C4D-ND	-2.88	1.33	1.37
24	AN	604	CLA	C3B-C4B	2.88	1.49	1.42
24	AB	604	CLA	C3B-C4B	2.88	1.49	1.42
24	AL	507	CLA	C3B-C4B	2.88	1.49	1.42
24	AS	304	CLA	C3B-C4B	2.88	1.49	1.42
24	AS	314	CLA	C3B-C4B	2.88	1.49	1.42
24	O	608	CLA	C4D-ND	-2.88	1.33	1.37
23	AF	608	CHL	C3B-C4B	2.88	1.49	1.42
24	0	612	CLA	C3B-C4B	2.88	1.49	1.42
29	AI	101	BCR	C30-C25	-2.88	1.49	1.53
24	9	603	CLA	C3B-C4B	2.88	1.49	1.42
24	v	304	CLA	C4D-ND	-2.88	1.33	1.37
24	AN	611	CLA	C4D-ND	-2.88	1.33	1.37
24	AK	609	CLA	C3B-C4B	2.88	1.49	1.42
24	9	604	CLA	C3B-C4B	2.88	1.49	1.42
27	AR	616	XAT	O24-C25	-2.88	1.42	1.46
24	9	612	CLA	C4D-ND	-2.87	1.33	1.37
24	AL	507	CLA	C4D-ND	-2.87	1.33	1.37
24	J	404	CLA	C4D-ND	-2.87	1.33	1.37
24	AE	604	CLA	C3B-C4B	2.87	1.49	1.42
27	AR	616	XAT	O4-C5	-2.87	1.42	1.46
24	AN	602	CLA	C3B-C4B	2.87	1.49	1.42
25	AQ	616	LUT	C8-C9	-2.87	1.39	1.45
24	AS	310	CLA	C4D-ND	-2.87	1.33	1.37
24	AU	602	CLA	C4D-ND	-2.87	1.33	1.37
24	P	506	CLA	C3B-C4B	2.87	1.49	1.42
24	9	614	CLA	C4D-ND	-2.87	1.33	1.37
23	AS	308	CHL	C1D-C2D	2.87	1.51	1.45
24	AD	310	CLA	C3B-C4B	2.87	1.49	1.42
23	AN	606	CHL	C3D-C2D	2.87	1.46	1.39
24	O	602	CLA	C3B-C4B	2.87	1.49	1.42
24	AL	513	CLA	C3B-C4B	2.87	1.49	1.42
24	AR	611	CLA	C4D-ND	-2.86	1.33	1.37
24	AA	612	CLA	C3B-C4B	2.86	1.49	1.42
24	AE	610	CLA	C4D-ND	-2.86	1.33	1.37
24	AS	313	CLA	C4D-ND	-2.86	1.33	1.37
24	O	607	CLA	C3B-C4B	2.86	1.49	1.42
24	AK	618	CLA	C4D-ND	-2.86	1.33	1.37
24	AH	604	CLA	C3B-C4B	2.86	1.49	1.42
24	AL	504	CLA	C3B-C4B	2.86	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AS	312	CLA	C4D-ND	-2.86	1.33	1.37
25	0	614	LUT	C8-C9	-2.86	1.39	1.45
25	p	615	LUT	C8-C9	-2.86	1.39	1.45
23	AS	306	CHL	OBD-CAD	2.86	1.28	1.22
24	v	312	CLA	C4D-ND	-2.86	1.33	1.37
23	AQ	605	CHL	C3D-C2D	2.86	1.46	1.39
27	AB	613	XAT	O4-C5	-2.86	1.42	1.46
24	q	609	CLA	C4D-ND	-2.86	1.33	1.37
24	AL	503	CLA	C4D-ND	-2.86	1.33	1.37
24	AD	312	CLA	C3B-C4B	2.86	1.49	1.42
24	AE	609	CLA	C4D-ND	-2.86	1.33	1.37
23	q	613	CHL	C3A-C2A	-2.86	1.51	1.54
23	V	601	CHL	C3D-C2D	2.86	1.46	1.39
24	AJ	405	CLA	C3B-C4B	2.86	1.49	1.42
23	AQ	607	CHL	C3D-C2D	2.85	1.46	1.39
24	AH	613	CLA	C3B-C4B	2.85	1.49	1.42
24	AL	508	CLA	C3B-C4B	2.85	1.49	1.42
27	AF	613	XAT	O24-C25	-2.85	1.42	1.46
27	q	617	XAT	O24-C25	-2.85	1.42	1.46
23	AD	306	CHL	C3D-C2D	2.85	1.46	1.39
24	O	616	CLA	C4D-ND	-2.85	1.33	1.37
24	P	502	CLA	C3B-C4B	2.85	1.49	1.42
24	V	603	CLA	C4D-ND	-2.85	1.33	1.37
24	P	509	CLA	C4D-ND	-2.85	1.33	1.37
23	AC	606	CHL	C1D-C2D	2.85	1.51	1.45
24	V	611	CLA	C3B-C4B	2.85	1.49	1.42
24	J	404	CLA	C3B-C4B	2.85	1.49	1.42
24	0	610	CLA	C1B-C2B	2.85	1.50	1.43
24	AD	313	CLA	C1B-C2B	2.85	1.50	1.43
23	AE	601	CHL	C3D-C2D	2.85	1.46	1.39
24	O	614	CLA	C1B-C2B	2.85	1.50	1.43
24	AK	615	CLA	C4D-ND	-2.85	1.33	1.37
24	q	604	CLA	C4D-ND	-2.85	1.33	1.37
24	AL	503	CLA	C3B-C4B	2.85	1.49	1.42
24	AC	602	CLA	C3B-C4B	2.85	1.49	1.42
24	O	603	CLA	C1B-C2B	2.85	1.50	1.43
24	q	602	CLA	C4D-ND	-2.85	1.33	1.37
23	AN	608	CHL	C1D-C2D	2.85	1.50	1.45
24	AK	614	CLA	C4D-ND	-2.85	1.33	1.37
23	v	307	CHL	C3D-C2D	2.84	1.46	1.39
24	v	314	CLA	C3B-C4B	2.84	1.49	1.42
24	P	510	CLA	C4D-ND	-2.84	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AD	302	CHL	C3B-C4B	2.84	1.49	1.42
24	AK	616	CLA	C3B-C4B	2.84	1.49	1.42
24	AB	610	CLA	C4D-ND	-2.84	1.33	1.37
24	v	313	CLA	C4D-ND	-2.84	1.33	1.37
24	AU	612	CLA	C3B-C4B	2.84	1.49	1.42
29	AK	602	BCR	C30-C25	-2.84	1.49	1.53
23	9	608	CHL	C3C-C2C	2.84	1.46	1.39
24	AK	611	CLA	C1B-C2B	2.84	1.49	1.43
38	F	102	HEM	CAC-C3C	2.84	1.55	1.47
23	AU	601	CHL	C1D-C2D	2.84	1.50	1.45
23	AS	302	CHL	CHC-C4B	2.83	1.47	1.40
23	AA	601	CHL	C3D-C2D	2.83	1.46	1.39
24	AA	611	CLA	C4D-ND	-2.83	1.33	1.37
24	AU	604	CLA	C3B-C4B	2.83	1.49	1.42
23	AC	607	CHL	C3C-C2C	2.83	1.46	1.39
24	AK	616	CLA	C1B-C2B	2.83	1.49	1.43
23	AB	608	CHL	OBD-CAD	2.83	1.28	1.23
24	P	507	CLA	C3B-C4B	2.83	1.49	1.42
24	AR	610	CLA	C3B-C4B	2.83	1.49	1.42
23	AA	605	CHL	C3B-C4B	2.83	1.49	1.42
23	AE	617	CHL	C3B-C4B	2.83	1.49	1.42
24	AD	305	CLA	C3B-C4B	2.83	1.49	1.42
24	9	602	CLA	C1B-C2B	2.83	1.49	1.43
23	V	607	CHL	C3D-C2D	2.83	1.46	1.39
24	q	611	CLA	C4D-ND	-2.83	1.33	1.37
24	AN	602	CLA	C1B-C2B	2.83	1.49	1.43
24	AR	617	CLA	C3B-C4B	2.83	1.49	1.42
24	9	612	CLA	C3B-C4B	2.83	1.49	1.42
24	AB	604	CLA	C4D-ND	-2.83	1.33	1.37
24	AE	603	CLA	C4D-ND	-2.83	1.33	1.37
24	0	604	CLA	C3B-C4B	2.83	1.49	1.42
24	0	609	CLA	C3B-C4B	2.83	1.49	1.42
24	AC	604	CLA	C3B-C4B	2.83	1.49	1.42
23	9	601	CHL	C3D-C2D	2.83	1.46	1.39
24	AK	605	CLA	C3B-C4B	2.83	1.49	1.42
24	AD	309	CLA	C3B-C4B	2.83	1.49	1.42
24	0	610	CLA	C4D-ND	-2.83	1.33	1.37
24	AA	610	CLA	C4D-ND	-2.83	1.33	1.37
24	AN	610	CLA	C4D-ND	-2.83	1.33	1.37
27	9	618	XAT	O24-C25	-2.83	1.42	1.46
24	9	603	CLA	C4D-ND	-2.83	1.33	1.37
24	AU	613	CLA	C3B-C4B	2.83	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AR	609	CLA	C1B-C2B	2.83	1.49	1.43
24	AD	304	CLA	C3B-C4B	2.82	1.49	1.42
23	AN	601	CHL	C3D-C2D	2.82	1.46	1.39
24	AH	602	CLA	C4D-ND	-2.82	1.33	1.37
24	AL	508	CLA	C4D-ND	-2.82	1.33	1.37
25	AQ	615	LUT	C8-C9	-2.82	1.39	1.45
24	AC	611	CLA	C3B-C4B	2.82	1.49	1.42
23	AH	605	CHL	C3D-C2D	2.82	1.46	1.39
23	AF	605	CHL	OBD-CAD	2.82	1.28	1.23
23	v	306	CHL	OBD-CAD	2.82	1.28	1.23
24	P	503	CLA	C3B-C4B	2.82	1.49	1.42
24	AK	614	CLA	C1B-C2B	2.82	1.49	1.43
24	AA	602	CLA	C4D-ND	-2.82	1.33	1.37
24	AR	603	CLA	C4D-ND	-2.82	1.33	1.37
23	v	302	CHL	CHC-C4B	2.82	1.47	1.40
24	O	602	CLA	C4D-ND	-2.82	1.33	1.37
24	AQ	611	CLA	C4D-ND	-2.82	1.33	1.37
25	v	316	LUT	C8-C9	-2.82	1.39	1.45
23	AC	601	CHL	C3D-C2D	2.82	1.46	1.39
23	AN	608	CHL	MG-NA	-2.81	1.99	2.06
24	Q	404	CLA	C3B-C4B	2.81	1.49	1.42
24	AC	602	CLA	C4D-ND	-2.81	1.33	1.37
24	AE	604	CLA	C4D-ND	-2.81	1.33	1.37
27	q	617	XAT	O4-C5	-2.81	1.42	1.46
24	AK	605	CLA	C1B-C2B	2.81	1.49	1.43
24	AS	310	CLA	C3B-C4B	2.81	1.49	1.42
24	AH	612	CLA	C3B-C4B	2.81	1.49	1.42
24	AD	303	CLA	C4D-ND	-2.81	1.33	1.37
23	AQ	609	CHL	C3D-C2D	2.81	1.46	1.39
24	AB	611	CLA	C3B-C4B	2.81	1.49	1.42
23	AB	605	CHL	C1D-C2D	2.81	1.50	1.45
23	AE	607	CHL	C3D-C2D	2.80	1.46	1.39
23	AR	613	CHL	C1D-C2D	2.80	1.50	1.45
23	AD	308	CHL	C3D-C2D	2.80	1.46	1.39
23	0	601	CHL	C1D-C2D	2.80	1.50	1.45
24	V	602	CLA	C3B-C4B	2.80	1.49	1.42
24	v	313	CLA	C3B-C4B	2.80	1.49	1.42
25	p	614	LUT	C8-C9	-2.80	1.39	1.45
24	AS	310	CLA	C1B-C2B	2.80	1.49	1.43
24	AA	609	CLA	C3B-C4B	2.80	1.49	1.42
24	AE	611	CLA	C3B-C4B	2.80	1.49	1.42
24	AQ	602	CLA	C4D-ND	-2.80	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AU	615	LUT	C8-C9	-2.80	1.39	1.45
23	AC	608	CHL	C3D-C2D	2.80	1.46	1.39
24	V	602	CLA	C1B-C2B	2.80	1.49	1.43
24	P	507	CLA	C4D-ND	-2.80	1.33	1.37
23	p	608	CHL	C3D-C2D	2.80	1.46	1.39
23	AB	601	CHL	C1D-C2D	2.80	1.50	1.45
24	O	603	CLA	C3B-C4B	2.80	1.49	1.42
24	P	502	CLA	C4D-ND	-2.80	1.33	1.37
23	AH	601	CHL	C1D-C2D	2.80	1.50	1.45
24	v	314	CLA	C4D-ND	-2.80	1.33	1.37
24	AF	610	CLA	C3B-C4B	2.80	1.49	1.42
24	p	602	CLA	C4D-ND	-2.80	1.33	1.37
25	AN	615	LUT	C8-C9	-2.79	1.39	1.45
23	V	608	CHL	C1D-C2D	2.79	1.50	1.45
25	AF	611	LUT	C32-C33	-2.79	1.39	1.45
23	AN	607	CHL	C3D-C2D	2.79	1.46	1.39
24	O	614	CLA	C4D-ND	-2.79	1.33	1.37
24	O	614	CLA	C3B-C4B	2.79	1.49	1.42
24	AH	603	CLA	C4D-ND	-2.79	1.33	1.37
24	AK	609	CLA	C4D-ND	-2.79	1.33	1.37
27	AB	613	XAT	O24-C25	-2.79	1.42	1.46
24	AR	612	CLA	C1B-C2B	2.79	1.49	1.43
24	AK	606	CLA	C3B-C4B	2.79	1.49	1.42
24	0	603	CLA	C3B-C4B	2.79	1.49	1.42
23	p	606	CHL	C3D-C2D	2.79	1.46	1.39
24	AE	612	CLA	C4D-ND	-2.79	1.33	1.37
24	AB	602	CLA	C1B-C2B	2.79	1.49	1.43
24	AL	511	CLA	C4D-ND	-2.79	1.33	1.37
24	O	604	CLA	C3B-C4B	2.79	1.49	1.42
24	P	508	CLA	C4D-ND	-2.79	1.33	1.37
24	p	613	CLA	C4D-ND	-2.79	1.33	1.37
23	AU	605	CHL	C3D-C2D	2.78	1.46	1.39
24	q	608	CLA	C4D-ND	-2.78	1.33	1.37
24	9	602	CLA	C4D-ND	-2.78	1.33	1.37
23	AF	608	CHL	C1B-C2B	2.78	1.49	1.43
24	AE	602	CLA	C4D-ND	-2.78	1.33	1.37
24	V	612	CLA	C1B-C2B	2.78	1.49	1.43
24	AK	613	CLA	C1B-C2B	2.78	1.49	1.43
23	AA	605	CHL	C3D-C2D	2.78	1.46	1.39
23	v	306	CHL	C1D-C2D	2.78	1.50	1.45
24	AA	613	CLA	C4D-ND	-2.78	1.33	1.37
23	AE	617	CHL	CHB-C1B	2.78	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	v	308	CHL	C1D-C2D	2.78	1.50	1.45
23	AQ	606	CHL	C3D-C2D	2.78	1.46	1.39
24	AF	614	CLA	C3B-C4B	2.78	1.49	1.42
24	AU	612	CLA	C4D-ND	-2.78	1.33	1.37
27	9	618	XAT	O4-C5	-2.78	1.42	1.46
23	0	605	CHL	C3D-C2D	2.78	1.46	1.39
24	9	612	CLA	C1B-C2B	2.78	1.49	1.43
23	AB	607	CHL	C1D-C2D	2.77	1.50	1.45
23	9	601	CHL	CHC-C4B	2.77	1.47	1.40
24	AK	610	CLA	C4D-ND	-2.77	1.33	1.37
24	AH	602	CLA	C1B-C2B	2.77	1.49	1.43
23	AE	606	CHL	C3D-C2D	2.77	1.46	1.39
25	AC	614	LUT	C8-C9	-2.77	1.40	1.45
24	O	612	CLA	C1B-C2B	2.77	1.49	1.43
24	AQ	613	CLA	C3B-C4B	2.77	1.49	1.42
24	9	611	CLA	C4D-ND	-2.77	1.33	1.37
24	AB	602	CLA	C3B-C4B	2.77	1.49	1.42
25	9	615	LUT	C8-C9	-2.77	1.40	1.45
25	AD	314	LUT	C8-C9	-2.77	1.40	1.45
24	AN	613	CLA	C1B-C2B	2.77	1.49	1.43
24	V	611	CLA	C4D-ND	-2.77	1.33	1.37
24	9	602	CLA	C3B-C4B	2.77	1.49	1.42
24	O	613	CLA	C4D-ND	-2.77	1.33	1.37
24	AM	404	CLA	C4D-ND	-2.77	1.33	1.37
25	AR	614	LUT	C8-C9	-2.77	1.40	1.45
23	p	607	CHL	C3B-C4B	2.77	1.49	1.42
24	AQ	613	CLA	C1B-C2B	2.77	1.49	1.43
24	AS	313	CLA	C1B-C2B	2.77	1.49	1.43
24	AL	509	CLA	C4D-ND	-2.77	1.33	1.37
24	AS	303	CLA	C4D-ND	-2.77	1.33	1.37
27	AF	613	XAT	O4-C5	-2.77	1.42	1.46
23	V	607	CHL	CHC-C4B	2.77	1.47	1.40
24	AR	609	CLA	C3B-C4B	2.77	1.49	1.42
24	AK	606	CLA	C4D-ND	-2.76	1.33	1.37
24	AK	612	CLA	C4D-ND	-2.76	1.33	1.37
23	AS	308	CHL	C3D-C2D	2.76	1.46	1.39
24	v	303	CLA	C4D-ND	-2.76	1.33	1.37
24	AF	603	CLA	C1B-C2B	2.76	1.49	1.43
25	AH	615	LUT	C8-C9	-2.76	1.40	1.45
24	AR	610	CLA	C1B-C2B	2.76	1.49	1.43
23	0	606	CHL	C3B-C4B	2.76	1.49	1.42
24	q	610	CLA	C4D-ND	-2.76	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AK	616	CLA	C4D-ND	-2.76	1.33	1.37
24	P	502	CLA	C1B-C2B	2.76	1.49	1.43
24	0	613	CLA	C4D-ND	-2.76	1.33	1.37
23	0	617	CHL	C4C-C3C	2.76	1.49	1.45
24	O	602	CLA	C1B-C2B	2.76	1.49	1.43
23	AE	616	CHL	C1B-NB	-2.75	1.34	1.37
23	AA	601	CHL	C3B-C4B	2.75	1.49	1.42
24	AL	503	CLA	C1B-C2B	2.75	1.49	1.43
23	AC	601	CHL	CHC-C4B	2.75	1.47	1.40
23	AA	617	CHL	C3B-C4B	2.75	1.49	1.42
24	AB	611	CLA	C1B-C2B	2.75	1.49	1.43
24	AS	305	CLA	C1B-C2B	2.75	1.49	1.43
24	AD	304	CLA	C4D-ND	-2.75	1.33	1.37
24	AL	506	CLA	C1B-C2B	2.75	1.49	1.43
24	AL	505	CLA	C1B-C2B	2.75	1.49	1.43
23	AD	317	CHL	C4C-C3C	2.75	1.49	1.45
23	AN	605	CHL	C3D-C2D	2.75	1.46	1.39
23	9	608	CHL	C3D-C2D	2.75	1.46	1.39
24	AS	314	CLA	C4D-ND	-2.75	1.33	1.37
24	AU	602	CLA	C1B-C2B	2.75	1.49	1.43
23	AR	605	CHL	C1D-C2D	2.75	1.50	1.45
24	AR	608	CLA	C4D-ND	-2.74	1.33	1.37
24	AS	309	CLA	C4D-ND	-2.74	1.33	1.37
24	q	612	CLA	C1B-C2B	2.74	1.49	1.43
24	9	614	CLA	C1B-C2B	2.74	1.49	1.43
24	AH	604	CLA	C1B-C2B	2.74	1.49	1.43
23	0	608	CHL	C1D-C2D	2.74	1.50	1.45
24	O	601	CLA	C4D-ND	-2.74	1.33	1.37
24	AU	604	CLA	C1B-C2B	2.74	1.49	1.43
23	AS	306	CHL	C3B-C4B	2.74	1.49	1.42
24	P	505	CLA	C3B-C4B	2.74	1.49	1.42
24	AR	604	CLA	C4D-ND	-2.74	1.33	1.37
24	P	503	CLA	C1B-C2B	2.74	1.49	1.43
23	AA	608	CHL	C3B-C4B	2.74	1.49	1.42
24	AQ	614	CLA	C4D-ND	-2.74	1.33	1.37
24	q	610	CLA	C1B-C2B	2.74	1.49	1.43
23	AR	607	CHL	C1D-C2D	2.74	1.50	1.45
24	p	612	CLA	C4D-ND	-2.74	1.33	1.37
23	AF	605	CHL	C3B-C4B	2.74	1.49	1.42
23	AC	605	CHL	C3D-C2D	2.74	1.46	1.39
24	0	602	CLA	C4D-ND	-2.74	1.33	1.37
24	P	504	CLA	C1B-C2B	2.74	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	609	CLA	C1B-C2B	2.73	1.49	1.43
24	AH	613	CLA	C4D-ND	-2.73	1.33	1.37
23	9	606	CHL	C3B-C4B	2.73	1.49	1.42
23	q	607	CHL	C1D-C2D	2.73	1.50	1.45
24	AR	610	CLA	C4D-ND	-2.73	1.33	1.37
23	AN	607	CHL	C3B-C4B	2.73	1.49	1.42
24	AH	612	CLA	C4D-ND	-2.73	1.33	1.37
24	AL	506	CLA	C3B-C4B	2.73	1.49	1.42
23	AU	608	CHL	C3D-C2D	2.73	1.46	1.39
24	AC	602	CLA	C1B-C2B	2.73	1.49	1.43
24	AA	604	CLA	C4D-ND	-2.73	1.33	1.37
24	AL	514	CLA	C4D-ND	-2.73	1.33	1.37
24	AK	618	CLA	C1B-C2B	2.73	1.49	1.43
24	0	612	CLA	C4D-ND	-2.73	1.33	1.37
24	AC	612	CLA	C3B-C4B	2.73	1.49	1.42
24	AH	613	CLA	C1B-C2B	2.73	1.49	1.43
24	AN	610	CLA	C1B-C2B	2.73	1.49	1.43
24	V	609	CLA	C1B-C2B	2.73	1.49	1.43
23	AH	601	CHL	C3B-C4B	2.73	1.49	1.42
24	AC	603	CLA	C1B-C2B	2.73	1.49	1.43
24	AR	612	CLA	C3B-C4B	2.73	1.49	1.42
24	AD	311	CLA	C1B-C2B	2.73	1.49	1.43
24	AU	603	CLA	C4D-ND	-2.73	1.33	1.37
23	9	605	CHL	C3D-C2D	2.73	1.46	1.39
24	O	612	CLA	C3B-C4B	2.73	1.49	1.42
23	AH	608	CHL	C3D-C2D	2.72	1.46	1.39
24	AB	610	CLA	C1B-C2B	2.72	1.49	1.43
24	O	604	CLA	C4D-ND	-2.72	1.33	1.37
24	AU	610	CLA	C4D-ND	-2.72	1.33	1.37
24	AK	609	CLA	C1B-C2B	2.72	1.49	1.43
24	V	609	CLA	C3B-C4B	2.72	1.49	1.42
24	9	603	CLA	C1B-C2B	2.72	1.49	1.43
24	AA	602	CLA	C1B-C2B	2.72	1.49	1.43
25	AF	611	LUT	C12-C13	-2.72	1.40	1.45
23	AC	606	CHL	C3B-C4B	2.72	1.49	1.42
24	9	613	CLA	C1B-C2B	2.72	1.49	1.43
23	AR	606	CHL	C1D-C2D	2.72	1.50	1.45
24	AH	604	CLA	C4D-ND	-2.72	1.33	1.37
23	p	608	CHL	C3B-C4B	2.72	1.49	1.42
24	O	607	CLA	C4D-ND	-2.72	1.33	1.37
23	AD	317	CHL	C1D-C2D	2.72	1.50	1.45
24	AK	606	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	O	607	CLA	C1B-C2B	2.72	1.49	1.43
24	AQ	604	CLA	C4D-ND	-2.72	1.34	1.37
23	AA	607	CHL	C3D-C2D	2.72	1.46	1.39
25	V	614	LUT	C8-C9	-2.72	1.40	1.45
23	AD	317	CHL	C3B-C4B	2.72	1.49	1.42
24	0	603	CLA	C1B-C2B	2.72	1.49	1.43
24	O	615	CLA	C4D-ND	-2.72	1.34	1.37
24	AS	312	CLA	C1B-C2B	2.72	1.49	1.43
23	0	605	CHL	C3B-C4B	2.72	1.49	1.42
23	AC	607	CHL	C3D-C2D	2.71	1.46	1.39
25	V	613	LUT	C28-C29	-2.71	1.40	1.45
24	O	604	CLA	C1B-C2B	2.71	1.49	1.43
24	AR	609	CLA	C4D-ND	-2.71	1.34	1.37
24	P	512	CLA	C4D-ND	-2.71	1.34	1.37
24	AD	305	CLA	C1B-C2B	2.71	1.49	1.43
24	AR	604	CLA	C1B-C2B	2.71	1.49	1.43
23	AQ	607	CHL	C3B-C4B	2.71	1.49	1.42
23	AQ	608	CHL	C3D-C2D	2.71	1.46	1.39
23	AE	605	CHL	C3B-C4B	2.71	1.49	1.42
24	AQ	610	CLA	C4D-ND	-2.71	1.34	1.37
23	AB	607	CHL	C3B-C4B	2.71	1.49	1.42
23	AQ	609	CHL	C1D-C2D	2.71	1.50	1.45
24	AU	612	CLA	C1B-C2B	2.71	1.49	1.43
24	AC	611	CLA	C1B-C2B	2.71	1.49	1.43
24	v	313	CLA	C1B-C2B	2.71	1.49	1.43
24	O	606	CLA	C4D-ND	-2.71	1.34	1.37
24	AK	614	CLA	C3B-C4B	2.71	1.49	1.42
24	AE	612	CLA	C1B-C2B	2.71	1.49	1.43
23	AE	617	CHL	C1B-NB	-2.71	1.34	1.37
24	AD	304	CLA	C1B-C2B	2.71	1.49	1.43
24	AJ	409	CLA	C1B-C2B	2.71	1.49	1.43
24	0	602	CLA	C1B-C2B	2.71	1.49	1.43
24	9	604	CLA	C1B-C2B	2.70	1.49	1.43
23	AN	606	CHL	C3B-C4B	2.70	1.49	1.42
25	AE	614	LUT	C8-C9	-2.70	1.40	1.45
24	AS	314	CLA	C1B-C2B	2.70	1.49	1.43
23	AE	616	CHL	C3B-C4B	2.70	1.49	1.42
24	AU	603	CLA	C1B-C2B	2.70	1.49	1.43
24	AD	312	CLA	C4D-ND	-2.70	1.34	1.37
24	AA	613	CLA	C1B-C2B	2.70	1.49	1.43
23	AE	606	CHL	C1D-C2D	2.70	1.50	1.45
23	AC	606	CHL	C3D-C2D	2.70	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AE	611	CLA	C4D-ND	-2.70	1.34	1.37
24	v	309	CLA	C4D-ND	-2.70	1.34	1.37
23	v	306	CHL	C3B-C4B	2.70	1.49	1.42
23	AU	601	CHL	C3B-C4B	2.70	1.49	1.42
24	P	505	CLA	C1B-C2B	2.70	1.49	1.43
24	AU	613	CLA	C1B-C2B	2.70	1.49	1.43
23	AF	601	CHL	C1D-C2D	2.70	1.50	1.45
24	AS	303	CLA	C1B-C2B	2.70	1.49	1.43
23	AE	601	CHL	C3B-C4B	2.70	1.49	1.42
23	v	308	CHL	C3B-C4B	2.70	1.49	1.42
24	O	616	CLA	C1B-C2B	2.70	1.49	1.43
24	AL	512	CLA	C1B-C2B	2.70	1.49	1.43
24	0	604	CLA	C1B-C2B	2.70	1.49	1.43
24	0	611	CLA	C1B-C2B	2.70	1.49	1.43
24	AA	604	CLA	C1B-C2B	2.70	1.49	1.43
24	AD	312	CLA	C1B-C2B	2.70	1.49	1.43
24	O	615	CLA	C1B-C2B	2.70	1.49	1.43
24	v	305	CLA	C1B-C2B	2.70	1.49	1.43
23	AE	605	CHL	C1D-C2D	2.70	1.50	1.45
23	p	601	CHL	C1D-C2D	2.70	1.50	1.45
23	9	606	CHL	C4C-C3C	2.70	1.49	1.45
24	p	602	CLA	C1B-C2B	2.69	1.49	1.43
24	AQ	602	CLA	C1B-C2B	2.69	1.49	1.43
24	O	605	CLA	C1B-C2B	2.69	1.49	1.43
24	0	613	CLA	C1B-C2B	2.69	1.49	1.43
24	AC	604	CLA	C1B-C2B	2.69	1.49	1.43
24	Q	404	CLA	C1B-C2B	2.69	1.49	1.43
24	AU	604	CLA	C4D-ND	-2.69	1.34	1.37
24	AK	607	CLA	C1B-C2B	2.69	1.49	1.43
24	AK	605	CLA	C4D-ND	-2.69	1.34	1.37
24	AQ	604	CLA	C1B-C2B	2.69	1.49	1.43
24	AU	610	CLA	C1B-C2B	2.69	1.49	1.43
24	AF	604	CLA	C4D-ND	-2.69	1.34	1.37
24	v	312	CLA	C1B-C2B	2.69	1.49	1.43
24	AR	611	CLA	C1B-C2B	2.69	1.49	1.43
25	AE	613	LUT	C32-C33	-2.69	1.40	1.45
24	O	609	CLA	C1B-C2B	2.69	1.49	1.43
25	AE	613	LUT	C12-C13	-2.69	1.40	1.45
23	AQ	601	CHL	C1D-C2D	2.69	1.50	1.45
24	AQ	613	CLA	C4D-ND	-2.68	1.34	1.37
24	J	407	CLA	C1B-C2B	2.68	1.49	1.43
24	V	612	CLA	C4D-ND	-2.68	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AL	504	CLA	C1B-C2B	2.68	1.49	1.43
23	AA	607	CHL	C1D-C2D	2.68	1.50	1.45
24	AL	510	CLA	C1B-C2B	2.68	1.49	1.43
24	v	314	CLA	C1B-C2B	2.68	1.49	1.43
23	V	605	CHL	C3D-C2D	2.68	1.46	1.39
23	AB	605	CHL	C3B-C4B	2.68	1.49	1.42
24	K	101	CLA	C1B-C2B	2.68	1.49	1.43
23	AC	608	CHL	C3B-C4B	2.68	1.49	1.42
24	P	509	CLA	C1B-C2B	2.68	1.49	1.43
24	p	604	CLA	C1B-C2B	2.68	1.49	1.43
24	AH	610	CLA	C1B-C2B	2.68	1.49	1.43
23	AQ	601	CHL	C3B-C4B	2.68	1.49	1.42
24	P	510	CLA	C1B-C2B	2.68	1.49	1.43
24	AJ	405	CLA	C1B-C2B	2.68	1.49	1.43
23	V	605	CHL	C1D-C2D	2.68	1.50	1.45
24	q	603	CLA	C4D-ND	-2.68	1.34	1.37
24	AN	604	CLA	C1B-C2B	2.68	1.49	1.43
24	J	404	CLA	C1B-C2B	2.67	1.49	1.43
24	AL	511	CLA	C1B-C2B	2.67	1.49	1.43
23	9	605	CHL	C1D-C2D	2.67	1.50	1.45
25	AA	614	LUT	C28-C29	-2.67	1.40	1.45
25	AA	614	LUT	C32-C33	-2.67	1.40	1.45
23	AR	606	CHL	C3B-C4B	2.67	1.49	1.42
24	p	603	CLA	C1B-C2B	2.67	1.49	1.43
23	AB	606	CHL	C1D-C2D	2.67	1.50	1.45
24	AC	613	CLA	C1B-C2B	2.67	1.49	1.43
24	p	611	CLA	C1B-C2B	2.67	1.49	1.43
24	AR	602	CLA	C1B-C2B	2.67	1.49	1.43
23	AQ	608	CHL	C1D-C2D	2.67	1.50	1.45
24	AA	612	CLA	C4D-ND	-2.67	1.34	1.37
24	AH	610	CLA	C4D-ND	-2.67	1.34	1.37
24	p	604	CLA	C4D-ND	-2.67	1.34	1.37
23	q	606	CHL	C1D-C2D	2.66	1.50	1.45
23	p	601	CHL	C3B-C4B	2.66	1.49	1.42
24	v	310	CLA	C1B-C2B	2.66	1.49	1.43
24	AD	303	CLA	C1B-C2B	2.66	1.49	1.43
24	AQ	614	CLA	C1B-C2B	2.66	1.49	1.43
23	AU	606	CHL	C3D-C2D	2.66	1.46	1.39
23	p	609	CHL	C1D-C2D	2.66	1.50	1.45
23	AN	608	CHL	C1B-C2B	2.66	1.49	1.43
25	0	615	LUT	C8-C9	-2.66	1.40	1.45
24	O	609	CLA	C4D-ND	-2.66	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	v	309	CLA	C1B-C2B	2.66	1.49	1.43
23	AB	601	CHL	C3B-C4B	2.66	1.49	1.42
24	P	504	CLA	C4D-ND	-2.66	1.34	1.37
23	AD	302	CHL	C1D-C2D	2.66	1.50	1.45
23	9	606	CHL	C3D-C2D	2.66	1.46	1.39
24	q	611	CLA	C1B-C2B	2.66	1.49	1.43
23	V	608	CHL	C3B-C4B	2.66	1.49	1.42
24	AB	604	CLA	C1B-C2B	2.66	1.49	1.43
24	AJ	406	CLA	C1B-C2B	2.66	1.49	1.43
23	AN	601	CHL	C1D-C2D	2.66	1.50	1.45
24	AE	608	CLA	C1B-C2B	2.65	1.49	1.43
24	AE	604	CLA	C1B-C2B	2.65	1.49	1.43
24	AK	603	CLA	C4D-ND	-2.65	1.34	1.37
23	q	613	CHL	C3B-C4B	2.65	1.49	1.42
24	AK	617	CLA	C1B-C2B	2.65	1.49	1.43
24	AA	611	CLA	C1B-C2B	2.65	1.49	1.43
24	AF	604	CLA	C1B-C2B	2.65	1.49	1.43
23	AS	302	CHL	C1D-C2D	2.65	1.50	1.45
24	AM	404	CLA	C1B-C2B	2.65	1.49	1.43
25	AC	615	LUT	C8-C9	-2.65	1.40	1.45
24	AR	612	CLA	C4D-ND	-2.65	1.34	1.37
24	AQ	603	CLA	C1B-C2B	2.65	1.49	1.43
24	AK	604	CLA	C4D-ND	-2.65	1.34	1.37
24	AH	603	CLA	C1B-C2B	2.65	1.49	1.43
24	AH	612	CLA	C1B-C2B	2.65	1.49	1.43
24	J	403	CLA	C4D-ND	-2.65	1.34	1.37
23	AB	608	CHL	C1B-C2B	2.65	1.49	1.43
23	AR	605	CHL	C1B-C2B	2.65	1.49	1.43
24	AE	610	CLA	C1B-C2B	2.65	1.49	1.43
24	AL	508	CLA	C1B-C2B	2.65	1.49	1.43
24	AL	509	CLA	C1B-C2B	2.65	1.49	1.43
23	AE	601	CHL	C1D-C2D	2.65	1.50	1.45
23	q	605	CHL	C1D-C2D	2.65	1.50	1.45
23	V	607	CHL	C1D-C2D	2.64	1.50	1.45
23	AQ	608	CHL	C3B-C4B	2.64	1.49	1.42
24	Q	401	CLA	C1B-C2B	2.64	1.49	1.43
23	p	608	CHL	C1D-C2D	2.64	1.50	1.45
24	AB	611	CLA	C4D-ND	-2.64	1.34	1.37
24	J	407	CLA	C4D-ND	-2.64	1.34	1.37
24	AS	305	CLA	C4D-ND	-2.64	1.34	1.37
23	V	606	CHL	C3B-C4B	2.64	1.48	1.42
23	AU	606	CHL	C3B-C4B	2.64	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	603	CLA	C1B-C2B	2.64	1.49	1.43
24	v	303	CLA	C1B-C2B	2.64	1.49	1.43
24	AE	602	CLA	C1B-C2B	2.64	1.49	1.43
24	O	603	CLA	C4D-ND	-2.64	1.34	1.37
23	AE	607	CHL	C1D-C2D	2.64	1.50	1.45
24	AS	304	CLA	C1B-C2B	2.64	1.49	1.43
24	9	604	CLA	C4D-ND	-2.64	1.34	1.37
23	AN	607	CHL	C1D-C2D	2.64	1.50	1.45
24	v	304	CLA	C1B-C2B	2.64	1.49	1.43
24	AR	601	CLA	C4D-ND	-2.64	1.34	1.37
23	9	609	CHL	C1D-C2D	2.64	1.50	1.45
24	AD	310	CLA	C1B-C2B	2.64	1.49	1.43
23	AA	608	CHL	C1B-C2B	2.64	1.49	1.43
23	AR	607	CHL	C3B-C4B	2.64	1.48	1.42
24	V	611	CLA	C1B-C2B	2.64	1.49	1.43
23	q	606	CHL	C3B-C4B	2.64	1.48	1.42
23	0	607	CHL	C1D-C2D	2.64	1.50	1.45
23	AC	608	CHL	C1D-C2D	2.64	1.50	1.45
23	0	607	CHL	C3D-C2D	2.63	1.46	1.39
23	AH	608	CHL	C3B-C4B	2.63	1.48	1.42
24	AS	309	CLA	C1B-C2B	2.63	1.49	1.43
23	AF	605	CHL	C1B-C2B	2.63	1.49	1.43
24	AA	610	CLA	C1B-C2B	2.63	1.49	1.43
24	P	508	CLA	C1B-C2B	2.63	1.49	1.43
23	AD	307	CHL	C3D-C2D	2.63	1.46	1.39
24	P	507	CLA	C1B-C2B	2.63	1.49	1.43
23	V	601	CHL	C1D-C2D	2.63	1.50	1.45
24	0	612	CLA	C1B-C2B	2.63	1.49	1.43
23	V	616	CHL	C4D-CHA	2.63	1.47	1.38
24	p	612	CLA	C1B-C2B	2.62	1.49	1.43
23	AB	608	CHL	C1D-C2D	2.62	1.50	1.45
24	AA	612	CLA	C1B-C2B	2.62	1.49	1.43
24	q	604	CLA	C1B-C2B	2.62	1.49	1.43
23	9	601	CHL	C1D-C2D	2.62	1.50	1.45
23	AU	605	CHL	C3B-C4B	2.62	1.48	1.42
23	AU	608	CHL	C1D-C2D	2.62	1.50	1.45
25	9	616	LUT	C8-C9	-2.62	1.40	1.45
23	9	607	CHL	C1D-C2D	2.62	1.50	1.45
23	p	606	CHL	C1D-C2D	2.62	1.50	1.45
24	O	610	CLA	C4D-ND	-2.62	1.34	1.37
24	AL	505	CLA	C4D-ND	-2.62	1.34	1.37
24	Q	403	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AE	603	CLA	C1B-C2B	2.62	1.49	1.43
24	P	506	CLA	C1B-C2B	2.62	1.49	1.43
24	AJ	409	CLA	C4D-ND	-2.62	1.34	1.37
24	O	611	CLA	C1B-C2B	2.61	1.49	1.43
23	AQ	606	CHL	C1D-C2D	2.61	1.50	1.45
23	v	302	CHL	C1D-C2D	2.61	1.50	1.45
24	AB	609	CLA	C1B-C2B	2.61	1.49	1.43
23	AC	601	CHL	C1D-C2D	2.61	1.50	1.45
24	AL	507	CLA	C1B-C2B	2.61	1.49	1.43
23	0	608	CHL	C1C-NC	-2.61	1.33	1.37
24	9	610	CLA	C1B-C2B	2.61	1.49	1.43
24	AJ	404	CLA	C4D-ND	-2.61	1.34	1.37
23	q	607	CHL	C1B-C2B	2.61	1.49	1.43
24	AA	609	CLA	C1B-C2B	2.61	1.49	1.43
24	q	612	CLA	C3B-C4B	2.61	1.48	1.42
24	q	609	CLA	C1B-C2B	2.61	1.49	1.43
23	AF	607	CHL	C4C-C3C	2.61	1.49	1.45
24	AD	309	CLA	C1B-C2B	2.61	1.49	1.43
23	AD	301	CHL	C1D-C2D	2.61	1.50	1.45
23	0	617	CHL	C3B-C4B	2.61	1.48	1.42
24	V	604	CLA	C1B-C2B	2.60	1.49	1.43
24	O	605	CLA	C4D-ND	-2.60	1.34	1.37
23	AQ	605	CHL	C1D-C2D	2.60	1.50	1.45
23	AS	307	CHL	C1B-C2B	2.60	1.49	1.43
24	q	618	CLA	C4D-ND	-2.60	1.34	1.37
24	0	603	CLA	C4D-ND	-2.60	1.34	1.37
24	AD	313	CLA	C4D-ND	-2.60	1.34	1.37
23	V	616	CHL	C1D-C2D	2.60	1.50	1.45
23	AU	607	CHL	C1D-C2D	2.60	1.50	1.45
24	AK	608	CLA	C1B-C2B	2.60	1.49	1.43
24	AM	403	CLA	C1B-C2B	2.60	1.49	1.43
24	Q	401	CLA	C4D-ND	-2.60	1.34	1.37
23	AB	605	CHL	C1B-NB	-2.60	1.34	1.37
23	AA	601	CHL	C1D-C2D	2.60	1.50	1.45
23	AH	605	CHL	C3B-C4B	2.60	1.48	1.42
23	9	608	CHL	C1D-C2D	2.60	1.50	1.45
23	AD	301	CHL	C3B-C4B	2.60	1.48	1.42
24	AK	607	CLA	C4D-ND	-2.60	1.34	1.37
24	AK	613	CLA	CMC-C2C	-2.60	1.45	1.50
23	0	601	CHL	C3B-C4B	2.60	1.48	1.42
23	V	605	CHL	C3B-C4B	2.60	1.48	1.42
23	AD	307	CHL	C1B-C2B	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AE	609	CLA	C1B-C2B	2.59	1.49	1.43
23	AF	601	CHL	C1B-C2B	2.59	1.49	1.43
23	p	607	CHL	C1D-C2D	2.59	1.50	1.45
23	AB	607	CHL	C1B-C2B	2.59	1.49	1.43
23	AH	608	CHL	C1D-C2D	2.59	1.50	1.45
25	AE	613	LUT	C28-C29	-2.59	1.40	1.45
23	AH	607	CHL	C3B-C4B	2.59	1.48	1.42
24	AK	603	CLA	C1B-C2B	2.59	1.49	1.43
24	v	305	CLA	C4D-ND	-2.59	1.34	1.37
23	AD	308	CHL	C3B-C4B	2.59	1.48	1.42
23	p	605	CHL	C1D-C2D	2.59	1.50	1.45
23	AS	308	CHL	C3B-C4B	2.59	1.48	1.42
23	AC	607	CHL	C1D-C2D	2.59	1.50	1.45
23	AA	606	CHL	C3B-C4B	2.59	1.48	1.42
23	AN	605	CHL	C3B-C4B	2.59	1.48	1.42
23	AH	605	CHL	C1D-C2D	2.59	1.50	1.45
24	AK	615	CLA	C1B-C2B	2.59	1.49	1.43
24	AN	611	CLA	C1B-C2B	2.59	1.49	1.43
23	9	601	CHL	C4C-C3C	2.58	1.49	1.45
24	AH	611	CLA	C1B-C2B	2.58	1.49	1.43
23	AU	607	CHL	C3B-C4B	2.58	1.48	1.42
23	AC	605	CHL	C1D-C2D	2.58	1.50	1.45
24	AH	609	CLA	C1B-C2B	2.58	1.49	1.43
23	v	307	CHL	C1D-C2D	2.58	1.50	1.45
24	q	602	CLA	C1B-C2B	2.58	1.49	1.43
24	AD	305	CLA	C4D-ND	-2.58	1.34	1.37
24	O	613	CLA	C1B-C2B	2.58	1.49	1.43
23	AQ	607	CHL	C1D-C2D	2.58	1.50	1.45
23	p	609	CHL	C3B-C4B	2.58	1.48	1.42
23	AH	606	CHL	C4C-C3C	2.58	1.49	1.45
24	AN	613	CLA	C4D-ND	-2.58	1.34	1.37
23	AS	302	CHL	C4C-C3C	2.58	1.49	1.45
24	AF	602	CLA	C1B-C2B	2.58	1.49	1.43
23	AU	608	CHL	C3B-C4B	2.58	1.48	1.42
25	AA	614	LUT	C12-C13	-2.58	1.40	1.45
25	AA	615	LUT	C8-C9	-2.58	1.40	1.45
23	0	617	CHL	C1D-C2D	2.57	1.50	1.45
23	AA	608	CHL	C4C-C3C	2.57	1.49	1.45
23	AU	605	CHL	C1D-C2D	2.57	1.50	1.45
24	AU	609	CLA	C1B-C2B	2.57	1.49	1.43
23	AN	601	CHL	C3B-C4B	2.57	1.48	1.42
23	q	605	CHL	C1B-C2B	2.57	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AK	604	CLA	C1B-C2B	2.57	1.49	1.43
23	AQ	605	CHL	C3B-C4B	2.57	1.48	1.42
23	0	606	CHL	C1D-C2D	2.57	1.50	1.45
24	AJ	406	CLA	C4D-ND	-2.57	1.34	1.37
23	9	607	CHL	C3B-C4B	2.57	1.48	1.42
24	AU	611	CLA	C1B-C2B	2.57	1.49	1.43
25	AN	614	LUT	C12-C13	-2.57	1.40	1.45
23	AF	607	CHL	C1B-C2B	2.57	1.49	1.43
23	0	605	CHL	C1D-C2D	2.57	1.50	1.45
23	AH	607	CHL	C1D-C2D	2.57	1.50	1.45
24	AK	612	CLA	C1B-C2B	2.57	1.49	1.43
23	q	613	CHL	C1B-C2B	2.56	1.49	1.43
24	AR	603	CLA	C1B-C2B	2.56	1.49	1.43
23	AF	605	CHL	C2C-C1C	2.56	1.49	1.43
24	AE	611	CLA	C1B-C2B	2.56	1.49	1.43
23	AA	605	CHL	C1D-C2D	2.56	1.50	1.45
23	AQ	609	CHL	C3B-C4B	2.56	1.48	1.42
23	AE	607	CHL	C1B-C2B	2.56	1.49	1.43
23	AA	617	CHL	C1D-C2D	2.56	1.50	1.45
24	q	603	CLA	C1B-C2B	2.56	1.49	1.43
25	AD	315	LUT	C8-C9	-2.56	1.40	1.45
23	9	609	CHL	C3B-C4B	2.56	1.48	1.42
24	AN	612	CLA	C1B-C2B	2.56	1.49	1.43
23	AH	606	CHL	C3B-C4B	2.56	1.48	1.42
24	O	611	CLA	C4D-ND	-2.55	1.34	1.37
24	P	501	CLA	C1B-C2B	2.55	1.49	1.43
23	AD	306	CHL	C1B-C2B	2.55	1.49	1.43
23	AB	608	CHL	C3B-C4B	2.55	1.48	1.42
23	V	601	CHL	C1B-C2B	2.55	1.49	1.43
24	AN	603	CLA	C1B-C2B	2.55	1.49	1.43
24	K	101	CLA	C4D-ND	-2.55	1.34	1.37
23	AD	308	CHL	C4C-C3C	2.55	1.49	1.45
23	AR	613	CHL	C1B-C2B	2.55	1.49	1.43
24	AL	512	CLA	C4D-ND	-2.55	1.34	1.37
23	AS	306	CHL	CHA-C1A	2.55	1.47	1.40
24	V	603	CLA	C1B-C2B	2.55	1.49	1.43
24	AQ	611	CLA	C1B-C2B	2.55	1.49	1.43
24	V	610	CLA	C1B-C2B	2.55	1.49	1.43
23	v	307	CHL	C1B-C2B	2.54	1.49	1.43
24	O	601	CLA	C1B-C2B	2.54	1.49	1.43
23	p	605	CHL	C3B-C4B	2.54	1.48	1.42
23	AN	608	CHL	CHC-C4B	2.54	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AU	606	CHL	C4C-C3C	2.54	1.49	1.45
23	9	607	CHL	C1B-C2B	2.54	1.49	1.43
23	AQ	606	CHL	C3B-C4B	2.54	1.48	1.42
23	AB	606	CHL	C1B-C2B	2.54	1.49	1.43
23	9	605	CHL	C3B-C4B	2.54	1.48	1.42
23	AE	601	CHL	C1B-C2B	2.54	1.49	1.43
24	0	609	CLA	C1B-C2B	2.54	1.49	1.43
23	AF	605	CHL	C3C-C4C	2.54	1.49	1.43
24	AL	502	CLA	C1B-C2B	2.54	1.49	1.43
23	AF	607	CHL	C3B-C4B	2.54	1.48	1.42
23	AN	605	CHL	C1D-C2D	2.54	1.50	1.45
23	AD	307	CHL	C1D-C2D	2.54	1.50	1.45
23	AC	606	CHL	C1B-NB	-2.53	1.34	1.37
23	AE	607	CHL	C3B-C4B	2.53	1.48	1.42
23	0	601	CHL	C1B-C2B	2.53	1.49	1.43
23	AN	606	CHL	C1B-C2B	2.53	1.49	1.43
23	AA	607	CHL	C3B-C4B	2.53	1.48	1.42
23	AC	605	CHL	C3B-C4B	2.53	1.48	1.42
23	q	613	CHL	C4C-C3C	2.53	1.49	1.45
23	AC	605	CHL	C1B-C2B	2.53	1.49	1.43
23	AR	607	CHL	C1B-C2B	2.53	1.49	1.43
23	AD	306	CHL	C1D-C2D	2.53	1.50	1.45
23	0	601	CHL	C4C-C3C	2.53	1.49	1.45
32	J	405	PHO	CMC-C2C	-2.53	1.46	1.50
32	AJ	407	PHO	CMC-C2C	-2.53	1.46	1.50
24	AL	506	CLA	C4D-ND	-2.53	1.34	1.37
24	AB	603	CLA	C1B-C2B	2.53	1.49	1.43
23	AD	301	CHL	C1B-C2B	2.52	1.49	1.43
23	AA	608	CHL	C1D-ND	-2.52	1.34	1.37
24	AF	609	CLA	C1B-C2B	2.52	1.49	1.43
23	v	307	CHL	C3B-C4B	2.52	1.48	1.42
23	AR	606	CHL	C1B-C2B	2.52	1.49	1.43
24	AL	513	CLA	C1B-C2B	2.52	1.49	1.43
23	0	607	CHL	C1B-C2B	2.52	1.49	1.43
23	AE	607	CHL	C4C-C3C	2.52	1.49	1.45
23	AB	606	CHL	C3B-C4B	2.52	1.48	1.42
24	AC	604	CLA	C4D-ND	-2.52	1.34	1.37
23	AN	601	CHL	C1B-C2B	2.52	1.49	1.43
24	P	505	CLA	C4D-ND	-2.52	1.34	1.37
25	q	614	LUT	C28-C29	-2.52	1.40	1.45
23	9	609	CHL	C1B-C2B	2.52	1.49	1.43
24	O	616	CLA	CMC-C2C	-2.52	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AN	608	CHL	C4C-C3C	2.51	1.49	1.45
24	AQ	612	CLA	C1B-C2B	2.51	1.49	1.43
24	P	511	CLA	C1B-C2B	2.51	1.49	1.43
23	AR	606	CHL	C4C-C3C	2.51	1.49	1.45
24	AK	613	CLA	C4D-ND	-2.51	1.34	1.37
24	AR	601	CLA	C1B-C2B	2.50	1.49	1.43
23	AE	616	CHL	C1D-C2D	2.50	1.50	1.45
23	p	606	CHL	C1B-C2B	2.50	1.49	1.43
23	V	601	CHL	C3B-C4B	2.50	1.48	1.42
23	AA	601	CHL	C1B-C2B	2.50	1.49	1.43
23	AN	601	CHL	C4C-C3C	2.50	1.49	1.45
24	P	501	CLA	C4D-ND	-2.50	1.34	1.37
23	V	606	CHL	C1B-C2B	2.50	1.49	1.43
24	AN	609	CLA	C1B-C2B	2.50	1.49	1.43
23	AF	601	CHL	C3B-C4B	2.50	1.48	1.42
23	9	605	CHL	C1B-C2B	2.49	1.49	1.43
23	v	302	CHL	C4C-C3C	2.49	1.49	1.45
23	v	308	CHL	C2C-C1C	2.49	1.49	1.43
25	AE	614	LUT	C32-C33	-2.49	1.40	1.45
23	AE	606	CHL	C3B-C4B	2.49	1.48	1.42
23	9	609	CHL	C1B-NB	-2.49	1.34	1.37
23	V	606	CHL	C1D-C2D	2.49	1.50	1.45
32	J	406	PHO	CMC-C2C	-2.48	1.46	1.50
23	AA	606	CHL	C1B-C2B	2.48	1.49	1.43
23	AN	617	CHL	C4D-CHA	2.48	1.47	1.38
23	AD	317	CHL	C1B-NB	-2.48	1.34	1.37
23	AD	307	CHL	C3B-C4B	2.48	1.48	1.42
23	AA	617	CHL	C4D-CHA	2.48	1.47	1.38
23	AU	606	CHL	C1B-C2B	2.48	1.49	1.43
23	AB	601	CHL	C1B-C2B	2.48	1.49	1.43
24	AR	608	CLA	C1B-C2B	2.48	1.49	1.43
24	AC	612	CLA	C4D-ND	-2.47	1.34	1.37
24	AS	311	CLA	C1B-C2B	2.47	1.49	1.43
32	AJ	408	PHO	CMC-C2C	-2.47	1.46	1.50
23	AH	605	CHL	C1B-C2B	2.47	1.49	1.43
23	AA	605	CHL	C1B-C2B	2.47	1.49	1.43
23	p	601	CHL	C1B-C2B	2.47	1.49	1.43
24	v	311	CLA	C1B-C2B	2.47	1.49	1.43
23	q	607	CHL	C3B-C4B	2.47	1.48	1.42
24	AL	502	CLA	C4D-ND	-2.47	1.34	1.37
23	AR	605	CHL	C3B-C4B	2.47	1.48	1.42
23	v	308	CHL	C3C-C4C	2.47	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AB	605	CHL	C1B-C2B	2.47	1.49	1.43
24	AQ	610	CLA	C1B-C2B	2.47	1.49	1.43
23	V	608	CHL	C4C-C3C	2.47	1.49	1.45
23	AC	608	CHL	C1B-C2B	2.46	1.49	1.43
23	AN	606	CHL	C1D-C2D	2.46	1.50	1.45
24	AJ	404	CLA	C1B-C2B	2.46	1.49	1.43
23	AQ	601	CHL	C1B-C2B	2.46	1.49	1.43
23	AU	607	CHL	C1B-C2B	2.46	1.49	1.43
25	AR	614	LUT	C28-C29	-2.46	1.40	1.45
24	AC	610	CLA	C1B-C2B	2.46	1.49	1.43
23	AN	617	CHL	C1D-C2D	2.46	1.50	1.45
23	0	607	CHL	C3B-C4B	2.46	1.48	1.42
23	0	606	CHL	C1B-C2B	2.46	1.49	1.43
23	AE	606	CHL	C1B-C2B	2.46	1.49	1.43
24	9	613	CLA	C4D-ND	-2.46	1.34	1.37
24	O	610	CLA	C1B-C2B	2.46	1.49	1.43
23	9	607	CHL	C4C-C3C	2.45	1.49	1.45
23	AS	307	CHL	C1D-C2D	2.45	1.50	1.45
23	p	601	CHL	C4C-C3C	2.45	1.49	1.45
24	J	403	CLA	C1B-C2B	2.45	1.49	1.43
23	AH	607	CHL	C1B-C2B	2.45	1.49	1.43
23	AD	308	CHL	C1B-C2B	2.45	1.49	1.43
23	AD	302	CHL	C4C-C3C	2.45	1.49	1.45
23	AN	617	CHL	C3B-C4B	2.45	1.48	1.42
23	AU	605	CHL	C1B-C2B	2.45	1.49	1.43
23	AC	608	CHL	C1B-NB	-2.45	1.34	1.37
25	q	614	LUT	C12-C13	-2.44	1.40	1.45
24	9	611	CLA	C1B-C2B	2.44	1.49	1.43
23	AR	613	CHL	C3B-C4B	2.44	1.48	1.42
25	p	615	LUT	C12-C13	-2.44	1.40	1.45
25	AN	615	LUT	C12-C13	-2.44	1.40	1.45
24	p	610	CLA	C4D-ND	-2.44	1.34	1.37
23	q	606	CHL	C1B-C2B	2.44	1.49	1.43
23	AS	306	CHL	C1D-ND	-2.44	1.34	1.37
23	p	605	CHL	C1B-C2B	2.44	1.49	1.43
23	AD	302	CHL	C1B-C2B	2.44	1.49	1.43
23	AA	606	CHL	C1D-C2D	2.43	1.50	1.45
25	AQ	616	LUT	C12-C13	-2.43	1.40	1.45
23	AA	607	CHL	C1B-C2B	2.43	1.49	1.43
32	J	405	PHO	CMB-C2B	-2.43	1.46	1.51
23	AE	617	CHL	CHB-C4A	-2.43	1.31	1.37
24	O	611	CLA	CMC-C2C	-2.43	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AQ	616	LUT	C32-C33	-2.43	1.40	1.45
23	AF	608	CHL	C4B-NB	-2.43	1.34	1.37
25	q	614	LUT	C32-C33	-2.43	1.40	1.45
32	J	406	PHO	C3D-C4D	2.43	1.44	1.41
23	AN	607	CHL	C1B-C2B	2.43	1.49	1.43
23	AQ	609	CHL	C1B-C2B	2.43	1.49	1.43
25	AN	614	LUT	C32-C33	-2.43	1.40	1.45
23	AF	605	CHL	CHD-C4C	2.43	1.48	1.40
23	AS	307	CHL	C3B-C4B	2.43	1.48	1.42
23	AE	616	CHL	C4D-CHA	2.43	1.47	1.38
32	AJ	407	PHO	CMB-C2B	-2.43	1.46	1.51
23	p	609	CHL	C1B-C2B	2.42	1.49	1.43
23	AS	306	CHL	CAD-C3D	2.42	1.50	1.45
24	AN	612	CLA	C4D-ND	-2.42	1.34	1.37
23	AN	607	CHL	C4C-C3C	2.42	1.49	1.45
32	J	405	PHO	CMD-C2D	-2.42	1.46	1.51
23	AB	608	CHL	C4C-C3C	2.42	1.49	1.45
23	AQ	605	CHL	C1B-C2B	2.42	1.49	1.43
23	AF	605	CHL	MG-NA	-2.42	2.00	2.06
23	AD	307	CHL	C1B-NB	-2.42	1.34	1.37
24	p	610	CLA	C1B-C2B	2.42	1.48	1.43
23	9	609	CHL	C4C-C3C	2.42	1.49	1.45
23	0	606	CHL	C1B-NB	-2.41	1.34	1.37
23	AE	605	CHL	C1B-NB	-2.41	1.34	1.37
23	AQ	601	CHL	C4C-C3C	2.41	1.49	1.45
23	p	606	CHL	C3B-C4B	2.41	1.48	1.42
23	AN	606	CHL	C4C-C3C	2.41	1.49	1.45
23	AS	308	CHL	C1B-C2B	2.41	1.48	1.43
32	AJ	408	PHO	CMD-C2D	-2.41	1.46	1.51
24	p	618	CLA	CMD-C2D	-2.41	1.45	1.50
25	AN	614	LUT	C28-C29	-2.41	1.40	1.45
23	V	601	CHL	C4C-C3C	2.41	1.49	1.45
23	AN	608	CHL	C1D-ND	-2.41	1.34	1.37
23	AU	601	CHL	C1B-C2B	2.41	1.48	1.43
23	AF	607	CHL	C1B-NB	-2.41	1.34	1.37
35	AL	518	DGD	O2G-C2G	-2.41	1.40	1.46
32	AJ	407	PHO	CMD-C2D	-2.40	1.46	1.51
23	9	608	CHL	C3B-C4B	2.40	1.48	1.42
24	p	613	CLA	C3B-C4B	2.40	1.48	1.42
23	AS	306	CHL	C4D-ND	2.40	1.40	1.37
23	AA	617	CHL	C4C-C3C	2.40	1.49	1.45
25	AS	316	LUT	C12-C13	-2.40	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AB	608	CHL	MG-NA	-2.40	2.00	2.06
25	v	315	LUT	C12-C13	-2.40	1.40	1.45
23	V	606	CHL	C4C-C3C	2.40	1.49	1.45
23	AA	601	CHL	C4C-C3C	2.40	1.49	1.45
23	AH	601	CHL	C1B-C2B	2.40	1.48	1.43
23	AH	601	CHL	C4C-C3C	2.40	1.49	1.45
25	0	615	LUT	C12-C13	-2.40	1.40	1.45
24	0	604	CLA	C4D-ND	-2.40	1.34	1.37
23	V	608	CHL	C1B-C2B	2.40	1.48	1.43
23	AB	601	CHL	C4C-C3C	2.40	1.49	1.45
23	AH	608	CHL	C4C-C3C	2.40	1.49	1.45
24	AB	609	CLA	CHC-C1C	2.39	1.43	1.38
23	V	605	CHL	C1B-C2B	2.39	1.48	1.43
23	p	609	CHL	C4C-C3C	2.39	1.49	1.45
23	9	608	CHL	C1B-C2B	2.39	1.48	1.43
23	AA	617	CHL	C1B-NB	-2.39	1.34	1.37
23	AB	605	CHL	MG-NA	-2.39	2.00	2.06
25	AU	614	LUT	C12-C13	-2.39	1.40	1.45
24	q	601	CLA	C4D-ND	-2.39	1.34	1.37
37	Q	405	PL9	C6-C1	-2.39	1.44	1.48
24	q	602	CLA	CHC-C1C	2.39	1.43	1.38
25	AR	614	LUT	C32-C33	-2.39	1.40	1.45
23	AC	606	CHL	C1B-C2B	2.39	1.48	1.43
25	p	615	LUT	C32-C33	-2.38	1.40	1.45
32	J	406	PHO	CMD-C2D	-2.38	1.46	1.51
24	AF	602	CLA	CMC-C2C	-2.38	1.45	1.50
25	AF	611	LUT	C28-C29	-2.38	1.40	1.45
24	AQ	610	CLA	CHC-C1C	2.38	1.43	1.38
23	AU	601	CHL	C4C-C3C	2.38	1.49	1.45
32	AJ	408	PHO	C3D-C4D	2.38	1.44	1.41
23	AQ	608	CHL	C1B-C2B	2.38	1.48	1.43
23	AE	605	CHL	C4C-C3C	2.38	1.49	1.45
23	AH	606	CHL	C1B-C2B	2.38	1.48	1.43
28	O	621	LHG	P-O6	2.38	1.68	1.59
25	AQ	615	LUT	C12-C13	-2.38	1.40	1.45
23	AD	306	CHL	C3B-C4B	2.38	1.48	1.42
24	AU	609	CLA	CHC-C1C	2.38	1.43	1.38
23	AD	301	CHL	C4C-C3C	2.38	1.49	1.45
23	AC	607	CHL	C1B-C2B	2.38	1.48	1.43
24	AR	602	CLA	CHC-C1C	2.38	1.43	1.38
23	AC	607	CHL	C3B-C4B	2.38	1.48	1.42
23	v	308	CHL	C1B-C2B	2.38	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	613	LUT	C32-C33	-2.38	1.40	1.45
25	AE	614	LUT	C28-C29	-2.37	1.40	1.45
23	AR	607	CHL	C1B-NB	-2.37	1.34	1.37
23	9	606	CHL	C1B-C2B	2.37	1.48	1.43
25	AU	615	LUT	C12-C13	-2.37	1.40	1.45
23	q	607	CHL	C4C-C3C	2.37	1.49	1.45
23	p	608	CHL	C1B-C2B	2.37	1.48	1.43
23	AQ	606	CHL	C1B-C2B	2.37	1.48	1.43
24	AF	610	CLA	C4D-ND	-2.37	1.34	1.37
37	AM	405	PL9	C6-C1	-2.37	1.44	1.48
24	O	606	CLA	C1B-C2B	2.37	1.48	1.43
23	AR	607	CHL	C4C-C3C	2.37	1.49	1.45
23	AN	605	CHL	C1B-C2B	2.37	1.48	1.43
23	0	606	CHL	C4C-C3C	2.37	1.49	1.45
25	V	614	LUT	C12-C13	-2.36	1.40	1.45
24	q	601	CLA	C1B-C2B	2.36	1.48	1.43
24	v	312	CLA	CHC-C1C	2.36	1.43	1.38
23	0	605	CHL	C1B-C2B	2.36	1.48	1.43
25	AH	615	LUT	C12-C13	-2.36	1.40	1.45
23	AQ	609	CHL	C4C-C3C	2.36	1.49	1.45
24	AH	609	CLA	CHC-C1C	2.36	1.43	1.38
23	q	613	CHL	MG-NA	-2.36	2.00	2.06
23	AU	608	CHL	C4C-C3C	2.36	1.49	1.45
24	v	310	CLA	CHC-C1C	2.36	1.43	1.38
24	AK	611	CLA	CMD-C2D	-2.36	1.45	1.50
23	AF	601	CHL	C4C-C3C	2.36	1.49	1.45
32	AJ	408	PHO	CMB-C2B	-2.36	1.46	1.51
23	AC	605	CHL	C4C-C3C	2.36	1.49	1.45
32	J	406	PHO	CMB-C2B	-2.35	1.46	1.51
24	9	614	CLA	CHC-C1C	2.35	1.43	1.38
23	q	607	CHL	C1B-NB	-2.35	1.34	1.37
23	AF	606	CHL	CHD-C4C	2.35	1.47	1.42
23	V	616	CHL	C3B-C4B	2.35	1.48	1.42
23	q	606	CHL	C1B-NB	-2.35	1.34	1.37
35	j	102	DGD	O2G-C2G	-2.35	1.40	1.46
24	O	611	CLA	CHC-C1C	2.35	1.43	1.38
23	AE	601	CHL	C4C-C3C	2.35	1.49	1.45
26	AS	317	NEX	C11-C10	-2.35	1.36	1.43
23	0	617	CHL	C1B-C2B	2.35	1.48	1.43
23	AU	607	CHL	C4C-C3C	2.35	1.49	1.45
25	V	614	LUT	C32-C33	-2.35	1.40	1.45
25	AN	615	LUT	C32-C33	-2.34	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	q	605	CHL	C3B-C4B	2.34	1.48	1.42
24	p	610	CLA	CHC-C1C	2.34	1.43	1.38
25	AS	315	LUT	C12-C13	-2.34	1.40	1.45
23	v	306	CHL	CHD-C4C	2.34	1.48	1.40
23	AH	607	CHL	C4C-C3C	2.34	1.49	1.45
23	9	605	CHL	C4C-C3C	2.34	1.49	1.45
25	AH	615	LUT	C32-C33	-2.34	1.40	1.45
25	v	315	LUT	C32-C33	-2.34	1.40	1.45
23	0	601	CHL	C1B-NB	-2.34	1.34	1.37
26	9	617	NEX	C12-C13	-2.34	1.40	1.45
25	AQ	615	LUT	C28-C29	-2.34	1.40	1.45
23	AD	306	CHL	C4C-C3C	2.33	1.49	1.45
23	AQ	609	CHL	C1B-NB	-2.33	1.34	1.37
23	q	605	CHL	C4C-C3C	2.33	1.49	1.45
23	AS	306	CHL	C1B-C2B	2.33	1.48	1.43
25	AS	315	LUT	C32-C33	-2.33	1.40	1.45
23	AR	606	CHL	C1B-NB	-2.33	1.34	1.37
24	AQ	612	CLA	CHC-C1C	2.33	1.43	1.38
23	AD	317	CHL	C1B-C2B	2.33	1.48	1.43
23	AH	608	CHL	C1B-C2B	2.33	1.48	1.43
25	AR	614	LUT	C12-C13	-2.33	1.40	1.45
24	AS	313	CLA	CHC-C1C	2.32	1.43	1.38
25	p	614	LUT	C12-C13	-2.32	1.41	1.45
23	AQ	605	CHL	C1B-NB	-2.32	1.34	1.37
25	AU	615	LUT	C32-C33	-2.32	1.41	1.45
23	AH	608	CHL	C1B-NB	-2.32	1.34	1.37
23	p	608	CHL	C1B-NB	-2.32	1.34	1.37
23	AR	605	CHL	CHD-C4C	2.32	1.48	1.40
25	p	614	LUT	C28-C29	-2.32	1.41	1.45
23	AN	608	CHL	C4D-CHA	2.32	1.46	1.38
24	q	609	CLA	CHC-C1C	2.32	1.43	1.38
24	O	612	CLA	CMD-C2D	-2.32	1.45	1.50
26	p	616	NEX	C32-C33	-2.32	1.41	1.45
23	AC	606	CHL	C4C-C3C	2.32	1.49	1.45
23	AR	613	CHL	C1D-ND	-2.32	1.34	1.37
23	0	617	CHL	C1B-NB	-2.31	1.34	1.37
25	p	615	LUT	C28-C29	-2.31	1.41	1.45
24	AN	602	CLA	CHC-C1C	2.31	1.43	1.38
24	AL	502	CLA	CHC-C1C	2.31	1.43	1.38
23	AQ	607	CHL	C1B-C2B	2.31	1.48	1.43
24	AA	613	CLA	CHC-C1C	2.31	1.43	1.38
24	AN	609	CLA	CHC-C1C	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AA	615	LUT	C12-C13	-2.31	1.41	1.45
24	P	501	CLA	CHC-C1C	2.31	1.43	1.38
23	p	605	CHL	C4C-C3C	2.31	1.49	1.45
24	AK	610	CLA	CHC-C1C	2.31	1.43	1.38
23	p	608	CHL	C4C-C3C	2.31	1.49	1.45
24	Q	403	CLA	CHC-C1C	2.31	1.43	1.38
25	V	613	LUT	C12-C13	-2.31	1.41	1.45
24	AK	604	CLA	CHC-C1C	2.31	1.43	1.38
24	AK	611	CLA	C4D-ND	-2.30	1.34	1.37
32	AJ	407	PHO	C3D-C4D	2.30	1.44	1.41
25	AH	614	LUT	C12-C13	-2.30	1.41	1.45
25	AD	315	LUT	C12-C13	-2.30	1.41	1.45
24	AS	312	CLA	CHC-C1C	2.30	1.43	1.38
24	AA	602	CLA	CHC-C1C	2.30	1.43	1.38
25	p	614	LUT	C32-C33	-2.30	1.41	1.45
25	AQ	616	LUT	C28-C29	-2.30	1.41	1.45
23	v	308	CHL	CHD-C4C	2.30	1.48	1.40
24	O	609	CLA	CHC-C1C	2.30	1.43	1.38
23	AB	607	CHL	C1B-NB	-2.30	1.35	1.37
24	AK	611	CLA	CHC-C1C	2.30	1.43	1.38
24	AQ	612	CLA	MG-NB	-2.29	2.01	2.05
35	AO	102	DGD	O2G-C2G	-2.29	1.40	1.46
23	AE	617	CHL	C4D-CHA	2.29	1.46	1.38
24	AB	610	CLA	CHC-C1C	2.29	1.43	1.38
25	V	614	LUT	C28-C29	-2.29	1.41	1.45
23	0	607	CHL	C1B-NB	-2.29	1.35	1.37
24	AF	602	CLA	C4C-C3C	2.29	1.49	1.45
25	AS	316	LUT	C32-C33	-2.29	1.41	1.45
25	AC	614	LUT	C12-C13	-2.29	1.41	1.45
25	AN	615	LUT	C28-C29	-2.29	1.41	1.45
24	AE	610	CLA	CHC-C1C	2.29	1.43	1.38
23	AN	607	CHL	C1B-NB	-2.29	1.35	1.37
23	p	607	CHL	C1B-C2B	2.29	1.48	1.43
24	AM	404	CLA	CHC-C1C	2.28	1.43	1.38
24	q	603	CLA	CHC-C1C	2.28	1.43	1.38
25	AQ	615	LUT	C32-C33	-2.28	1.41	1.45
25	9	615	LUT	C32-C33	-2.28	1.41	1.45
24	O	616	CLA	CHC-C1C	2.28	1.43	1.38
24	AR	603	CLA	CHC-C1C	2.28	1.43	1.38
25	AC	615	LUT	C32-C33	-2.28	1.41	1.45
24	AB	604	CLA	CHC-C1C	2.28	1.43	1.38
24	AK	618	CLA	CHC-C1C	2.28	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	p	609	CHL	C1B-NB	-2.28	1.35	1.37
23	AU	608	CHL	C1B-NB	-2.28	1.35	1.37
24	AC	613	CLA	CHC-C1C	2.28	1.43	1.38
24	V	612	CLA	CHC-C1C	2.28	1.43	1.38
23	AE	616	CHL	CHB-C4A	-2.28	1.32	1.37
23	AU	608	CHL	C1B-C2B	2.28	1.48	1.43
23	AU	605	CHL	C1B-NB	-2.28	1.35	1.37
24	AM	403	CLA	CHC-C1C	2.28	1.43	1.38
24	AK	613	CLA	CHC-C1C	2.27	1.43	1.38
23	V	608	CHL	C1B-NB	-2.27	1.35	1.37
23	p	605	CHL	C1B-NB	-2.27	1.35	1.37
23	AD	308	CHL	C1B-NB	-2.27	1.35	1.37
23	p	607	CHL	C1B-NB	-2.27	1.35	1.37
24	P	509	CLA	CHC-C1C	2.27	1.43	1.38
25	AS	316	LUT	C28-C29	-2.27	1.41	1.45
24	AC	609	CLA	CHC-C1C	2.27	1.43	1.38
24	O	613	CLA	CHC-C1C	2.27	1.43	1.38
25	v	316	LUT	C12-C13	-2.27	1.41	1.45
23	p	607	CHL	C4C-C3C	2.27	1.48	1.45
23	v	306	CHL	C1B-C2B	2.27	1.48	1.43
26	p	616	NEX	C28-C29	-2.27	1.41	1.45
32	J	405	PHO	CAC-C3C	-2.27	1.47	1.51
25	AH	614	LUT	C32-C33	-2.27	1.41	1.45
25	AU	614	LUT	C32-C33	-2.27	1.41	1.45
24	P	506	CLA	CHC-C1C	2.27	1.43	1.38
24	AK	615	CLA	CHC-C1C	2.27	1.43	1.38
24	P	511	CLA	CHC-C1C	2.26	1.43	1.38
24	AL	511	CLA	CHC-C1C	2.26	1.43	1.38
35	J	411	DGD	O1G-C1G	-2.26	1.40	1.45
25	9	616	LUT	C32-C33	-2.26	1.41	1.45
23	AQ	608	CHL	C4C-C3C	2.26	1.48	1.45
24	O	602	CLA	CHC-C1C	2.26	1.43	1.38
24	AA	611	CLA	CHC-C1C	2.26	1.43	1.38
23	AQ	605	CHL	C4C-C3C	2.26	1.48	1.45
25	v	316	LUT	C28-C29	-2.26	1.41	1.45
24	v	314	CLA	CHC-C1C	2.26	1.43	1.38
25	0	615	LUT	C28-C29	-2.26	1.41	1.45
32	AJ	408	PHO	CAC-C3C	-2.26	1.47	1.51
24	AL	513	CLA	CHC-C1C	2.26	1.43	1.38
23	AA	617	CHL	CHB-C4A	-2.26	1.32	1.37
25	AC	615	LUT	C28-C29	-2.26	1.41	1.45
23	AR	613	CHL	C4C-C3C	2.26	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	V	604	CLA	CHC-C1C	2.26	1.43	1.38
35	j	102	DGD	O1G-C1G	-2.25	1.40	1.45
23	AH	605	CHL	C1B-NB	-2.25	1.35	1.37
23	AC	608	CHL	C4C-C3C	2.25	1.48	1.45
24	0	610	CLA	CHC-C1C	2.25	1.43	1.38
24	AE	612	CLA	CHC-C1C	2.25	1.43	1.38
26	AQ	617	NEX	C12-C13	-2.25	1.41	1.45
24	0	602	CLA	CHC-C1C	2.25	1.43	1.38
23	AA	601	CHL	C1B-NB	-2.25	1.35	1.37
23	AE	606	CHL	C4C-C3C	2.25	1.48	1.45
24	AM	403	CLA	CMD-C2D	-2.25	1.46	1.50
25	AH	614	LUT	C28-C29	-2.25	1.41	1.45
23	0	617	CHL	C4D-CHA	2.25	1.46	1.38
24	AK	614	CLA	CMD-C2D	-2.25	1.46	1.50
24	AF	604	CLA	CHC-C1C	2.25	1.43	1.38
23	AB	607	CHL	MG-NA	-2.25	2.00	2.06
24	V	612	CLA	CMD-C2D	-2.25	1.46	1.50
24	AL	507	CLA	CHC-C1C	2.25	1.43	1.38
24	q	610	CLA	CHC-C1C	2.25	1.43	1.38
25	AE	614	LUT	C12-C13	-2.25	1.41	1.45
23	v	307	CHL	C1B-NB	-2.25	1.35	1.37
24	p	612	CLA	CHC-C1C	2.25	1.43	1.38
23	0	605	CHL	C1B-NB	-2.25	1.35	1.37
24	AK	608	CLA	CHC-C1C	2.25	1.43	1.38
24	AN	604	CLA	CHC-C1C	2.25	1.43	1.38
23	AQ	607	CHL	C1B-NB	-2.25	1.35	1.37
24	AA	603	CLA	CHC-C1C	2.25	1.43	1.38
24	AK	617	CLA	CHC-C1C	2.25	1.43	1.38
24	q	601	CLA	CMD-C2D	-2.25	1.46	1.50
32	J	405	PHO	C3D-C4D	2.24	1.44	1.41
24	AN	613	CLA	CHC-C1C	2.24	1.43	1.38
25	0	614	LUT	C12-C13	-2.24	1.41	1.45
32	J	406	PHO	CAC-C3C	-2.24	1.47	1.51
24	AE	604	CLA	CHC-C1C	2.24	1.43	1.38
24	O	609	CLA	CMD-C2D	-2.24	1.46	1.50
24	AQ	603	CLA	CHC-C1C	2.24	1.43	1.38
24	AJ	406	CLA	CHC-C1C	2.24	1.43	1.38
24	O	615	CLA	CHC-C1C	2.24	1.43	1.38
24	q	611	CLA	CHC-C1C	2.24	1.43	1.38
24	P	504	CLA	CHC-C1C	2.24	1.43	1.38
24	AS	311	CLA	CHC-C1C	2.24	1.43	1.38
26	AQ	617	NEX	C32-C33	-2.24	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AS	303	CLA	CHC-C1C	2.24	1.43	1.38
23	AA	608	CHL	C4D-CHA	2.24	1.46	1.38
25	v	316	LUT	C32-C33	-2.24	1.41	1.45
23	AQ	608	CHL	C1B-NB	-2.24	1.35	1.37
24	AJ	409	CLA	CHC-C1C	2.24	1.43	1.38
24	AL	510	CLA	CHC-C1C	2.24	1.43	1.38
24	AD	311	CLA	CHC-C1C	2.24	1.43	1.38
24	P	502	CLA	CHC-C1C	2.24	1.43	1.38
23	AC	607	CHL	CHD-C4C	2.24	1.47	1.40
24	AE	602	CLA	CHC-C1C	2.24	1.43	1.38
24	v	303	CLA	CHC-C1C	2.24	1.43	1.38
24	p	603	CLA	CHC-C1C	2.24	1.43	1.38
24	AU	603	CLA	CHC-C1C	2.24	1.43	1.38
24	AL	504	CLA	CHC-C1C	2.23	1.43	1.38
23	AQ	607	CHL	C4C-C3C	2.23	1.48	1.45
34	M	101	SQD	O9-S	2.23	1.51	1.45
24	9	604	CLA	CHC-C1C	2.23	1.43	1.38
25	AH	615	LUT	C28-C29	-2.23	1.41	1.45
24	Q	403	CLA	CMD-C2D	-2.23	1.46	1.50
24	q	604	CLA	CMD-C2D	-2.23	1.46	1.50
23	AU	607	CHL	C1B-NB	-2.23	1.35	1.37
24	AU	604	CLA	CHC-C1C	2.23	1.43	1.38
25	AU	615	LUT	C28-C29	-2.23	1.41	1.45
35	AJ	412	DGD	O1G-C1G	-2.23	1.40	1.45
25	9	615	LUT	C28-C29	-2.23	1.41	1.45
28	0	616	LHG	O7-C5	-2.23	1.41	1.46
35	J	413	DGD	O1G-C1G	-2.23	1.40	1.45
24	V	610	CLA	CHC-C1C	2.23	1.43	1.38
28	O	623	LHG	O7-C5	-2.23	1.41	1.46
24	AA	609	CLA	CHC-C1C	2.23	1.43	1.38
24	AK	612	CLA	CHC-C1C	2.23	1.43	1.38
23	AA	606	CHL	C4C-C3C	2.23	1.48	1.45
24	9	610	CLA	CHC-C1C	2.23	1.43	1.38
24	AB	603	CLA	CHC-C1C	2.23	1.43	1.38
24	Q	401	CLA	CHC-C1C	2.23	1.43	1.38
24	v	311	CLA	CHC-C1C	2.23	1.43	1.38
24	0	611	CLA	CHC-C1C	2.23	1.43	1.38
24	J	407	CLA	CHC-C1C	2.23	1.43	1.38
32	AJ	407	PHO	CAC-C3C	-2.23	1.47	1.51
24	p	604	CLA	CHC-C1C	2.23	1.43	1.38
24	AH	603	CLA	CHC-C1C	2.23	1.43	1.38
23	AN	605	CHL	C4C-C3C	2.23	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	508	CLA	CHC-C1C	2.23	1.43	1.38
24	v	305	CLA	CHC-C1C	2.23	1.43	1.38
25	0	615	LUT	C32-C33	-2.23	1.41	1.45
23	AB	608	CHL	C1D-ND	-2.22	1.35	1.37
23	AU	605	CHL	C4C-C3C	2.22	1.48	1.45
24	AE	603	CLA	CHC-C1C	2.22	1.43	1.38
24	AQ	611	CLA	CHC-C1C	2.22	1.43	1.38
24	AU	610	CLA	CHC-C1C	2.22	1.43	1.38
23	AD	302	CHL	C1B-NB	-2.22	1.35	1.37
25	AU	614	LUT	C28-C29	-2.22	1.41	1.45
24	AR	603	CLA	MG-NB	-2.22	2.01	2.05
24	AQ	614	CLA	CHC-C1C	2.22	1.43	1.38
23	AB	606	CHL	C1B-NB	-2.22	1.35	1.37
26	AC	616	NEX	C12-C13	-2.22	1.41	1.45
24	q	608	CLA	CHC-C1C	2.22	1.43	1.38
24	AH	604	CLA	CHC-C1C	2.22	1.43	1.38
23	AB	606	CHL	CHD-C4C	2.22	1.47	1.40
35	AJ	401	DGD	O1G-C1G	-2.22	1.40	1.45
28	AK	624	LHG	O7-C5	-2.22	1.41	1.46
24	AR	610	CLA	CHC-C1C	2.22	1.43	1.38
25	0	614	LUT	C28-C29	-2.22	1.41	1.45
24	AR	611	CLA	CHC-C1C	2.22	1.43	1.38
23	9	608	CHL	CHD-C4C	2.22	1.47	1.40
25	9	615	LUT	C12-C13	-2.22	1.41	1.45
24	p	602	CLA	CHC-C1C	2.22	1.43	1.38
23	AR	613	CHL	C1B-NB	-2.22	1.35	1.37
23	AS	307	CHL	C1B-NB	-2.22	1.35	1.37
24	O	605	CLA	CHC-C1C	2.22	1.43	1.38
23	AQ	606	CHL	C4C-C3C	2.22	1.48	1.45
24	AS	305	CLA	CHC-C1C	2.22	1.43	1.38
25	AD	315	LUT	C28-C29	-2.22	1.41	1.45
27	9	618	XAT	C18-C5	2.22	1.55	1.51
24	AE	608	CLA	CHC-C1C	2.22	1.43	1.38
24	AS	304	CLA	CHC-C1C	2.22	1.43	1.38
34	AJ	411	SQD	O9-S	2.21	1.51	1.45
23	AB	608	CHL	C4B-NB	-2.21	1.35	1.37
25	9	616	LUT	C12-C13	-2.21	1.41	1.45
24	AL	509	CLA	CHC-C1C	2.21	1.43	1.38
24	q	604	CLA	CHC-C1C	2.21	1.43	1.38
23	V	605	CHL	C4C-C3C	2.21	1.48	1.45
26	v	317	NEX	C28-C29	-2.21	1.41	1.45
24	AA	604	CLA	CHC-C1C	2.21	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AR	604	CLA	CHC-C1C	2.21	1.43	1.38
24	p	613	CLA	CMB-C2B	-2.21	1.46	1.50
24	P	510	CLA	CHC-C1C	2.21	1.43	1.38
23	AE	605	CHL	C1B-C2B	2.21	1.48	1.43
23	V	616	CHL	C1B-C2B	2.21	1.48	1.43
24	AU	609	CLA	MG-NB	-2.21	2.01	2.05
23	v	307	CHL	C4C-C3C	2.21	1.48	1.45
24	O	612	CLA	CHC-C1C	2.21	1.43	1.38
24	P	507	CLA	CHC-C1C	2.20	1.43	1.38
34	o	101	SQD	O9-S	2.20	1.51	1.45
37	Q	405	PL9	C53-C6	-2.20	1.46	1.50
24	AS	314	CLA	CHC-C1C	2.20	1.43	1.38
24	AK	616	CLA	CHC-C1C	2.20	1.43	1.38
24	AE	611	CLA	CMB-C2B	-2.20	1.46	1.50
25	AC	615	LUT	C12-C13	-2.20	1.41	1.45
23	AD	317	CHL	C4D-CHA	2.20	1.46	1.38
24	v	310	CLA	CMD-C2D	-2.20	1.46	1.50
24	AS	303	CLA	CMD-C2D	-2.20	1.46	1.50
24	AR	608	CLA	CHC-C1C	2.20	1.43	1.38
23	AE	617	CHL	C2C-C1C	2.20	1.49	1.44
24	AC	611	CLA	CHC-C1C	2.20	1.43	1.38
34	AP	101	SQD	O9-S	2.20	1.51	1.45
24	q	608	CLA	MG-NB	-2.20	2.01	2.05
24	AN	611	CLA	CHC-C1C	2.20	1.43	1.38
23	AH	607	CHL	C1B-NB	-2.20	1.35	1.37
23	AR	613	CHL	MG-NA	-2.20	2.01	2.06
34	J	410	SQD	O9-S	2.20	1.51	1.45
23	AR	607	CHL	C4D-CHA	2.20	1.46	1.38
24	q	603	CLA	CMD-C2D	-2.20	1.46	1.50
23	9	607	CHL	C1B-NB	-2.20	1.35	1.37
24	AN	612	CLA	CHC-C1C	2.20	1.43	1.38
24	v	304	CLA	CHC-C1C	2.19	1.43	1.38
34	m	101	SQD	O9-S	2.19	1.51	1.45
23	AN	606	CHL	C1B-NB	-2.19	1.35	1.37
24	AA	610	CLA	CHC-C1C	2.19	1.43	1.38
24	AN	609	CLA	MG-NB	-2.19	2.01	2.05
23	AE	607	CHL	C1B-NB	-2.19	1.35	1.37
23	AR	605	CHL	C1B-NB	-2.19	1.35	1.37
24	AF	614	CLA	CMD-C2D	-2.19	1.46	1.50
26	q	615	NEX	C28-C29	-2.19	1.41	1.45
24	AH	613	CLA	CHC-C1C	2.19	1.43	1.38
24	AU	611	CLA	CHC-C1C	2.19	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AF	609	CLA	CHC-C1C	2.19	1.43	1.38
26	AS	317	NEX	C28-C29	-2.19	1.41	1.45
23	AH	601	CHL	C1B-NB	-2.19	1.35	1.37
24	V	611	CLA	CHC-C1C	2.19	1.43	1.38
24	AR	617	CLA	C4D-ND	-2.19	1.34	1.37
24	AR	601	CLA	CHC-C1C	2.19	1.43	1.38
24	O	606	CLA	CHC-C1C	2.19	1.43	1.38
24	AS	310	CLA	CHC-C1C	2.19	1.43	1.38
24	P	503	CLA	CHC-C1C	2.19	1.43	1.38
23	AA	606	CHL	C1B-NB	-2.19	1.35	1.37
35	AL	518	DGD	O1G-C1G	-2.19	1.40	1.45
26	p	616	NEX	C12-C13	-2.19	1.41	1.45
24	O	603	CLA	CHC-C1C	2.19	1.43	1.38
24	AK	609	CLA	CHC-C1C	2.19	1.43	1.38
34	Q	402	SQD	O9-S	2.19	1.51	1.45
24	AC	604	CLA	CMB-C2B	-2.19	1.46	1.50
24	AR	603	CLA	CMD-C2D	-2.19	1.46	1.50
24	AR	612	CLA	CMD-C2D	-2.19	1.46	1.50
24	0	613	CLA	CHC-C1C	2.18	1.43	1.38
25	9	616	LUT	C28-C29	-2.18	1.41	1.45
24	q	601	CLA	CMB-C2B	-2.18	1.46	1.50
24	AL	505	CLA	CHC-C1C	2.18	1.43	1.38
24	AK	615	CLA	MG-NB	-2.18	2.01	2.05
23	0	605	CHL	C4C-C3C	2.18	1.48	1.45
23	AS	308	CHL	C1B-NB	-2.18	1.35	1.37
23	AU	601	CHL	C1B-NB	-2.18	1.35	1.37
25	0	614	LUT	C32-C33	-2.18	1.41	1.45
24	AL	503	CLA	CHC-C1C	2.18	1.43	1.38
25	AD	314	LUT	C28-C29	-2.18	1.41	1.45
23	q	613	CHL	C1B-NB	-2.18	1.35	1.37
24	AL	508	CLA	CHC-C1C	2.18	1.43	1.38
23	AC	605	CHL	C1B-NB	-2.18	1.35	1.37
26	AQ	617	NEX	C28-C29	-2.18	1.41	1.45
24	AD	304	CLA	CHC-C1C	2.18	1.43	1.38
24	AQ	604	CLA	CHC-C1C	2.18	1.43	1.38
23	AQ	601	CHL	C1B-NB	-2.18	1.35	1.37
23	AS	306	CHL	CHD-C4C	2.18	1.47	1.40
24	AD	304	CLA	MG-NB	-2.18	2.01	2.05
24	AE	609	CLA	CHC-C1C	2.18	1.42	1.38
23	p	601	CHL	C1B-NB	-2.18	1.35	1.37
24	9	603	CLA	CHC-C1C	2.18	1.42	1.38
24	AN	610	CLA	CHC-C1C	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AC	614	LUT	C28-C29	-2.18	1.41	1.45
25	AD	314	LUT	C12-C13	-2.17	1.41	1.45
24	AA	604	CLA	CMD-C2D	-2.17	1.46	1.50
23	AA	607	CHL	C4C-C3C	2.17	1.48	1.45
23	AH	605	CHL	C4C-C3C	2.17	1.48	1.45
23	V	601	CHL	C1B-NB	-2.17	1.35	1.37
24	AF	603	CLA	CHC-C1C	2.17	1.42	1.38
25	v	315	LUT	C28-C29	-2.17	1.41	1.45
24	0	612	CLA	CHC-C1C	2.17	1.42	1.38
23	AQ	607	CHL	CHB-C4A	-2.17	1.32	1.37
25	AD	315	LUT	C32-C33	-2.17	1.41	1.45
23	p	606	CHL	C4C-C3C	2.17	1.48	1.45
23	p	607	CHL	CHB-C4A	-2.17	1.32	1.37
24	p	610	CLA	C2A-C1A	2.17	1.54	1.50
23	AD	307	CHL	C4C-C3C	2.17	1.48	1.45
24	AJ	405	CLA	CHC-C1C	2.17	1.42	1.38
24	AH	611	CLA	CHC-C1C	2.17	1.42	1.38
24	AK	607	CLA	CHC-C1C	2.17	1.42	1.38
23	AH	606	CHL	C1B-NB	-2.17	1.35	1.37
24	0	609	CLA	MG-NB	-2.17	2.01	2.05
24	AK	607	CLA	CMD-C2D	-2.17	1.46	1.50
24	O	607	CLA	CHC-C1C	2.17	1.42	1.38
24	p	611	CLA	CHC-C1C	2.17	1.42	1.38
23	q	606	CHL	CHD-C4C	2.17	1.47	1.40
24	AD	311	CLA	CMD-C2D	-2.17	1.46	1.50
24	AH	602	CLA	CHC-C1C	2.17	1.42	1.38
24	q	612	CLA	CMB-C2B	-2.17	1.46	1.50
24	9	612	CLA	CHC-C1C	2.17	1.42	1.38
24	AC	603	CLA	CHC-C1C	2.17	1.42	1.38
23	9	609	CHL	C4D-CHA	2.17	1.46	1.38
35	AO	102	DGD	O1G-C1G	-2.17	1.40	1.45
28	AD	316	LHG	O7-C5	-2.17	1.41	1.46
35	P	516	DGD	O2G-C2G	-2.17	1.41	1.46
24	9	614	CLA	CBD-CAD	2.17	1.56	1.51
24	Q	404	CLA	CHC-C1C	2.17	1.42	1.38
24	AC	610	CLA	CHC-C1C	2.17	1.42	1.38
24	AH	610	CLA	CHC-C1C	2.17	1.42	1.38
24	AJ	404	CLA	CHC-C1C	2.17	1.42	1.38
24	AU	613	CLA	CHC-C1C	2.17	1.42	1.38
34	J	410	SQD	O7-S	2.16	1.51	1.45
24	AK	614	CLA	MG-NB	-2.16	2.01	2.05
24	AF	609	CLA	CMC-C2C	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	611	CLA	CHC-C1C	2.16	1.42	1.38
24	O	610	CLA	CHC-C1C	2.16	1.42	1.38
24	V	603	CLA	CHC-C1C	2.16	1.42	1.38
23	9	605	CHL	C1B-NB	-2.16	1.35	1.37
23	AB	601	CHL	C1B-NB	-2.16	1.35	1.37
25	AA	615	LUT	C32-C33	-2.16	1.41	1.45
24	AD	309	CLA	MG-NB	-2.16	2.01	2.05
24	V	604	CLA	CBD-CAD	2.16	1.56	1.51
23	AN	601	CHL	C1B-NB	-2.16	1.35	1.37
35	AL	517	DGD	O1G-C1G	-2.16	1.40	1.45
34	o	101	SQD	O7-S	2.16	1.51	1.45
24	O	608	CLA	CHC-C1C	2.16	1.42	1.38
24	K	101	CLA	CHC-C1C	2.16	1.42	1.38
26	9	617	NEX	C28-C29	-2.16	1.41	1.45
23	AS	307	CHL	C4C-C3C	2.16	1.48	1.45
26	v	317	NEX	C32-C33	-2.16	1.41	1.45
24	AK	608	CLA	CMD-C2D	-2.16	1.46	1.50
24	AU	602	CLA	CHC-C1C	2.16	1.42	1.38
35	P	516	DGD	O1G-C1G	-2.16	1.40	1.45
24	O	613	CLA	MG-NB	-2.16	2.01	2.05
23	AA	605	CHL	C4C-C3C	2.16	1.48	1.45
24	AD	303	CLA	CHC-C1C	2.16	1.42	1.38
24	AA	612	CLA	CHC-C1C	2.15	1.42	1.38
24	v	310	CLA	CMC-C2C	-2.15	1.46	1.50
27	q	617	XAT	C18-C5	2.15	1.55	1.51
23	9	608	CHL	C1B-NB	-2.15	1.35	1.37
24	p	604	CLA	CMD-C2D	-2.15	1.46	1.50
24	v	303	CLA	CMD-C2D	-2.15	1.46	1.50
24	AK	616	CLA	CMD-C2D	-2.15	1.46	1.50
23	AH	606	CHL	CHB-C4A	-2.15	1.32	1.37
23	AC	607	CHL	C1B-NB	-2.15	1.35	1.37
23	AS	302	CHL	C4D-CHA	2.15	1.46	1.38
23	AN	617	CHL	C1B-C2B	2.15	1.48	1.43
24	AD	303	CLA	CMD-C2D	-2.15	1.46	1.50
34	AM	401	SQD	O7-S	2.15	1.51	1.45
24	AH	609	CLA	MG-NB	-2.15	2.01	2.05
34	AJ	411	SQD	O7-S	2.15	1.51	1.45
24	O	614	CLA	CHC-C1C	2.15	1.42	1.38
35	AJ	412	DGD	O2G-C2G	-2.15	1.41	1.46
24	AC	603	CLA	MG-NB	-2.15	2.01	2.05
24	V	604	CLA	MG-NB	-2.15	2.01	2.05
24	O	612	CLA	MG-NB	-2.15	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AD	312	CLA	CHC-C1C	2.15	1.42	1.38
23	AN	617	CHL	CHB-C4A	-2.15	1.32	1.37
26	AA	616	NEX	C28-C29	-2.15	1.41	1.45
23	AN	605	CHL	C1B-NB	-2.15	1.35	1.37
34	AP	101	SQD	O7-S	2.15	1.51	1.45
24	9	603	CLA	MG-NB	-2.15	2.01	2.05
23	AU	606	CHL	C1B-NB	-2.15	1.35	1.37
24	AQ	603	CLA	MG-NB	-2.15	2.01	2.05
24	O	605	CLA	CMD-C2D	-2.15	1.46	1.50
34	M	101	SQD	O7-S	2.15	1.51	1.45
34	AM	401	SQD	O9-S	2.14	1.51	1.45
24	AN	603	CLA	MG-NB	-2.14	2.01	2.05
27	AB	613	XAT	C18-C5	2.14	1.55	1.51
23	AE	601	CHL	C1B-NB	-2.14	1.35	1.37
24	AF	614	CLA	O2A-CGA	2.14	1.37	1.30
28	O	622	LHG	O7-C5	-2.14	1.41	1.46
25	AS	315	LUT	C28-C29	-2.14	1.41	1.45
24	p	603	CLA	MG-NB	-2.14	2.01	2.05
24	AN	604	CLA	CMD-C2D	-2.14	1.46	1.50
28	AK	623	LHG	O7-C5	-2.14	1.41	1.46
24	AH	612	CLA	MG-NB	-2.14	2.01	2.05
35	AL	517	DGD	O2G-C2G	-2.14	1.41	1.46
23	AF	608	CHL	C4C-C3C	2.14	1.48	1.45
37	AM	405	PL9	C53-C6	-2.14	1.46	1.50
24	P	512	CLA	CHC-C1C	2.14	1.42	1.38
24	J	403	CLA	CHC-C1C	2.14	1.42	1.38
24	q	602	CLA	CMD-C2D	-2.14	1.46	1.50
24	p	611	CLA	MG-NB	-2.14	2.01	2.05
26	AR	615	NEX	C28-C29	-2.14	1.41	1.45
24	AE	602	CLA	CMD-C2D	-2.13	1.46	1.50
24	p	613	CLA	MG-NB	-2.13	2.01	2.05
24	AC	604	CLA	CHC-C1C	2.13	1.42	1.38
35	J	413	DGD	O2G-C2G	-2.13	1.41	1.46
26	AC	616	NEX	C28-C29	-2.13	1.41	1.45
24	q	604	CLA	MG-NB	-2.13	2.01	2.05
24	AF	602	CLA	C4D-ND	-2.13	1.34	1.37
23	AD	301	CHL	C1B-NB	-2.13	1.35	1.37
26	9	617	NEX	C32-C33	-2.13	1.41	1.45
23	AR	613	CHL	C4B-NB	-2.13	1.35	1.37
23	v	302	CHL	C4D-CHA	2.13	1.46	1.38
24	AR	601	CLA	CMD-C2D	-2.13	1.46	1.50
24	0	604	CLA	CHC-C1C	2.13	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	v	308	CHL	C1B-NB	-2.13	1.35	1.37
24	V	611	CLA	MG-NB	-2.13	2.01	2.05
24	0	611	CLA	CMD-C2D	-2.13	1.46	1.50
24	AC	610	CLA	MG-NB	-2.13	2.01	2.05
24	q	603	CLA	MG-NB	-2.13	2.01	2.05
24	AK	603	CLA	CHC-C1C	2.13	1.42	1.38
24	9	613	CLA	CHC-C1C	2.13	1.42	1.38
24	AC	613	CLA	MG-NB	-2.13	2.01	2.05
26	AU	616	NEX	C28-C29	-2.13	1.41	1.45
27	AF	613	XAT	C18-C5	2.12	1.55	1.51
24	AS	311	CLA	MG-NB	-2.12	2.01	2.05
24	AS	309	CLA	CHC-C1C	2.12	1.42	1.38
24	AE	604	CLA	CMD-C2D	-2.12	1.46	1.50
35	J	411	DGD	O2G-C2G	-2.12	1.41	1.46
24	AD	313	CLA	CHC-C1C	2.12	1.42	1.38
24	O	601	CLA	CHC-C1C	2.12	1.42	1.38
38	F	102	HEM	FE-NC	2.12	2.02	1.95
24	AD	309	CLA	CHC-C1C	2.12	1.42	1.38
32	J	405	PHO	C4D-ND	-2.12	1.35	1.38
34	m	101	SQD	O7-S	2.12	1.51	1.45
23	AD	306	CHL	C1B-NB	-2.12	1.35	1.37
24	P	511	CLA	MG-NB	-2.12	2.01	2.05
23	AA	607	CHL	C1B-NB	-2.12	1.35	1.37
24	AS	310	CLA	CMD-C2D	-2.12	1.46	1.50
24	AL	510	CLA	MG-NB	-2.12	2.01	2.05
24	P	503	CLA	MG-NB	-2.12	2.01	2.05
24	AD	305	CLA	CHC-C1C	2.12	1.42	1.38
23	AE	605	CHL	CHB-C4A	-2.12	1.32	1.37
24	q	608	CLA	C1B-C2B	2.12	1.48	1.43
35	AJ	401	DGD	O2G-C2G	-2.12	1.41	1.46
24	AF	602	CLA	C1D-C2D	2.12	1.49	1.45
24	AK	618	CLA	MG-NB	-2.12	2.01	2.05
24	AU	613	CLA	MG-NB	-2.12	2.01	2.05
26	AU	616	NEX	C32-C33	-2.12	1.41	1.45
24	AL	511	CLA	MG-NB	-2.12	2.01	2.05
23	q	607	CHL	MG-NA	-2.12	2.01	2.06
23	0	601	CHL	C4D-CHA	2.12	1.45	1.38
24	AK	605	CLA	CHC-C1C	2.12	1.42	1.38
25	AC	614	LUT	C32-C33	-2.12	1.41	1.45
24	AB	610	CLA	CMC-C2C	-2.12	1.46	1.50
24	AD	305	CLA	CMD-C2D	-2.12	1.46	1.50
24	AF	603	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	611	CLA	MG-NB	-2.11	2.01	2.05
24	AJ	406	CLA	CMD-C2D	-2.11	1.46	1.50
24	q	612	CLA	MG-NB	-2.11	2.01	2.05
34	Q	402	SQD	O7-S	2.11	1.51	1.45
24	AL	503	CLA	MG-NB	-2.11	2.01	2.05
24	P	507	CLA	MG-NB	-2.11	2.01	2.05
24	P	510	CLA	MG-NB	-2.11	2.01	2.05
24	AL	513	CLA	MG-NB	-2.11	2.01	2.05
24	AB	603	CLA	MG-NB	-2.11	2.01	2.05
24	AB	609	CLA	MG-NB	-2.11	2.01	2.05
24	O	601	CLA	CMD-C2D	-2.11	1.46	1.50
24	O	614	CLA	CMD-C2D	-2.11	1.46	1.50
24	0	609	CLA	CHC-C1C	2.11	1.42	1.38
24	AH	613	CLA	CMB-C2B	-2.11	1.46	1.50
24	AL	514	CLA	CHC-C1C	2.11	1.42	1.38
24	AH	611	CLA	CMC-C2C	-2.11	1.46	1.50
24	p	612	CLA	MG-NB	-2.11	2.01	2.05
28	AM	406	LHG	O7-C5	-2.11	1.41	1.46
24	v	304	CLA	MG-NB	-2.11	2.01	2.05
24	Q	404	CLA	MG-NB	-2.11	2.01	2.05
23	AR	607	CHL	C2C-C1C	2.11	1.49	1.44
24	AL	506	CLA	CHC-C1C	2.11	1.42	1.38
24	v	313	CLA	CHC-C1C	2.11	1.42	1.38
23	V	606	CHL	C1B-NB	-2.11	1.35	1.37
24	AL	512	CLA	CHC-C1C	2.11	1.42	1.38
23	AR	607	CHL	MG-NA	-2.10	2.01	2.06
24	Q	401	CLA	CMD-C2D	-2.10	1.46	1.50
23	9	606	CHL	CHB-C4A	-2.10	1.32	1.37
24	AE	604	CLA	MG-NB	-2.10	2.01	2.05
24	V	609	CLA	MG-NB	-2.10	2.01	2.05
32	AJ	407	PHO	C4D-ND	-2.10	1.35	1.38
23	AE	606	CHL	C1B-NB	-2.10	1.35	1.37
24	J	404	CLA	CHC-C1C	2.10	1.42	1.38
24	v	309	CLA	CHC-C1C	2.10	1.42	1.38
23	AR	613	CHL	C2C-C1C	2.10	1.49	1.44
24	AL	506	CLA	MG-NB	-2.10	2.01	2.05
24	AF	614	CLA	C4D-ND	-2.10	1.34	1.37
24	AS	304	CLA	MG-NB	-2.10	2.01	2.05
24	AU	613	CLA	CMB-C2B	-2.10	1.46	1.50
23	AA	605	CHL	C1B-NB	-2.10	1.35	1.37
24	AF	609	CLA	MG-NB	-2.10	2.01	2.05
24	AD	310	CLA	CHC-C1C	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AU	608	CHL	CHB-C4A	-2.10	1.32	1.37
24	AF	610	CLA	C3D-C4D	2.10	1.48	1.44
24	AE	609	CLA	MG-NB	-2.10	2.01	2.05
28	p	617	LHG	O7-C5	-2.10	1.41	1.46
24	AQ	604	CLA	CMD-C2D	-2.10	1.46	1.50
24	q	601	CLA	CHC-C1C	2.10	1.42	1.38
23	AC	601	CHL	C1D-ND	-2.09	1.35	1.37
24	AE	611	CLA	MG-NB	-2.09	2.01	2.05
24	9	603	CLA	CMD-C2D	-2.09	1.46	1.50
24	AM	403	CLA	CMC-C2C	-2.09	1.46	1.50
24	v	312	CLA	CMC-C2C	-2.09	1.46	1.50
24	AR	601	CLA	CMB-C2B	-2.09	1.46	1.50
24	P	505	CLA	MG-NB	-2.09	2.01	2.05
23	V	605	CHL	C1B-NB	-2.09	1.35	1.37
27	q	617	XAT	C38-C25	2.09	1.55	1.51
26	q	615	NEX	C32-C33	-2.09	1.41	1.45
28	Q	406	LHG	O7-C5	-2.09	1.41	1.46
24	0	609	CLA	CMD-C2D	-2.09	1.46	1.50
24	AU	604	CLA	CMD-C2D	-2.09	1.46	1.50
24	AR	609	CLA	CHC-C1C	2.09	1.42	1.38
23	AA	617	CHL	CMC-C2C	2.09	1.49	1.45
24	AN	611	CLA	CMB-C2B	-2.09	1.46	1.50
24	v	311	CLA	MG-NB	-2.09	2.01	2.05
24	P	505	CLA	CHC-C1C	2.09	1.42	1.38
23	AE	607	CHL	C4D-CHA	2.09	1.45	1.38
24	AB	604	CLA	MG-NB	-2.09	2.01	2.05
23	AR	606	CHL	C4D-CHA	2.08	1.45	1.38
24	v	313	CLA	CMB-C2B	-2.08	1.46	1.50
24	0	611	CLA	MG-NB	-2.08	2.01	2.05
24	AC	602	CLA	CHC-C1C	2.08	1.42	1.38
26	AA	616	NEX	C11-C12	2.08	1.39	1.34
24	O	612	CLA	CMC-C2C	-2.08	1.46	1.50
23	q	605	CHL	C1B-NB	-2.08	1.35	1.37
24	AJ	405	CLA	CMD-C2D	-2.08	1.46	1.50
24	AN	603	CLA	CMB-C2B	-2.08	1.46	1.50
24	V	603	CLA	MG-NB	-2.08	2.01	2.05
27	AR	616	XAT	C18-C5	2.08	1.55	1.51
24	V	611	CLA	CMB-C2B	-2.08	1.46	1.50
24	p	602	CLA	CMD-C2D	-2.08	1.46	1.50
24	AQ	612	CLA	CMD-C2D	-2.08	1.46	1.50
24	V	609	CLA	CHC-C1C	2.08	1.42	1.38
23	AF	607	CHL	C4D-CHA	2.08	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	610	CLA	MG-NB	-2.08	2.01	2.05
24	P	508	CLA	MG-NB	-2.08	2.01	2.05
24	AQ	604	CLA	MG-NB	-2.08	2.01	2.05
24	O	604	CLA	CMB-C2B	-2.08	1.46	1.50
23	AE	617	CHL	C4C-C3C	2.08	1.48	1.45
24	AK	615	CLA	CMB-C2B	-2.08	1.46	1.50
24	AS	312	CLA	CMC-C2C	-2.08	1.46	1.50
25	AF	611	LUT	C15-C14	-2.08	1.37	1.43
26	AE	615	NEX	C31-C32	2.08	1.39	1.34
24	AA	603	CLA	MG-NB	-2.08	2.01	2.05
23	V	607	CHL	C4D-CHA	2.08	1.45	1.38
24	AE	611	CLA	CHC-C1C	2.08	1.42	1.38
23	AC	605	CHL	C4D-CHA	2.08	1.45	1.38
24	AQ	613	CLA	CHC-C1C	2.08	1.42	1.38
24	AQ	602	CLA	CHC-C1C	2.08	1.42	1.38
24	AL	509	CLA	CMC-C2C	-2.07	1.46	1.50
24	AC	609	CLA	CMC-C2C	-2.07	1.46	1.50
24	9	612	CLA	MG-NB	-2.07	2.01	2.05
23	AF	601	CHL	C1B-NB	-2.07	1.35	1.37
24	AA	604	CLA	MG-NB	-2.07	2.01	2.05
24	AK	615	CLA	CMD-C2D	-2.07	1.46	1.50
24	AN	609	CLA	CMC-C2C	-2.07	1.46	1.50
24	AL	504	CLA	MG-NB	-2.07	2.01	2.05
24	AH	604	CLA	CMD-C2D	-2.07	1.46	1.50
24	AN	613	CLA	CMD-C2D	-2.07	1.46	1.50
24	AK	614	CLA	CHC-C1C	2.07	1.42	1.38
24	AF	614	CLA	CHC-C1C	2.07	1.42	1.38
24	AH	612	CLA	CHC-C1C	2.07	1.42	1.38
24	AK	603	CLA	CMD-C2D	-2.07	1.46	1.50
24	v	310	CLA	MG-NB	-2.07	2.01	2.05
23	AF	605	CHL	C4B-NB	-2.07	1.35	1.37
24	O	616	CLA	MG-NB	-2.07	2.01	2.05
24	AR	617	CLA	CMD-C2D	-2.07	1.46	1.50
23	AB	607	CHL	C4D-CHA	2.07	1.45	1.38
24	v	312	CLA	MG-NB	-2.07	2.01	2.05
24	AN	609	CLA	CMD-C2D	-2.07	1.46	1.50
24	AH	603	CLA	MG-NB	-2.07	2.01	2.05
24	0	602	CLA	CMD-C2D	-2.07	1.46	1.50
26	AU	616	NEX	C12-C13	-2.07	1.41	1.45
24	AM	403	CLA	MG-NB	-2.07	2.01	2.05
24	O	613	CLA	CMB-C2B	-2.07	1.46	1.50
24	O	613	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AR	611	CLA	MG-NB	-2.07	2.01	2.05
24	9	603	CLA	CMB-C2B	-2.07	1.46	1.50
24	AB	611	CLA	CHC-C1C	2.07	1.42	1.38
24	AQ	613	CLA	MG-NB	-2.07	2.01	2.05
26	AE	615	NEX	C11-C12	2.07	1.39	1.34
24	0	611	CLA	CMC-C2C	-2.07	1.46	1.50
23	AF	605	CHL	C1D-ND	-2.07	1.35	1.37
24	AU	604	CLA	MG-NB	-2.07	2.01	2.05
28	w	201	LHG	O7-C5	-2.06	1.41	1.46
24	AS	311	CLA	CMD-C2D	-2.06	1.46	1.50
23	AE	607	CHL	C2C-C1C	2.06	1.49	1.44
23	q	606	CHL	C4D-CHA	2.06	1.45	1.38
24	Q	403	CLA	MG-NB	-2.06	2.01	2.05
27	AB	613	XAT	C38-C25	2.06	1.55	1.51
24	p	603	CLA	CMB-C2B	-2.06	1.46	1.50
24	p	603	CLA	CMD-C2D	-2.06	1.46	1.50
24	AD	305	CLA	MG-NB	-2.06	2.01	2.05
24	O	610	CLA	MG-NB	-2.06	2.01	2.05
23	AA	617	CHL	C1B-C2B	2.06	1.48	1.43
24	9	604	CLA	CMD-C2D	-2.06	1.46	1.50
24	AL	502	CLA	CMD-C2D	-2.06	1.46	1.50
23	V	608	CHL	CHB-C4A	-2.06	1.32	1.37
25	AD	314	LUT	C32-C33	-2.06	1.41	1.45
24	AR	610	CLA	MG-NB	-2.06	2.01	2.05
23	V	616	CHL	CHB-C4A	-2.06	1.32	1.37
23	9	605	CHL	C4D-CHA	2.06	1.45	1.38
26	AA	616	NEX	C32-C33	-2.06	1.41	1.45
24	AL	508	CLA	MG-NB	-2.06	2.01	2.05
23	0	607	CHL	C4D-CHA	2.06	1.45	1.38
24	AU	603	CLA	CMB-C2B	-2.06	1.46	1.50
24	AM	404	CLA	MG-NB	-2.06	2.01	2.05
23	AF	601	CHL	C2C-C1C	2.06	1.49	1.44
24	AA	610	CLA	CMD-C2D	-2.06	1.46	1.50
24	AU	611	CLA	CMC-C2C	-2.06	1.46	1.50
24	AE	602	CLA	MG-NB	-2.06	2.01	2.05
24	P	502	CLA	MG-NB	-2.06	2.01	2.05
24	v	313	CLA	MG-NB	-2.06	2.01	2.05
24	v	303	CLA	MG-NB	-2.06	2.01	2.05
27	AR	616	XAT	C38-C25	2.06	1.55	1.51
24	AH	611	CLA	CMD-C2D	-2.06	1.46	1.50
24	O	604	CLA	MG-NB	-2.06	2.01	2.05
23	AB	608	CHL	C1B-NB	-2.06	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AQ	610	CLA	MG-NB	-2.06	2.01	2.05
24	AA	603	CLA	CMD-C2D	-2.06	1.46	1.50
24	AS	304	CLA	CMD-C2D	-2.06	1.46	1.50
24	AU	612	CLA	MG-NB	-2.06	2.01	2.05
24	Q	403	CLA	CMC-C2C	-2.06	1.46	1.50
24	q	618	CLA	CMD-C2D	-2.06	1.46	1.50
24	O	604	CLA	CHC-C1C	2.06	1.42	1.38
24	AK	606	CLA	CHC-C1C	2.06	1.42	1.38
24	P	506	CLA	MG-NB	-2.06	2.01	2.05
24	AC	603	CLA	CMD-C2D	-2.06	1.46	1.50
24	AK	606	CLA	MG-NB	-2.06	2.01	2.05
24	AK	614	CLA	CMC-C2C	-2.06	1.46	1.50
23	0	606	CHL	C1D-ND	-2.06	1.35	1.37
24	p	611	CLA	CBD-CAD	2.06	1.56	1.51
28	V	615	LHG	O7-C5	-2.06	1.41	1.46
24	AL	506	CLA	CMD-C2D	-2.06	1.46	1.50
24	AQ	602	CLA	CMD-C2D	-2.06	1.46	1.50
24	AU	604	CLA	CMB-C2B	-2.06	1.46	1.50
24	Q	401	CLA	MG-NB	-2.06	2.01	2.05
24	AC	604	CLA	MG-NB	-2.06	2.01	2.05
24	P	504	CLA	MG-NB	-2.06	2.01	2.05
24	P	501	CLA	CMD-C2D	-2.05	1.46	1.50
24	AS	314	CLA	MG-NB	-2.05	2.01	2.05
23	AQ	606	CHL	C1B-NB	-2.05	1.35	1.37
26	AS	317	NEX	C32-C33	-2.05	1.41	1.45
23	AN	607	CHL	C4D-CHA	2.05	1.45	1.38
24	AK	616	CLA	MG-NB	-2.05	2.01	2.05
24	AU	603	CLA	MG-NB	-2.05	2.01	2.05
23	AN	617	CHL	C1A-CHA	2.05	1.51	1.43
28	AU	617	LHG	O7-C5	-2.05	1.41	1.46
24	p	604	CLA	MG-NB	-2.05	2.01	2.05
24	AN	602	CLA	CMD-C2D	-2.05	1.46	1.50
26	v	317	NEX	C11-C12	2.05	1.39	1.34
24	0	612	CLA	MG-NB	-2.05	2.01	2.05
24	AD	303	CLA	MG-NB	-2.05	2.01	2.05
24	AN	612	CLA	MG-NB	-2.05	2.01	2.05
23	p	607	CHL	C2C-C1C	2.05	1.49	1.44
24	AR	602	CLA	MG-NB	-2.05	2.01	2.05
26	v	317	NEX	C12-C13	-2.05	1.41	1.45
24	AN	610	CLA	CMD-C2D	-2.05	1.46	1.50
24	AR	602	CLA	CMD-C2D	-2.05	1.46	1.50
24	AR	617	CLA	CMB-C2B	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	V	602	CLA	CHC-C1C	2.05	1.42	1.38
24	O	606	CLA	C1D-C2D	2.05	1.49	1.45
26	AC	616	NEX	C32-C33	-2.05	1.41	1.45
24	O	603	CLA	MG-NB	-2.05	2.01	2.05
24	AA	604	CLA	CMB-C2B	-2.05	1.46	1.50
24	AR	604	CLA	CMD-C2D	-2.05	1.46	1.50
24	P	508	CLA	CMC-C2C	-2.05	1.46	1.50
24	AS	313	CLA	CMD-C2D	-2.05	1.46	1.50
24	O	614	CLA	MG-NB	-2.05	2.01	2.05
24	AD	305	CLA	CMB-C2B	-2.05	1.46	1.50
24	AD	312	CLA	MG-NB	-2.05	2.01	2.05
23	AH	608	CHL	CHB-C4A	-2.05	1.32	1.37
24	AJ	405	CLA	MG-NB	-2.05	2.01	2.05
24	AH	610	CLA	CMD-C2D	-2.05	1.46	1.50
24	AC	610	CLA	CMB-C2B	-2.05	1.46	1.50
24	P	505	CLA	CMD-C2D	-2.05	1.46	1.50
24	AQ	604	CLA	CMB-C2B	-2.05	1.46	1.50
23	AA	601	CHL	C4D-CHA	2.05	1.45	1.38
24	AU	612	CLA	CHC-C1C	2.05	1.42	1.38
24	AK	609	CLA	CMD-C2D	-2.05	1.46	1.50
24	AS	312	CLA	CMD-C2D	-2.05	1.46	1.50
23	p	606	CHL	C4D-CHA	2.05	1.45	1.38
23	v	307	CHL	C4D-CHA	2.04	1.45	1.38
26	AE	615	NEX	C28-C29	-2.04	1.41	1.45
24	V	603	CLA	CMB-C2B	-2.04	1.46	1.50
24	AR	609	CLA	CMD-C2D	-2.04	1.46	1.50
24	p	618	CLA	C4D-ND	-2.04	1.34	1.37
23	q	607	CHL	C4D-CHA	2.04	1.45	1.38
24	AH	611	CLA	CMB-C2B	-2.04	1.46	1.50
24	0	604	CLA	CMD-C2D	-2.04	1.46	1.50
24	v	314	CLA	CMD-C2D	-2.04	1.46	1.50
24	AS	305	CLA	CMD-C2D	-2.04	1.46	1.50
24	AF	609	CLA	CMB-C2B	-2.04	1.46	1.50
24	q	610	CLA	CMD-C2D	-2.04	1.46	1.50
24	q	601	CLA	MG-NB	-2.04	2.01	2.05
24	AQ	602	CLA	MG-NB	-2.04	2.01	2.05
24	AH	603	CLA	CMB-C2B	-2.04	1.46	1.50
26	q	615	NEX	C12-C13	-2.04	1.41	1.45
24	AK	609	CLA	MG-NB	-2.04	2.01	2.05
24	AN	602	CLA	MG-NB	-2.04	2.01	2.05
24	AA	602	CLA	CMD-C2D	-2.04	1.46	1.50
23	AQ	605	CHL	C4D-CHA	2.04	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	W	201	LHG	O7-C5	-2.04	1.41	1.46
24	AB	603	CLA	CMD-C2D	-2.04	1.46	1.50
24	AR	612	CLA	MG-NB	-2.04	2.01	2.05
24	AD	309	CLA	CMD-C2D	-2.04	1.46	1.50
24	AA	609	CLA	MG-NB	-2.04	2.01	2.05
24	AL	511	CLA	CMD-C2D	-2.04	1.46	1.50
24	AS	312	CLA	MG-NB	-2.04	2.01	2.05
24	AE	604	CLA	CMB-C2B	-2.04	1.46	1.50
24	O	616	CLA	CMD-C2D	-2.04	1.46	1.50
24	9	610	CLA	MG-NB	-2.04	2.01	2.05
24	J	404	CLA	CMD-C2D	-2.04	1.46	1.50
23	0	606	CHL	C2C-C1C	2.04	1.48	1.44
24	AN	604	CLA	MG-NB	-2.04	2.01	2.05
24	AN	603	CLA	CHC-C1C	2.04	1.42	1.38
24	AA	602	CLA	MG-NB	-2.04	2.01	2.05
23	0	605	CHL	CHB-C4A	-2.04	1.32	1.37
23	q	607	CHL	C2C-C1C	2.04	1.48	1.44
24	9	611	CLA	MG-NB	-2.04	2.01	2.05
24	q	611	CLA	MG-NB	-2.04	2.01	2.05
24	9	611	CLA	CMB-C2B	-2.04	1.46	1.50
24	P	507	CLA	CMD-C2D	-2.04	1.46	1.50
24	AR	611	CLA	CMD-C2D	-2.04	1.46	1.50
24	q	611	CLA	CMD-C2D	-2.04	1.46	1.50
24	q	602	CLA	MG-NB	-2.04	2.01	2.05
24	AC	604	CLA	CMD-C2D	-2.04	1.46	1.50
24	Q	401	CLA	CMB-C2B	-2.04	1.46	1.50
24	AK	605	CLA	MG-NB	-2.04	2.01	2.05
24	AQ	611	CLA	MG-NB	-2.04	2.01	2.05
24	AR	612	CLA	CMB-C2B	-2.04	1.46	1.50
23	AE	616	CHL	C1A-CHA	2.04	1.51	1.43
23	AE	616	CHL	C1B-C2B	2.04	1.48	1.43
24	AD	310	CLA	MG-NB	-2.04	2.01	2.05
28	AQ	618	LHG	O7-C5	-2.04	1.41	1.46
24	P	509	CLA	MG-NB	-2.03	2.01	2.05
24	P	510	CLA	CMD-C2D	-2.03	1.46	1.50
24	AC	602	CLA	O2D-CGD	2.03	1.38	1.33
24	AC	602	CLA	MG-NB	-2.03	2.01	2.05
24	V	612	CLA	MG-NB	-2.03	2.01	2.05
24	AQ	603	CLA	CMB-C2B	-2.03	1.46	1.50
24	AS	314	CLA	CMD-C2D	-2.03	1.46	1.50
24	p	612	CLA	CMD-C2D	-2.03	1.46	1.50
24	AU	610	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AR	612	CLA	C3D-C4D	2.03	1.48	1.44
24	AL	510	CLA	CMD-C2D	-2.03	1.46	1.50
24	AS	313	CLA	CMC-C2C	-2.03	1.46	1.50
24	AN	611	CLA	MG-NB	-2.03	2.01	2.05
23	q	613	CHL	C1D-ND	-2.03	1.35	1.37
24	AA	611	CLA	CMB-C2B	-2.03	1.46	1.50
24	AR	610	CLA	CMD-C2D	-2.03	1.46	1.50
24	AL	509	CLA	MG-NB	-2.03	2.01	2.05
24	AL	507	CLA	MG-NB	-2.03	2.01	2.05
24	q	618	CLA	CMB-C2B	-2.03	1.46	1.50
24	AU	611	CLA	MG-NB	-2.03	2.01	2.05
24	V	609	CLA	CMD-C2D	-2.03	1.46	1.50
38	F	102	HEM	C2A-C3A	-2.03	1.33	1.38
23	AB	605	CHL	C1D-ND	-2.03	1.35	1.37
24	AF	610	CLA	C1B-NB	-2.03	1.35	1.37
24	AC	603	CLA	CMB-C2B	-2.03	1.46	1.50
24	0	613	CLA	MG-NB	-2.03	2.01	2.05
24	q	609	CLA	CMB-C2B	-2.03	1.46	1.50
24	AL	508	CLA	CMD-C2D	-2.03	1.46	1.50
24	P	506	CLA	CMB-C2B	-2.03	1.46	1.50
24	V	602	CLA	CMC-C2C	-2.03	1.46	1.50
24	AH	611	CLA	MG-NB	-2.03	2.01	2.05
24	O	615	CLA	CMB-C2B	-2.03	1.46	1.50
24	AU	602	CLA	CMD-C2D	-2.03	1.46	1.50
33	Q	407	LMG	O7-C8	-2.03	1.41	1.46
24	AE	608	CLA	CMB-C2B	-2.03	1.46	1.50
28	AS	301	LHG	O7-C5	-2.03	1.41	1.46
24	O	604	CLA	CMD-C2D	-2.03	1.46	1.50
24	AQ	613	CLA	CMB-C2B	-2.03	1.46	1.50
24	AS	309	CLA	CMD-C2D	-2.03	1.46	1.50
23	AE	605	CHL	C4D-CHA	2.03	1.45	1.38
24	P	509	CLA	CMD-C2D	-2.03	1.46	1.50
25	AA	615	LUT	C28-C29	-2.03	1.41	1.45
24	q	608	CLA	O2A-CGA	2.03	1.37	1.30
24	V	604	CLA	CMD-C2D	-2.03	1.46	1.50
24	9	612	CLA	CMD-C2D	-2.03	1.46	1.50
24	v	312	CLA	CMD-C2D	-2.03	1.46	1.50
28	AH	616	LHG	O7-C5	-2.03	1.41	1.46
24	O	608	CLA	C3D-C4D	2.03	1.48	1.44
24	AU	612	CLA	CMB-C2B	-2.03	1.46	1.50
24	AC	610	CLA	CMD-C2D	-2.02	1.46	1.50
23	p	608	CHL	C4D-CHA	2.02	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	q	618	CLA	C3D-C4D	2.02	1.48	1.44
24	AD	311	CLA	CMC-C2C	-2.02	1.46	1.50
24	AE	609	CLA	CMD-C2D	-2.02	1.46	1.50
24	q	608	CLA	CMB-C2B	-2.02	1.46	1.50
32	J	406	PHO	C1A-C2A	2.02	1.54	1.51
24	9	613	CLA	CMD-C2D	-2.02	1.46	1.50
24	AJ	406	CLA	CMB-C2B	-2.02	1.46	1.50
24	AU	612	CLA	CMD-C2D	-2.02	1.46	1.50
23	AS	306	CHL	CHB-C4A	-2.02	1.32	1.37
24	O	609	CLA	MG-NB	-2.02	2.01	2.05
24	AR	609	CLA	MG-NB	-2.02	2.01	2.05
24	AE	603	CLA	CMD-C2D	-2.02	1.46	1.50
24	AE	608	CLA	MG-NB	-2.02	2.01	2.05
24	AH	604	CLA	CMB-C2B	-2.02	1.46	1.50
24	AN	611	CLA	CMD-C2D	-2.02	1.46	1.50
24	AH	610	CLA	MG-NB	-2.02	2.01	2.05
24	AK	617	CLA	MG-NB	-2.02	2.01	2.05
24	AR	612	CLA	CHC-C1C	2.02	1.42	1.38
27	9	618	XAT	C20-C13	2.02	1.55	1.50
24	O	602	CLA	CMD-C2D	-2.02	1.46	1.50
23	q	613	CHL	C4B-NB	-2.02	1.35	1.37
24	AK	613	CLA	CMD-C2D	-2.02	1.46	1.50
24	AL	510	CLA	CMB-C2B	-2.02	1.46	1.50
23	p	605	CHL	C4D-CHA	2.02	1.45	1.38
24	AC	609	CLA	CMD-C2D	-2.02	1.46	1.50
24	AA	612	CLA	MG-NB	-2.02	2.01	2.05
24	v	314	CLA	MG-NB	-2.02	2.01	2.05
24	AH	602	CLA	MG-NB	-2.02	2.01	2.05
24	AC	611	CLA	CMD-C2D	-2.02	1.46	1.50
24	p	604	CLA	CMB-C2B	-2.02	1.46	1.50
24	AL	502	CLA	CMB-C2B	-2.02	1.46	1.50
28	AU	617	LHG	P-O6	2.02	1.67	1.59
23	AA	617	CHL	C1A-CHA	2.02	1.51	1.43
24	O	607	CLA	MG-NB	-2.02	2.01	2.05
28	q	616	LHG	P-O6	2.02	1.67	1.59
28	AN	616	LHG	O7-C5	-2.02	1.41	1.46
23	AB	605	CHL	C4B-NB	-2.02	1.35	1.37
24	AB	604	CLA	CMD-C2D	-2.02	1.46	1.50
24	AD	311	CLA	MG-NB	-2.02	2.01	2.05
24	O	610	CLA	CMD-C2D	-2.02	1.46	1.50
24	AN	612	CLA	CMB-C2B	-2.02	1.46	1.50
24	AK	606	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	602	CLA	MG-NB	-2.02	2.01	2.05
24	V	610	CLA	CMB-C2B	-2.02	1.46	1.50
38	f	102	HEM	CMB-C2B	2.02	1.55	1.50
24	0	611	CLA	CMB-C2B	-2.02	1.46	1.50
24	AS	310	CLA	CMC-C2C	-2.02	1.46	1.50
24	AF	602	CLA	CHC-C1C	2.02	1.42	1.38
24	AE	603	CLA	MG-NB	-2.02	2.01	2.05
24	AS	303	CLA	MG-NB	-2.02	2.01	2.05
23	AN	608	CHL	C1C-NC	-2.02	1.34	1.37
24	AD	310	CLA	CMD-C2D	-2.02	1.46	1.50
24	K	101	CLA	CMD-C2D	-2.02	1.46	1.50
23	AH	605	CHL	C4D-CHA	2.02	1.45	1.38
23	AQ	608	CHL	CHB-C4A	-2.02	1.32	1.37
24	AC	602	CLA	CMD-C2D	-2.02	1.46	1.50
24	AK	618	CLA	CMD-C2D	-2.02	1.46	1.50
24	AF	603	CLA	CMB-C2B	-2.01	1.46	1.50
23	v	306	CHL	CHB-C4A	-2.01	1.32	1.37
24	q	604	CLA	CMB-C2B	-2.01	1.46	1.50
24	p	610	CLA	MG-NB	-2.01	2.01	2.05
24	q	609	CLA	MG-NB	-2.01	2.01	2.05
24	AH	602	CLA	CMD-C2D	-2.01	1.46	1.50
23	p	608	CHL	CHB-C4A	-2.01	1.32	1.37
24	AU	611	CLA	CMD-C2D	-2.01	1.46	1.50
23	0	606	CHL	MG-NA	-2.01	2.01	2.06
24	AC	612	CLA	CMD-C2D	-2.01	1.46	1.50
24	O	607	CLA	CMD-C2D	-2.01	1.46	1.50
24	P	501	CLA	CMB-C2B	-2.01	1.46	1.50
24	AU	613	CLA	CMD-C2D	-2.01	1.46	1.50
24	9	614	CLA	MG-NB	-2.01	2.01	2.05
24	O	602	CLA	MG-NB	-2.01	2.01	2.05
23	q	605	CHL	C2C-C1C	2.01	1.48	1.44
24	AK	604	CLA	MG-NB	-2.01	2.01	2.05
24	AE	609	CLA	CMB-C2B	-2.01	1.46	1.50
24	AK	608	CLA	CMB-C2B	-2.01	1.46	1.50
24	AL	507	CLA	CMB-C2B	-2.01	1.46	1.50
23	AB	607	CHL	C2C-C1C	2.01	1.48	1.44
23	AU	605	CHL	C4D-CHA	2.01	1.45	1.38
24	AL	513	CLA	CMD-C2D	-2.01	1.46	1.50
23	AR	605	CHL	C4D-CHA	2.01	1.45	1.38
24	AA	603	CLA	CMB-C2B	-2.01	1.46	1.50
24	V	610	CLA	MG-NB	-2.01	2.01	2.05
24	AR	609	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AK	614	CLA	CMB-C2B	-2.01	1.46	1.50
24	AK	617	CLA	CMB-C2B	-2.01	1.46	1.50
24	AS	312	CLA	CMB-C2B	-2.01	1.46	1.50
23	AA	608	CHL	C4B-NB	-2.01	1.35	1.37
23	AE	617	CHL	C1D-ND	-2.01	1.35	1.37
24	AU	610	CLA	MG-NB	-2.01	2.01	2.05
24	AD	309	CLA	CMB-C2B	-2.01	1.46	1.50
24	AK	612	CLA	CMB-C2B	-2.01	1.46	1.50
24	9	612	CLA	CMB-C2B	-2.01	1.46	1.50
24	AH	613	CLA	MG-NB	-2.01	2.01	2.05
23	AD	308	CHL	CHB-C4A	-2.01	1.32	1.37
24	0	603	CLA	CMD-C2D	-2.01	1.46	1.50
23	V	606	CHL	C4D-CHA	2.01	1.45	1.38
24	AL	511	CLA	CMB-C2B	-2.01	1.46	1.50
23	q	605	CHL	C4D-CHA	2.01	1.45	1.38
24	9	604	CLA	CMB-C2B	-2.01	1.46	1.50
24	AD	313	CLA	CMD-C2D	-2.01	1.46	1.50
24	P	506	CLA	CMD-C2D	-2.01	1.46	1.50
24	v	304	CLA	CMD-C2D	-2.01	1.46	1.50
24	AU	611	CLA	CMB-C2B	-2.01	1.46	1.50
23	AB	607	CHL	C1D-ND	-2.01	1.35	1.37
23	AF	605	CHL	C1B-NB	-2.01	1.35	1.37
23	AE	601	CHL	C4D-CHA	2.00	1.45	1.38
24	AE	603	CLA	CMB-C2B	-2.00	1.46	1.50
24	AK	606	CLA	CMB-C2B	-2.00	1.46	1.50
26	AR	615	NEX	C32-C33	-2.00	1.41	1.45
24	0	612	CLA	CMB-C2B	-2.00	1.46	1.50
24	AE	610	CLA	CMB-C2B	-2.00	1.46	1.50
24	O	611	CLA	CMD-C2D	-2.00	1.46	1.50
24	AC	609	CLA	MG-NB	-2.00	2.01	2.05
24	AD	311	CLA	CMB-C2B	-2.00	1.46	1.50
24	O	612	CLA	CMB-C2B	-2.00	1.46	1.50
24	AK	607	CLA	CMC-C2C	-2.00	1.46	1.50
24	AL	506	CLA	CMB-C2B	-2.00	1.46	1.50
23	AR	606	CHL	C2C-C1C	2.00	1.48	1.44
23	9	607	CHL	C4D-CHA	2.00	1.45	1.38
24	AH	609	CLA	CMD-C2D	-2.00	1.46	1.50
24	J	404	CLA	MG-NB	-2.00	2.01	2.05
24	AN	610	CLA	MG-NB	-2.00	2.01	2.05
24	P	511	CLA	CMD-C2D	-2.00	1.46	1.50
24	AJ	406	CLA	MG-NB	-2.00	2.01	2.05
34	AJ	411	SQD	C8-C7	2.00	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	K	101	CLA	C3D-C4D	2.00	1.48	1.44
27	AB	613	XAT	C39-C29	2.00	1.55	1.50
24	AR	604	CLA	MG-NB	-2.00	2.01	2.05
27	q	617	XAT	C20-C13	2.00	1.55	1.50
24	AB	603	CLA	CMB-C2B	-2.00	1.46	1.50
24	AU	603	CLA	CMD-C2D	-2.00	1.46	1.50

All (4822) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	9	618	XAT	O4-C5-C4	32.84	138.05	113.38
27	9	618	XAT	O24-C25-C24	32.41	137.73	113.38
27	AB	613	XAT	O4-C5-C4	32.27	137.62	113.38
27	q	617	XAT	O4-C5-C4	32.17	137.55	113.38
27	AR	616	XAT	O4-C5-C4	32.12	137.51	113.38
27	AB	613	XAT	O24-C25-C24	31.98	137.41	113.38
27	AF	613	XAT	O24-C25-C24	31.57	137.10	113.38
27	AF	613	XAT	O4-C5-C4	31.44	137.00	113.38
27	AR	616	XAT	O24-C25-C24	30.99	136.66	113.38
27	q	617	XAT	O24-C25-C24	30.93	136.62	113.38
23	0	607	CHL	C1C-NC-C4C	-11.81	101.40	106.71
23	v	308	CHL	C1C-NC-C4C	-11.17	101.68	106.71
23	p	607	CHL	C2B-C1B-NB	11.17	117.72	110.23
23	AQ	607	CHL	C2B-C1B-NB	11.11	117.68	110.23
23	AE	605	CHL	C2B-C1B-NB	11.05	117.64	110.23
23	0	608	CHL	C2C-C3C-C4C	-10.96	98.68	106.49
23	0	608	CHL	CMD-C2D-C1D	10.79	143.74	124.71
23	V	607	CHL	C1C-NC-C4C	-10.76	101.87	106.71
23	AS	308	CHL	C1C-NC-C4C	-10.71	101.89	106.71
23	AH	606	CHL	C2B-C1B-NB	10.66	117.38	110.23
23	AU	608	CHL	C2B-C1B-NB	10.62	117.35	110.23
23	AC	606	CHL	C2B-C1B-NB	10.61	117.34	110.23
23	AQ	605	CHL	C2B-C1B-NB	10.57	117.32	110.23
23	9	606	CHL	C2B-C1B-NB	10.52	117.28	110.23
27	AB	613	XAT	C15-C14-C13	-10.48	112.36	127.31
23	p	605	CHL	C2B-C1B-NB	10.46	117.25	110.23
23	AH	608	CHL	C2B-C1B-NB	10.46	117.25	110.23
27	9	618	XAT	C31-C30-C29	-10.40	112.47	127.31
23	AN	608	CHL	C2B-C1B-NB	10.40	117.20	110.23
23	AD	308	CHL	C2B-C1B-NB	10.39	117.20	110.23
23	AC	607	CHL	C1C-NC-C4C	-10.37	102.05	106.71
23	0	605	CHL	C2B-C1B-NB	10.36	117.18	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AA	607	CHL	C2B-C1B-NB	10.36	117.18	110.23
23	9	608	CHL	C1C-NC-C4C	-10.36	102.05	106.71
23	p	608	CHL	C2B-C1B-NB	10.34	117.17	110.23
23	AQ	606	CHL	C2B-C1B-NB	10.33	117.15	110.23
23	q	606	CHL	C1C-NC-C4C	-10.33	102.06	106.71
23	V	608	CHL	C2B-C1B-NB	10.31	117.14	110.23
23	9	607	CHL	C2B-C1B-NB	10.30	117.14	110.23
23	AE	607	CHL	C2B-C1B-NB	10.30	117.13	110.23
23	AD	302	CHL	C2B-C1B-NB	10.27	117.12	110.23
23	AE	606	CHL	C2B-C1B-NB	10.27	117.12	110.23
23	AQ	608	CHL	C2B-C1B-NB	10.27	117.12	110.23
23	AU	606	CHL	C2B-C1B-NB	10.26	117.11	110.23
23	AA	606	CHL	C2B-C1B-NB	10.24	117.10	110.23
23	AN	606	CHL	C2B-C1B-NB	10.17	117.05	110.23
23	V	606	CHL	C2B-C1B-NB	10.17	117.05	110.23
23	AU	605	CHL	C2B-C1B-NB	10.13	117.02	110.23
23	AC	607	CHL	C2B-C1B-NB	10.11	117.01	110.23
23	AH	605	CHL	C2B-C1B-NB	10.11	117.01	110.23
23	AB	601	CHL	C2B-C1B-NB	10.10	117.00	110.23
24	O	608	CLA	C4A-NA-C1A	10.10	111.25	106.71
23	9	608	CHL	C2B-C1B-NB	10.09	117.00	110.23
23	AD	301	CHL	C2B-C1B-NB	10.07	116.98	110.23
23	AN	607	CHL	C2B-C1B-NB	10.05	116.97	110.23
27	9	618	XAT	C15-C14-C13	-10.04	112.98	127.31
23	AE	617	CHL	C2B-C1B-NB	10.04	116.96	110.23
23	AC	608	CHL	C2B-C1B-NB	10.03	116.96	110.23
23	AH	607	CHL	C2B-C1B-NB	10.03	116.95	110.23
27	AF	613	XAT	C15-C14-C13	-10.02	113.01	127.31
23	v	307	CHL	C2B-C1B-NB	10.02	116.95	110.23
23	AA	605	CHL	C2B-C1B-NB	10.01	116.94	110.23
23	p	609	CHL	C2B-C1B-NB	9.99	116.93	110.23
23	AQ	601	CHL	C2B-C1B-NB	9.98	116.92	110.23
23	AS	308	CHL	C2B-C1B-NB	9.97	116.92	110.23
23	0	601	CHL	C2B-C1B-NB	9.96	116.91	110.23
23	0	607	CHL	C2B-C1B-NB	9.95	116.90	110.23
23	AE	601	CHL	C2B-C1B-NB	9.95	116.90	110.23
23	AR	606	CHL	C2B-C1B-NB	9.94	116.90	110.23
23	AU	607	CHL	C2B-C1B-NB	9.94	116.90	110.23
23	p	601	CHL	C2B-C1B-NB	9.94	116.89	110.23
23	AC	605	CHL	C2B-C1B-NB	9.94	116.89	110.23
23	q	606	CHL	C2B-C1B-NB	9.93	116.89	110.23
27	AR	616	XAT	C11-C10-C9	-9.92	113.15	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	v	308	CHL	C2B-C1B-NB	9.92	116.88	110.23
23	AQ	609	CHL	C2B-C1B-NB	9.90	116.87	110.23
23	v	306	CHL	C2B-C1B-NB	9.87	116.85	110.23
23	9	605	CHL	C2B-C1B-NB	9.86	116.84	110.23
23	AH	601	CHL	C2B-C1B-NB	9.81	116.81	110.23
23	AN	601	CHL	C2B-C1B-NB	9.80	116.80	110.23
23	AD	306	CHL	C2B-C1B-NB	9.80	116.80	110.23
23	AE	616	CHL	C2B-C1B-NB	9.79	116.79	110.23
23	AF	601	CHL	C2B-C1B-NB	9.79	116.79	110.23
23	AB	606	CHL	C1C-NC-C4C	-9.77	102.31	106.71
23	V	601	CHL	C2B-C1B-NB	9.76	116.77	110.23
27	q	617	XAT	C11-C10-C9	-9.75	113.39	127.31
23	AU	601	CHL	C2B-C1B-NB	9.75	116.77	110.23
23	AS	306	CHL	C2B-C1B-NB	9.74	116.76	110.23
23	9	609	CHL	C2B-C1B-NB	9.73	116.76	110.23
23	AD	307	CHL	C2B-C1B-NB	9.72	116.75	110.23
27	q	617	XAT	C35-C34-C33	-9.71	113.45	127.31
23	AB	606	CHL	C2B-C1B-NB	9.70	116.74	110.23
23	AN	605	CHL	C2B-C1B-NB	9.69	116.73	110.23
27	AR	616	XAT	C35-C34-C33	-9.68	113.49	127.31
27	AF	613	XAT	C31-C30-C29	-9.66	113.52	127.31
23	AA	617	CHL	C2B-C1B-NB	9.64	116.69	110.23
23	V	605	CHL	C2B-C1B-NB	9.62	116.68	110.23
23	AS	307	CHL	C2B-C1B-NB	9.59	116.66	110.23
23	AA	601	CHL	C2B-C1B-NB	9.55	116.63	110.23
27	9	618	XAT	C11-C10-C9	-9.52	113.72	127.31
27	AB	613	XAT	C31-C30-C29	-9.46	113.82	127.31
23	AR	605	CHL	C1C-NC-C4C	-9.43	102.47	106.71
27	AR	616	XAT	C15-C14-C13	-9.33	114.00	127.31
23	9	606	CHL	CMD-C2D-C1D	9.32	141.14	124.71
27	q	617	XAT	C15-C14-C13	-9.30	114.04	127.31
23	p	606	CHL	C2B-C1B-NB	9.29	116.46	110.23
23	v	306	CHL	C1C-NC-C4C	-9.22	102.56	106.71
23	q	605	CHL	C2B-C1B-NB	9.15	116.37	110.23
23	AF	608	CHL	C2B-C1B-NB	9.08	116.32	110.23
23	0	606	CHL	C2B-C1B-NB	9.07	116.31	110.23
27	9	618	XAT	C35-C34-C33	-9.06	114.38	127.31
27	AB	613	XAT	C11-C10-C9	-8.95	114.53	127.31
23	9	601	CHL	C2B-C1B-NB	8.95	116.23	110.23
23	AR	605	CHL	C2B-C1B-NB	8.92	116.21	110.23
23	AC	606	CHL	CMD-C2D-C1D	8.86	140.34	124.71
23	AS	302	CHL	C2B-C1B-NB	8.86	116.17	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AK	610	CLA	C4A-NA-C1A	8.84	110.68	106.71
23	v	302	CHL	C2B-C1B-NB	8.83	116.15	110.23
23	AC	601	CHL	C2B-C1B-NB	8.83	116.15	110.23
27	AR	616	XAT	C31-C30-C29	-8.78	114.77	127.31
23	AB	608	CHL	C2B-C1B-NB	8.73	116.08	110.23
27	q	617	XAT	C31-C30-C29	-8.73	114.86	127.31
23	V	605	CHL	CMD-C2D-C1D	8.70	140.04	124.71
23	0	607	CHL	CMD-C2D-C1D	8.69	140.03	124.71
23	AU	606	CHL	CMD-C2D-C1D	8.67	140.00	124.71
23	AA	608	CHL	CHD-C1D-ND	-8.67	116.49	124.45
23	AC	601	CHL	C2C-C3C-C4C	-8.66	100.32	106.49
24	AK	613	CLA	C4A-NA-C1A	8.66	110.60	106.71
23	AC	607	CHL	C3C-C4C-NC	8.65	117.86	109.95
23	q	613	CHL	C2B-C1B-NB	8.65	116.03	110.23
23	AN	617	CHL	C2B-C1B-NB	8.62	116.01	110.23
23	q	607	CHL	C2B-C1B-NB	8.62	116.01	110.23
23	AR	613	CHL	C2B-C1B-NB	8.61	116.00	110.23
23	AN	608	CHL	CMD-C2D-C1D	8.56	139.80	124.71
23	9	608	CHL	C3C-C4C-NC	8.55	117.77	109.95
23	AD	317	CHL	C2B-C1B-NB	8.55	115.96	110.23
23	AF	607	CHL	C2B-C1B-NB	8.53	115.95	110.23
27	AF	613	XAT	C35-C34-C33	-8.51	115.16	127.31
23	AD	308	CHL	CMD-C2D-C1D	8.51	139.71	124.71
23	AS	308	CHL	CMD-C2D-C1D	8.51	139.71	124.71
23	AQ	608	CHL	CMD-C2D-C1D	8.46	139.62	124.71
23	AC	607	CHL	CMD-C2D-C1D	8.44	139.59	124.71
23	q	606	CHL	C3C-C4C-NC	8.44	117.68	109.95
23	0	617	CHL	C2B-C1B-NB	8.42	115.88	110.23
23	AD	307	CHL	CMD-C2D-C1D	8.42	139.55	124.71
23	AS	306	CHL	C1C-NC-C4C	-8.42	102.92	106.71
23	AR	607	CHL	C2B-C1B-NB	8.41	115.87	110.23
23	V	607	CHL	C2B-C1B-NB	8.41	115.87	110.23
23	AU	606	CHL	C2C-C3C-C4C	-8.40	100.50	106.49
23	AA	606	CHL	C2C-C3C-C4C	-8.39	100.50	106.49
23	AE	617	CHL	C2C-C3C-C4C	-8.39	100.51	106.49
23	AC	605	CHL	CMD-C2D-C1D	8.38	139.48	124.71
23	9	606	CHL	C2C-C3C-C4C	-8.37	100.53	106.49
23	AH	606	CHL	CMD-C2D-C1D	8.35	139.43	124.71
23	AH	608	CHL	CMD-C2D-C1D	8.35	139.43	124.71
23	AB	605	CHL	C2B-C1B-NB	8.35	115.83	110.23
23	AE	606	CHL	CMD-C2D-C1D	8.34	139.41	124.71
23	9	605	CHL	CMD-C2D-C1D	8.33	139.40	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	9	608	CHL	CMD-C2D-C1D	8.33	139.39	124.71
23	AA	607	CHL	CMD-C2D-C1D	8.32	139.38	124.71
23	AF	607	CHL	CMD-C2D-C1D	8.32	139.38	124.71
23	AB	606	CHL	C3C-C4C-NC	8.32	117.56	109.95
23	AE	607	CHL	CMD-C2D-C1D	8.30	139.35	124.71
23	q	607	CHL	CMD-C2D-C1D	8.30	139.35	124.71
23	AU	608	CHL	CMD-C2D-C1D	8.29	139.32	124.71
27	9	618	XAT	C27-C28-C29	-8.28	112.68	125.53
23	AR	605	CHL	C3C-C4C-NC	8.28	117.53	109.95
23	p	608	CHL	CMD-C2D-C1D	8.26	139.28	124.71
23	V	607	CHL	CMD-C2D-C1D	8.26	139.26	124.71
23	AQ	609	CHL	CMD-C2D-C1D	8.25	139.25	124.71
32	J	406	PHO	C4D-CHA-CBD	-8.24	104.79	108.52
24	AF	614	CLA	C4A-NA-C1A	8.24	110.41	106.71
23	AQ	606	CHL	CMD-C2D-C1D	8.24	139.24	124.71
23	AR	607	CHL	CMD-C2D-C1D	8.23	139.22	124.71
23	AB	607	CHL	CMD-C2D-C1D	8.22	139.20	124.71
23	AH	606	CHL	C2C-C3C-C4C	-8.20	100.64	106.49
23	AF	605	CHL	C1C-NC-C4C	-8.17	103.03	106.71
23	p	606	CHL	CMD-C2D-C1D	8.16	139.10	124.71
27	9	618	XAT	C39-C29-C30	-8.16	111.50	122.92
23	AU	605	CHL	CMD-C2D-C1D	8.15	139.08	124.71
23	AA	601	CHL	CMD-C2D-C1D	8.15	139.07	124.71
23	V	605	CHL	C2C-C3C-C4C	-8.14	100.68	106.49
23	AH	605	CHL	CMD-C2D-C1D	8.14	139.06	124.71
23	9	601	CHL	CMD-C2D-C1D	8.14	139.06	124.71
23	AC	608	CHL	CMD-C2D-C1D	8.14	139.05	124.71
23	AH	608	CHL	C2C-C3C-C4C	-8.12	100.70	106.49
23	AQ	607	CHL	C2C-C3C-C4C	-8.12	100.70	106.49
23	AN	607	CHL	CMD-C2D-C1D	8.11	139.01	124.71
23	p	606	CHL	C2C-C3C-C4C	-8.11	100.71	106.49
23	AU	608	CHL	C2C-C3C-C4C	-8.10	100.72	106.49
23	AF	607	CHL	C2C-C3C-C4C	-8.10	100.72	106.49
23	V	608	CHL	CMD-C2D-C1D	8.10	138.99	124.71
23	AA	608	CHL	CMD-C2D-C1D	8.10	138.98	124.71
23	9	607	CHL	C2C-C3C-C4C	-8.09	100.72	106.49
23	AN	607	CHL	C2C-C3C-C4C	-8.08	100.73	106.49
23	AC	601	CHL	CMD-C2D-C1D	8.08	138.95	124.71
23	V	601	CHL	CMD-C2D-C1D	8.08	138.95	124.71
23	AF	605	CHL	C2B-C1B-NB	8.06	115.64	110.23
23	AE	601	CHL	CMD-C2D-C1D	8.06	138.92	124.71
23	AS	306	CHL	C3C-C4C-NC	8.06	117.33	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AQ	608	CHL	C2C-C3C-C4C	-8.06	100.74	106.49
23	AR	613	CHL	C2C-C3C-C4C	-8.06	100.74	106.49
23	AS	302	CHL	C2C-C3C-C4C	-8.06	100.74	106.49
23	AN	601	CHL	CMD-C2D-C1D	8.06	138.92	124.71
23	0	605	CHL	CMD-C2D-C1D	8.06	138.91	124.71
23	v	308	CHL	CMD-C2D-C1D	8.06	138.91	124.71
32	AJ	408	PHO	C4D-CHA-CBD	-8.06	104.87	108.52
23	V	607	CHL	C4B-C3B-C2B	-8.05	101.15	108.69
23	0	605	CHL	C2C-C3C-C4C	-8.05	100.75	106.49
27	AF	613	XAT	C38-C25-C26	-8.04	108.78	122.26
23	AQ	606	CHL	C2C-C3C-C4C	-8.04	100.76	106.49
23	AH	605	CHL	C2C-C3C-C4C	-8.03	100.76	106.49
23	0	601	CHL	CMD-C2D-C1D	8.02	138.85	124.71
23	AN	605	CHL	CMD-C2D-C1D	8.02	138.85	124.71
23	AN	605	CHL	C2C-C3C-C4C	-8.02	100.77	106.49
23	v	307	CHL	CMD-C2D-C1D	8.02	138.84	124.71
23	AR	605	CHL	CMD-C2D-C1D	8.01	138.83	124.71
23	q	605	CHL	CMD-C2D-C1D	8.01	138.83	124.71
23	AU	601	CHL	CMD-C2D-C1D	8.01	138.82	124.71
23	v	302	CHL	C2C-C3C-C4C	-8.01	100.78	106.49
23	p	607	CHL	CMD-C2D-C1D	8.00	138.82	124.71
27	AR	616	XAT	C7-C8-C9	-8.00	113.11	125.53
23	AH	601	CHL	CMD-C2D-C1D	8.00	138.81	124.71
23	AD	307	CHL	C2C-C3C-C4C	-8.00	100.79	106.49
23	v	306	CHL	C3C-C4C-NC	7.99	117.26	109.95
23	AE	607	CHL	O2D-CGD-CBD	7.99	125.46	111.27
23	AU	605	CHL	C2C-C3C-C4C	-7.99	100.80	106.49
23	p	605	CHL	CMD-C2D-C1D	7.98	138.78	124.71
23	AC	607	CHL	C2C-C3C-C4C	-7.97	99.46	108.58
23	AB	607	CHL	C2B-C1B-NB	7.97	115.58	110.23
23	AA	607	CHL	C2C-C3C-C4C	-7.97	100.81	106.49
23	AB	606	CHL	CMD-C2D-C1D	7.96	138.74	124.71
23	AQ	607	CHL	CMD-C2D-C1D	7.96	138.74	124.71
23	AD	301	CHL	CMD-C2D-C1D	7.95	138.72	124.71
23	9	607	CHL	CMD-C2D-C1D	7.95	138.72	124.71
23	9	601	CHL	C2C-C3C-C4C	-7.95	100.83	106.49
23	p	608	CHL	C2C-C3C-C4C	-7.94	100.83	106.49
23	AC	605	CHL	C2C-C3C-C4C	-7.94	100.83	106.49
23	AB	605	CHL	CMD-C2D-C1D	7.93	138.70	124.71
27	q	617	XAT	C7-C8-C9	-7.93	113.22	125.53
23	V	616	CHL	C2B-C1B-NB	7.93	115.55	110.23
24	AB	611	CLA	C4A-NA-C1A	7.93	110.27	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	9	609	CHL	CMD-C2D-C1D	7.92	138.68	124.71
23	AF	601	CHL	CMD-C2D-C1D	7.92	138.68	124.71
23	AE	616	CHL	C2C-C3C-C4C	-7.92	100.84	106.49
23	AQ	605	CHL	CMD-C2D-C1D	7.92	138.67	124.71
23	AB	601	CHL	CMD-C2D-C1D	7.91	138.66	124.71
23	9	608	CHL	C2C-C3C-C4C	-7.89	99.55	108.58
27	9	618	XAT	C7-C8-C9	-7.88	113.31	125.53
23	AE	606	CHL	C2C-C3C-C4C	-7.88	100.87	106.49
23	AN	617	CHL	C2C-C3C-C4C	-7.88	100.87	106.49
23	0	606	CHL	C2C-C3C-C4C	-7.87	100.88	106.49
23	AA	605	CHL	CMD-C2D-C1D	7.87	138.58	124.71
23	AU	607	CHL	C2C-C3C-C4C	-7.87	100.88	106.49
24	AL	514	CLA	C4A-NA-C1A	7.87	110.24	106.71
23	AH	607	CHL	C2C-C3C-C4C	-7.87	100.88	106.49
23	AF	606	CHL	C2C-C3C-C4C	-7.87	99.58	108.58
23	p	609	CHL	CMD-C2D-C1D	7.86	138.57	124.71
23	AR	606	CHL	CMD-C2D-C1D	7.86	138.57	124.71
23	AB	605	CHL	C1C-NC-C4C	-7.85	103.17	106.71
23	p	601	CHL	CMD-C2D-C1D	7.84	138.53	124.71
23	AN	606	CHL	C2C-C3C-C4C	-7.84	100.90	106.49
23	AC	601	CHL	C4B-C3B-C2B	-7.84	101.35	108.69
23	AQ	601	CHL	CMD-C2D-C1D	7.83	138.52	124.71
23	AE	605	CHL	CMD-C2D-C1D	7.83	138.51	124.71
23	AH	607	CHL	CMD-C2D-C1D	7.82	138.50	124.71
23	AR	605	CHL	C2C-C3C-C4C	-7.82	99.63	108.58
23	AU	607	CHL	CMD-C2D-C1D	7.81	138.49	124.71
23	AD	302	CHL	CMD-C2D-C1D	7.80	138.47	124.71
23	AQ	609	CHL	C2C-C3C-C4C	-7.80	100.93	106.49
23	AA	605	CHL	C2C-C3C-C4C	-7.80	100.93	106.49
23	p	609	CHL	C2C-C3C-C4C	-7.80	100.93	106.49
23	V	606	CHL	C2C-C3C-C4C	-7.80	100.93	106.49
27	AF	613	XAT	C11-C10-C9	-7.79	116.19	127.31
24	P	512	CLA	C4A-NA-C1A	7.79	110.21	106.71
23	AB	601	CHL	C2C-C3C-C4C	-7.78	100.94	106.49
24	AD	313	CLA	C4A-NA-C1A	7.78	110.20	106.71
23	v	302	CHL	CMD-C2D-C1D	7.77	138.41	124.71
23	9	601	CHL	C4B-C3B-C2B	-7.77	101.42	108.69
23	q	606	CHL	CMD-C2D-C1D	7.77	138.40	124.71
23	AB	606	CHL	C2C-C3C-C4C	-7.76	99.70	108.58
23	AS	302	CHL	CMD-C2D-C1D	7.76	138.39	124.71
23	AF	605	CHL	CMD-C2D-C1D	7.75	138.37	124.71
23	p	607	CHL	C2C-C3C-C4C	-7.75	100.97	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AS	307	CHL	C2C-C3C-C4C	-7.74	100.97	106.49
23	q	605	CHL	C2C-C3C-C4C	-7.74	100.97	106.49
23	AF	606	CHL	C3C-C4C-NC	7.73	117.02	109.95
23	AF	608	CHL	C2C-C3C-C4C	-7.72	100.99	106.49
23	AN	606	CHL	CMD-C2D-C1D	7.71	138.31	124.71
23	AE	601	CHL	C2C-C3C-C4C	-7.71	100.99	106.49
23	AQ	601	CHL	C2C-C3C-C4C	-7.71	100.99	106.49
23	9	605	CHL	C2C-C3C-C4C	-7.71	100.99	106.49
23	q	613	CHL	CMD-C2D-C1D	7.71	138.29	124.71
23	AC	608	CHL	C2C-C3C-C4C	-7.70	101.00	106.49
23	p	601	CHL	C2C-C3C-C4C	-7.70	101.00	106.49
23	0	617	CHL	C2C-C3C-C4C	-7.70	101.00	106.49
23	AS	306	CHL	C2C-C3C-C4C	-7.69	99.77	108.58
23	v	306	CHL	CMD-C2D-C1D	7.69	138.26	124.71
23	AC	606	CHL	C2C-C3C-C4C	-7.69	101.01	106.49
23	AD	306	CHL	CMD-C2D-C1D	7.68	138.25	124.71
23	v	307	CHL	C2C-C3C-C4C	-7.67	101.02	106.49
23	0	601	CHL	C2C-C3C-C4C	-7.66	101.03	106.49
23	AD	317	CHL	C2C-C3C-C4C	-7.66	101.03	106.49
23	AS	307	CHL	CMD-C2D-C1D	7.65	138.19	124.71
23	AR	606	CHL	C2C-C3C-C4C	-7.65	101.04	106.49
23	AD	302	CHL	C2C-C3C-C4C	-7.64	101.04	106.49
23	p	605	CHL	C2C-C3C-C4C	-7.64	101.05	106.49
23	AD	306	CHL	C2C-C3C-C4C	-7.63	101.05	106.49
23	V	606	CHL	CMD-C2D-C1D	7.63	138.17	124.71
24	q	618	CLA	C4A-NA-C1A	7.63	110.14	106.71
23	q	606	CHL	C2C-C3C-C4C	-7.63	99.85	108.58
23	AN	601	CHL	C2C-C3C-C4C	-7.63	101.05	106.49
23	AQ	605	CHL	C2C-C3C-C4C	-7.62	101.06	106.49
23	AF	601	CHL	C2C-C3C-C4C	-7.61	101.07	106.49
23	V	601	CHL	C2C-C3C-C4C	-7.59	101.08	106.49
23	AB	608	CHL	C2C-C3C-C4C	-7.59	101.08	106.49
27	AF	613	XAT	C19-C9-C10	-7.58	112.31	122.92
23	0	608	CHL	CAC-C3C-C4C	7.57	134.63	124.81
23	AA	601	CHL	C2C-C3C-C4C	-7.57	101.10	106.49
23	AA	606	CHL	CMD-C2D-C1D	7.56	138.03	124.71
23	AD	301	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
23	v	302	CHL	C4B-C3B-C2B	-7.54	101.63	108.69
24	O	611	CLA	C4A-NA-C1A	7.54	110.10	106.71
24	AL	503	CLA	C4A-NA-C1A	7.54	110.10	106.71
23	AE	605	CHL	C2C-C3C-C4C	-7.53	101.12	106.49
23	v	306	CHL	C2C-C3C-C4C	-7.52	99.97	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AS	302	CHL	C4B-C3B-C2B	-7.52	101.64	108.69
24	AR	612	CLA	C4A-NA-C1A	7.52	110.09	106.71
23	9	609	CHL	C2C-C3C-C4C	-7.51	101.14	106.49
24	AL	512	CLA	C4A-NA-C1A	7.50	110.08	106.71
23	AE	607	CHL	C2C-C3C-C4C	-7.49	101.15	106.49
23	0	606	CHL	CMD-C2D-C1D	7.48	137.89	124.71
23	V	616	CHL	C2C-C3C-C4C	-7.47	101.16	106.49
27	9	618	XAT	C38-C25-C26	-7.45	109.77	122.26
27	AB	613	XAT	C19-C9-C10	-7.45	112.49	122.92
23	AH	601	CHL	C2C-C3C-C4C	-7.39	101.22	106.49
23	q	607	CHL	C2C-C3C-C4C	-7.39	101.22	106.49
27	AF	613	XAT	C40-C33-C34	-7.39	112.58	122.92
24	K	101	CLA	C4A-NA-C1A	7.38	110.03	106.71
23	AN	608	CHL	C2C-C3C-C4C	-7.38	101.23	106.49
24	0	610	CLA	C4A-NA-C1A	7.36	110.01	106.71
24	AH	613	CLA	C4A-NA-C1A	7.35	110.01	106.71
27	AF	613	XAT	C18-C5-C6	-7.35	109.94	122.26
24	AR	609	CLA	C4A-NA-C1A	7.35	110.01	106.71
24	AS	313	CLA	C4A-NA-C1A	7.35	110.01	106.71
24	p	618	CLA	C4A-NA-C1A	7.34	110.01	106.71
24	P	502	CLA	C4A-NA-C1A	7.34	110.00	106.71
24	AR	604	CLA	C4A-NA-C1A	7.33	110.00	106.71
23	AD	308	CHL	C2C-C3C-C4C	-7.33	101.26	106.49
23	AU	601	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
24	AB	602	CLA	C4A-NA-C1A	7.31	109.99	106.71
27	AB	613	XAT	C35-C34-C33	-7.30	116.89	127.31
23	q	613	CHL	C2C-C3C-C4C	-7.29	101.29	106.49
27	AF	613	XAT	C6-C7-C8	-7.29	110.59	125.99
24	AD	303	CLA	C4A-NA-C1A	7.28	109.98	106.71
23	AN	608	CHL	CHD-C1D-ND	-7.25	117.79	124.45
24	AK	606	CLA	C4A-NA-C1A	7.24	109.96	106.71
24	O	604	CLA	C4A-NA-C1A	7.23	109.96	106.71
24	v	305	CLA	C4A-NA-C1A	7.23	109.95	106.71
23	AF	606	CHL	C2B-C1B-NB	7.22	115.08	110.23
23	AS	302	CHL	O2D-CGD-CBD	7.22	124.10	111.27
27	AF	613	XAT	C39-C29-C30	-7.22	112.81	122.92
23	AN	608	CHL	CHB-C1B-NB	-7.22	116.62	124.26
23	AR	607	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
24	V	609	CLA	C4A-NA-C1A	7.21	109.95	106.71
24	AS	305	CLA	C4A-NA-C1A	7.21	109.95	106.71
24	0	602	CLA	C4A-NA-C1A	7.20	109.94	106.71
23	AD	317	CHL	CMD-C2D-C1D	7.20	137.40	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AB	605	CHL	CHD-C1D-ND	-7.19	117.84	124.45
27	AB	613	XAT	C27-C28-C29	-7.18	114.38	125.53
24	0	604	CLA	C4A-NA-C1A	7.18	109.93	106.71
23	V	608	CHL	C2C-C3C-C4C	-7.17	101.38	106.49
24	AD	310	CLA	C4A-NA-C1A	7.17	109.93	106.71
23	V	601	CHL	O2D-CGD-CBD	7.17	124.00	111.27
23	AF	606	CHL	C4B-C3B-C2B	-7.17	101.98	108.69
24	J	407	CLA	C4A-NA-C1A	7.16	109.92	106.71
27	AR	616	XAT	C27-C28-C29	-7.15	114.44	125.53
23	AR	613	CHL	CMD-C2D-C1D	7.15	137.31	124.71
24	O	609	CLA	C4A-NA-C1A	7.14	109.92	106.71
24	V	602	CLA	C4A-NA-C1A	7.14	109.92	106.71
23	AF	608	CHL	CMD-C2D-C1D	7.14	137.30	124.71
24	J	404	CLA	C4A-NA-C1A	7.14	109.92	106.71
24	AU	604	CLA	C4A-NA-C1A	7.14	109.92	106.71
27	q	617	XAT	C27-C28-C29	-7.13	114.46	125.53
23	v	302	CHL	O2D-CGD-CBD	7.13	123.93	111.27
24	P	505	CLA	C4A-NA-C1A	7.12	109.91	106.71
24	9	602	CLA	C4A-NA-C1A	7.12	109.91	106.71
23	9	606	CHL	CHD-C1D-ND	-7.12	117.92	124.45
24	v	309	CLA	C4A-NA-C1A	7.11	109.90	106.71
24	AC	609	CLA	C4A-NA-C1A	7.11	109.90	106.71
24	AJ	409	CLA	C4A-NA-C1A	7.10	109.90	106.71
23	v	308	CHL	C3C-C4C-NC	7.10	116.52	109.97
24	O	601	CLA	C4A-NA-C1A	7.09	109.89	106.71
23	AN	601	CHL	O2D-CGD-CBD	7.08	123.85	111.27
24	AH	604	CLA	C4A-NA-C1A	7.08	109.89	106.71
24	AL	506	CLA	C4A-NA-C1A	7.08	109.89	106.71
24	p	604	CLA	C4A-NA-C1A	7.07	109.89	106.71
23	AB	607	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
24	AL	505	CLA	C4A-NA-C1A	7.06	109.88	106.71
27	q	617	XAT	C19-C9-C10	-7.05	113.05	122.92
24	AA	612	CLA	C4A-NA-C1A	7.04	109.87	106.71
24	AJ	405	CLA	C4A-NA-C1A	7.04	109.87	106.71
24	0	613	CLA	C4A-NA-C1A	7.03	109.87	106.71
24	O	602	CLA	C4A-NA-C1A	7.03	109.87	106.71
24	AS	310	CLA	C4A-NA-C1A	7.02	109.86	106.71
23	AC	601	CHL	CAC-C3C-C4C	7.01	133.91	124.81
24	AS	309	CLA	C4A-NA-C1A	7.01	109.86	106.71
24	AU	602	CLA	C4A-NA-C1A	7.00	109.85	106.71
24	AH	602	CLA	C4A-NA-C1A	6.99	109.85	106.71
24	AK	616	CLA	C4A-NA-C1A	6.99	109.85	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	O	607	CLA	C4A-NA-C1A	6.99	109.85	106.71
24	q	612	CLA	C4A-NA-C1A	6.98	109.85	106.71
24	AN	613	CLA	C4A-NA-C1A	6.98	109.85	106.71
24	q	601	CLA	C4A-NA-C1A	6.98	109.84	106.71
27	AB	613	XAT	C18-C5-C6	-6.98	110.56	122.26
24	AD	305	CLA	C4A-NA-C1A	6.98	109.84	106.71
24	AN	610	CLA	C4A-NA-C1A	6.98	109.84	106.71
27	AR	616	XAT	C26-C27-C28	-6.97	111.25	125.99
24	AK	603	CLA	C4A-NA-C1A	6.96	109.84	106.71
24	AR	601	CLA	C4A-NA-C1A	6.95	109.83	106.71
24	O	614	CLA	C4A-NA-C1A	6.95	109.83	106.71
27	AR	616	XAT	C18-C5-C6	-6.95	110.62	122.26
24	P	501	CLA	C4A-NA-C1A	6.94	109.83	106.71
27	AR	616	XAT	C19-C9-C10	-6.93	113.21	122.92
27	9	618	XAT	C19-C9-C10	-6.91	113.24	122.92
24	AF	609	CLA	C4A-NA-C1A	6.91	109.81	106.71
24	q	604	CLA	C4A-NA-C1A	6.91	109.81	106.71
27	q	617	XAT	C18-C5-C6	-6.91	110.67	122.26
24	p	613	CLA	C4A-NA-C1A	6.91	109.81	106.71
24	v	313	CLA	C4A-NA-C1A	6.90	109.81	106.71
24	V	611	CLA	C4A-NA-C1A	6.89	109.80	106.71
27	q	617	XAT	C26-C27-C28	-6.88	111.45	125.99
24	AK	607	CLA	C4A-NA-C1A	6.88	109.80	106.71
23	AS	307	CHL	O2D-CGD-CBD	6.86	123.46	111.27
24	O	612	CLA	C4A-NA-C1A	6.86	109.79	106.71
24	AK	611	CLA	C4A-NA-C1A	6.86	109.79	106.71
24	AK	609	CLA	C4A-NA-C1A	6.86	109.79	106.71
24	AL	502	CLA	C4A-NA-C1A	6.84	109.78	106.71
23	9	607	CHL	O2D-CGD-CBD	6.84	123.42	111.27
23	q	613	CHL	CHD-C1D-ND	-6.83	118.18	124.45
24	v	310	CLA	C4A-NA-C1A	6.82	109.77	106.71
23	AB	608	CHL	CMD-C2D-C1D	6.82	136.73	124.71
24	AC	604	CLA	C4A-NA-C1A	6.81	109.77	106.71
24	P	508	CLA	C4A-NA-C1A	6.80	109.76	106.71
27	9	618	XAT	C20-C13-C14	-6.80	113.40	122.92
24	9	604	CLA	C4A-NA-C1A	6.79	109.76	106.71
27	AB	613	XAT	C6-C7-C8	-6.79	111.64	125.99
24	AU	613	CLA	C4A-NA-C1A	6.78	109.75	106.71
24	AK	614	CLA	C4A-NA-C1A	6.78	109.75	106.71
23	AE	617	CHL	C3C-C4C-NC	6.78	118.17	110.57
24	AH	610	CLA	C4A-NA-C1A	6.77	109.75	106.71
24	AL	509	CLA	C4A-NA-C1A	6.77	109.75	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AE	608	CLA	C4A-NA-C1A	6.76	109.74	106.71
24	9	612	CLA	C4A-NA-C1A	6.76	109.74	106.71
24	AQ	604	CLA	C4A-NA-C1A	6.76	109.74	106.71
24	AR	602	CLA	C4A-NA-C1A	6.75	109.74	106.71
23	0	617	CHL	CMD-C2D-C1D	6.75	136.61	124.71
27	AF	613	XAT	C7-C8-C9	-6.74	115.07	125.53
23	AE	601	CHL	O2D-CGD-CBD	6.74	123.25	111.27
24	P	504	CLA	C4A-NA-C1A	6.73	109.73	106.71
24	AD	312	CLA	C4A-NA-C1A	6.73	109.73	106.71
24	AA	609	CLA	C4A-NA-C1A	6.72	109.73	106.71
23	AA	608	CHL	O2D-CGD-CBD	6.70	123.18	111.27
24	O	616	CLA	C4A-NA-C1A	6.70	109.72	106.71
27	AR	616	XAT	C20-C13-C14	-6.69	113.55	122.92
23	AD	301	CHL	O2D-CGD-CBD	6.69	123.15	111.27
24	AK	605	CLA	C4A-NA-C1A	6.69	109.71	106.71
24	O	605	CLA	C4A-NA-C1A	6.68	109.71	106.71
24	AR	608	CLA	C4A-NA-C1A	6.68	109.71	106.71
27	q	617	XAT	C20-C13-C14	-6.67	113.58	122.92
23	AF	605	CHL	CHD-C1D-ND	-6.66	118.33	124.45
24	AE	611	CLA	C4A-NA-C1A	6.66	109.70	106.71
24	p	602	CLA	C4A-NA-C1A	6.66	109.70	106.71
23	V	616	CHL	CMD-C2D-C1D	6.66	136.44	124.71
24	q	609	CLA	C4A-NA-C1A	6.65	109.69	106.71
24	V	612	CLA	C4A-NA-C1A	6.65	109.69	106.71
27	AR	616	XAT	C38-C25-C26	-6.65	111.12	122.26
23	AE	617	CHL	CMD-C2D-C1D	6.64	136.42	124.71
24	Q	404	CLA	C4A-NA-C1A	6.63	109.69	106.71
27	q	617	XAT	C38-C25-C26	-6.63	111.15	122.26
24	9	610	CLA	C4A-NA-C1A	6.63	109.69	106.71
24	AB	610	CLA	C4A-NA-C1A	6.63	109.69	106.71
27	AB	613	XAT	C7-C8-C9	-6.63	115.25	125.53
23	9	609	CHL	O2D-CGD-CBD	6.63	123.04	111.27
24	Q	401	CLA	C4A-NA-C1A	6.62	109.68	106.71
24	p	610	CLA	C2A-C1A-CHA	6.62	130.37	120.38
24	AN	612	CLA	C4A-NA-C1A	6.62	109.68	106.71
24	AR	610	CLA	C4A-NA-C1A	6.62	109.68	106.71
24	AC	611	CLA	C4A-NA-C1A	6.62	109.68	106.71
27	9	618	XAT	C18-C5-C6	-6.62	111.17	122.26
27	AF	613	XAT	C27-C28-C29	-6.61	115.27	125.53
23	AA	601	CHL	O2D-CGD-CBD	6.61	123.01	111.27
24	AN	604	CLA	C4A-NA-C1A	6.61	109.68	106.71
27	q	617	XAT	C40-C33-C34	-6.61	113.67	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	J	405	PHO	C4D-CHA-CBD	-6.60	105.53	108.52
24	AQ	602	CLA	C4A-NA-C1A	6.60	109.67	106.71
24	AA	604	CLA	C4A-NA-C1A	6.57	109.66	106.71
24	Q	403	CLA	C4A-NA-C1A	6.57	109.66	106.71
27	9	618	XAT	C40-C33-C34	-6.57	113.72	122.92
23	AC	608	CHL	O2D-CGD-CBD	6.56	122.93	111.27
23	0	607	CHL	O2D-CGD-CBD	6.56	122.92	111.27
24	AN	602	CLA	C4A-NA-C1A	6.56	109.65	106.71
24	AQ	614	CLA	C4A-NA-C1A	6.56	109.65	106.71
24	AQ	613	CLA	C4A-NA-C1A	6.55	109.65	106.71
32	AJ	407	PHO	C4D-CHA-CBD	-6.55	105.55	108.52
24	0	612	CLA	C4A-NA-C1A	6.55	109.65	106.71
24	AH	611	CLA	C4A-NA-C1A	6.55	109.65	106.71
24	q	602	CLA	C4A-NA-C1A	6.54	109.65	106.71
24	P	503	CLA	C4A-NA-C1A	6.53	109.64	106.71
24	AM	403	CLA	C4A-NA-C1A	6.53	109.64	106.71
27	9	618	XAT	C6-C7-C8	-6.53	112.19	125.99
23	AA	617	CHL	C2C-C3C-C4C	-6.52	101.84	106.49
24	O	603	CLA	C4A-NA-C1A	6.52	109.64	106.71
24	AU	612	CLA	C4A-NA-C1A	6.52	109.64	106.71
27	AR	616	XAT	C40-C33-C34	-6.52	113.80	122.92
24	AF	604	CLA	C4A-NA-C1A	6.51	109.64	106.71
24	q	610	CLA	C4A-NA-C1A	6.51	109.63	106.71
27	AF	613	XAT	C20-C13-C14	-6.51	113.81	122.92
24	AU	610	CLA	C4A-NA-C1A	6.50	109.63	106.71
24	J	403	CLA	C4A-NA-C1A	6.49	109.62	106.71
27	AB	613	XAT	C26-C27-C28	-6.49	112.27	125.99
24	AE	612	CLA	C4A-NA-C1A	6.49	109.62	106.71
23	AA	617	CHL	CMD-C2D-C1D	6.49	136.15	124.71
24	v	303	CLA	C4A-NA-C1A	6.49	109.62	106.71
24	9	613	CLA	C4A-NA-C1A	6.48	109.62	106.71
24	AJ	406	CLA	C4A-NA-C1A	6.47	109.62	106.71
24	AK	612	CLA	C4A-NA-C1A	6.47	109.62	106.71
24	AL	513	CLA	C4A-NA-C1A	6.47	109.61	106.71
27	AR	616	XAT	C39-C29-C30	-6.47	113.86	122.92
24	9	611	CLA	C4A-NA-C1A	6.47	109.61	106.71
24	AD	309	CLA	C4A-NA-C1A	6.47	109.61	106.71
24	P	511	CLA	C4A-NA-C1A	6.46	109.61	106.71
24	AQ	610	CLA	C4A-NA-C1A	6.45	109.61	106.71
24	AL	504	CLA	C4A-NA-C1A	6.45	109.60	106.71
27	q	617	XAT	C39-C29-C30	-6.44	113.91	122.92
24	O	613	CLA	C4A-NA-C1A	6.43	109.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AB	607	CHL	CHD-C1D-ND	-6.43	118.54	124.45
24	AA	613	CLA	C4A-NA-C1A	6.43	109.60	106.71
24	AH	612	CLA	C4A-NA-C1A	6.43	109.60	106.71
24	AJ	404	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	AR	613	CHL	CHD-C1D-ND	-6.41	118.56	124.45
24	AB	604	CLA	C4A-NA-C1A	6.41	109.59	106.71
24	AK	604	CLA	C4A-NA-C1A	6.41	109.59	106.71
24	0	609	CLA	C4A-NA-C1A	6.38	109.58	106.71
24	v	314	CLA	C4A-NA-C1A	6.38	109.58	106.71
24	AK	608	CLA	C4A-NA-C1A	6.38	109.57	106.71
24	AM	404	CLA	C4A-NA-C1A	6.36	109.57	106.71
24	AD	311	CLA	C4A-NA-C1A	6.36	109.57	106.71
24	0	603	CLA	C4A-NA-C1A	6.36	109.56	106.71
24	AE	604	CLA	C4A-NA-C1A	6.36	109.56	106.71
24	AA	602	CLA	C4A-NA-C1A	6.36	109.56	106.71
27	AB	613	XAT	C20-C13-C14	-6.36	114.02	122.92
24	AC	612	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	P	507	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	q	611	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	V	604	CLA	C2A-C1A-NA	-6.35	111.78	120.66
24	AA	610	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	AK	615	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	p	611	CLA	C4A-NA-C1A	6.34	109.56	106.71
23	v	307	CHL	O2D-CGD-CBD	6.33	122.52	111.27
24	AC	602	CLA	C4A-NA-C1A	6.33	109.55	106.71
23	V	607	CHL	O2D-CGD-CBD	6.33	122.51	111.27
27	AR	616	XAT	C6-C7-C8	-6.33	112.62	125.99
24	AQ	611	CLA	C4A-NA-C1A	6.32	109.55	106.71
27	q	617	XAT	C6-C7-C8	-6.32	112.62	125.99
23	AH	606	CHL	CHD-C1D-ND	-6.32	118.64	124.45
23	AF	608	CHL	CHD-C1D-ND	-6.32	118.64	124.45
27	AF	613	XAT	C15-C35-C34	-6.31	110.54	123.47
24	AF	610	CLA	C4A-NA-C1A	6.31	109.55	106.71
24	AS	303	CLA	C4A-NA-C1A	6.31	109.54	106.71
24	AR	611	CLA	C4A-NA-C1A	6.30	109.54	106.71
23	AD	307	CHL	O2D-CGD-CBD	6.29	122.45	111.27
27	AB	613	XAT	C39-C29-C30	-6.29	114.11	122.92
24	AN	609	CLA	C4A-NA-C1A	6.29	109.53	106.71
24	9	614	CLA	C4A-NA-C1A	6.28	109.53	106.71
24	AC	610	CLA	C4A-NA-C1A	6.28	109.53	106.71
24	O	615	CLA	C4A-NA-C1A	6.28	109.53	106.71
23	AF	607	CHL	CHD-C1D-ND	-6.28	118.69	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AS	314	CLA	C4A-NA-C1A	6.28	109.53	106.71
24	AA	603	CLA	C4A-NA-C1A	6.26	109.52	106.71
24	AL	508	CLA	C4A-NA-C1A	6.26	109.52	106.71
24	AU	611	CLA	C4A-NA-C1A	6.26	109.52	106.71
24	O	606	CLA	C4A-NA-C1A	6.25	109.52	106.71
24	P	506	CLA	C4A-NA-C1A	6.24	109.51	106.71
24	P	509	CLA	C4A-NA-C1A	6.24	109.51	106.71
24	AC	613	CLA	C4A-NA-C1A	6.24	109.51	106.71
24	AE	609	CLA	C4A-NA-C1A	6.23	109.51	106.71
24	v	312	CLA	C4A-NA-C1A	6.23	109.51	106.71
24	AN	611	CLA	C4A-NA-C1A	6.23	109.51	106.71
24	AS	312	CLA	C4A-NA-C1A	6.23	109.51	106.71
24	AN	603	CLA	C4A-NA-C1A	6.20	109.50	106.71
23	AR	607	CHL	CHD-C1D-ND	-6.20	118.76	124.45
24	V	610	CLA	C4A-NA-C1A	6.19	109.49	106.71
24	AL	507	CLA	C4A-NA-C1A	6.18	109.49	106.71
24	AE	603	CLA	C4A-NA-C1A	6.18	109.48	106.71
24	AK	617	CLA	C4A-NA-C1A	6.18	109.48	106.71
24	AL	510	CLA	C4A-NA-C1A	6.17	109.48	106.71
23	AF	605	CHL	C3C-C4C-NC	6.16	115.66	109.97
24	AE	602	CLA	C4A-NA-C1A	6.16	109.48	106.71
23	AN	617	CHL	C3C-C4C-NC	6.14	117.46	110.57
24	AS	304	CLA	C4A-NA-C1A	6.14	109.47	106.71
24	v	304	CLA	C4A-NA-C1A	6.14	109.47	106.71
23	AF	608	CHL	CHB-C1B-NB	-6.14	117.76	124.26
24	AA	611	CLA	C4A-NA-C1A	6.11	109.45	106.71
23	AU	606	CHL	CHD-C1D-ND	-6.10	118.85	124.45
24	AC	602	CLA	O2D-CGD-CBD	6.07	122.06	111.27
23	0	617	CHL	C3C-C4C-NC	6.07	117.37	110.57
23	AE	616	CHL	CMD-C2D-C1D	6.04	135.36	124.71
24	P	510	CLA	C4A-NA-C1A	6.04	109.42	106.71
23	AA	608	CHL	C2C-C3C-C4C	-6.03	102.19	106.49
23	AS	308	CHL	CHD-C1D-ND	-6.02	118.92	124.45
24	q	603	CLA	C4A-NA-C1A	6.01	109.41	106.71
24	AH	603	CLA	C4A-NA-C1A	6.01	109.41	106.71
23	AA	608	CHL	C2B-C1B-NB	6.00	114.25	110.23
23	AR	607	CHL	O2D-CGD-CBD	6.00	121.92	111.27
24	AF	603	CLA	C4A-NA-C1A	5.99	109.40	106.71
23	AC	606	CHL	CHD-C1D-ND	-5.98	118.95	124.45
23	AF	606	CHL	C1D-CHD-C4C	5.98	126.51	120.75
24	AH	609	CLA	C4A-NA-C1A	5.97	109.39	106.71
24	AC	603	CLA	C4A-NA-C1A	5.96	109.39	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AU	609	CLA	C4A-NA-C1A	5.96	109.39	106.71
24	V	603	CLA	C4A-NA-C1A	5.96	109.39	106.71
23	v	306	CHL	CHD-C1D-ND	-5.95	118.99	124.45
24	AK	618	CLA	C4A-NA-C1A	5.94	109.38	106.71
23	AN	608	CHL	C3B-C2B-C1B	-5.93	100.01	107.16
24	AD	304	CLA	C4A-NA-C1A	5.92	109.37	106.71
24	AL	511	CLA	C4A-NA-C1A	5.91	109.36	106.71
23	0	608	CHL	C3C-C4C-NC	5.90	117.19	110.57
23	AR	613	CHL	O2D-CGD-CBD	5.90	121.75	111.27
23	q	607	CHL	O2D-CGD-CBD	5.89	121.73	111.27
24	0	604	CLA	O2D-CGD-CBD	5.89	121.73	111.27
24	0	611	CLA	C4A-NA-C1A	5.88	109.35	106.71
23	0	605	CHL	C3C-C4C-NC	5.88	117.17	110.57
24	p	612	CLA	C4A-NA-C1A	5.88	109.35	106.71
27	AF	613	XAT	C32-C33-C34	-5.87	109.94	118.94
23	AS	306	CHL	CHA-C4D-ND	5.87	129.85	124.45
23	AA	606	CHL	C3C-C4C-NC	5.86	117.14	110.57
23	q	607	CHL	CHD-C1D-ND	-5.85	119.08	124.45
23	AN	607	CHL	O2D-CGD-CBD	5.85	121.66	111.27
23	AD	317	CHL	CAA-CBA-CGA	-5.84	97.00	112.51
24	AE	610	CLA	C4A-NA-C1A	5.84	109.33	106.71
23	AQ	607	CHL	C3B-C2B-C1B	-5.83	100.12	107.16
24	AU	603	CLA	C4A-NA-C1A	5.83	109.33	106.71
23	AU	606	CHL	C3C-C4C-NC	5.83	117.11	110.57
23	AH	605	CHL	C3C-C4C-NC	5.82	117.10	110.57
24	9	603	CLA	C4A-NA-C1A	5.82	109.32	106.71
23	p	607	CHL	C3B-C2B-C1B	-5.81	100.15	107.16
23	0	606	CHL	CHD-C1D-ND	-5.81	119.12	124.45
23	p	606	CHL	C3C-C4C-NC	5.80	117.08	110.57
27	9	618	XAT	C15-C35-C34	-5.79	111.61	123.47
23	AN	617	CHL	CMD-C2D-C1D	5.79	134.91	124.71
23	AU	605	CHL	C3C-C4C-NC	5.78	117.06	110.57
24	AR	603	CLA	C4A-NA-C1A	5.78	109.30	106.71
23	AQ	606	CHL	C3C-C4C-NC	5.78	117.05	110.57
23	AD	307	CHL	C3C-C4C-NC	5.78	117.05	110.57
23	V	608	CHL	CHD-C1D-ND	-5.77	119.15	124.45
23	AD	308	CHL	CHD-C1D-ND	-5.76	119.16	124.45
23	v	308	CHL	CHD-C1D-ND	-5.75	119.17	124.45
27	9	618	XAT	C26-C27-C28	-5.74	113.85	125.99
24	AS	311	CLA	C4A-NA-C1A	5.74	109.29	106.71
23	AU	601	CHL	CHD-C1D-ND	-5.74	119.18	124.45
23	0	601	CHL	CHD-C1D-ND	-5.74	119.18	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	V	616	CHL	C3C-C4C-NC	5.73	117.00	110.57
23	AA	608	CHL	CBD-CHA-C1A	5.73	135.26	128.50
23	9	606	CHL	C3B-C2B-C1B	-5.72	100.25	107.16
24	AB	609	CLA	C4A-NA-C1A	5.72	109.28	106.71
23	AC	608	CHL	CHD-C1D-ND	-5.72	119.20	124.45
23	AD	306	CHL	C3C-C4C-NC	5.72	116.98	110.57
23	AH	601	CHL	CHD-C1D-ND	-5.71	119.21	124.45
23	AC	605	CHL	C3C-C4C-NC	5.70	116.97	110.57
23	AD	317	CHL	C3C-C4C-NC	5.69	116.95	110.57
23	AF	608	CHL	C3B-C2B-C1B	-5.69	100.29	107.16
23	AR	606	CHL	CHD-C1D-ND	-5.68	119.23	124.45
23	AE	616	CHL	C3C-C4C-NC	5.68	116.94	110.57
23	AQ	605	CHL	C3C-C4C-NC	5.68	116.94	110.57
23	AF	606	CHL	C1C-NC-C4C	-5.68	104.15	106.71
23	9	605	CHL	C3C-C4C-NC	5.67	116.93	110.57
23	v	302	CHL	C3C-C4C-NC	5.67	116.92	110.57
24	v	311	CLA	C4A-NA-C1A	5.67	109.25	106.71
23	AC	607	CHL	C3B-C2B-C1B	-5.64	100.35	107.16
23	9	608	CHL	C3B-C2B-C1B	-5.63	100.36	107.16
23	AS	307	CHL	C3C-C4C-NC	5.63	116.89	110.57
23	AN	606	CHL	C3C-C4C-NC	5.63	116.89	110.57
23	AF	601	CHL	C3C-C4C-NC	5.63	116.89	110.57
23	9	609	CHL	CHD-C1D-ND	-5.63	119.28	124.45
23	V	606	CHL	C3C-C4C-NC	5.63	116.89	110.57
23	AE	607	CHL	C3C-C4C-NC	5.62	116.88	110.57
23	AS	302	CHL	C3C-C4C-NC	5.62	116.87	110.57
23	p	605	CHL	C3C-C4C-NC	5.62	116.87	110.57
24	AB	603	CLA	C4A-NA-C1A	5.62	109.23	106.71
23	AH	607	CHL	C3C-C4C-NC	5.61	116.87	110.57
23	AC	606	CHL	C3B-C2B-C1B	-5.61	100.39	107.16
23	AE	601	CHL	C3C-C4C-NC	5.61	116.86	110.57
23	AA	605	CHL	C3C-C4C-NC	5.61	116.86	110.57
36	AM	402	BCT	O2-C-O1	5.60	134.08	119.55
23	p	608	CHL	C3C-C4C-NC	5.60	116.85	110.57
23	AU	607	CHL	C3C-C4C-NC	5.60	116.85	110.57
23	AB	601	CHL	CHD-C1D-ND	-5.60	119.31	124.45
27	AB	613	XAT	C38-C25-C26	-5.59	112.88	122.26
24	O	610	CLA	C4A-NA-C1A	5.59	109.22	106.71
23	AA	606	CHL	C3B-C2B-C1B	-5.59	100.42	107.16
23	q	605	CHL	C3C-C4C-NC	5.58	116.83	110.57
23	AH	606	CHL	C3B-C2B-C1B	-5.58	100.42	107.16
23	AE	607	CHL	C3B-C2B-C1B	-5.58	100.42	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AH	606	CHL	C3C-C4C-NC	5.57	116.82	110.57
23	AQ	606	CHL	C3B-C2B-C1B	-5.57	100.43	107.16
23	AQ	608	CHL	C3C-C4C-NC	5.57	116.82	110.57
23	AB	601	CHL	C3C-C4C-NC	5.57	116.82	110.57
23	AC	606	CHL	C3C-C4C-NC	5.57	116.82	110.57
23	v	307	CHL	C3C-C4C-NC	5.56	116.81	110.57
24	AQ	603	CLA	C4A-NA-C1A	5.56	109.21	106.71
23	0	617	CHL	CAA-CBA-CGA	-5.56	97.75	112.51
23	AE	606	CHL	CHD-C1D-ND	-5.56	119.34	124.45
23	AE	605	CHL	C3B-C2B-C1B	-5.56	100.45	107.16
27	AB	613	XAT	C40-C33-C34	-5.56	115.14	122.92
23	V	601	CHL	C3C-C4C-NC	5.56	116.80	110.57
24	AF	602	CLA	CAC-C3C-C4C	5.56	132.02	124.81
23	AA	607	CHL	CHD-C1D-ND	-5.55	119.35	124.45
24	p	603	CLA	C4A-NA-C1A	5.55	109.20	106.71
23	AU	608	CHL	C3B-C2B-C1B	-5.55	100.46	107.16
23	AB	608	CHL	CHD-C1D-ND	-5.55	119.36	124.45
23	9	607	CHL	C3C-C4C-NC	5.54	116.78	110.57
23	AF	601	CHL	CHD-C1D-ND	-5.53	119.37	124.45
23	9	601	CHL	C3C-C4C-NC	5.53	116.77	110.57
23	AQ	609	CHL	C3C-C4C-NC	5.52	116.76	110.57
23	AR	605	CHL	CHD-C1D-ND	-5.52	119.39	124.45
23	AN	601	CHL	C3C-C4C-NC	5.51	116.75	110.57
23	9	601	CHL	CHD-C1D-ND	-5.51	119.39	124.45
23	AB	606	CHL	CHD-C1D-ND	-5.51	119.39	124.45
23	V	605	CHL	CHD-C1D-ND	-5.51	119.39	124.45
23	AE	606	CHL	C3B-C2B-C1B	-5.51	100.52	107.16
23	AQ	605	CHL	C3B-C2B-C1B	-5.50	100.52	107.16
23	p	601	CHL	C3C-C4C-NC	5.50	116.74	110.57
23	AC	601	CHL	CHD-C1D-ND	-5.50	119.40	124.45
23	q	606	CHL	CHD-C1D-ND	-5.50	119.40	124.45
23	AA	607	CHL	C3B-C2B-C1B	-5.49	100.53	107.16
23	V	605	CHL	C3C-C4C-NC	5.49	116.73	110.57
23	AN	605	CHL	C3C-C4C-NC	5.49	116.73	110.57
24	AF	602	CLA	C4A-NA-C1A	5.49	109.17	106.71
23	AC	601	CHL	C3C-C4C-NC	5.49	116.73	110.57
23	AU	608	CHL	C3C-C4C-NC	5.49	116.73	110.57
23	AD	302	CHL	C3C-C4C-NC	5.49	116.72	110.57
23	AR	606	CHL	C3B-C2B-C1B	-5.49	100.54	107.16
23	9	607	CHL	C3B-C2B-C1B	-5.48	100.54	107.16
23	p	605	CHL	C3B-C2B-C1B	-5.48	100.55	107.16
23	AE	605	CHL	CHD-C1D-ND	-5.48	119.42	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	p	609	CHL	C3C-C4C-NC	5.48	116.71	110.57
23	AQ	607	CHL	C3C-C4C-NC	5.48	116.71	110.57
23	AQ	601	CHL	C3C-C4C-NC	5.47	116.71	110.57
23	AQ	609	CHL	CHD-C1D-ND	-5.47	119.42	124.45
23	V	616	CHL	CHD-C1D-ND	-5.46	119.43	124.45
23	V	607	CHL	CHD-C1D-ND	-5.46	119.44	124.45
23	AC	608	CHL	C3C-C4C-NC	5.45	116.69	110.57
36	J	412	BCT	O2-C-O1	5.45	133.69	119.55
23	p	607	CHL	C3C-C4C-NC	5.45	116.69	110.57
23	p	609	CHL	CHD-C1D-ND	-5.45	119.44	124.45
23	AQ	607	CHL	CHD-C1D-ND	-5.45	119.44	124.45
23	AR	613	CHL	C3C-C4C-NC	5.45	116.68	110.57
23	q	605	CHL	CHD-C1D-ND	-5.45	119.45	124.45
23	AS	306	CHL	OBD-CAD-C3D	-5.45	113.37	125.69
23	q	605	CHL	C3B-C2B-C1B	-5.45	100.59	107.16
23	AB	608	CHL	C3B-C2B-C1B	-5.44	100.60	107.16
23	AS	306	CHL	C3D-C2D-C1D	-5.44	101.89	107.08
23	AH	608	CHL	C3C-C4C-NC	5.44	116.67	110.57
23	0	607	CHL	CHD-C1D-ND	-5.43	119.46	124.45
23	AD	301	CHL	C3C-C4C-NC	5.43	116.66	110.57
23	AS	306	CHL	CMD-C2D-C1D	5.43	134.28	124.71
23	0	601	CHL	C3C-C4C-NC	5.43	116.66	110.57
23	p	601	CHL	CHD-C1D-ND	-5.43	119.47	124.45
23	AS	306	CHL	C3B-C2B-C1B	-5.43	100.61	107.16
23	AD	301	CHL	C3B-C2B-C1B	-5.42	100.61	107.16
23	AN	605	CHL	C3B-C2B-C1B	-5.41	100.63	107.16
23	AE	605	CHL	C3C-C4C-NC	5.41	116.64	110.57
23	0	606	CHL	C3C-C4C-NC	5.41	116.64	110.57
23	AF	606	CHL	CHB-C1B-NB	-5.41	118.53	124.26
23	AA	617	CHL	C3C-C4C-NC	5.41	116.64	110.57
23	AQ	606	CHL	CHD-C1D-ND	-5.40	119.49	124.45
23	AN	608	CHL	C3C-C4C-NC	5.40	116.63	110.57
23	AA	607	CHL	C3C-C4C-NC	5.40	116.62	110.57
23	9	608	CHL	CHD-C1D-ND	-5.39	119.50	124.45
23	AH	608	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
23	AQ	601	CHL	CHD-C1D-ND	-5.38	119.51	124.45
23	AC	607	CHL	CHD-C1D-ND	-5.38	119.51	124.45
23	V	616	CHL	C3D-C2D-C1D	-5.38	98.49	105.83
23	0	605	CHL	C3B-C2B-C1B	-5.38	100.67	107.16
23	AN	608	CHL	C3B-C4B-NB	5.37	115.50	110.52
23	0	601	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
23	AN	607	CHL	C3B-C2B-C1B	-5.37	100.68	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AA	601	CHL	C3C-C4C-NC	5.37	116.59	110.57
23	p	607	CHL	CHD-C1D-ND	-5.36	119.53	124.45
23	AS	306	CHL	C4D-CHA-C1A	-5.36	116.16	125.89
23	AB	606	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
24	AK	606	CLA	O2D-CGD-CBD	5.36	120.79	111.27
23	AD	307	CHL	CHD-C1D-ND	-5.35	119.53	124.45
23	9	609	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
23	AQ	608	CHL	C3B-C2B-C1B	-5.35	100.71	107.16
23	AR	613	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
23	AH	607	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
23	p	606	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
24	V	604	CLA	C2A-C1A-CHA	5.34	124.77	117.33
23	AS	308	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
23	AQ	608	CHL	CHD-C1D-ND	-5.34	119.55	124.45
23	AB	601	CHL	C3B-C2B-C1B	-5.33	100.72	107.16
24	AR	617	CLA	C4A-NA-C1A	5.33	109.10	106.71
23	p	606	CHL	CHD-C1D-ND	-5.33	119.55	124.45
23	AR	606	CHL	C3C-C4C-NC	5.33	116.55	110.57
23	AF	601	CHL	C3B-C2B-C1B	-5.33	100.72	107.16
23	V	605	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
23	AH	601	CHL	C1-C2-C3	-5.33	116.83	126.04
23	v	306	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
23	AU	606	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
23	AD	302	CHL	CHD-C1D-ND	-5.32	119.56	124.45
23	V	606	CHL	C3B-C2B-C1B	-5.32	100.74	107.16
23	p	605	CHL	CHD-C1D-ND	-5.32	119.57	124.45
23	AB	607	CHL	CHB-C1B-NB	-5.32	118.63	124.26
24	q	612	CLA	O2D-CGD-CBD	5.31	120.71	111.27
23	V	608	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
27	AF	613	XAT	C8-C9-C10	-5.31	110.80	118.94
23	v	307	CHL	CHD-C1D-ND	-5.31	119.58	124.45
23	AU	607	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
23	AC	608	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
23	AD	306	CHL	CHD-C1D-ND	-5.30	119.59	124.45
23	AH	608	CHL	CHD-C1D-ND	-5.30	119.59	124.45
23	AH	601	CHL	C3C-C4C-NC	5.30	116.51	110.57
23	AD	306	CHL	C3B-C2B-C1B	-5.30	100.77	107.16
23	q	606	CHL	C3B-C2B-C1B	-5.30	100.77	107.16
23	AC	605	CHL	CHD-C1D-ND	-5.29	119.59	124.45
23	v	307	CHL	C3B-C2B-C1B	-5.29	100.78	107.16
23	AU	601	CHL	C3C-C4C-NC	5.29	116.50	110.57
23	9	606	CHL	C3C-C4C-NC	5.28	116.50	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AE	606	CHL	C3C-C4C-NC	5.28	116.50	110.57
23	AD	301	CHL	CHD-C1D-ND	-5.28	119.60	124.45
23	AE	601	CHL	CHD-C1D-ND	-5.28	119.60	124.45
23	AN	605	CHL	CHD-C1D-ND	-5.28	119.60	124.45
23	AH	605	CHL	CHD-C1D-ND	-5.27	119.61	124.45
23	AN	606	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
23	AD	308	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
23	9	609	CHL	C3C-C4C-NC	5.27	116.48	110.57
23	AN	607	CHL	C3C-C4C-NC	5.26	116.47	110.57
27	AB	613	XAT	C15-C35-C34	-5.26	112.69	123.47
23	AC	605	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
23	AU	605	CHL	CHD-C1D-ND	-5.26	119.62	124.45
23	p	608	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
23	v	308	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
23	AU	601	CHL	C1-C2-C3	-5.26	116.95	126.04
23	9	605	CHL	CHD-C1D-ND	-5.25	119.63	124.45
23	AN	607	CHL	CHD-C1D-ND	-5.25	119.63	124.45
23	AU	608	CHL	CHD-C1D-ND	-5.24	119.64	124.45
23	AH	605	CHL	C3B-C2B-C1B	-5.24	100.83	107.16
27	q	617	XAT	C35-C15-C14	-5.24	112.74	123.47
23	AE	607	CHL	CHD-C1D-ND	-5.24	119.64	124.45
23	AQ	605	CHL	CHD-C1D-ND	-5.24	119.64	124.45
23	AR	605	CHL	C3B-C2B-C1B	-5.24	100.84	107.16
23	9	605	CHL	C3B-C2B-C1B	-5.24	100.84	107.16
27	AR	616	XAT	C35-C15-C14	-5.23	112.75	123.47
23	0	607	CHL	C3B-C2B-C1B	-5.23	100.85	107.16
23	V	601	CHL	CHD-C1D-ND	-5.22	119.65	124.45
23	AS	307	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
23	AD	317	CHL	CHD-C1D-ND	-5.22	119.66	124.45
23	AN	601	CHL	CHD-C1D-ND	-5.21	119.66	124.45
23	AH	607	CHL	CHD-C1D-ND	-5.21	119.66	124.45
23	AA	601	CHL	CHD-C1D-ND	-5.21	119.67	124.45
23	0	605	CHL	CHD-C1D-ND	-5.21	119.67	124.45
23	AB	608	CHL	CHB-C1B-NB	-5.21	118.74	124.26
23	AU	605	CHL	C3B-C2B-C1B	-5.21	100.88	107.16
23	AU	607	CHL	CHD-C1D-ND	-5.21	119.67	124.45
23	p	608	CHL	CHD-C1D-ND	-5.20	119.67	124.45
23	AQ	609	CHL	C3B-C2B-C1B	-5.20	100.88	107.16
23	AE	601	CHL	C3B-C2B-C1B	-5.20	100.89	107.16
23	V	601	CHL	C3B-C2B-C1B	-5.19	100.89	107.16
23	q	613	CHL	C3B-C2B-C1B	-5.19	100.89	107.16
23	AD	308	CHL	C3C-C4C-NC	5.19	116.39	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AD	307	CHL	C3B-C2B-C1B	-5.19	100.90	107.16
37	AM	405	PL9	C7-C3-C4	5.17	121.08	116.88
23	q	607	CHL	C3B-C2B-C1B	-5.17	100.92	107.16
24	P	503	CLA	O2D-CGD-CBD	5.17	120.46	111.27
23	p	601	CHL	C3B-C2B-C1B	-5.17	100.92	107.16
27	AB	613	XAT	C8-C9-C10	-5.17	111.01	118.94
27	AB	613	XAT	O24-C25-C38	-5.16	108.87	115.06
23	v	302	CHL	CHD-C1D-ND	-5.16	119.71	124.45
23	AQ	601	CHL	C3B-C2B-C1B	-5.15	100.94	107.16
23	p	609	CHL	C3B-C2B-C1B	-5.15	100.94	107.16
23	AE	617	CHL	CHD-C4C-C3C	-5.14	117.28	124.84
23	AC	601	CHL	C1B-NB-C4B	-5.14	102.68	106.33
23	AF	607	CHL	C3C-C4C-NC	5.13	116.33	110.57
23	AN	601	CHL	C3B-C2B-C1B	-5.13	100.97	107.16
23	AA	617	CHL	CHD-C1D-ND	-5.12	119.75	124.45
23	AS	307	CHL	CHD-C1D-ND	-5.12	119.75	124.45
37	Q	405	PL9	C7-C3-C4	5.12	121.04	116.88
23	0	608	CHL	C2A-C3A-C4A	-5.12	93.60	101.87
23	AH	608	CHL	C1-C2-C3	-5.10	117.22	126.04
23	AS	302	CHL	CHD-C1D-ND	-5.10	119.77	124.45
23	9	607	CHL	CHD-C1D-ND	-5.10	119.77	124.45
23	AA	605	CHL	C3B-C2B-C1B	-5.09	101.02	107.16
23	V	608	CHL	C3C-C4C-NC	5.09	116.28	110.57
23	AD	302	CHL	C3B-C2B-C1B	-5.08	101.03	107.16
23	9	601	CHL	C1B-NB-C4B	-5.07	102.73	106.33
23	0	606	CHL	C3B-C2B-C1B	-5.07	101.04	107.16
23	AE	617	CHL	C3D-C2D-C1D	-5.07	98.92	105.83
23	0	608	CHL	CHD-C1D-ND	-5.07	119.80	124.45
23	AU	608	CHL	C1-C2-C3	-5.06	117.28	126.04
24	AK	606	CLA	O2D-CGD-O1D	-5.06	113.94	123.84
23	AF	605	CHL	C3B-C2B-C1B	-5.06	101.05	107.16
24	AJ	406	CLA	O2D-CGD-CBD	5.06	120.25	111.27
23	AC	606	CHL	O2D-CGD-CBD	5.06	120.25	111.27
24	O	604	CLA	O2D-CGD-CBD	5.06	120.25	111.27
23	AB	605	CHL	CHB-C1B-NB	-5.05	118.91	124.26
23	AA	605	CHL	CHD-C1D-ND	-5.03	119.83	124.45
24	AR	612	CLA	O2D-CGD-CBD	5.01	120.17	111.27
23	AF	606	CHL	C4A-NA-C1A	4.99	108.95	106.71
23	AA	601	CHL	C3B-C2B-C1B	-4.99	101.14	107.16
23	q	607	CHL	C3C-C4C-NC	4.99	116.16	110.57
23	AN	608	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
23	AH	601	CHL	C3B-C2B-C1B	-4.98	101.15	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	q	617	XAT	C15-C35-C34	-4.98	113.27	123.47
23	AQ	601	CHL	C6-C7-C8	-4.97	99.85	115.92
23	AU	601	CHL	C3B-C2B-C1B	-4.97	101.16	107.16
23	AB	605	CHL	C4A-NA-C1A	4.96	108.94	106.71
27	AR	616	XAT	C15-C35-C34	-4.96	113.31	123.47
24	p	610	CLA	CBD-CHA-C1A	4.96	134.35	128.50
23	0	617	CHL	CHD-C1D-ND	-4.96	119.90	124.45
23	AR	607	CHL	C3B-C2B-C1B	-4.96	101.18	107.16
23	AS	302	CHL	C1B-NB-C4B	-4.94	102.82	106.33
23	AB	607	CHL	C3B-C2B-C1B	-4.94	101.20	107.16
23	AA	606	CHL	CHD-C1D-ND	-4.93	119.92	124.45
23	0	601	CHL	C1-C2-C3	-4.93	117.52	126.04
23	v	302	CHL	C1B-NB-C4B	-4.92	102.84	106.33
23	0	605	CHL	C3D-C2D-C1D	-4.91	99.12	105.83
24	O	604	CLA	O2D-CGD-O1D	-4.91	114.23	123.84
23	AF	607	CHL	C3B-C2B-C1B	-4.91	101.23	107.16
27	AF	613	XAT	C26-C27-C28	-4.91	115.61	125.99
23	AN	606	CHL	CHD-C1D-ND	-4.91	119.94	124.45
23	0	607	CHL	C3C-C4C-NC	4.91	116.07	110.57
23	AE	616	CHL	CHD-C1D-ND	-4.91	119.95	124.45
23	AH	605	CHL	C3D-C2D-C1D	-4.90	99.14	105.83
23	9	601	CHL	C3D-C2D-C1D	-4.89	99.16	105.83
23	9	609	CHL	CHB-C1B-NB	-4.89	119.08	124.26
23	0	607	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
23	AD	307	CHL	C3D-C2D-C1D	-4.87	99.18	105.83
23	AB	605	CHL	C3B-C2B-C1B	-4.87	101.28	107.16
23	AU	606	CHL	C3D-C2D-C1D	-4.87	99.19	105.83
23	v	307	CHL	C3D-C2D-C1D	-4.86	99.20	105.83
24	O	614	CLA	O2D-CGD-CBD	4.86	119.90	111.27
23	0	608	CHL	CAA-C2A-C1A	4.85	122.88	112.14
23	AD	302	CHL	C1-C2-C3	-4.85	117.65	126.04
23	p	605	CHL	C3D-C2D-C1D	-4.85	99.21	105.83
27	9	618	XAT	C11-C12-C13	-4.85	112.80	126.42
23	AC	601	CHL	C3D-C2D-C1D	-4.84	99.22	105.83
23	AQ	605	CHL	C3D-C2D-C1D	-4.84	99.23	105.83
23	AR	607	CHL	C3C-C4C-NC	4.83	115.99	110.57
23	V	605	CHL	C3D-C2D-C1D	-4.83	99.24	105.83
23	AH	605	CHL	CHD-C4C-C3C	-4.83	117.74	124.84
23	0	608	CHL	CMD-C2D-C3D	-4.83	116.50	127.61
23	V	605	CHL	O2D-CGD-CBD	4.83	119.84	111.27
23	AS	306	CHL	CHA-C4D-C3D	-4.82	117.02	125.26
23	p	607	CHL	C3D-C2D-C1D	-4.82	99.26	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	AR	616	XAT	C28-C29-C30	-4.82	111.55	118.94
23	AU	605	CHL	C3D-C2D-C1D	-4.81	99.27	105.83
23	AB	605	CHL	C3D-C2D-C1D	-4.81	99.27	105.83
23	AB	608	CHL	C3C-C4C-NC	4.80	115.96	110.57
23	V	606	CHL	CHD-C1D-ND	-4.80	120.04	124.45
23	9	605	CHL	C3D-C2D-C1D	-4.80	99.28	105.83
23	AQ	606	CHL	C3D-C2D-C1D	-4.80	99.28	105.83
23	9	606	CHL	O2D-CGD-CBD	4.80	119.80	111.27
23	0	607	CHL	C2C-C1C-NC	4.79	117.64	109.51
23	V	616	CHL	CHB-C1B-NB	-4.79	119.18	124.26
23	AU	605	CHL	CHD-C4C-C3C	-4.79	117.80	124.84
24	AQ	612	CLA	C4A-NA-C1A	4.79	108.86	106.71
24	0	604	CLA	O2D-CGD-O1D	-4.79	114.48	123.84
23	p	608	CHL	C3D-C2D-C1D	-4.79	99.30	105.83
23	AQ	607	CHL	C3D-C2D-C1D	-4.78	99.31	105.83
23	AS	307	CHL	C3D-C2D-C1D	-4.77	99.32	105.83
23	AS	308	CHL	C3D-C2D-C1D	-4.77	99.32	105.83
23	AB	601	CHL	C3D-C2D-C1D	-4.77	99.32	105.83
23	AE	617	CHL	C3B-C2B-C1B	-4.76	101.41	107.16
27	AR	616	XAT	C18-C5-C4	-4.76	108.92	114.28
27	q	617	XAT	C28-C29-C30	-4.76	111.64	118.94
23	p	606	CHL	C3D-C2D-C1D	-4.76	99.34	105.83
23	AB	607	CHL	C3C-C4C-NC	4.75	115.90	110.57
27	AR	616	XAT	C11-C12-C13	-4.75	113.06	126.42
23	AA	617	CHL	C3D-C2D-C1D	-4.75	99.35	105.83
23	AH	606	CHL	C3D-C2D-C1D	-4.75	99.35	105.83
23	AC	605	CHL	C3D-C2D-C1D	-4.75	99.35	105.83
23	AB	606	CHL	C3D-C2D-C1D	-4.75	99.35	105.83
23	0	605	CHL	CHD-C4C-C3C	-4.74	117.87	124.84
23	AA	606	CHL	C3D-C2D-C1D	-4.74	99.36	105.83
23	V	607	CHL	C1B-NB-C4B	-4.74	102.97	106.33
23	AE	601	CHL	C3D-C2D-C1D	-4.73	99.38	105.83
23	q	605	CHL	C3D-C2D-C1D	-4.73	99.38	105.83
23	AN	605	CHL	C3D-C2D-C1D	-4.73	99.38	105.83
23	9	607	CHL	C3D-C2D-C1D	-4.72	99.39	105.83
27	q	617	XAT	C11-C12-C13	-4.72	113.16	126.42
23	AQ	608	CHL	C3D-C2D-C1D	-4.72	99.39	105.83
23	V	601	CHL	C3D-C2D-C1D	-4.72	99.39	105.83
23	AN	601	CHL	C3D-C2D-C1D	-4.72	99.39	105.83
23	V	605	CHL	CHD-C4C-C3C	-4.72	117.91	124.84
23	AQ	606	CHL	CHD-C4C-C3C	-4.71	117.91	124.84
24	q	608	CLA	C4A-NA-C1A	4.70	108.82	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AA	601	CHL	C3D-C2D-C1D	-4.70	99.41	105.83
23	AH	608	CHL	C3D-C2D-C1D	-4.70	99.42	105.83
23	AD	302	CHL	C3D-C2D-C1D	-4.70	99.42	105.83
23	AF	601	CHL	C3D-C2D-C1D	-4.70	99.42	105.83
23	q	613	CHL	CHB-C1B-NB	-4.70	119.28	124.26
23	p	601	CHL	C3D-C2D-C1D	-4.70	99.42	105.83
23	AH	607	CHL	C3D-C2D-C1D	-4.69	99.42	105.83
24	AB	602	CLA	O2D-CGD-CBD	4.69	119.60	111.27
27	9	618	XAT	C35-C15-C14	-4.68	113.89	123.47
23	v	308	CHL	C3D-C2D-C1D	-4.68	99.45	105.83
23	AU	608	CHL	C3D-C2D-C1D	-4.68	99.45	105.83
23	AS	307	CHL	CHD-C4C-C3C	-4.67	117.98	124.84
23	AD	306	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
23	AR	606	CHL	CHB-C1B-NB	-4.67	119.32	124.26
23	AR	613	CHL	CHB-C1B-NB	-4.67	119.32	124.26
23	AB	607	CHL	C3D-C2D-C1D	-4.66	99.47	105.83
27	AF	613	XAT	C38-C25-C24	-4.66	109.04	114.28
27	9	618	XAT	O4-C5-C18	-4.66	109.47	115.06
23	AU	607	CHL	C3D-C2D-C1D	-4.66	99.47	105.83
23	AD	301	CHL	C3D-C2D-C1D	-4.66	99.48	105.83
23	AS	302	CHL	C3D-C2D-C1D	-4.66	99.48	105.83
24	P	504	CLA	O2D-CGD-CBD	4.65	119.54	111.27
23	AC	606	CHL	C3D-C2D-C1D	-4.65	99.48	105.83
24	Q	401	CLA	O2D-CGD-CBD	4.65	119.52	111.27
23	AA	607	CHL	C3D-C2D-C1D	-4.65	99.49	105.83
23	AA	606	CHL	CHD-C4C-C3C	-4.65	118.01	124.84
23	AQ	601	CHL	C3D-C2D-C1D	-4.64	99.49	105.83
23	V	606	CHL	C3D-C2D-C1D	-4.64	99.50	105.83
23	9	608	CHL	C3D-C2D-C1D	-4.64	99.50	105.83
23	AE	617	CHL	C2D-C1D-ND	4.64	113.52	110.10
23	V	607	CHL	C2C-C1C-NC	4.64	117.38	109.51
23	q	613	CHL	C3C-C4C-NC	4.64	115.77	110.57
23	v	302	CHL	C3D-C2D-C1D	-4.63	99.51	105.83
23	q	607	CHL	C3D-C2D-C1D	-4.63	99.52	105.83
23	p	606	CHL	CHD-C4C-C3C	-4.63	118.04	124.84
27	9	618	XAT	C8-C9-C10	-4.63	111.84	118.94
23	AC	607	CHL	C3D-C2D-C1D	-4.63	99.52	105.83
23	AE	616	CHL	C3D-C2D-C1D	-4.62	99.52	105.83
23	AN	606	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
23	AQ	609	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
23	AS	308	CHL	C2C-C1C-NC	4.62	117.34	109.51
23	V	607	CHL	C3D-C2D-C1D	-4.62	99.53	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	p	609	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
23	AC	608	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
23	AU	601	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
23	AR	607	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
23	AF	607	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
23	0	617	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
23	AH	601	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
23	AE	606	CHL	C3D-C2D-C1D	-4.61	99.55	105.83
23	0	601	CHL	C3D-C2D-C1D	-4.60	99.55	105.83
23	AA	605	CHL	C3D-C2D-C1D	-4.60	99.56	105.83
23	AN	607	CHL	C3D-C2D-C1D	-4.60	99.56	105.83
24	AJ	405	CLA	O2D-CGD-CBD	4.60	119.44	111.27
23	AE	605	CHL	C3D-C2D-C1D	-4.60	99.56	105.83
23	AE	607	CHL	C3D-C2D-C1D	-4.59	99.56	105.83
23	q	607	CHL	CHB-C1B-NB	-4.59	119.40	124.26
27	q	617	XAT	C18-C5-C4	-4.59	109.12	114.28
23	AA	617	CHL	O2D-CGD-CBD	4.58	119.41	111.27
23	9	609	CHL	C3D-C2D-C1D	-4.57	99.59	105.83
23	V	607	CHL	C3C-C4C-NC	4.57	115.70	110.57
23	AA	617	CHL	C3B-C2B-C1B	-4.56	101.65	107.16
23	AH	605	CHL	C2D-C1D-ND	4.56	113.47	110.10
24	AC	602	CLA	O2D-CGD-O1D	-4.56	114.92	123.84
23	AQ	605	CHL	CHD-C4C-C3C	-4.56	118.14	124.84
23	p	605	CHL	CHD-C4C-C3C	-4.56	118.14	124.84
23	AS	308	CHL	C3C-C4C-NC	4.56	115.68	110.57
23	AR	605	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
23	9	605	CHL	CHD-C4C-C3C	-4.56	118.14	124.84
23	p	607	CHL	CHD-C4C-C3C	-4.55	118.14	124.84
27	9	618	XAT	O24-C25-C38	-4.55	109.60	115.06
27	AB	613	XAT	C31-C32-C33	-4.55	113.64	126.42
23	AD	307	CHL	CHD-C4C-C3C	-4.55	118.16	124.84
23	0	606	CHL	CHB-C1B-NB	-4.54	119.45	124.26
23	V	607	CHL	C1C-C2C-C3C	-4.54	101.41	107.65
23	AQ	607	CHL	CHD-C4C-C3C	-4.53	118.18	124.84
23	0	607	CHL	C1C-C2C-C3C	-4.53	101.41	107.65
23	q	606	CHL	C3D-C2D-C1D	-4.53	99.65	105.83
23	AD	306	CHL	CHD-C4C-C3C	-4.53	118.19	124.84
23	V	608	CHL	C3D-C2D-C1D	-4.52	99.66	105.83
23	AA	605	CHL	CHD-C4C-C3C	-4.52	118.20	124.84
26	AE	615	NEX	C39-C29-C30	-4.51	116.61	122.92
27	AB	613	XAT	C18-C5-C4	-4.51	109.21	114.28
23	AE	617	CHL	CHD-C1D-ND	-4.50	120.31	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AD	308	CHL	C3D-C2D-C1D	-4.50	99.69	105.83
23	9	606	CHL	C3D-C2D-C1D	-4.50	99.69	105.83
23	AN	606	CHL	CHD-C4C-C3C	-4.49	118.23	124.84
26	v	317	NEX	C35-C15-C14	4.49	132.68	123.47
23	AF	607	CHL	CHB-C1B-NB	-4.49	119.50	124.26
23	q	613	CHL	C3D-C2D-C1D	-4.49	99.71	105.83
23	AC	605	CHL	CHD-C4C-C3C	-4.49	118.25	124.84
23	AA	607	CHL	CHD-C4C-C3C	-4.48	118.25	124.84
23	AF	605	CHL	CHB-C1B-NB	-4.48	119.51	124.26
23	AF	601	CHL	CHD-C4C-C3C	-4.48	118.26	124.84
23	0	606	CHL	C3D-C2D-C1D	-4.48	99.72	105.83
23	AQ	606	CHL	C2D-C1D-ND	4.47	113.40	110.10
23	AN	617	CHL	C3D-C2D-C1D	-4.47	99.73	105.83
23	V	606	CHL	CHD-C4C-C3C	-4.46	118.28	124.84
23	AB	601	CHL	CHD-C4C-C3C	-4.46	118.28	124.84
27	AR	616	XAT	C31-C32-C33	-4.46	113.88	126.42
23	AE	616	CHL	O2D-CGD-CBD	4.46	119.19	111.27
27	9	618	XAT	C18-C5-C4	-4.46	109.27	114.28
23	AF	605	CHL	C3D-C2D-C1D	-4.45	99.75	105.83
24	AJ	406	CLA	O2D-CGD-O1D	-4.45	115.14	123.84
23	9	601	CHL	CAC-C3C-C4C	4.45	130.58	124.81
23	0	608	CHL	C3D-C2D-C1D	-4.45	99.76	105.83
23	AC	601	CHL	C2D-C1D-ND	4.44	113.38	110.10
23	AN	605	CHL	CHD-C4C-C3C	-4.44	118.31	124.84
23	q	605	CHL	CHD-C4C-C3C	-4.44	118.31	124.84
23	AF	608	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
23	AR	607	CHL	CHB-C1B-NB	-4.44	119.56	124.26
26	AR	615	NEX	C39-C29-C30	-4.44	116.71	122.92
23	AE	616	CHL	C3B-C4B-NB	4.44	114.63	110.52
23	p	605	CHL	C2D-C1D-ND	4.43	113.37	110.10
27	q	617	XAT	C31-C32-C33	-4.43	113.97	126.42
24	AB	602	CLA	O2D-CGD-O1D	-4.43	115.19	123.84
23	p	608	CHL	CHD-C4C-C3C	-4.43	118.33	124.84
23	v	308	CHL	C2C-C1C-NC	4.42	117.02	109.51
23	AN	617	CHL	CHD-C1D-ND	-4.42	120.39	124.45
23	AA	617	CHL	C1C-C2C-C3C	-4.42	103.61	107.11
23	AR	606	CHL	C3D-C2D-C1D	-4.42	99.80	105.83
23	AD	317	CHL	C3D-C2D-C1D	-4.42	99.81	105.83
23	v	306	CHL	C3D-C2D-C1D	-4.41	99.81	105.83
24	AF	602	CLA	CAC-C3C-C2C	-4.41	119.99	127.53
23	AQ	608	CHL	CHD-C4C-C3C	-4.40	118.37	124.84
23	AE	601	CHL	CHD-C4C-C3C	-4.40	118.37	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AS	308	CHL	C1C-C2C-C3C	-4.40	101.60	107.65
23	AU	606	CHL	CHD-C4C-C3C	-4.39	118.38	124.84
23	AE	606	CHL	CAC-C3C-C4C	4.39	130.51	124.81
23	v	307	CHL	CHD-C4C-C3C	-4.39	118.39	124.84
23	AF	601	CHL	C2D-C1D-ND	4.38	113.33	110.10
24	AJ	405	CLA	O2D-CGD-O1D	-4.38	115.27	123.84
23	AA	605	CHL	C2D-C1D-ND	4.38	113.33	110.10
23	AS	307	CHL	C2D-C1D-ND	4.38	113.33	110.10
23	AE	617	CHL	O2D-CGD-CBD	4.37	119.04	111.27
23	AN	607	CHL	CAC-C3C-C4C	4.37	130.48	124.81
23	AN	608	CHL	CAC-C3C-C4C	4.37	130.48	124.81
35	J	411	DGD	O3G-C3G-C2G	-4.37	100.36	110.90
35	AJ	412	DGD	O3G-C3G-C2G	-4.37	100.36	110.90
23	0	605	CHL	C2D-C1D-ND	4.36	113.32	110.10
23	0	601	CHL	CHB-C1B-NB	-4.36	119.64	124.26
23	AU	605	CHL	C2D-C1D-ND	4.36	113.32	110.10
26	q	615	NEX	C39-C29-C30	-4.36	116.82	122.92
23	p	609	CHL	CHD-C4C-C3C	-4.35	118.44	124.84
26	q	615	NEX	C35-C15-C14	4.35	132.39	123.47
23	AC	608	CHL	CHB-C1B-NB	-4.35	119.65	124.26
23	V	616	CHL	C2A-C3A-C4A	-4.35	94.85	101.87
35	AL	517	DGD	O3G-C3G-C2G	-4.34	100.43	110.90
23	AA	606	CHL	C2D-C1D-ND	4.34	113.30	110.10
23	AQ	605	CHL	C2D-C1D-ND	4.34	113.30	110.10
23	p	601	CHL	CHD-C4C-C3C	-4.33	118.47	124.84
23	AD	302	CHL	CHD-C4C-C3C	-4.33	118.47	124.84
23	v	307	CHL	C2D-C1D-ND	4.33	113.30	110.10
35	P	516	DGD	O3G-C3G-C2G	-4.33	100.45	110.90
23	AA	608	CHL	C3B-C2B-C1B	-4.33	101.94	107.16
26	AR	615	NEX	C15-C35-C34	4.33	132.34	123.47
24	AR	612	CLA	O2D-CGD-O1D	-4.33	115.38	123.84
23	AR	613	CHL	C3D-C2D-C1D	-4.32	99.93	105.83
23	AB	601	CHL	C2D-C1D-ND	4.32	113.29	110.10
23	AD	306	CHL	C2D-C1D-ND	4.32	113.29	110.10
23	AD	307	CHL	C2D-C1D-ND	4.32	113.29	110.10
23	AN	601	CHL	CHD-C4C-C3C	-4.32	118.49	124.84
23	AU	606	CHL	C2D-C1D-ND	4.32	113.28	110.10
23	AB	606	CHL	CHB-C1B-NB	-4.31	119.69	124.26
26	AQ	617	NEX	C15-C35-C34	4.31	132.30	123.47
24	p	618	CLA	O1D-CGD-CBD	4.31	133.30	124.48
23	AE	601	CHL	C2D-C1D-ND	4.31	113.28	110.10
23	AD	302	CHL	C2D-C1D-ND	4.31	113.28	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AA	616	NEX	C39-C29-C30	-4.31	116.89	122.92
23	AQ	601	CHL	CHD-C4C-C3C	-4.30	118.52	124.84
23	AE	606	CHL	CHD-C4C-C3C	-4.30	118.52	124.84
23	AH	608	CHL	CAC-C3C-C4C	4.30	130.39	124.81
23	AB	605	CHL	C1C-C2C-C3C	-4.30	101.73	107.65
23	9	601	CHL	C2D-C1D-ND	4.30	113.27	110.10
32	AJ	408	PHO	C2B-C1B-NB	-4.30	106.56	109.53
23	AD	317	CHL	C3B-C4B-NB	4.29	114.50	110.52
23	AH	607	CHL	CHD-C4C-C3C	-4.29	118.53	124.84
26	AU	616	NEX	C39-C29-C30	-4.29	116.91	122.92
24	O	614	CLA	O2D-CGD-O1D	-4.29	115.45	123.84
23	AB	608	CHL	C3D-C2D-C1D	-4.29	99.98	105.83
23	AN	606	CHL	C2D-C1D-ND	4.28	113.26	110.10
23	V	601	CHL	CHD-C4C-C3C	-4.28	118.55	124.84
23	AQ	609	CHL	CHD-C4C-C3C	-4.28	118.55	124.84
23	p	607	CHL	C2D-C1D-ND	4.28	113.26	110.10
23	AF	608	CHL	C3C-C4C-NC	4.28	115.37	110.57
27	AB	613	XAT	O4-C5-C18	-4.27	109.94	115.06
26	AS	317	NEX	C35-C15-C14	4.27	132.23	123.47
23	AD	308	CHL	C3B-C4B-NB	4.27	114.48	110.52
23	AH	601	CHL	CHD-C4C-C3C	-4.27	118.56	124.84
25	9	615	LUT	C19-C9-C10	-4.26	116.95	122.92
23	AU	608	CHL	CHD-C4C-C3C	-4.26	118.57	124.84
23	AC	606	CHL	CHD-C4C-C3C	-4.26	118.58	124.84
27	9	618	XAT	C31-C32-C33	-4.26	114.45	126.42
23	V	606	CHL	C2D-C1D-ND	4.25	113.24	110.10
26	9	617	NEX	C39-C29-C30	-4.25	116.96	122.92
32	J	406	PHO	C2B-C1B-NB	-4.25	106.59	109.53
27	AB	613	XAT	C32-C33-C34	-4.25	112.41	118.94
23	AU	607	CHL	CHD-C4C-C3C	-4.25	118.59	124.84
32	J	405	PHO	C2B-C1B-NB	-4.25	106.59	109.53
27	q	617	XAT	O24-C25-C38	-4.25	109.96	115.06
24	AC	602	CLA	CED-O2D-CGD	4.25	125.55	115.94
35	AL	518	DGD	O3G-C3G-C2G	-4.25	100.65	110.90
23	AD	301	CHL	CHD-C4C-C3C	-4.25	118.60	124.84
25	AF	611	LUT	C39-C29-C30	-4.24	116.98	122.92
27	9	618	XAT	C38-C25-C24	-4.24	109.51	114.28
26	AQ	617	NEX	C39-C29-C30	-4.24	116.98	122.92
27	AF	613	XAT	C30-C31-C32	-4.24	109.98	123.22
23	V	607	CHL	CBA-CAA-C2A	4.24	126.38	113.86
32	AJ	407	PHO	C2B-C1B-NB	-4.24	106.60	109.53
23	0	607	CHL	C3B-C4B-NB	4.23	114.44	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AD	301	CHL	C2D-C1D-ND	4.23	113.22	110.10
23	AU	601	CHL	CHD-C4C-C3C	-4.23	118.62	124.84
27	9	618	XAT	C12-C13-C14	-4.23	112.45	118.94
23	AN	617	CHL	C4D-CHA-C1A	-4.23	116.10	121.25
23	AU	608	CHL	CAC-C3C-C4C	4.23	130.30	124.81
26	AS	317	NEX	C39-C29-C30	-4.23	117.00	122.92
23	AE	605	CHL	CHD-C4C-C3C	-4.23	118.63	124.84
24	q	612	CLA	O2D-CGD-O1D	-4.22	115.58	123.84
26	p	616	NEX	C17-C1-C6	4.22	114.25	110.47
26	p	616	NEX	C39-C29-C30	-4.22	117.01	122.92
23	AN	607	CHL	C1-C2-C3	-4.22	118.75	126.04
26	v	317	NEX	C39-C29-C30	-4.22	117.02	122.92
23	AE	616	CHL	C3B-C2B-C1B	-4.22	102.07	107.16
23	9	607	CHL	CHD-C4C-C3C	-4.22	118.64	124.84
24	J	404	CLA	O2D-CGD-O1D	-4.22	115.60	123.84
26	AC	616	NEX	C39-C29-C30	-4.21	117.02	122.92
28	AK	624	LHG	O4-P-O5	4.21	133.06	112.24
28	P	517	LHG	O4-P-O5	4.21	133.06	112.24
26	AC	616	NEX	C15-C35-C34	4.21	132.10	123.47
28	AL	519	LHG	O4-P-O5	4.21	133.05	112.24
28	O	623	LHG	O4-P-O5	4.21	133.03	112.24
23	AN	617	CHL	C3B-C4B-NB	4.20	114.41	110.52
28	AQ	618	LHG	O4-P-O5	4.20	133.02	112.24
23	AR	605	CHL	CHB-C1B-NB	-4.20	119.81	124.26
23	V	616	CHL	C2D-C1D-ND	4.20	113.20	110.10
23	AC	608	CHL	CHD-C4C-C3C	-4.20	118.66	124.84
23	AD	306	CHL	C3B-C4B-NB	4.20	114.41	110.52
23	AS	302	CHL	CHD-C4C-C3C	-4.20	118.67	124.84
23	AF	606	CHL	O2D-CGD-CBD	4.20	118.73	111.27
27	q	617	XAT	O4-C5-C18	-4.19	110.03	115.06
23	AH	608	CHL	CHD-C4C-C3C	-4.19	118.68	124.84
28	AD	316	LHG	O4-P-O5	4.19	132.96	112.24
28	V	615	LHG	O4-P-O5	4.19	132.95	112.24
23	p	606	CHL	C2D-C1D-ND	4.18	113.19	110.10
28	AS	301	LHG	O4-P-O5	4.18	132.92	112.24
23	0	617	CHL	O2D-CGD-CBD	4.18	118.70	111.27
28	0	616	LHG	O4-P-O5	4.18	132.91	112.24
28	q	616	LHG	O4-P-O5	4.18	132.91	112.24
28	AM	406	LHG	O4-P-O5	4.18	132.91	112.24
28	AK	623	LHG	O4-P-O5	4.18	132.90	112.24
23	v	302	CHL	CHD-C4C-C3C	-4.18	118.70	124.84
24	J	404	CLA	O2D-CGD-CBD	4.18	118.69	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Q	406	LHG	O4-P-O5	4.18	132.90	112.24
23	AA	608	CHL	C3D-C2D-C1D	-4.18	100.13	105.83
28	v	301	LHG	O4-P-O5	4.18	132.89	112.24
28	O	622	LHG	O4-P-O5	4.17	132.88	112.24
28	w	201	LHG	O4-P-O5	4.17	132.87	112.24
28	AU	617	LHG	O4-P-O5	4.17	132.87	112.24
28	AN	616	LHG	O4-P-O5	4.17	132.87	112.24
28	W	201	LHG	O4-P-O5	4.17	132.86	112.24
26	q	615	NEX	C15-C35-C34	4.17	132.02	123.47
24	Q	401	CLA	O2D-CGD-O1D	-4.17	115.69	123.84
26	AS	317	NEX	C20-C13-C14	-4.17	117.09	122.92
35	j	102	DGD	O3G-C3G-C2G	-4.17	100.85	110.90
27	AR	616	XAT	O24-C25-C38	-4.16	110.07	115.06
28	AH	616	LHG	O4-P-O5	4.16	132.82	112.24
23	AA	607	CHL	C2D-C1D-ND	4.16	113.17	110.10
23	0	617	CHL	CHD-C4C-C3C	-4.16	118.73	124.84
23	0	617	CHL	C2D-C1D-ND	4.16	113.17	110.10
23	V	616	CHL	C4D-CHA-C1A	-4.15	116.19	121.25
23	AU	601	CHL	C2D-C1D-ND	4.15	113.16	110.10
23	AA	607	CHL	CAC-C3C-C4C	4.15	130.20	124.81
23	AQ	607	CHL	C2D-C1D-ND	4.15	113.16	110.10
23	AN	605	CHL	C2D-C1D-ND	4.14	113.16	110.10
23	p	608	CHL	C2D-C1D-ND	4.14	113.15	110.10
25	9	616	LUT	C19-C9-C10	-4.14	117.13	122.92
23	V	601	CHL	C3B-C4B-NB	4.14	114.35	110.52
23	AB	608	CHL	CAC-C3C-C4C	4.13	130.18	124.81
23	v	308	CHL	C2D-C1D-ND	4.13	113.15	110.10
23	V	616	CHL	O2D-CGD-CBD	4.13	118.61	111.27
25	AC	614	LUT	C19-C9-C10	-4.13	117.14	122.92
27	9	618	XAT	C32-C33-C34	-4.13	112.60	118.94
23	AN	607	CHL	CHB-C1B-NB	-4.13	119.88	124.26
23	AA	617	CHL	CHD-C4C-C3C	-4.13	118.77	124.84
23	AN	601	CHL	C3B-C4B-NB	4.13	114.34	110.52
26	AU	616	NEX	C15-C35-C34	4.13	131.93	123.47
23	v	307	CHL	C3B-C4B-NB	4.13	114.34	110.52
27	AF	613	XAT	C12-C13-C14	-4.12	112.61	118.94
23	9	607	CHL	C2D-C1D-ND	4.12	113.14	110.10
23	V	601	CHL	C2D-C1D-ND	4.12	113.14	110.10
24	p	618	CLA	CAA-C2A-C1A	4.12	125.48	111.97
23	AR	606	CHL	CAC-C3C-C4C	4.12	130.16	124.81
23	p	601	CHL	C2D-C1D-ND	4.12	113.14	110.10
23	AH	601	CHL	C2D-C1D-ND	4.12	113.14	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	0	617	CHL	C3B-C2B-C1B	-4.12	102.19	107.16
27	q	617	XAT	C12-C13-C14	-4.12	112.62	118.94
26	AA	616	NEX	C15-C35-C34	4.12	131.91	123.47
23	AE	607	CHL	CHD-C4C-C3C	-4.11	118.79	124.84
25	AC	615	LUT	C19-C9-C10	-4.11	117.17	122.92
23	V	607	CHL	C1-C2-C3	-4.11	118.93	126.04
23	9	605	CHL	C2D-C1D-ND	4.11	113.13	110.10
23	q	605	CHL	C2D-C1D-ND	4.11	113.13	110.10
27	AR	616	XAT	C12-C13-C14	-4.11	112.64	118.94
23	AC	606	CHL	C2D-C1D-ND	4.11	113.13	110.10
23	AC	605	CHL	C2D-C1D-ND	4.10	113.13	110.10
26	v	317	NEX	C19-C9-C10	-4.10	117.18	122.92
23	AE	606	CHL	C2D-C1D-ND	4.10	113.12	110.10
24	q	612	CLA	C1D-CHD-C4C	4.10	125.03	120.68
25	V	614	LUT	C19-C9-C10	-4.09	117.19	122.92
23	AH	606	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
25	AN	615	LUT	C19-C9-C10	-4.09	117.19	122.92
25	AQ	616	LUT	C19-C9-C10	-4.09	117.20	122.92
27	q	617	XAT	C8-C9-C10	-4.09	112.67	118.94
23	V	606	CHL	C3B-C4B-NB	4.09	114.31	110.52
23	AD	307	CHL	C3B-C4B-NB	4.08	114.30	110.52
23	AS	307	CHL	C3B-C4B-NB	4.08	114.30	110.52
25	AD	315	LUT	C19-C9-C10	-4.08	117.21	122.92
25	0	615	LUT	C19-C9-C10	-4.08	117.21	122.92
25	AA	614	LUT	C35-C15-C14	4.08	131.83	123.47
23	AC	605	CHL	C3B-C4B-NB	4.08	114.30	110.52
23	AB	605	CHL	C2C-C1C-NC	4.07	116.42	109.51
35	AO	102	DGD	O3G-C3G-C2G	-4.07	101.08	110.90
27	AB	613	XAT	C11-C12-C13	-4.06	115.00	126.42
23	V	605	CHL	C2D-C1D-ND	4.06	113.10	110.10
23	AH	607	CHL	C2D-C1D-ND	4.06	113.10	110.10
23	AH	608	CHL	C2D-C1D-ND	4.06	113.09	110.10
26	AE	615	NEX	C15-C35-C34	4.06	131.79	123.47
23	9	607	CHL	C3B-C4B-NB	4.06	114.28	110.52
23	v	308	CHL	C3C-C2C-C1C	-4.06	102.35	107.21
23	AN	601	CHL	C2D-C1D-ND	4.06	113.09	110.10
23	AQ	601	CHL	C2D-C1D-ND	4.05	113.09	110.10
28	O	621	LHG	O4-P-O5	4.05	132.28	112.24
25	AF	611	LUT	C19-C9-C10	-4.05	117.25	122.92
23	AC	608	CHL	C2D-C1D-ND	4.05	113.09	110.10
25	AD	315	LUT	C39-C29-C30	-4.05	117.25	122.92
25	0	615	LUT	C39-C29-C30	-4.05	117.25	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AA	601	CHL	CHD-C4C-C3C	-4.05	118.89	124.84
23	AS	308	CHL	C2D-C1D-ND	4.05	113.09	110.10
23	AD	307	CHL	CHB-C1B-NB	-4.04	119.97	124.26
23	AQ	608	CHL	CAC-C3C-C4C	4.04	130.06	124.81
23	AN	617	CHL	O2D-CGD-CBD	4.04	118.45	111.27
23	9	606	CHL	CAC-C3C-C4C	4.03	130.04	124.81
23	AU	605	CHL	C3B-C4B-NB	4.02	114.25	110.52
26	AR	615	NEX	C35-C15-C14	4.02	131.71	123.47
26	9	617	NEX	C15-C35-C34	4.02	131.71	123.47
23	0	607	CHL	C2D-C1D-ND	4.02	113.06	110.10
23	AN	606	CHL	C3B-C4B-NB	4.01	114.24	110.52
23	AA	601	CHL	C2D-C1D-ND	4.01	113.06	110.10
25	AR	614	LUT	C19-C9-C10	-4.01	117.31	122.92
23	AD	302	CHL	C3B-C4B-NB	4.01	114.23	110.52
23	AU	607	CHL	C2D-C1D-ND	4.01	113.06	110.10
25	p	615	LUT	C19-C9-C10	-4.01	117.31	122.92
23	V	601	CHL	CAC-C3C-C4C	4.01	130.01	124.81
24	9	602	CLA	O2D-CGD-O1D	-4.00	116.01	123.84
23	AQ	601	CHL	C3B-C4B-NB	4.00	114.23	110.52
23	9	607	CHL	CAC-C3C-C4C	4.00	130.00	124.81
23	V	616	CHL	C3B-C4B-NB	4.00	114.22	110.52
23	AE	607	CHL	CAC-C3C-C4C	4.00	130.00	124.81
23	AB	606	CHL	C2D-C1D-ND	4.00	113.05	110.10
23	p	609	CHL	C2D-C1D-ND	3.99	113.05	110.10
23	v	308	CHL	C2C-C3C-C4C	-3.99	102.43	107.21
23	AQ	608	CHL	C2D-C1D-ND	3.99	113.04	110.10
27	AR	616	XAT	O4-C5-C18	-3.99	110.28	115.06
23	AN	601	CHL	CAC-C3C-C4C	3.99	129.98	124.81
27	AF	613	XAT	C10-C11-C12	-3.98	110.79	123.22
27	AF	613	XAT	C18-C5-C4	-3.98	109.80	114.28
23	p	605	CHL	C3B-C4B-NB	3.98	114.21	110.52
23	AF	601	CHL	C3B-C4B-NB	3.98	114.20	110.52
23	AH	605	CHL	C3B-C4B-NB	3.98	114.20	110.52
25	AU	615	LUT	C19-C9-C10	-3.98	117.35	122.92
24	AN	613	CLA	O2D-CGD-O1D	-3.98	116.07	123.84
23	AE	601	CHL	C3B-C4B-NB	3.97	114.20	110.52
23	AU	601	CHL	O2D-CGD-CBD	3.97	118.33	111.27
26	AA	616	NEX	C35-C15-C14	3.97	131.61	123.47
23	0	605	CHL	O2D-CGD-CBD	3.97	118.32	111.27
25	AH	615	LUT	C39-C29-C30	-3.96	117.37	122.92
23	p	609	CHL	C3B-C4B-NB	3.96	114.19	110.52
23	AQ	605	CHL	C3B-C4B-NB	3.96	114.19	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	AR	616	XAT	C8-C9-C10	-3.96	112.86	118.94
23	p	601	CHL	C3B-C4B-NB	3.96	114.19	110.52
24	AK	616	CLA	O2D-CGD-CBD	3.96	118.30	111.27
23	AU	608	CHL	C2D-C1D-ND	3.96	113.02	110.10
23	9	601	CHL	CHD-C4C-C3C	-3.95	119.03	124.84
25	AH	615	LUT	C19-C9-C10	-3.95	117.39	122.92
24	q	618	CLA	O1D-CGD-CBD	3.95	132.57	124.48
24	AF	614	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
26	9	617	NEX	C35-C15-C14	3.95	131.56	123.47
25	AU	615	LUT	C39-C29-C30	-3.95	117.39	122.92
23	q	605	CHL	CAC-C3C-C4C	3.95	129.93	124.81
23	q	606	CHL	CHB-C1B-NB	-3.95	120.08	124.26
24	P	504	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
23	0	606	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
23	AH	601	CHL	C3B-C4B-NB	3.94	114.17	110.52
23	AN	617	CHL	C3B-C2B-C1B	-3.94	102.41	107.16
23	AF	608	CHL	CAC-C3C-C4C	3.94	129.92	124.81
23	AU	601	CHL	C3B-C4B-NB	3.94	114.17	110.52
25	AA	614	LUT	C19-C9-C10	-3.94	117.41	122.92
25	AD	314	LUT	C15-C35-C34	3.94	131.53	123.47
23	AS	306	CHL	C2D-C1D-ND	3.93	113.00	110.10
23	AN	607	CHL	CHD-C4C-C3C	-3.93	119.06	124.84
27	AF	613	XAT	O4-C5-C18	-3.93	110.34	115.06
26	AE	615	NEX	C35-C15-C14	3.93	131.53	123.47
23	AH	601	CHL	O2D-CGD-CBD	3.93	118.25	111.27
23	p	606	CHL	CAC-C3C-C4C	3.93	129.91	124.81
25	V	614	LUT	C39-C29-C30	-3.92	117.43	122.92
27	AF	613	XAT	C28-C29-C30	-3.92	112.92	118.94
25	AE	613	LUT	C19-C9-C10	-3.92	117.43	122.92
23	AR	613	CHL	CHD-C4C-C3C	-3.92	119.08	124.84
27	AB	613	XAT	C28-C29-C30	-3.92	112.93	118.94
23	V	616	CHL	C1C-C2C-C3C	-3.92	104.00	107.11
23	AB	607	CHL	C4A-NA-C1A	3.92	108.47	106.71
25	p	614	LUT	C19-C9-C10	-3.91	117.44	122.92
24	J	403	CLA	O2D-CGD-O1D	-3.91	116.20	123.84
34	o	101	SQD	O47-C7-C8	3.91	119.92	111.50
24	AH	602	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
34	AM	401	SQD	O47-C7-C8	3.90	119.91	111.50
25	AA	615	LUT	C19-C9-C10	-3.90	117.46	122.92
24	AU	602	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
23	0	601	CHL	CHD-C4C-C3C	-3.90	119.11	124.84
24	AK	616	CLA	O2D-CGD-O1D	-3.90	116.21	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AD	302	CHL	CAC-C3C-C4C	3.90	129.87	124.81
23	V	608	CHL	C3B-C4B-NB	3.90	114.13	110.52
34	AP	101	SQD	O47-C7-C8	3.90	119.90	111.50
23	AB	607	CHL	O2D-CGD-CBD	3.90	118.19	111.27
34	Q	402	SQD	O47-C7-C8	3.89	119.89	111.50
23	AB	605	CHL	C3C-C4C-NC	3.89	114.94	110.57
23	AD	317	CHL	CHD-C4C-C3C	-3.89	119.12	124.84
25	AD	314	LUT	C19-C9-C10	-3.89	117.47	122.92
23	AE	607	CHL	C3B-C4B-NB	3.89	114.12	110.52
25	AC	614	LUT	C39-C29-C30	-3.89	117.47	122.92
23	AD	317	CHL	C3B-C2B-C1B	-3.89	102.47	107.16
23	AA	617	CHL	C2D-C1D-ND	3.89	112.97	110.10
26	p	616	NEX	C15-C35-C34	3.89	131.43	123.47
23	AU	606	CHL	C3B-C4B-NB	3.88	114.12	110.52
23	0	617	CHL	C3B-C4B-NB	3.88	114.12	110.52
24	P	502	CLA	O2D-CGD-CBD	3.88	118.17	111.27
23	AE	605	CHL	C2D-C1D-ND	3.88	112.96	110.10
23	V	608	CHL	CAC-C3C-C4C	3.88	129.84	124.81
24	P	501	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
26	p	616	NEX	C2-C1-C6	-3.88	105.44	109.21
23	AF	605	CHL	C2C-C1C-NC	3.88	116.08	109.51
23	AD	308	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
26	AU	616	NEX	C35-C15-C14	3.87	131.41	123.47
25	AQ	615	LUT	C19-C9-C10	-3.87	117.50	122.92
23	0	601	CHL	C3B-C4B-NB	3.87	114.11	110.52
27	AB	613	XAT	C10-C11-C12	-3.87	111.14	123.22
27	AR	616	XAT	C38-C25-C24	-3.87	109.93	114.28
23	AF	605	CHL	C2C-C3C-C4C	-3.87	102.58	107.21
23	V	608	CHL	CHD-C4C-C3C	-3.87	119.16	124.84
24	AB	611	CLA	CAA-CBA-CGA	-3.86	102.25	112.51
25	9	615	LUT	C39-C29-C30	-3.86	117.51	122.92
25	AC	614	LUT	C35-C15-C14	3.86	131.39	123.47
24	K	101	CLA	O2D-CGD-CBD	3.86	118.12	111.27
25	p	615	LUT	C39-C29-C30	-3.86	117.52	122.92
23	AN	605	CHL	O2D-CGD-CBD	3.86	118.12	111.27
23	AC	607	CHL	C2D-C1D-ND	3.86	112.95	110.10
23	V	616	CHL	C3B-C2B-C1B	-3.86	102.50	107.16
25	AQ	616	LUT	C39-C29-C30	-3.86	117.52	122.92
23	AD	301	CHL	CAC-C3C-C4C	3.86	129.81	124.81
23	AH	607	CHL	C3B-C4B-NB	3.86	114.09	110.52
23	AD	317	CHL	O2D-CGD-CBD	3.86	118.12	111.27
34	m	101	SQD	O47-C7-C8	3.86	119.81	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	9	606	CHL	CHD-C4C-C3C	-3.85	119.18	124.84
23	AF	608	CHL	CHC-C4B-NB	-3.85	120.18	124.26
23	9	605	CHL	C3B-C4B-NB	3.84	114.08	110.52
24	P	503	CLA	O2D-CGD-O1D	-3.84	116.32	123.84
23	AS	302	CHL	CHB-C1B-NB	-3.84	120.19	124.26
24	AL	512	CLA	O2D-CGD-CBD	3.84	118.10	111.27
23	AS	306	CHL	C2A-C1A-CHA	-3.84	114.81	122.75
23	AA	605	CHL	O2D-CGD-CBD	3.84	118.09	111.27
23	9	608	CHL	C2D-C1D-ND	3.84	112.93	110.10
25	9	615	LUT	C35-C15-C14	3.84	131.34	123.47
23	AQ	601	CHL	CAC-C3C-C4C	3.84	129.79	124.81
25	AA	615	LUT	C39-C29-C30	-3.84	117.55	122.92
23	p	608	CHL	CAC-C3C-C4C	3.84	129.79	124.81
25	AN	615	LUT	C39-C29-C30	-3.84	117.55	122.92
23	AD	301	CHL	C3B-C4B-NB	3.84	114.07	110.52
23	0	607	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
23	v	307	CHL	CAC-C3C-C4C	3.83	129.78	124.81
23	v	302	CHL	CHB-C1B-NB	-3.83	120.20	124.26
23	AA	605	CHL	CAC-C3C-C4C	3.83	129.78	124.81
34	M	101	SQD	O47-C7-C8	3.83	119.76	111.50
23	AU	607	CHL	C3B-C4B-NB	3.83	114.07	110.52
25	AE	614	LUT	C19-C9-C10	-3.83	117.56	122.92
23	9	601	CHL	CAA-C2A-C1A	3.83	120.62	112.14
23	AF	608	CHL	CMB-C2B-C1B	3.83	131.20	125.37
27	AF	613	XAT	C11-C12-C13	-3.83	115.66	126.42
23	v	306	CHL	C2D-C1D-ND	3.83	112.92	110.10
27	AB	613	XAT	C35-C15-C14	-3.83	115.64	123.47
25	q	614	LUT	C19-C9-C10	-3.82	117.57	122.92
23	AE	607	CHL	CHB-C1B-NB	-3.82	120.21	124.26
23	AE	607	CHL	C2D-C1D-ND	3.82	112.92	110.10
25	v	315	LUT	C39-C29-C30	-3.82	117.57	122.92
23	AE	616	CHL	C2D-C1D-ND	3.82	112.92	110.10
23	AH	606	CHL	C2D-C1D-ND	3.82	112.92	110.10
26	v	317	NEX	C15-C35-C34	3.81	131.28	123.47
23	AE	606	CHL	C3B-C4B-NB	3.81	114.05	110.52
24	O	611	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
24	AJ	404	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
23	AF	605	CHL	C3C-C2C-C1C	-3.81	102.65	107.21
23	0	601	CHL	C4-C3-C5	3.81	121.67	115.27
23	9	607	CHL	CHB-C1B-NB	-3.80	120.23	124.26
23	p	601	CHL	CAC-C3C-C4C	3.80	129.74	124.81
23	0	601	CHL	O2D-CGD-CBD	3.80	118.02	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AA	616	NEX	C19-C9-C10	-3.80	117.60	122.92
23	AH	606	CHL	O2D-CGD-CBD	3.80	118.02	111.27
25	0	614	LUT	C19-C9-C10	-3.80	117.60	122.92
23	AA	607	CHL	C3B-C4B-NB	3.80	114.04	110.52
25	AU	614	LUT	C39-C29-C30	-3.79	117.61	122.92
23	AU	607	CHL	CAC-C3C-C4C	3.79	129.73	124.81
23	AQ	606	CHL	CAC-C3C-C4C	3.79	129.73	124.81
23	0	601	CHL	O2A-CGA-CBA	3.79	123.80	111.91
23	9	609	CHL	CHD-C4C-C3C	-3.79	119.28	124.84
24	AL	502	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
25	AH	614	LUT	C39-C29-C30	-3.78	117.62	122.92
23	AH	606	CHL	C3B-C4B-NB	3.78	114.02	110.52
25	AC	615	LUT	C39-C29-C30	-3.78	117.62	122.92
23	AE	605	CHL	CAC-C3C-C4C	3.78	129.72	124.81
24	O	601	CLA	CAA-C2A-C3A	-3.78	102.42	112.78
23	AN	606	CHL	C1-C2-C3	-3.78	119.50	126.04
23	0	607	CHL	CHB-C1B-NB	-3.78	120.25	124.26
23	q	613	CHL	CAC-C3C-C4C	3.78	129.71	124.81
23	AH	607	CHL	CAC-C3C-C4C	3.78	129.71	124.81
24	p	602	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
23	AA	606	CHL	CAC-C3C-C4C	3.77	129.71	124.81
27	q	617	XAT	C38-C25-C24	-3.77	110.04	114.28
23	AD	301	CHL	CHB-C1B-NB	-3.77	120.27	124.26
23	v	308	CHL	O2D-CGD-CBD	3.77	117.97	111.27
23	q	606	CHL	O2D-CGD-CBD	3.77	117.97	111.27
23	q	607	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
23	AN	606	CHL	O2D-CGD-CBD	3.77	117.96	111.27
25	AN	614	LUT	C19-C9-C10	-3.76	117.65	122.92
24	AS	303	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
27	AF	613	XAT	C35-C15-C14	-3.76	115.77	123.47
25	9	616	LUT	C39-C29-C30	-3.76	117.65	122.92
26	AE	615	NEX	C19-C9-C10	-3.76	117.65	122.92
23	p	609	CHL	CAC-C3C-C4C	3.76	129.69	124.81
25	AS	315	LUT	C39-C29-C30	-3.76	117.66	122.92
24	AK	603	CLA	CAA-C2A-C3A	-3.76	102.49	112.78
23	AQ	609	CHL	C3B-C4B-NB	3.75	114.00	110.52
23	AB	607	CHL	CHD-C4C-C3C	-3.75	119.33	124.84
23	AS	307	CHL	CAC-C3C-C4C	3.75	129.68	124.81
23	V	606	CHL	C1-C2-C3	-3.75	119.56	126.04
23	AN	608	CHL	C1C-C2C-C3C	-3.75	104.14	107.11
34	o	101	SQD	O9-S-C6	3.75	111.39	106.94
23	p	608	CHL	CAA-C2A-C1A	3.74	124.25	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	v	316	LUT	C39-C29-C30	-3.74	117.68	122.92
23	AQ	609	CHL	C2D-C1D-ND	3.74	112.86	110.10
24	AB	611	CLA	CBA-CAA-C2A	3.74	124.91	113.86
23	AH	607	CHL	CHB-C1B-NB	-3.74	120.30	124.26
23	AU	607	CHL	CHB-C1B-NB	-3.74	120.30	124.26
25	AF	611	LUT	C7-C8-C9	-3.74	120.58	126.23
24	0	613	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
23	V	608	CHL	CHB-C1B-NB	-3.74	120.30	124.26
24	p	618	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
34	AM	401	SQD	O9-S-O7	-3.74	101.01	113.95
25	AQ	615	LUT	C39-C29-C30	-3.74	117.69	122.92
25	AE	614	LUT	C15-C35-C34	3.74	131.13	123.47
23	AR	605	CHL	C2D-C1D-ND	3.74	112.86	110.10
25	AS	316	LUT	C39-C29-C30	-3.73	117.69	122.92
24	AK	613	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
23	AD	307	CHL	CAC-C3C-C4C	3.73	129.66	124.81
23	V	606	CHL	O2D-CGD-CBD	3.73	117.90	111.27
24	AD	305	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
34	M	101	SQD	O9-S-C6	3.73	111.37	106.94
25	p	614	LUT	C39-C29-C30	-3.73	117.70	122.92
23	AN	607	CHL	C2D-C1D-ND	3.73	112.85	110.10
23	AB	606	CHL	C3B-C4B-NB	3.73	113.97	110.52
23	AQ	609	CHL	O2D-CGD-CBD	3.72	117.89	111.27
23	AC	608	CHL	C3B-C4B-NB	3.72	113.97	110.52
23	AB	601	CHL	C3B-C4B-NB	3.72	113.97	110.52
23	V	608	CHL	C2D-C1D-ND	3.72	112.85	110.10
23	v	306	CHL	C1D-ND-C4D	-3.72	103.69	106.33
23	AQ	609	CHL	CAC-C3C-C4C	3.72	129.64	124.81
23	p	601	CHL	C11-C12-C13	-3.72	103.90	115.92
23	AB	601	CHL	CAC-C3C-C4C	3.72	129.63	124.81
23	AR	607	CHL	CAC-C3C-C4C	3.72	129.63	124.81
23	AE	607	CHL	O2D-CGD-O1D	-3.72	116.57	123.84
23	AD	308	CHL	CAC-C3C-C4C	3.72	129.63	124.81
24	9	612	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
23	AU	601	CHL	C1D-ND-C4D	-3.71	103.70	106.33
34	AP	101	SQD	O9-S-C6	3.71	111.35	106.94
34	m	101	SQD	O9-S-C6	3.71	111.35	106.94
23	v	302	CHL	C2D-C1D-ND	3.71	112.84	110.10
23	AF	601	CHL	C1D-ND-C4D	-3.71	103.70	106.33
35	AJ	401	DGD	O3G-C3G-C2G	-3.71	101.95	110.90
25	v	315	LUT	C19-C9-C10	-3.71	117.73	122.92
23	9	609	CHL	C3B-C4B-NB	3.71	113.96	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	J	413	DGD	O3G-C3G-C2G	-3.71	101.95	110.90
23	AC	605	CHL	O2D-CGD-CBD	3.71	117.86	111.27
24	AN	602	CLA	O2D-CGD-O1D	-3.71	116.59	123.84
24	V	602	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
25	AD	314	LUT	C35-C15-C14	3.70	131.06	123.47
23	AE	616	CHL	CAC-C3C-C4C	3.70	129.61	124.81
23	AE	606	CHL	O2D-CGD-CBD	3.70	117.84	111.27
23	AA	601	CHL	C3B-C4B-NB	3.70	113.94	110.52
23	p	607	CHL	C6-C7-C8	-3.69	103.98	115.92
25	AH	614	LUT	C15-C35-C34	3.69	131.03	123.47
23	AD	302	CHL	O2D-CGD-CBD	3.69	117.83	111.27
23	AF	607	CHL	O2D-CGD-CBD	3.69	117.82	111.27
25	AD	314	LUT	C39-C29-C30	-3.69	117.75	122.92
23	AE	601	CHL	CHB-C1B-NB	-3.69	120.35	124.26
23	p	608	CHL	C1-C2-C3	-3.69	119.67	126.04
34	J	410	SQD	O47-C7-C8	3.69	119.45	111.50
34	AJ	411	SQD	O47-C7-C8	3.69	119.45	111.50
23	9	609	CHL	CAC-C3C-C4C	3.69	129.59	124.81
23	q	605	CHL	CHB-C1B-NB	-3.69	120.35	124.26
23	v	307	CHL	CHB-C1B-NB	-3.69	120.35	124.26
25	0	614	LUT	C39-C29-C30	-3.69	117.76	122.92
34	Q	402	SQD	O9-S-O7	-3.69	101.19	113.95
25	AE	613	LUT	C35-C15-C14	3.68	131.02	123.47
34	AJ	411	SQD	O9-S-O7	-3.68	101.20	113.95
23	AF	607	CHL	CAC-C3C-C4C	3.68	129.59	124.81
34	AM	401	SQD	O8-S-C6	3.68	111.61	105.74
23	AD	302	CHL	C4-C3-C5	3.68	121.46	115.27
25	AN	614	LUT	C39-C29-C30	-3.68	117.77	122.92
34	J	410	SQD	O9-S-O7	-3.68	101.22	113.95
23	9	605	CHL	O2D-CGD-CBD	3.68	117.80	111.27
23	AC	606	CHL	C1D-ND-C4D	-3.68	103.72	106.33
23	AH	601	CHL	C1D-ND-C4D	-3.68	103.72	106.33
23	V	607	CHL	C2D-C1D-ND	3.67	112.81	110.10
25	AD	315	LUT	C35-C15-C14	3.67	131.00	123.47
24	AE	609	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
23	9	606	CHL	CMD-C2D-C3D	-3.67	119.17	127.61
25	AA	614	LUT	C39-C29-C30	-3.67	117.78	122.92
26	AE	615	NEX	C40-C33-C34	-3.67	117.78	122.92
34	M	101	SQD	O9-S-O7	-3.67	101.26	113.95
23	AR	606	CHL	CHD-C4C-C3C	-3.67	119.45	124.84
23	AA	605	CHL	C3B-C4B-NB	3.67	113.92	110.52
25	AU	614	LUT	C15-C35-C34	3.66	130.98	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	0	614	LUT	C35-C15-C14	3.66	130.98	123.47
26	AS	317	NEX	C12-C13-C14	3.66	124.56	118.94
23	AH	608	CHL	C3B-C4B-NB	3.66	113.91	110.52
34	m	101	SQD	O9-S-O7	-3.66	101.28	113.95
23	0	605	CHL	CAC-C3C-C4C	3.66	129.56	124.81
24	AL	505	CLA	O2D-CGD-CBD	3.66	117.77	111.27
24	AA	604	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
23	AA	601	CHL	CAC-C3C-C4C	3.66	129.56	124.81
34	AJ	411	SQD	O7-S-C6	3.66	111.28	106.94
23	AS	308	CHL	CHD-C4C-C3C	-3.65	119.47	124.84
23	AS	307	CHL	CHB-C1B-NB	-3.65	120.39	124.26
24	AC	604	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
23	AS	302	CHL	C2D-C1D-ND	3.65	112.80	110.10
23	p	608	CHL	C3B-C4B-NB	3.65	113.90	110.52
23	AB	606	CHL	O2D-CGD-CBD	3.65	117.75	111.27
24	v	303	CLA	O2D-CGD-O1D	-3.65	116.71	123.84
23	0	617	CHL	C1C-C2C-C3C	-3.64	104.22	107.11
23	AE	605	CHL	O2D-CGD-CBD	3.64	117.74	111.27
25	AE	614	LUT	C39-C29-C30	-3.64	117.83	122.92
25	v	316	LUT	C19-C9-C10	-3.64	117.83	122.92
34	AJ	411	SQD	O9-S-C6	3.64	111.26	106.94
23	q	607	CHL	CAC-C3C-C4C	3.64	129.53	124.81
23	AU	606	CHL	C1D-ND-C4D	-3.64	103.75	106.33
34	M	101	SQD	O7-S-C6	3.63	111.26	106.94
23	AD	308	CHL	C2D-C1D-ND	3.63	112.78	110.10
24	AQ	602	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
23	AQ	608	CHL	CAA-C2A-C1A	3.63	123.87	111.97
34	AP	101	SQD	O9-S-O7	-3.63	101.39	113.95
34	o	101	SQD	O9-S-O7	-3.63	101.40	113.95
27	9	618	XAT	C20-C13-C12	-3.62	112.37	118.08
23	AU	601	CHL	CAC-C3C-C4C	3.62	129.51	124.81
25	AR	614	LUT	C39-C29-C30	-3.62	117.85	122.92
25	AS	315	LUT	C19-C9-C10	-3.62	117.86	122.92
23	0	606	CHL	C2D-C1D-ND	3.62	112.77	110.10
23	AD	308	CHL	CHB-C1B-NB	-3.62	120.43	124.26
25	AC	615	LUT	C35-C15-C14	3.61	130.88	123.47
23	AQ	609	CHL	CHB-C1B-NB	-3.61	120.44	124.26
23	AN	617	CHL	CAC-C3C-C4C	3.61	129.49	124.81
23	AA	606	CHL	O2D-CGD-CBD	3.60	117.67	111.27
23	AE	601	CHL	CAC-C3C-C4C	3.60	129.48	124.81
23	AQ	608	CHL	C3B-C4B-NB	3.60	113.86	110.52
26	q	615	NEX	C20-C13-C14	-3.60	117.88	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	9	618	XAT	C10-C11-C12	-3.60	111.98	123.22
34	m	101	SQD	O7-S-C6	3.60	111.22	106.94
25	0	614	LUT	C15-C35-C34	3.60	130.84	123.47
34	J	410	SQD	O7-S-C6	3.60	111.21	106.94
23	AU	607	CHL	O2D-CGD-CBD	3.60	117.66	111.27
25	V	613	LUT	C19-C9-C10	-3.60	117.89	122.92
25	9	616	LUT	C35-C15-C14	3.60	130.84	123.47
25	AE	613	LUT	C39-C29-C30	-3.60	117.89	122.92
25	AH	614	LUT	C19-C9-C10	-3.60	117.89	122.92
23	AA	605	CHL	C1D-ND-C4D	-3.59	103.78	106.33
34	J	410	SQD	O9-S-C6	3.59	111.21	106.94
23	q	606	CHL	C3B-C4B-NB	3.59	113.85	110.52
23	v	306	CHL	C3D-C4D-ND	3.59	116.04	110.24
23	AH	607	CHL	O2D-CGD-CBD	3.59	117.64	111.27
23	AH	601	CHL	CAC-C3C-C4C	3.58	129.46	124.81
26	AC	616	NEX	C12-C13-C14	3.58	124.44	118.94
24	AF	602	CLA	C2D-C1D-ND	-3.58	107.47	110.10
23	AU	607	CHL	C1-C2-C3	-3.58	119.85	126.04
23	AD	306	CHL	CHB-C1B-NB	-3.58	120.47	124.26
23	9	601	CHL	O2D-CGD-CBD	3.58	117.63	111.27
27	AR	616	XAT	C32-C33-C34	-3.58	113.45	118.94
24	AE	604	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
23	V	607	CHL	CHD-C4C-C3C	-3.58	119.58	124.84
26	p	616	NEX	C19-C9-C10	-3.58	117.91	122.92
23	AA	607	CHL	C1D-ND-C4D	-3.58	103.80	106.33
23	AA	606	CHL	C3B-C4B-NB	3.57	113.83	110.52
23	AQ	607	CHL	C6-C7-C8	-3.57	104.37	115.92
24	AF	614	CLA	CHB-C4A-NA	3.57	129.45	124.51
25	AU	614	LUT	C19-C9-C10	-3.57	117.92	122.92
26	p	616	NEX	C35-C15-C14	3.57	130.79	123.47
23	AH	605	CHL	O2D-CGD-CBD	3.57	117.62	111.27
24	AF	602	CLA	C3C-C4C-NC	-3.57	106.57	110.57
25	V	613	LUT	C39-C29-C30	-3.57	117.92	122.92
23	AR	605	CHL	O2D-CGD-CBD	3.57	117.61	111.27
27	AB	613	XAT	C38-C25-C24	-3.57	110.27	114.28
23	AB	601	CHL	C1D-ND-C4D	-3.57	103.80	106.33
24	AL	512	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
24	O	612	CLA	O2D-CGD-O1D	-3.57	116.87	123.84
23	AA	617	CHL	C3B-C4B-NB	3.56	113.82	110.52
34	Q	402	SQD	O7-S-C6	3.56	111.17	106.94
23	AU	606	CHL	O2D-CGD-CBD	3.56	117.60	111.27
23	AH	607	CHL	C1-C2-C3	-3.56	119.89	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	q	617	XAT	C30-C31-C32	-3.56	112.12	123.22
27	AR	616	XAT	C30-C31-C32	-3.55	112.13	123.22
23	0	605	CHL	C3B-C4B-NB	3.55	113.81	110.52
23	AN	617	CHL	C2D-C1D-ND	3.55	112.72	110.10
23	V	606	CHL	CAC-C3C-C4C	3.55	129.42	124.81
23	AU	608	CHL	C3B-C4B-NB	3.55	113.81	110.52
23	AU	605	CHL	O2D-CGD-CBD	3.55	117.58	111.27
23	AE	606	CHL	C1D-ND-C4D	-3.55	103.81	106.33
25	q	614	LUT	C39-C29-C30	-3.55	117.95	122.92
24	AK	614	CLA	O2D-CGD-O1D	-3.55	116.91	123.84
27	AF	613	XAT	O24-C25-C38	-3.54	110.81	115.06
23	v	308	CHL	C1D-ND-C4D	-3.54	103.82	106.33
23	AE	605	CHL	C3B-C4B-NB	3.54	113.80	110.52
23	AN	617	CHL	C1C-C2C-C3C	-3.54	104.31	107.11
25	0	615	LUT	C35-C15-C14	3.54	130.72	123.47
27	9	618	XAT	C39-C29-C28	-3.54	112.50	118.08
26	AR	615	NEX	C20-C13-C14	-3.54	117.97	122.92
23	AQ	608	CHL	C1-C2-C3	-3.53	119.93	126.04
27	q	617	XAT	C32-C33-C34	-3.53	113.52	118.94
23	AS	308	CHL	C3B-C4B-NB	3.53	113.79	110.52
23	AD	317	CHL	C2D-C1D-ND	3.53	112.71	110.10
26	v	317	NEX	C12-C13-C14	3.53	124.36	118.94
27	AB	613	XAT	C25-C24-C23	-3.53	105.76	112.75
26	AC	616	NEX	C35-C15-C14	3.53	130.70	123.47
24	q	601	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
23	AC	601	CHL	O2D-CGD-CBD	3.53	117.54	111.27
23	AF	601	CHL	CAC-C3C-C4C	3.53	129.39	124.81
23	AQ	607	CHL	CAC-C3C-C4C	3.53	129.38	124.81
23	p	605	CHL	O2D-CGD-CBD	3.52	117.52	111.27
24	P	502	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
23	AR	606	CHL	O2A-CGA-CBA	3.52	122.95	111.91
23	AR	605	CHL	CMB-C2B-C1B	3.52	130.73	125.37
27	AR	616	XAT	C39-C29-C28	-3.52	112.54	118.08
23	0	601	CHL	C2D-C1D-ND	3.51	112.69	110.10
23	AH	606	CHL	CAC-C3C-C4C	3.51	129.37	124.81
26	q	615	NEX	C40-C33-C34	-3.51	118.00	122.92
23	AQ	605	CHL	CHB-C4A-NA	3.51	129.37	124.51
24	K	101	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
23	AN	606	CHL	CAC-C3C-C4C	3.51	129.36	124.81
24	AQ	614	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
23	AQ	605	CHL	O2D-CGD-CBD	3.51	117.50	111.27
24	AH	609	CLA	C3B-C4B-NB	-3.51	107.26	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	v	315	LUT	C15-C35-C34	3.51	130.65	123.47
27	9	618	XAT	C30-C31-C32	-3.50	112.28	123.22
24	AE	612	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
23	0	606	CHL	O2D-CGD-CBD	3.50	117.49	111.27
23	0	606	CHL	CAC-C3C-C4C	3.50	129.35	124.81
25	AS	315	LUT	C15-C35-C34	3.50	130.64	123.47
26	AR	615	NEX	C40-C33-C34	-3.50	118.03	122.92
23	AB	608	CHL	CHD-C4C-C3C	-3.50	119.70	124.84
26	AC	616	NEX	C20-C13-C14	-3.49	118.03	122.92
23	AR	606	CHL	C2D-C1D-ND	3.49	112.68	110.10
23	AF	608	CHL	CHD-C4C-C3C	-3.49	119.71	124.84
23	AC	608	CHL	CAC-C3C-C4C	3.49	129.34	124.81
25	AS	316	LUT	C19-C9-C10	-3.49	118.03	122.92
34	AM	401	SQD	O7-S-C6	3.49	111.08	106.94
27	q	617	XAT	C39-C29-C28	-3.49	112.58	118.08
26	v	317	NEX	C20-C13-C14	-3.49	118.04	122.92
24	O	601	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
23	AC	606	CHL	C3B-C4B-NB	3.48	113.74	110.52
23	AC	607	CHL	C3C-C4C-CHD	-3.48	117.53	125.23
35	AL	518	DGD	O6D-C1D-O3G	-3.48	101.74	109.97
23	AQ	601	CHL	O2D-CGD-CBD	3.48	117.44	111.27
23	p	607	CHL	C1-C2-C3	-3.48	120.03	126.04
35	AJ	412	DGD	O6D-C1D-O3G	-3.47	101.75	109.97
23	AU	605	CHL	CAC-C3C-C4C	3.47	129.32	124.81
24	AL	505	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
23	AU	606	CHL	CAC-C3C-C4C	3.47	129.31	124.81
23	v	308	CHL	C3B-C4B-NB	3.47	113.74	110.52
23	AD	306	CHL	CAC-C3C-C4C	3.47	129.31	124.81
23	AQ	607	CHL	O2D-CGD-CBD	3.47	117.44	111.27
25	AQ	615	LUT	C15-C35-C34	3.47	130.58	123.47
23	AB	605	CHL	C2D-C1D-ND	3.47	112.66	110.10
23	p	606	CHL	O2D-CGD-CBD	3.47	117.43	111.27
23	9	601	CHL	CHB-C1B-C2B	-3.46	122.83	130.42
23	AA	607	CHL	O2D-CGD-CBD	3.46	117.42	111.27
23	9	609	CHL	CAA-C2A-C1A	3.46	123.31	111.97
25	AN	614	LUT	C35-C15-C14	3.46	130.56	123.47
23	AQ	606	CHL	O2D-CGD-CBD	3.46	117.41	111.27
23	q	605	CHL	O2D-CGD-CBD	3.45	117.40	111.27
23	AQ	606	CHL	C1D-ND-C4D	-3.45	103.88	106.33
23	AA	606	CHL	CHB-C1B-NB	-3.45	120.60	124.26
37	AM	405	PL9	C7-C3-C2	-3.45	118.76	123.30
25	AU	615	LUT	C35-C15-C14	3.45	130.54	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AF	610	CLA	CAA-C2A-C3A	-3.45	103.33	112.78
35	J	411	DGD	O6D-C1D-O3G	-3.45	101.81	109.97
23	AR	607	CHL	CHD-C4C-C3C	-3.45	119.77	124.84
27	9	618	XAT	C28-C29-C30	-3.45	113.65	118.94
23	v	306	CHL	CAD-CBD-CHA	-3.45	101.26	105.14
23	9	608	CHL	C3C-C4C-CHD	-3.44	117.61	125.23
26	q	615	NEX	C12-C13-C14	3.44	124.22	118.94
25	AH	615	LUT	C35-C15-C14	3.44	130.53	123.47
24	AB	611	CLA	CAA-C2A-C1A	3.44	123.25	111.97
26	AU	616	NEX	C20-C13-C14	-3.44	118.11	122.92
24	q	608	CLA	C3B-C4B-NB	-3.44	107.33	110.52
23	q	605	CHL	CMB-C2B-C1B	3.44	130.60	125.37
27	AR	616	XAT	C20-C13-C12	-3.44	112.66	118.08
25	AS	316	LUT	C19-C9-C8	3.43	123.49	118.08
23	V	601	CHL	O2D-CGD-O1D	-3.43	117.12	123.84
24	AD	313	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
24	AR	617	CLA	C2D-C1D-ND	-3.43	107.58	110.10
25	p	615	LUT	C35-C15-C14	3.43	130.50	123.47
23	AC	605	CHL	CAC-C3C-C4C	3.43	129.26	124.81
23	AQ	605	CHL	CAC-C3C-C4C	3.43	129.26	124.81
23	9	606	CHL	CHB-C1B-NB	-3.43	120.63	124.26
23	AD	302	CHL	C1D-ND-C4D	-3.42	103.91	106.33
23	AS	302	CHL	CAC-C3C-C4C	3.42	129.25	124.81
23	AC	607	CHL	C3B-C4B-NB	3.42	113.69	110.52
37	Q	405	PL9	C7-C3-C2	-3.42	118.80	123.30
23	p	601	CHL	O2D-CGD-CBD	3.42	117.34	111.27
23	p	607	CHL	O2D-CGD-CBD	3.42	117.34	111.27
23	AR	606	CHL	C3B-C4B-NB	3.42	113.68	110.52
23	AF	607	CHL	CHD-C4C-C3C	-3.41	119.82	124.84
23	AA	608	CHL	CHD-C1D-C2D	3.41	132.63	125.48
34	o	101	SQD	O7-S-C6	3.41	110.99	106.94
23	AA	608	CHL	CAC-C3C-C4C	3.41	129.24	124.81
26	AA	616	NEX	C20-C13-C14	-3.41	118.15	122.92
25	V	614	LUT	C15-C35-C34	3.41	130.46	123.47
23	q	606	CHL	C2D-C1D-ND	3.41	112.62	110.10
23	v	302	CHL	CAC-C3C-C4C	3.41	129.23	124.81
27	q	617	XAT	C10-C11-C12	-3.41	112.58	123.22
23	AA	617	CHL	CHB-C4A-NA	3.41	129.22	124.51
23	AE	617	CHL	CHB-C4A-NA	3.40	129.22	124.51
26	AS	317	NEX	C15-C35-C34	3.40	130.45	123.47
23	AE	616	CHL	C2A-C3A-C4A	-3.40	96.38	101.87
23	p	605	CHL	CHB-C4A-NA	3.40	129.22	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	q	617	XAT	C20-C13-C12	-3.40	112.72	118.08
26	AU	616	NEX	C40-C33-C34	-3.40	118.17	122.92
34	AP	101	SQD	O7-S-C6	3.40	110.97	106.94
24	AQ	611	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
23	0	608	CHL	CHD-C4C-C3C	-3.39	119.86	124.84
23	AQ	607	CHL	C1-C2-C3	-3.39	120.18	126.04
23	p	606	CHL	CMB-C2B-C1B	3.39	130.53	125.37
23	AN	607	CHL	C3B-C4B-NB	3.39	113.66	110.52
24	AK	603	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
23	V	607	CHL	O2D-CGD-O1D	-3.38	117.23	123.84
23	9	609	CHL	C2D-C1D-ND	3.37	112.59	110.10
25	AR	614	LUT	C35-C15-C14	3.37	130.38	123.47
23	9	605	CHL	CAC-C3C-C4C	3.37	129.19	124.81
23	AH	605	CHL	C1D-ND-C4D	-3.37	103.94	106.33
23	V	605	CHL	CAC-C3C-C4C	3.37	129.18	124.81
23	AF	607	CHL	C3B-C4B-NB	3.37	113.64	110.52
23	AC	605	CHL	CHB-C1B-NB	-3.37	120.69	124.26
24	q	608	CLA	CHB-C1B-NB	3.36	127.82	124.26
23	AF	606	CHL	CHC-C4B-NB	-3.36	120.87	124.27
25	q	614	LUT	C15-C35-C34	3.36	130.37	123.47
23	p	607	CHL	CAC-C3C-C4C	3.36	129.18	124.81
23	AA	608	CHL	C4D-CHA-C1A	-3.36	117.16	121.25
23	9	609	CHL	C4-C3-C5	3.36	120.93	115.27
24	q	603	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
26	AQ	617	NEX	C40-C33-C34	-3.36	118.21	122.92
23	AC	601	CHL	CHB-C1B-C2B	-3.36	123.05	130.42
24	AA	613	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
27	AR	616	XAT	C10-C11-C12	-3.36	112.73	123.22
24	AQ	614	CLA	CBD-CHA-C1A	3.36	132.46	128.50
26	AA	616	NEX	C40-C33-C34	-3.36	118.22	122.92
23	AD	306	CHL	C1D-ND-C4D	-3.36	103.95	106.33
23	9	608	CHL	O2D-CGD-CBD	3.36	117.24	111.27
23	AU	605	CHL	C1D-ND-C4D	-3.36	103.95	106.33
35	P	516	DGD	O6D-C1D-O3G	-3.36	102.03	109.97
23	p	605	CHL	CAC-C3C-C4C	3.35	129.16	124.81
24	AH	603	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
23	AH	605	CHL	CAC-C3C-C4C	3.35	129.16	124.81
23	9	608	CHL	C3B-C4B-NB	3.35	113.62	110.52
25	AA	615	LUT	C15-C35-C34	3.35	130.34	123.47
25	AF	611	LUT	C35-C15-C14	3.35	130.34	123.47
25	AD	315	LUT	C15-C35-C34	3.35	130.34	123.47
23	q	606	CHL	O2A-CGA-CBA	3.35	122.42	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AU	609	CLA	C3B-C4B-NB	-3.35	107.41	110.52
23	AA	601	CHL	CHB-C1B-NB	-3.35	120.72	124.26
24	AF	602	CLA	CHD-C4C-C3C	3.35	129.76	124.84
24	P	503	CLA	CED-O2D-CGD	3.35	123.50	115.94
24	9	604	CLA	C1-C2-C3	-3.34	121.34	126.75
25	V	613	LUT	C35-C15-C14	3.34	130.32	123.47
25	p	614	LUT	C15-C35-C34	3.34	130.32	123.47
26	9	617	NEX	C40-C33-C34	-3.34	118.24	122.92
23	AR	606	CHL	O2D-CGD-CBD	3.34	117.20	111.27
24	9	604	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
25	AS	316	LUT	C1-C6-C7	3.34	125.22	115.78
24	P	505	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
24	0	604	CLA	CED-O2D-CGD	3.33	123.48	115.94
23	9	609	CHL	O2D-CGD-O1D	-3.33	117.33	123.84
23	p	601	CHL	C1D-ND-C4D	-3.33	103.97	106.33
25	AS	316	LUT	C1-C6-C5	-3.33	117.93	122.61
23	AN	601	CHL	O2D-CGD-O1D	-3.33	117.33	123.84
23	AQ	606	CHL	C3B-C4B-NB	3.33	113.60	110.52
27	9	618	XAT	C19-C9-C8	-3.33	112.84	118.08
24	q	612	CLA	OBD-CAD-C3D	3.33	130.11	125.86
24	O	610	CLA	O2D-CGD-O1D	-3.33	117.34	123.84
35	AL	517	DGD	O6D-C1D-O3G	-3.32	102.10	109.97
26	AS	317	NEX	C40-C33-C34	-3.32	118.27	122.92
23	AU	606	CHL	CHB-C1B-NB	-3.32	120.74	124.26
24	AA	602	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
23	V	607	CHL	CHB-C1B-NB	-3.32	120.74	124.26
24	AL	506	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
23	AN	601	CHL	CHB-C1B-NB	-3.32	120.75	124.26
23	AC	607	CHL	O2D-CGD-CBD	3.32	117.16	111.27
26	AC	616	NEX	C40-C33-C34	-3.32	118.28	122.92
24	AU	603	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
23	AS	308	CHL	C1D-ND-C4D	-3.32	103.98	106.33
25	AS	316	LUT	C7-C8-C9	3.32	131.25	126.23
23	AC	608	CHL	O2D-CGD-O1D	-3.32	117.36	123.84
23	AR	613	CHL	C2D-C1D-ND	3.32	112.55	110.10
25	v	316	LUT	C15-C35-C34	3.31	130.26	123.47
23	AU	601	CHL	C3D-C4D-ND	3.31	115.60	110.24
23	AF	601	CHL	CHB-C1B-NB	-3.31	120.75	124.26
23	AQ	607	CHL	C3B-C4B-NB	3.31	113.59	110.52
23	AB	608	CHL	C2D-C1D-ND	3.31	112.54	110.10
23	q	607	CHL	C2D-C1D-ND	3.31	112.54	110.10
24	AF	614	CLA	O1D-CGD-CBD	3.31	131.25	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AS	308	CHL	O2D-CGD-CBD	3.31	117.15	111.27
23	q	607	CHL	C3B-C4B-NB	3.30	113.58	110.52
24	p	618	CLA	CBA-CAA-C2A	3.30	123.61	113.86
23	AU	608	CHL	CHB-C4A-NA	3.30	129.08	124.51
23	q	607	CHL	O2D-CGD-O1D	-3.30	117.38	123.84
23	AS	302	CHL	C3B-C2B-C1B	-3.30	102.92	106.35
34	Q	402	SQD	O9-S-C6	3.30	110.86	106.94
23	v	302	CHL	C3B-C2B-C1B	-3.30	102.93	106.35
23	AQ	601	CHL	C1D-ND-C4D	-3.30	103.99	106.33
23	AR	605	CHL	C3B-C4B-NB	3.30	113.57	110.52
23	AE	601	CHL	C1D-ND-C4D	-3.30	103.99	106.33
23	p	606	CHL	CHB-C1B-NB	-3.30	120.77	124.26
26	v	317	NEX	C40-C33-C34	-3.30	118.31	122.92
24	AK	612	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
24	AR	612	CLA	CED-O2D-CGD	-3.29	108.49	115.94
23	AN	617	CHL	CHD-C4C-C3C	-3.29	120.00	124.84
23	AD	306	CHL	O2D-CGD-CBD	3.29	117.11	111.27
24	AN	612	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	AN	606	CHL	C1D-ND-C4D	-3.29	104.00	106.33
25	v	316	LUT	C35-C15-C14	3.29	130.21	123.47
24	AK	609	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	AB	607	CHL	C2D-C1D-ND	3.29	112.53	110.10
23	AH	605	CHL	CHB-C4A-NA	3.28	129.05	124.51
26	9	617	NEX	C20-C13-C14	-3.28	118.32	122.92
24	v	311	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
26	AR	615	NEX	C12-C13-C14	3.28	123.98	118.94
23	AA	605	CHL	CMB-C2B-C1B	3.28	130.37	125.37
23	AF	605	CHL	C3D-C4D-ND	3.28	115.55	110.24
24	AQ	612	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
27	AF	613	XAT	C19-C9-C8	-3.28	112.91	118.08
23	AU	605	CHL	CHB-C4A-NA	3.28	129.04	124.51
29	AK	602	BCR	C2-C1-C6	3.28	115.53	110.48
23	AA	608	CHL	C2A-C1A-CHA	3.28	125.33	120.38
24	V	603	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
23	AN	605	CHL	CAC-C3C-C4C	3.27	129.06	124.81
23	AH	601	CHL	C3D-C4D-ND	3.27	115.53	110.24
27	AB	613	XAT	C40-C33-C32	-3.27	112.92	118.08
23	p	608	CHL	O2D-CGD-CBD	3.27	117.08	111.27
26	AQ	617	NEX	C20-C13-C14	-3.27	118.34	122.92
23	V	616	CHL	CAC-C3C-C4C	3.27	129.05	124.81
23	AS	306	CHL	CHB-C1B-NB	-3.27	120.80	124.26
34	Q	402	SQD	O8-S-C6	3.27	110.95	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	O	625	BCR	C2-C1-C6	3.26	115.51	110.48
23	AN	606	CHL	CHB-C4A-NA	3.26	129.03	124.51
25	V	614	LUT	C35-C15-C14	3.26	130.16	123.47
23	AC	601	CHL	CHB-C1B-NB	-3.26	120.80	124.26
23	AQ	605	CHL	CHB-C1B-NB	-3.26	120.80	124.26
26	AE	615	NEX	C32-C33-C34	3.26	123.95	118.94
25	AD	314	LUT	C40-C33-C34	-3.26	118.36	122.92
23	AN	607	CHL	O2D-CGD-O1D	-3.26	117.47	123.84
23	V	605	CHL	C3B-C4B-NB	3.26	113.54	110.52
25	AN	615	LUT	C15-C35-C34	3.26	130.15	123.47
23	AQ	607	CHL	CHB-C1B-NB	-3.26	120.81	124.26
24	O	609	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
23	AH	608	CHL	C4-C3-C5	3.26	120.75	115.27
26	AQ	617	NEX	C35-C15-C14	3.26	130.14	123.47
23	V	601	CHL	C1D-ND-C4D	-3.25	104.02	106.33
24	AK	604	CLA	CAA-C2A-C3A	-3.25	103.87	112.78
23	v	306	CHL	C3C-C4C-CHD	-3.25	118.04	125.23
23	9	606	CHL	C3D-C4D-ND	3.25	115.50	110.24
27	AF	613	XAT	C31-C32-C33	-3.25	117.28	126.42
24	AK	604	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
25	9	615	LUT	C20-C13-C14	-3.25	118.37	122.92
25	AD	315	LUT	C20-C13-C14	-3.25	118.37	122.92
23	V	606	CHL	CHB-C1B-NB	-3.25	120.82	124.26
23	p	605	CHL	CHB-C1B-NB	-3.25	120.82	124.26
25	AC	614	LUT	C20-C13-C14	-3.25	118.37	122.92
23	AF	607	CHL	C2D-C1D-ND	3.25	112.50	110.10
23	AR	613	CHL	CAC-C3C-C4C	3.25	129.02	124.81
23	q	606	CHL	C3C-C4C-CHD	-3.25	118.05	125.23
23	p	606	CHL	C3B-C4B-NB	3.25	113.53	110.52
23	AD	301	CHL	C1D-ND-C4D	-3.24	104.03	106.33
23	AN	606	CHL	CHB-C1B-NB	-3.24	120.82	124.26
24	O	615	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
23	AC	601	CHL	C1D-ND-C4D	-3.24	104.03	106.33
23	AE	616	CHL	CHD-C4C-C3C	-3.24	120.08	124.84
23	AB	606	CHL	C3C-C4C-CHD	-3.24	118.06	125.23
23	V	601	CHL	CHB-C1B-NB	-3.24	120.83	124.26
23	V	606	CHL	CHB-C4A-NA	3.24	128.99	124.51
23	V	605	CHL	C1D-ND-C4D	-3.24	104.03	106.33
23	p	607	CHL	C3B-C4B-NB	3.24	113.52	110.52
25	0	615	LUT	C15-C35-C34	3.24	130.10	123.47
23	AE	606	CHL	CHB-C4A-NA	3.23	128.98	124.51
25	AU	614	LUT	C35-C15-C14	3.23	130.09	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AU	602	CLA	O2D-CGD-CBD	3.23	117.01	111.27
23	AC	606	CHL	CMD-C2D-C3D	-3.23	120.18	127.61
23	0	605	CHL	C1D-ND-C4D	-3.23	104.04	106.33
24	O	607	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
23	AD	317	CHL	C1C-C2C-C3C	-3.23	104.55	107.11
24	AQ	610	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
25	AQ	616	LUT	C35-C15-C14	3.23	130.08	123.47
23	AU	608	CHL	C4-C3-C5	3.23	120.70	115.27
26	AU	616	NEX	C12-C13-C14	3.23	123.89	118.94
24	AN	603	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
25	V	613	LUT	C20-C13-C14	-3.22	118.41	122.92
25	AF	611	LUT	C39-C29-C28	3.22	123.15	118.08
26	AE	615	NEX	C20-C13-C14	-3.22	118.41	122.92
26	p	616	NEX	C40-C33-C34	-3.22	118.41	122.92
23	AR	606	CHL	CMB-C2B-C1B	3.22	130.28	125.37
25	0	614	LUT	C40-C33-C34	-3.22	118.41	122.92
24	9	602	CLA	O2D-CGD-CBD	3.22	116.99	111.27
24	AU	610	CLA	C1-C2-C3	-3.22	120.48	126.04
23	AF	606	CHL	C3B-C2B-C1B	-3.22	103.01	106.35
24	AR	603	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
25	0	615	LUT	C20-C13-C14	-3.22	118.42	122.92
23	AH	608	CHL	CAA-C2A-C1A	3.22	122.51	111.97
23	V	606	CHL	C1D-ND-C4D	-3.22	104.05	106.33
23	9	601	CHL	C3B-C2B-C1B	-3.21	103.01	106.35
27	q	617	XAT	C19-C9-C8	-3.21	113.01	118.08
24	AS	314	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
23	9	606	CHL	C1D-ND-C4D	-3.21	104.05	106.33
23	AH	608	CHL	CHB-C4A-NA	3.21	128.95	124.51
23	V	607	CHL	CHB-C1B-C2B	-3.21	123.38	130.42
23	AS	308	CHL	CHB-C1B-NB	-3.21	120.86	124.26
25	AA	614	LUT	C7-C8-C9	-3.21	121.39	126.23
23	AR	613	CHL	C3D-C4D-ND	3.21	115.42	110.24
24	q	604	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
25	9	616	LUT	C15-C35-C34	3.20	130.04	123.47
23	v	308	CHL	C3D-C4D-ND	3.20	115.42	110.24
23	p	608	CHL	CHB-C4A-NA	3.20	128.94	124.51
25	AE	614	LUT	C39-C29-C28	3.20	123.12	118.08
23	AD	302	CHL	CHB-C4A-NA	3.20	128.94	124.51
23	AH	606	CHL	O2A-CGA-CBA	3.20	121.95	111.91
23	AE	607	CHL	CHB-C4A-NA	3.20	128.93	124.51
24	AR	608	CLA	C3B-C4B-NB	-3.20	107.55	110.52
24	AU	604	CLA	O2D-CGD-O1D	-3.20	117.59	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AE	616	CHL	CHB-C4A-NA	3.20	128.93	124.51
26	p	616	NEX	C20-C13-C14	-3.20	118.45	122.92
25	AC	614	LUT	C15-C35-C34	3.19	130.02	123.47
25	AS	316	LUT	C35-C15-C14	3.19	130.02	123.47
23	AU	605	CHL	CHB-C1B-NB	-3.19	120.88	124.26
24	AH	602	CLA	O2D-CGD-CBD	3.19	116.94	111.27
25	AH	614	LUT	C35-C15-C14	3.19	130.01	123.47
25	AN	615	LUT	C35-C15-C14	3.19	130.01	123.47
23	p	605	CHL	C1D-ND-C4D	-3.19	104.07	106.33
24	p	602	CLA	O2D-CGD-CBD	3.19	116.93	111.27
23	AC	601	CHL	C3B-C2B-C1B	-3.19	103.04	106.35
25	AR	614	LUT	C15-C35-C34	3.19	130.00	123.47
24	V	612	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
25	v	316	LUT	C40-C33-C34	-3.19	118.46	122.92
23	AE	607	CHL	O1D-CGD-CBD	-3.19	117.97	124.48
23	9	606	CHL	C3B-C4B-NB	3.18	113.47	110.52
27	AR	616	XAT	C19-C9-C8	-3.18	113.06	118.08
23	AE	616	CHL	C1C-C2C-C3C	-3.18	104.59	107.11
23	AE	606	CHL	CHB-C1B-NB	-3.18	120.89	124.26
23	AF	606	CHL	OBD-CAD-CBD	-3.18	121.94	124.98
25	AD	315	LUT	C40-C33-C34	-3.18	118.47	122.92
24	AK	603	CLA	CHB-C4A-NA	3.18	128.91	124.51
23	0	605	CHL	CHB-C1B-NB	-3.18	120.89	124.26
24	p	613	CLA	CBD-CHA-C1A	3.18	132.25	128.50
23	AQ	608	CHL	CHB-C4A-NA	3.18	128.91	124.51
26	AR	615	NEX	C19-C9-C10	-3.18	118.47	122.92
23	AD	308	CHL	C1D-ND-C4D	-3.18	104.08	106.33
23	AF	605	CHL	CAD-CBD-CHA	-3.18	101.56	105.14
23	AS	307	CHL	C1D-ND-C4D	-3.18	104.08	106.33
23	AA	607	CHL	CHB-C4A-NA	3.18	128.90	124.51
23	q	605	CHL	C3B-C4B-NB	3.17	113.46	110.52
23	AN	617	CHL	C2A-C3A-C4A	-3.17	96.75	101.87
25	AD	314	LUT	C20-C13-C14	-3.17	118.48	122.92
29	P	515	BCR	C15-C16-C17	-3.17	116.98	123.47
23	p	607	CHL	C1D-ND-C4D	-3.17	104.08	106.33
23	AH	606	CHL	C1D-ND-C4D	-3.17	104.08	106.33
25	0	614	LUT	C20-C13-C14	-3.17	118.48	122.92
24	O	606	CLA	CHD-C1D-ND	-3.17	121.54	124.45
23	0	608	CHL	C4A-NA-C1A	3.17	108.13	106.71
23	AD	307	CHL	C1D-ND-C4D	-3.17	104.09	106.33
25	v	315	LUT	C40-C33-C34	-3.16	118.49	122.92
24	0	610	CLA	C1-C2-C3	-3.16	120.57	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AN	601	CHL	C1D-ND-C4D	-3.16	104.09	106.33
23	AF	601	CHL	C3D-C4D-ND	3.16	115.36	110.24
23	0	606	CHL	C3B-C4B-NB	3.16	113.45	110.52
23	AR	605	CHL	O2A-CGA-CBA	3.16	121.83	111.91
23	AD	308	CHL	CHB-C4A-NA	3.16	128.88	124.51
35	j	102	DGD	O6D-C1D-O3G	-3.16	102.49	109.97
24	AN	609	CLA	C3B-C4B-NB	-3.16	107.58	110.52
23	AF	605	CHL	C2D-C1D-ND	3.16	112.43	110.10
23	q	613	CHL	C2D-C1D-ND	3.16	112.43	110.10
24	O	606	CLA	CHB-C4A-NA	3.16	128.88	124.51
25	AC	615	LUT	C15-C35-C34	3.16	129.94	123.47
25	9	615	LUT	C15-C35-C34	3.16	129.94	123.47
23	AN	605	CHL	C1D-ND-C4D	-3.16	104.09	106.33
23	AN	605	CHL	C3B-C4B-NB	3.16	113.44	110.52
23	AA	608	CHL	C4-C3-C5	3.15	120.58	115.27
23	AE	607	CHL	C4-C3-C5	3.15	120.58	115.27
26	9	617	NEX	C12-C13-C14	3.15	123.78	118.94
34	AP	101	SQD	O8-S-C6	3.15	110.76	105.74
25	9	616	LUT	C40-C33-C34	-3.15	118.51	122.92
24	AL	503	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
23	0	617	CHL	C4D-CHA-C1A	-3.15	117.42	121.25
23	AH	605	CHL	CHB-C1B-NB	-3.15	120.92	124.26
25	p	614	LUT	C35-C15-C14	3.15	129.92	123.47
23	AN	607	CHL	O2A-CGA-CBA	3.15	121.79	111.91
24	AU	604	CLA	C1-C2-C3	-3.15	121.66	126.75
25	AU	615	LUT	C15-C35-C34	3.15	129.92	123.47
23	9	605	CHL	C1D-ND-C4D	-3.15	104.10	106.33
24	AL	508	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
26	AA	616	NEX	C28-C29-C30	3.15	123.77	118.94
27	AF	613	XAT	C20-C13-C12	-3.15	113.12	118.08
24	AF	609	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
23	AN	608	CHL	OMC-CMC-C2C	-3.14	118.58	125.69
23	v	306	CHL	C2A-C1A-CHA	-3.14	117.84	122.71
23	9	605	CHL	CHB-C1B-NB	-3.14	120.93	124.26
23	AS	307	CHL	O2A-CGA-CBA	3.14	121.77	111.91
24	AE	603	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
24	v	310	CLA	C3B-C4B-NB	-3.14	107.60	110.52
26	AA	616	NEX	C32-C33-C34	3.14	123.76	118.94
24	AH	604	CLA	C1-C2-C3	-3.14	121.67	126.75
23	9	601	CHL	C1D-ND-C4D	-3.14	104.11	106.33
25	V	614	LUT	C40-C33-C34	-3.14	118.53	122.92
25	q	614	LUT	C40-C33-C34	-3.14	118.53	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AE	602	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
26	AS	317	NEX	C32-C33-C34	3.14	123.76	118.94
23	AA	605	CHL	CHB-C1B-NB	-3.14	120.94	124.26
23	p	609	CHL	CHB-C1B-NB	-3.14	120.94	124.26
26	p	616	NEX	C12-C13-C14	3.14	123.75	118.94
23	AB	601	CHL	C3D-C4D-ND	3.13	115.31	110.24
23	AQ	605	CHL	C1D-ND-C4D	-3.13	104.11	106.33
23	v	306	CHL	C3B-C4B-NB	3.13	113.42	110.52
23	p	607	CHL	CMB-C2B-C1B	3.13	130.14	125.37
23	AQ	601	CHL	C4-C3-C5	3.13	120.54	115.27
23	9	606	CHL	C2D-C1D-ND	3.13	112.41	110.10
23	0	608	CHL	C1D-ND-C4D	-3.13	104.11	106.33
23	9	601	CHL	CHB-C1B-NB	-3.13	120.94	124.26
24	O	601	CLA	CHB-C4A-NA	3.13	128.84	124.51
25	0	615	LUT	C40-C33-C34	-3.13	118.54	122.92
23	AC	601	CHL	CHD-C4C-C3C	-3.13	120.24	124.84
23	AA	606	CHL	C1D-ND-C4D	-3.13	104.11	106.33
23	AR	605	CHL	C3C-C4C-CHD	-3.13	118.31	125.23
23	p	609	CHL	C1D-ND-C4D	-3.13	104.11	106.33
24	AF	610	CLA	C2A-C1A-CHA	3.13	129.33	123.86
24	O	611	CLA	O2D-CGD-CBD	3.12	116.82	111.27
23	AU	608	CHL	CAA-C2A-C1A	3.12	122.21	111.97
25	AH	615	LUT	C15-C35-C34	3.12	129.87	123.47
23	v	302	CHL	CMB-C2B-C1B	3.12	129.00	125.81
23	AS	302	CHL	O1D-CGD-CBD	-3.12	118.09	124.48
23	p	601	CHL	CHB-C1B-NB	-3.12	120.95	124.26
23	AF	608	CHL	C3D-C4D-ND	3.12	115.29	110.24
24	AU	609	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
34	o	101	SQD	O8-S-C6	3.12	110.71	105.74
23	AU	606	CHL	CHB-C4A-NA	3.12	128.83	124.51
24	P	512	CLA	CHB-C4A-NA	3.12	128.83	124.51
23	AA	607	CHL	CHB-C1B-NB	-3.12	120.95	124.26
23	AQ	601	CHL	CHB-C1B-NB	-3.12	120.95	124.26
23	v	307	CHL	C1D-ND-C4D	-3.12	104.12	106.33
23	9	607	CHL	O2D-CGD-O1D	-3.12	117.75	123.84
24	AA	603	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
23	AN	601	CHL	CHB-C4A-NA	3.12	128.82	124.51
24	AL	514	CLA	CHB-C4A-NA	3.12	128.82	124.51
24	v	311	CLA	C3B-C4B-NB	-3.12	107.62	110.52
25	AC	615	LUT	C40-C33-C34	-3.11	118.56	122.92
35	AO	102	DGD	O6D-C1D-O3G	-3.11	102.60	109.97
23	AR	607	CHL	C3B-C4B-NB	3.11	113.40	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AN	605	CHL	CHB-C1B-NB	-3.11	120.96	124.26
24	AC	612	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
25	AN	614	LUT	C20-C13-C14	-3.11	118.56	122.92
23	AA	608	CHL	CMB-C2B-C1B	3.11	130.11	125.37
24	AS	311	CLA	C3B-C4B-NB	-3.11	107.63	110.52
24	AD	304	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
26	AU	616	NEX	C32-C33-C34	3.11	123.71	118.94
25	AN	615	LUT	C40-C33-C34	-3.11	118.57	122.92
23	p	607	CHL	CHB-C4A-NA	3.11	128.81	124.51
24	q	610	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
24	P	507	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
24	AH	604	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
24	O	610	CLA	C3B-C4B-NB	-3.11	107.63	110.52
26	AQ	617	NEX	C12-C13-C14	3.11	123.71	118.94
23	AC	606	CHL	C3D-C4D-ND	3.11	115.26	110.24
27	AB	613	XAT	C12-C13-C14	-3.11	114.18	118.94
27	AF	613	XAT	C40-C33-C32	-3.10	113.19	118.08
25	9	616	LUT	C20-C13-C14	-3.10	118.58	122.92
23	AS	307	CHL	CMB-C2B-C1B	3.10	130.10	125.37
23	AR	607	CHL	C2D-C1D-ND	3.10	112.39	110.10
23	V	601	CHL	CHB-C4A-NA	3.10	128.80	124.51
23	V	606	CHL	C6-C7-C8	-3.10	105.89	115.92
23	AD	302	CHL	CHB-C1B-NB	-3.10	120.97	124.26
25	AU	615	LUT	C20-C13-C14	-3.10	118.58	122.92
26	AE	615	NEX	C28-C29-C30	3.10	123.70	118.94
25	AH	615	LUT	C20-C13-C14	-3.10	118.58	122.92
23	AE	606	CHL	C3D-C4D-ND	3.10	115.25	110.24
24	O	611	CLA	CAA-CBA-CGA	-3.10	104.20	113.25
26	AA	616	NEX	C12-C13-C14	3.10	123.69	118.94
23	AQ	607	CHL	CMB-C2B-C1B	3.10	130.09	125.37
24	p	618	CLA	CHB-C4A-NA	3.10	128.79	124.51
23	AB	607	CHL	CMB-C2B-C1B	3.10	130.09	125.37
23	v	302	CHL	O2D-CGD-O1D	-3.09	117.79	123.84
23	AC	606	CHL	C1C-C2C-C3C	-3.09	104.66	107.11
23	AS	307	CHL	CHB-C4A-NA	3.09	128.79	124.51
23	AC	608	CHL	C1D-ND-C4D	-3.09	104.14	106.33
23	AS	302	CHL	CHB-C1B-C2B	-3.09	123.64	130.42
24	q	604	CLA	O2D-CGD-CBD	3.09	116.76	111.27
29	AB	612	BCR	C15-C14-C13	-3.09	122.90	127.31
23	q	605	CHL	O2A-CGA-CBA	3.09	121.61	111.91
23	v	302	CHL	CHB-C1B-C2B	-3.09	123.64	130.42
25	AS	315	LUT	C40-C33-C34	-3.09	118.60	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	p	606	CHL	O2A-CGA-CBA	3.09	121.60	111.91
25	AQ	615	LUT	C40-C33-C34	-3.09	118.60	122.92
25	AS	316	LUT	C40-C33-C34	-3.09	118.60	122.92
23	AN	606	CHL	C6-C7-C8	-3.09	105.94	115.92
23	AN	617	CHL	CHB-C1B-NB	-3.09	120.99	124.26
24	AH	609	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
34	AM	401	SQD	O9-S-C6	3.09	110.61	106.94
25	AR	614	LUT	C20-C13-C14	-3.09	118.60	122.92
23	AS	302	CHL	O2D-CGD-O1D	-3.08	117.81	123.84
25	AQ	615	LUT	C35-C15-C14	3.08	129.79	123.47
25	v	316	LUT	C20-C13-C14	-3.08	118.61	122.92
25	AH	614	LUT	C40-C33-C34	-3.08	118.61	122.92
24	AL	502	CLA	C3B-C4B-NB	-3.08	107.66	110.52
23	q	605	CHL	C1D-ND-C4D	-3.08	104.15	106.33
23	AH	606	CHL	C3D-C4D-ND	3.08	115.22	110.24
25	AU	614	LUT	C20-C13-C14	-3.08	118.61	122.92
23	AH	608	CHL	C1D-ND-C4D	-3.08	104.15	106.33
23	AC	607	CHL	CHB-C4A-NA	3.08	128.77	124.51
24	AR	601	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
24	0	613	CLA	O2D-CGD-CBD	3.08	116.73	111.27
23	q	613	CHL	CHD-C4C-C3C	-3.08	120.32	124.84
23	AQ	601	CHL	C3D-C4D-ND	3.07	115.21	110.24
23	AQ	607	CHL	C1D-ND-C4D	-3.07	104.15	106.33
23	AN	617	CHL	O2D-CGD-O1D	-3.07	117.83	123.84
24	AB	603	CLA	C3B-C4B-NB	-3.07	107.67	110.52
25	AC	615	LUT	C20-C13-C14	-3.07	118.62	122.92
24	AN	602	CLA	O2D-CGD-CBD	3.07	116.72	111.27
23	p	608	CHL	C1D-ND-C4D	-3.07	104.16	106.33
23	AA	608	CHL	O2A-CGA-CBA	3.07	121.53	111.91
23	AQ	606	CHL	CHB-C1B-NB	-3.07	121.01	124.26
26	q	615	NEX	C32-C33-C34	3.07	123.65	118.94
24	AK	616	CLA	C1-C2-C3	-3.07	120.74	126.04
24	p	610	CLA	C3B-C4B-NB	-3.07	107.67	110.52
25	AU	614	LUT	C40-C33-C34	-3.06	118.63	122.92
23	AB	608	CHL	C3D-C4D-ND	3.06	115.19	110.24
23	AS	302	CHL	CMB-C2B-C1B	3.06	128.94	125.81
23	AU	608	CHL	O2D-CGD-CBD	3.06	116.71	111.27
23	AQ	608	CHL	C1D-ND-C4D	-3.06	104.16	106.33
25	q	614	LUT	C35-C15-C14	3.06	129.74	123.47
23	AC	605	CHL	C1D-ND-C4D	-3.06	104.16	106.33
27	AB	613	XAT	C20-C13-C12	-3.06	113.26	118.08
24	AQ	603	CLA	O2D-CGD-O1D	-3.06	117.86	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AQ	616	LUT	C20-C13-C14	-3.06	118.64	122.92
23	AC	607	CHL	C1D-ND-C4D	-3.06	104.16	106.33
24	P	510	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
23	AN	607	CHL	CMB-C2B-C1B	3.06	130.02	125.37
24	v	314	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	AH	610	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
23	AB	608	CHL	C3B-C4B-NB	3.05	113.35	110.52
24	0	602	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
25	q	614	LUT	C20-C13-C14	-3.05	118.64	122.92
25	p	614	LUT	C40-C33-C34	-3.05	118.65	122.92
23	9	607	CHL	C1D-ND-C4D	-3.05	104.17	106.33
23	AD	308	CHL	CMD-C2D-C3D	-3.05	120.60	127.61
23	AB	601	CHL	CHB-C1B-NB	-3.05	121.03	124.26
26	v	317	NEX	C17-C1-C6	-3.05	107.75	110.47
23	AA	608	CHL	CHC-C4B-NB	-3.05	121.03	124.26
24	AB	609	CLA	CMA-C3A-C2A	-3.05	105.61	114.44
23	p	606	CHL	C1D-ND-C4D	-3.04	104.17	106.33
25	AR	614	LUT	C40-C33-C34	-3.04	118.66	122.92
23	p	601	CHL	C3D-C4D-ND	3.04	115.16	110.24
23	AE	617	CHL	O2D-CGD-O1D	-3.04	117.89	123.84
24	q	603	CLA	O2D-CGD-CBD	3.04	116.67	111.27
23	AN	607	CHL	CBA-CAA-C2A	3.04	122.84	113.86
26	9	617	NEX	C32-C33-C34	3.04	123.61	118.94
29	k	101	BCR	C15-C16-C17	-3.04	117.25	123.47
25	AU	615	LUT	C40-C33-C34	-3.04	118.67	122.92
26	AC	616	NEX	C32-C33-C34	3.04	123.60	118.94
24	p	603	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
25	V	614	LUT	C20-C13-C14	-3.04	118.67	122.92
25	AH	615	LUT	C40-C33-C34	-3.04	118.67	122.92
23	AH	608	CHL	OMC-CMC-C2C	-3.04	118.82	125.69
23	0	605	CHL	CHB-C4A-NA	3.04	128.71	124.51
26	v	317	NEX	C32-C33-C34	3.04	123.60	118.94
23	9	608	CHL	C1D-ND-C4D	-3.03	104.18	106.33
23	AA	607	CHL	C3D-C4D-ND	3.03	115.15	110.24
24	9	613	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
23	v	302	CHL	O1D-CGD-CBD	-3.03	118.28	124.48
23	AE	616	CHL	C4D-CHA-C1A	-3.03	117.56	121.25
29	P	514	BCR	C15-C16-C17	-3.03	117.27	123.47
23	AR	607	CHL	O2D-CGD-O1D	-3.03	117.91	123.84
23	AU	606	CHL	C3D-C4D-ND	3.03	115.14	110.24
24	AR	604	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
23	AN	606	CHL	O2A-C1-C2	3.03	116.60	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AB	605	CHL	C3B-C4B-NB	3.03	113.32	110.52
24	AE	611	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
25	AC	614	LUT	C40-C33-C34	-3.03	118.68	122.92
24	AA	611	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
25	v	316	LUT	C19-C9-C8	3.02	122.84	118.08
23	v	308	CHL	C3C-C4C-CHD	-3.02	118.60	125.22
25	AQ	615	LUT	C20-C13-C14	-3.02	118.69	122.92
25	v	315	LUT	C20-C13-C14	-3.02	118.69	122.92
23	AA	608	CHL	C3C-C4C-NC	3.02	113.96	110.57
24	J	403	CLA	CHB-C4A-NA	3.02	128.69	124.51
24	AB	609	CLA	C3B-C4B-NB	-3.02	107.71	110.52
24	AE	609	CLA	O2D-CGD-CBD	3.02	116.63	111.27
23	AS	306	CHL	CMB-C2B-C1B	3.02	129.97	125.37
23	p	607	CHL	CHB-C1B-NB	-3.02	121.06	124.26
25	AS	315	LUT	C35-C15-C14	3.02	129.66	123.47
25	AQ	616	LUT	C40-C33-C34	-3.02	118.69	122.92
24	AK	611	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	AN	614	LUT	C40-C33-C34	-3.02	118.70	122.92
24	AN	613	CLA	O2D-CGD-CBD	3.02	116.63	111.27
24	AL	511	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
23	AB	608	CHL	CMB-C2B-C1B	3.02	129.96	125.37
23	AD	308	CHL	C3D-C4D-ND	3.02	115.12	110.24
37	Q	405	PL9	C40-C39-C41	3.02	120.35	115.27
23	AC	608	CHL	C1-C2-C3	-3.01	120.83	126.04
23	AA	608	CHL	O2D-CGD-O1D	-3.01	117.95	123.84
23	AD	302	CHL	O2A-CGA-CBA	3.01	121.36	111.91
24	AE	610	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
29	AL	516	BCR	C15-C16-C17	-3.01	117.30	123.47
23	AD	306	CHL	CHB-C4A-NA	3.01	128.68	124.51
24	V	603	CLA	C3B-C4B-NB	-3.01	107.72	110.52
25	AH	614	LUT	C20-C13-C14	-3.01	118.71	122.92
24	O	612	CLA	O2D-CGD-CBD	3.01	116.62	111.27
24	AR	603	CLA	C3B-C4B-NB	-3.01	107.72	110.52
23	0	605	CHL	CMB-C2B-C1B	3.01	129.95	125.37
23	AS	307	CHL	C6-C5-C3	-3.01	105.57	113.45
23	AQ	608	CHL	CHB-C1B-NB	-3.01	121.08	124.26
23	AD	302	CHL	C3D-C4D-ND	3.00	115.10	110.24
23	AD	301	CHL	O2D-CGD-O1D	-3.00	117.97	123.84
24	AS	312	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
23	AR	613	CHL	C3B-C4B-NB	3.00	113.30	110.52
23	0	607	CHL	CHB-C4A-NA	3.00	128.66	124.51
24	O	602	CLA	O2D-CGD-O1D	-3.00	117.97	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	610	CLA	C3B-C4B-NB	-3.00	107.73	110.52
37	AM	405	PL9	C40-C39-C41	3.00	120.32	115.27
23	AQ	607	CHL	CHB-C4A-NA	3.00	128.66	124.51
29	j	101	BCR	C24-C23-C22	-3.00	121.70	126.23
29	AK	619	BCR	C15-C16-C17	-3.00	117.33	123.47
23	AN	605	CHL	O2A-CGA-CBA	3.00	121.32	111.91
23	q	613	CHL	C3D-C4D-ND	3.00	115.09	110.24
23	AR	613	CHL	O2D-CGD-O1D	-3.00	117.98	123.84
23	0	608	CHL	C2D-C1D-ND	3.00	112.31	110.10
24	AK	614	CLA	O2D-CGD-CBD	3.00	116.59	111.27
24	AK	615	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
24	AJ	404	CLA	CHB-C4A-NA	3.00	128.66	124.51
24	AL	504	CLA	O2D-CGD-CBD	3.00	116.59	111.27
24	q	609	CLA	C3B-C4B-NB	-3.00	107.73	110.52
23	V	605	CHL	CMD-C2D-C3D	-3.00	120.72	127.61
25	9	615	LUT	C40-C33-C34	-3.00	118.73	122.92
23	AF	608	CHL	C2D-C1D-ND	2.99	112.31	110.10
24	O	613	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
23	AF	608	CHL	C2A-C3A-C4A	-2.99	97.03	101.87
25	AE	614	LUT	C40-C33-C34	-2.99	118.73	122.92
24	O	614	CLA	C1-C2-C3	-2.99	120.87	126.04
24	O	616	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
23	p	608	CHL	CHB-C1B-NB	-2.99	121.09	124.26
35	AJ	401	DGD	O6D-C1D-O3G	-2.99	102.89	109.97
24	AM	403	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
23	0	607	CHL	O2D-CGD-O1D	-2.99	117.99	123.84
23	AA	607	CHL	OMC-CMC-C2C	-2.99	118.93	125.69
23	q	613	CHL	C3B-C4B-NB	2.99	113.29	110.52
25	p	614	LUT	C20-C13-C14	-2.99	118.74	122.92
24	AK	607	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
24	v	310	CLA	C1-C2-C3	-2.99	120.88	126.04
23	AH	606	CHL	CHB-C1B-NB	-2.99	121.09	124.26
24	0	603	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
23	V	616	CHL	CHD-C4C-C3C	-2.99	120.45	124.84
24	AF	610	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
23	AR	607	CHL	C4A-NA-C1A	2.99	108.05	106.71
25	p	615	LUT	C20-C13-C14	-2.98	118.74	122.92
23	AU	608	CHL	OMC-CMC-C2C	-2.98	118.94	125.69
23	p	609	CHL	CHB-C4A-NA	2.98	128.64	124.51
25	v	315	LUT	C35-C15-C14	2.98	129.58	123.47
23	V	608	CHL	C1D-ND-C4D	-2.98	104.22	106.33
26	AQ	617	NEX	C32-C33-C34	2.98	123.52	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AD	308	CHL	C1C-C2C-C3C	-2.98	104.75	107.11
24	AA	612	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
29	AB	612	BCR	C15-C16-C17	-2.98	117.37	123.47
24	AC	610	CLA	C3B-C4B-NB	-2.98	107.75	110.52
23	AB	606	CHL	CMB-C2B-C1B	2.98	129.91	125.37
23	AE	605	CHL	CHB-C4A-NA	2.98	128.63	124.51
23	p	601	CHL	CHB-C4A-NA	2.98	128.63	124.51
24	P	510	CLA	C3B-C4B-NB	-2.98	107.75	110.52
24	P	511	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
24	AL	513	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
23	AU	608	CHL	C1D-ND-C4D	-2.98	104.22	106.33
23	AA	608	CHL	CHB-C1B-NB	-2.98	120.53	124.17
29	AO	101	BCR	C24-C23-C22	-2.98	121.74	126.23
23	AE	606	CHL	OMC-CMC-C2C	-2.98	118.96	125.69
35	J	413	DGD	O6D-C1D-O3G	-2.97	102.93	109.97
23	q	606	CHL	CMB-C2B-C1B	2.97	129.90	125.37
23	V	608	CHL	C3D-C4D-ND	2.97	115.05	110.24
24	O	601	CLA	O2D-CGD-CBD	2.97	116.55	111.27
23	AE	606	CHL	CMB-C2B-C1B	2.97	129.90	125.37
25	p	615	LUT	C40-C33-C34	-2.97	118.76	122.92
23	AE	607	CHL	CMB-C2B-C1B	2.97	129.90	125.37
23	AQ	608	CHL	CMB-C2B-C1B	2.97	129.90	125.37
24	q	618	CLA	CHB-C4A-NA	2.97	128.62	124.51
23	AH	606	CHL	CMB-C2B-C1B	2.97	129.89	125.37
29	O	617	BCR	C15-C16-C17	-2.97	117.39	123.47
24	O	613	CLA	C3B-C4B-NB	-2.97	107.76	110.52
24	AB	609	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	AA	605	CHL	CAA-CBA-CGA	-2.97	104.63	112.51
23	0	601	CHL	C1C-C2C-C3C	-2.97	104.76	107.11
24	AS	304	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
25	AC	614	LUT	C12-C13-C14	2.97	123.50	118.94
24	AQ	603	CLA	C3B-C4B-NB	-2.97	107.76	110.52
25	9	615	LUT	C12-C13-C14	2.97	123.49	118.94
23	V	606	CHL	O2A-C1-C2	2.97	116.43	108.64
24	P	506	CLA	C3B-C4B-NB	-2.97	107.76	110.52
23	AH	608	CHL	O2D-CGD-CBD	2.97	116.54	111.27
23	AN	608	CHL	CHD-C4C-C3C	-2.97	120.48	124.84
24	AQ	610	CLA	C3B-C4B-NB	-2.97	107.76	110.52
23	0	607	CHL	CMD-C2D-C3D	-2.97	120.79	127.61
23	9	608	CHL	CHB-C1B-NB	-2.96	121.12	124.26
24	v	312	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	V	605	CHL	O2A-CGA-CBA	2.96	121.20	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	p	609	CHL	C3D-C4D-ND	2.96	115.03	110.24
26	AR	615	NEX	C32-C33-C34	2.96	123.48	118.94
24	AF	610	CLA	CHB-C4A-NA	2.96	128.60	124.51
25	AS	315	LUT	C20-C13-C14	-2.96	118.78	122.92
24	AC	603	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
24	p	612	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
23	AQ	606	CHL	CHB-C4A-NA	2.96	128.60	124.51
23	AU	606	CHL	CMD-C2D-C3D	-2.96	120.81	127.61
23	AS	307	CHL	O2D-CGD-O1D	-2.95	118.06	123.84
24	V	610	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
24	AK	617	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
24	AL	508	CLA	C3B-C4B-NB	-2.95	107.78	110.52
24	AK	618	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	AU	606	CHL	CMB-C2B-C1B	2.95	129.87	125.37
24	AE	603	CLA	C3B-C4B-NB	-2.95	107.78	110.52
24	v	314	CLA	C3B-C4B-NB	-2.95	107.78	110.52
24	AL	507	CLA	C3B-C4B-NB	-2.95	107.78	110.52
24	AU	610	CLA	C3B-C4B-NB	-2.95	107.78	110.52
23	p	608	CHL	CMB-C2B-C1B	2.95	129.86	125.37
23	p	608	CHL	CBA-CAA-C2A	2.95	122.57	113.86
25	AS	316	LUT	C20-C13-C14	-2.95	118.79	122.92
24	J	403	CLA	O2D-CGD-CBD	2.95	116.51	111.27
24	AK	613	CLA	CAA-CBA-CGA	-2.95	104.63	113.25
23	0	607	CHL	C1D-ND-C4D	-2.95	104.24	106.33
23	9	608	CHL	CHB-C4A-NA	2.95	128.59	124.51
25	AN	615	LUT	C20-C13-C14	-2.95	118.79	122.92
24	AR	617	CLA	CHD-C1D-ND	-2.95	121.75	124.45
24	p	603	CLA	C3B-C4B-NB	-2.94	107.78	110.52
24	v	304	CLA	C3B-C4B-NB	-2.94	107.78	110.52
24	AS	304	CLA	C3B-C4B-NB	-2.94	107.78	110.52
24	v	304	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
23	AQ	606	CHL	O2A-CGA-CBA	2.94	121.15	111.91
28	p	617	LHG	O6-C4-C5	-2.94	103.98	111.78
24	AK	618	CLA	C3B-C4B-NB	-2.94	107.78	110.52
23	AQ	601	CHL	CHB-C4A-NA	2.94	128.58	124.51
26	AQ	617	NEX	C19-C9-C10	-2.94	118.80	122.92
23	AN	608	CHL	CMB-C2B-C1B	2.94	129.85	125.37
23	AC	606	CHL	CHB-C1B-NB	-2.94	121.14	124.26
24	V	610	CLA	C3B-C4B-NB	-2.94	107.79	110.52
23	AA	605	CHL	C3D-C4D-ND	2.94	114.99	110.24
23	AS	307	CHL	O1D-CGD-CBD	-2.94	118.47	124.48
24	AA	603	CLA	C3B-C4B-NB	-2.94	107.79	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AS	308	CHL	C3D-C4D-ND	2.93	114.98	110.24
23	0	608	CHL	C3D-C4D-ND	2.93	114.98	110.24
23	AA	605	CHL	CHB-C4A-NA	2.93	128.57	124.51
23	AQ	606	CHL	CMB-C2B-C1B	2.93	129.83	125.37
23	V	607	CHL	CHB-C4A-NA	2.93	128.56	124.51
32	AJ	408	PHO	O2D-CGD-O1D	-2.93	118.11	123.84
23	AA	608	CHL	CMD-C2D-C3D	-2.93	120.88	127.61
23	AH	606	CHL	CHB-C4A-NA	2.93	128.56	124.51
24	AL	511	CLA	C3B-C4B-NB	-2.93	107.80	110.52
24	AD	303	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
23	AS	308	CHL	CHB-C4A-NA	2.93	128.56	124.51
24	AK	613	CLA	CHB-C4A-NA	2.93	128.56	124.51
23	AA	606	CHL	CMB-C2B-C1B	2.93	129.82	125.37
23	AH	608	CHL	CHB-C1B-NB	-2.92	121.16	124.26
23	AC	607	CHL	CMD-C2D-C3D	-2.92	120.89	127.61
24	AR	610	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
23	AD	317	CHL	CAC-C3C-C4C	2.92	128.60	124.81
23	AQ	608	CHL	OMC-CMC-C2C	-2.92	119.08	125.69
24	AK	615	CLA	C3B-C4B-NB	-2.92	107.81	110.52
29	k	101	BCR	C24-C23-C22	-2.92	121.82	126.23
24	P	501	CLA	C3B-C4B-NB	-2.92	107.81	110.52
24	AS	314	CLA	C3B-C4B-NB	-2.92	107.81	110.52
23	V	616	CHL	O2D-CGD-O1D	-2.92	118.13	123.84
23	AN	608	CHL	C1-C2-C3	-2.92	121.00	126.04
24	AL	509	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
24	0	611	CLA	C3B-C4B-NB	-2.92	107.81	110.52
27	AB	613	XAT	C30-C31-C32	-2.92	114.12	123.22
24	AD	313	CLA	CAA-CBA-CGA	-2.91	104.73	113.25
23	p	609	CHL	CMB-C2B-C1B	2.91	129.81	125.37
24	AB	602	CLA	CHB-C4A-NA	2.91	128.54	124.51
23	AQ	601	CHL	O2A-CGA-CBA	2.91	121.05	111.91
23	AH	601	CHL	CHB-C1B-NB	-2.91	121.17	124.26
24	q	603	CLA	C3B-C4B-NB	-2.91	107.81	110.52
29	AF	612	BCR	C11-C10-C9	-2.91	123.16	127.31
23	AE	601	CHL	O2D-CGD-O1D	-2.91	118.15	123.84
23	AH	607	CHL	C6-C7-C8	-2.91	106.51	115.92
25	AS	316	LUT	C15-C35-C34	2.91	129.44	123.47
26	q	615	NEX	C19-C9-C10	-2.91	118.85	122.92
23	v	307	CHL	O1D-CGD-CBD	-2.91	118.53	124.48
23	AA	617	CHL	O2D-CGD-O1D	-2.91	118.15	123.84
23	AF	601	CHL	CHB-C4A-NA	2.91	128.53	124.51
23	V	607	CHL	C3B-C2B-C1B	-2.91	103.33	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AS	308	CHL	CMB-C2B-C1B	2.91	129.80	125.37
23	9	607	CHL	CHB-C4A-NA	2.91	128.53	124.51
24	p	613	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	AQ	609	CHL	CMB-C2B-C1B	2.91	129.80	125.37
25	AN	614	LUT	C15-C35-C34	2.91	129.43	123.47
24	q	618	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
23	AD	307	CHL	CMB-C2B-C1B	2.91	129.79	125.37
23	AC	608	CHL	C4-C3-C5	2.90	120.16	115.27
23	AE	607	CHL	C1C-C2C-C3C	-2.90	104.81	107.11
23	AQ	609	CHL	C1D-ND-C4D	-2.90	104.27	106.33
23	AU	607	CHL	C1D-ND-C4D	-2.90	104.27	106.33
23	AD	306	CHL	C3D-C4D-ND	2.90	114.94	110.24
24	AC	604	CLA	C1-C2-C3	-2.90	122.05	126.75
23	AA	607	CHL	CMB-C2B-C1B	2.90	129.79	125.37
24	AJ	406	CLA	C3B-C4B-NB	-2.90	107.82	110.52
23	AU	607	CHL	C6-C7-C8	-2.90	106.55	115.92
24	q	602	CLA	C3B-C4B-NB	-2.90	107.83	110.52
24	9	603	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	AF	602	CLA	CHB-C4A-NA	2.90	128.52	124.51
24	p	611	CLA	C3B-C4B-NB	-2.90	107.83	110.52
24	AS	312	CLA	C3B-C4B-NB	-2.90	107.83	110.52
23	AH	607	CHL	C1D-ND-C4D	-2.90	104.28	106.33
24	0	613	CLA	CAA-CBA-CGA	-2.90	104.78	113.25
23	9	607	CHL	CMB-C2B-C1B	2.90	129.78	125.37
23	0	607	CHL	CMB-C2B-C1B	2.90	129.78	125.37
24	Q	403	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	AN	603	CLA	C3B-C4B-NB	-2.90	107.83	110.52
24	AN	611	CLA	C3B-C4B-NB	-2.90	107.83	110.52
24	AR	602	CLA	C3B-C4B-NB	-2.90	107.83	110.52
24	P	504	CLA	CED-O2D-CGD	2.89	122.48	115.94
23	AE	617	CHL	C1C-C2C-C3C	-2.89	104.82	107.11
23	9	608	CHL	CMB-C2B-C1B	2.89	129.78	125.37
23	AQ	608	CHL	CBA-CAA-C2A	2.89	122.40	113.86
23	q	607	CHL	C4-C3-C5	2.89	119.29	115.98
23	AB	606	CHL	C1D-ND-C4D	-2.89	104.28	106.33
24	AB	610	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
23	AB	601	CHL	CHB-C4A-NA	2.89	128.51	124.51
24	q	611	CLA	C3B-C4B-NB	-2.89	107.83	110.52
24	AU	603	CLA	C3B-C4B-NB	-2.89	107.83	110.52
23	AS	308	CHL	CMD-C2D-C3D	-2.89	120.97	127.61
24	P	508	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
32	J	406	PHO	O2D-CGD-O1D	-2.89	118.20	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AF	609	CLA	CAC-C3C-C4C	2.88	128.55	124.81
24	O	605	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	AD	301	CHL	CMB-C2B-C1B	2.88	129.76	125.37
26	p	616	NEX	C32-C33-C34	2.88	123.37	118.94
24	P	507	CLA	C3B-C4B-NB	-2.88	107.84	110.52
24	AS	303	CLA	C3B-C4B-NB	-2.88	107.84	110.52
23	AU	608	CHL	CHB-C1B-NB	-2.88	121.20	124.26
24	AR	611	CLA	C3B-C4B-NB	-2.88	107.84	110.52
23	AE	607	CHL	C1D-ND-C4D	-2.88	104.29	106.33
24	AE	610	CLA	C3B-C4B-NB	-2.88	107.84	110.52
24	AL	510	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	9	605	CHL	CHB-C4A-NA	2.88	128.49	124.51
35	AJ	412	DGD	O5D-C6D-C5D	-2.88	103.72	109.05
23	AQ	608	CHL	CMD-C2D-C3D	-2.88	120.99	127.61
23	V	601	CHL	C3D-C4D-ND	2.88	114.89	110.24
35	J	411	DGD	O5D-C6D-C5D	-2.88	103.72	109.05
23	AE	601	CHL	O1D-CGD-CBD	-2.88	118.60	124.48
24	AB	611	CLA	CAA-C2A-C3A	2.88	120.65	112.78
23	AQ	608	CHL	O2D-CGD-CBD	2.88	116.38	111.27
23	AF	601	CHL	CMB-C2B-C1B	2.88	129.75	125.37
24	v	312	CLA	C3B-C4B-NB	-2.87	107.85	110.52
24	AS	305	CLA	C1-C2-C3	-2.87	122.10	126.75
23	AD	301	CHL	C3D-C4D-ND	2.87	114.89	110.24
23	AD	317	CHL	C4D-CHA-C1A	-2.87	117.75	121.25
23	AS	307	CHL	C4-C3-C5	2.87	120.10	115.27
23	AU	601	CHL	C1C-C2C-C3C	-2.87	104.83	107.11
25	AF	611	LUT	C40-C33-C34	-2.87	118.90	122.92
26	9	617	NEX	C19-C9-C10	-2.87	118.90	122.92
23	AR	613	CHL	CMB-C2B-C1B	2.87	129.74	125.37
24	AS	303	CLA	O2D-CGD-CBD	2.87	116.37	111.27
23	AQ	605	CHL	CAA-CBA-CGA	-2.87	104.87	113.25
24	0	612	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	AC	609	CLA	C3B-C4B-NB	-2.87	107.85	110.52
23	AB	601	CHL	CMB-C2B-C1B	2.87	129.74	125.37
24	V	602	CLA	O2D-CGD-CBD	2.87	116.36	111.27
24	p	610	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	0	603	CLA	CHB-C4A-NA	2.87	128.48	124.51
24	AN	611	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	AA	610	CLA	C3B-C4B-NB	-2.87	107.86	110.52
24	AD	309	CLA	C3B-C4B-NB	-2.87	107.86	110.52
29	AK	619	BCR	C15-C14-C13	-2.87	123.22	127.31
24	9	611	CLA	C3B-C4B-NB	-2.87	107.86	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	9	606	CHL	O2D-CGD-O1D	-2.86	118.24	123.84
33	J	409	LMG	O6-C1-O1	-2.86	103.19	109.97
23	AS	306	CHL	C3B-C4B-NB	2.86	113.17	110.52
23	AC	605	CHL	CMB-C2B-C1B	2.86	129.73	125.37
33	AL	501	LMG	O6-C1-O1	-2.86	103.20	109.97
24	q	608	CLA	O2A-CGA-O1A	-2.86	116.17	123.30
24	AH	603	CLA	C3B-C4B-NB	-2.86	107.86	110.52
23	V	601	CHL	CMB-C2B-C1B	2.86	129.72	125.37
24	AC	604	CLA	O2D-CGD-CBD	2.86	116.35	111.27
23	AC	607	CHL	CHB-C1B-NB	-2.86	121.23	124.26
24	AB	603	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	AA	601	CHL	C1D-ND-C4D	-2.86	104.31	106.33
24	Q	401	CLA	C3B-C4B-NB	-2.86	107.86	110.52
23	q	613	CHL	CMB-C2B-C1B	2.86	129.72	125.37
24	AE	609	CLA	C3B-C4B-NB	-2.86	107.86	110.52
23	AD	306	CHL	C1-C2-C3	-2.86	121.10	126.04
23	AD	306	CHL	C1C-C2C-C3C	-2.86	104.85	107.11
23	AE	606	CHL	CMD-C2D-C3D	-2.86	121.05	127.61
24	AA	611	CLA	C3B-C4B-NB	-2.85	107.87	110.52
24	AU	610	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
24	AE	608	CLA	C3B-C4B-NB	-2.85	107.87	110.52
24	AR	611	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	AH	601	CHL	C1C-C2C-C3C	-2.85	104.85	107.11
23	AR	605	CHL	C3D-C4D-ND	2.85	114.85	110.24
23	9	609	CHL	C11-C12-C13	-2.85	106.70	115.92
29	O	617	BCR	C15-C14-C13	-2.85	123.24	127.31
24	P	512	CLA	CHB-C1B-C2B	-2.85	124.17	130.42
23	AE	605	CHL	C1D-ND-C4D	-2.85	104.31	106.33
32	AJ	407	PHO	O2D-CGD-O1D	-2.85	118.27	123.84
24	O	611	CLA	CHB-C4A-NA	2.85	128.45	124.51
23	AC	607	CHL	CMB-C2B-C1B	2.85	129.71	125.37
23	v	307	CHL	CMB-C2B-C1B	2.85	129.71	125.37
28	O	621	LHG	O8-C23-C24	2.85	120.85	111.91
24	AA	609	CLA	C3B-C4B-NB	-2.85	107.87	110.52
24	AL	514	CLA	CHB-C1B-C2B	-2.85	124.17	130.42
24	AD	304	CLA	C3B-C4B-NB	-2.85	107.87	110.52
23	AN	601	CHL	C3D-C4D-ND	2.85	114.84	110.24
25	AQ	616	LUT	C15-C35-C34	2.85	129.30	123.47
34	m	101	SQD	O8-S-C6	2.85	110.28	105.74
23	9	608	CHL	C3D-C4D-ND	2.85	114.84	110.24
23	AE	601	CHL	CMB-C2B-C1B	2.85	129.70	125.37
23	AN	601	CHL	CMB-C2B-C1B	2.85	129.70	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	V	604	CLA	C3B-C4B-NB	-2.84	107.88	110.52
23	AE	616	CHL	CAA-C2A-C1A	2.84	121.30	111.97
23	AC	601	CHL	CHB-C4A-NA	2.84	128.44	124.51
25	AA	614	LUT	C20-C13-C14	-2.84	118.94	122.92
38	f	102	HEM	C4D-ND-C1D	2.84	108.01	105.07
24	q	601	CLA	CHB-C4A-NA	2.84	128.44	124.51
24	p	610	CLA	C4A-CHB-C1B	2.84	125.54	120.10
34	M	101	SQD	O8-S-C6	2.84	110.27	105.74
24	AA	602	CLA	C3B-C4B-NB	-2.84	107.88	110.52
24	P	509	CLA	C3B-C4B-NB	-2.84	107.88	110.52
23	p	601	CHL	O2A-CGA-CBA	2.84	120.82	111.91
23	0	606	CHL	C3D-C4D-ND	2.84	114.83	110.24
24	AK	604	CLA	CHB-C4A-NA	2.84	128.44	124.51
23	AF	605	CHL	CMB-C2B-C1B	2.84	129.69	125.37
23	AF	607	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
29	O	617	BCR	C29-C30-C25	2.84	114.85	110.48
29	P	515	BCR	C15-C14-C13	-2.84	123.26	127.31
24	AL	510	CLA	C3B-C4B-NB	-2.84	107.88	110.52
29	AK	619	BCR	C29-C30-C25	2.84	114.85	110.48
23	AD	306	CHL	CMB-C2B-C1B	2.84	129.69	125.37
24	0	609	CLA	C3B-C4B-NB	-2.84	107.88	110.52
23	AA	601	CHL	O2D-CGD-O1D	-2.84	118.29	123.84
24	P	506	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
23	AE	607	CHL	CMD-C2D-C3D	-2.84	121.09	127.61
23	AA	601	CHL	CMB-C2B-C1B	2.84	129.69	125.37
24	V	604	CLA	C4A-CHB-C1B	2.84	125.53	120.10
29	P	513	BCR	C33-C5-C6	-2.83	121.34	124.53
38	f	102	HEM	C4C-NC-C1C	2.83	108.12	105.35
23	AF	608	CHL	C3B-C4B-NB	2.83	113.14	110.52
35	AJ	401	DGD	C3G-C2G-C1G	-2.83	105.09	111.79
23	AU	601	CHL	CHB-C1B-NB	-2.83	121.26	124.26
24	AB	604	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
23	v	308	CHL	CAA-C2A-C3A	-2.83	109.50	116.10
23	AA	601	CHL	O1D-CGD-CBD	-2.83	118.70	124.48
23	AC	607	CHL	C3D-C4D-ND	2.83	114.81	110.24
24	P	511	CLA	C3B-C4B-NB	-2.83	107.89	110.52
23	9	608	CHL	CMD-C2D-C3D	-2.83	121.11	127.61
38	F	102	HEM	C4D-ND-C1D	2.83	107.99	105.07
24	9	602	CLA	CHB-C4A-NA	2.83	128.42	124.51
23	AH	605	CHL	CMB-C2B-C1B	2.83	129.67	125.37
28	AS	301	LHG	O8-C23-C24	2.83	120.78	111.91
29	AF	612	BCR	C33-C5-C6	-2.83	121.35	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AS	307	CHL	C3D-C4D-ND	2.83	114.81	110.24
24	AL	513	CLA	C3B-C4B-NB	-2.83	107.89	110.52
23	0	606	CHL	C1-C2-C3	-2.82	121.16	126.04
24	AS	305	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	9	609	CHL	CMB-C2B-C1B	2.82	129.67	125.37
24	AQ	613	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	p	605	CHL	CMB-C2B-C1B	2.82	129.67	125.37
24	AH	610	CLA	C3B-C4B-NB	-2.82	107.90	110.52
24	AR	608	CLA	CHB-C4A-NA	2.82	128.41	124.51
23	V	606	CHL	C3D-C4D-ND	2.82	114.80	110.24
23	AF	606	CHL	OBD-CAD-C3D	-2.82	122.27	125.86
23	AA	607	CHL	CMD-C2D-C3D	-2.82	121.13	127.61
25	V	613	LUT	C40-C33-C34	-2.82	118.97	122.92
26	AE	615	NEX	C12-C13-C14	2.82	123.27	118.94
32	J	405	PHO	O2D-CGD-O1D	-2.82	118.33	123.84
29	P	515	BCR	C24-C23-C22	-2.82	121.97	126.23
29	j	101	BCR	C2-C1-C6	2.82	114.82	110.48
23	q	613	CHL	O2D-CGD-CBD	2.82	116.28	111.27
23	AQ	605	CHL	CMB-C2B-C1B	2.82	129.66	125.37
23	q	607	CHL	CMD-C2D-C3D	-2.82	121.13	127.61
24	AL	507	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
24	AC	611	CLA	C3B-C4B-NB	-2.82	107.90	110.52
24	AK	617	CLA	C3B-C4B-NB	-2.82	107.90	110.52
23	0	601	CHL	CMB-C2B-C1B	2.82	129.66	125.37
23	AU	605	CHL	CMB-C2B-C1B	2.82	129.66	125.37
24	AQ	602	CLA	O2D-CGD-CBD	2.81	116.27	111.27
34	J	410	SQD	O8-S-C6	2.81	110.22	105.74
24	AC	603	CLA	C3B-C4B-NB	-2.81	107.91	110.52
23	9	605	CHL	CMB-C2B-C1B	2.81	129.65	125.37
23	0	601	CHL	CAC-C3C-C4C	2.81	128.46	124.81
23	AN	606	CHL	C3D-C4D-ND	2.81	114.79	110.24
23	AU	607	CHL	CMB-C2B-C1B	2.81	129.65	125.37
24	AK	608	CLA	C3B-C4B-NB	-2.81	107.91	110.52
26	AS	317	NEX	C19-C9-C10	-2.81	118.99	122.92
24	9	603	CLA	C3B-C4B-NB	-2.81	107.91	110.52
23	AE	601	CHL	C3D-C4D-ND	2.81	114.78	110.24
29	O	617	BCR	C33-C5-C6	-2.81	121.37	124.53
24	v	303	CLA	O2D-CGD-CBD	2.81	116.26	111.27
23	AC	608	CHL	C3D-C4D-ND	2.81	114.78	110.24
23	AD	307	CHL	O2D-CGD-O1D	-2.81	118.35	123.84
25	AD	315	LUT	C12-C13-C14	2.81	123.25	118.94
24	AQ	611	CLA	C3B-C4B-NB	-2.81	107.91	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AN	608	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
23	q	605	CHL	C3D-C4D-ND	2.81	114.78	110.24
23	AH	608	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
23	v	302	CHL	CHB-C4A-NA	2.81	128.39	124.51
23	AS	302	CHL	CHB-C4A-NA	2.81	128.39	124.51
24	AQ	614	CLA	C3B-C4B-NB	-2.80	107.91	110.52
33	O	624	LMG	O6-C1-O1	-2.80	103.33	109.97
24	AJ	404	CLA	CGD-CBD-CAD	2.80	119.82	110.73
33	AK	601	LMG	O6-C1-O1	-2.80	103.33	109.97
23	AC	601	CHL	C3D-C4D-ND	2.80	114.77	110.24
24	AR	603	CLA	O2D-CGD-CBD	2.80	116.25	111.27
23	AC	605	CHL	CMD-C2D-C3D	-2.80	121.17	127.61
23	p	601	CHL	C6-C7-C8	-2.80	106.86	115.92
24	q	611	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
29	AL	515	BCR	C33-C5-C6	-2.80	121.38	124.53
24	9	612	CLA	C3B-C4B-NB	-2.80	107.92	110.52
28	v	301	LHG	O8-C23-C24	2.80	120.70	111.91
23	0	606	CHL	C6-C5-C3	-2.80	110.04	114.62
23	AR	605	CHL	C1D-ND-C4D	-2.80	104.35	106.33
23	AH	607	CHL	CMB-C2B-C1B	2.80	129.63	125.37
24	AL	506	CLA	C3B-C4B-NB	-2.80	107.92	110.52
24	AQ	612	CLA	O2D-CGD-CBD	2.80	116.24	111.27
24	AD	311	CLA	C3B-C4B-NB	-2.80	107.92	110.52
24	AB	610	CLA	C3B-C4B-NB	-2.80	107.92	110.52
35	J	413	DGD	C3G-C2G-C1G	-2.80	105.17	111.79
27	AB	613	XAT	C39-C29-C28	-2.80	113.67	118.08
24	v	311	CLA	O1D-CGD-CBD	2.80	130.20	124.48
23	AU	608	CHL	CMB-C2B-C1B	2.80	129.63	125.37
24	q	604	CLA	C3B-C4B-NB	-2.80	107.92	110.52
23	9	601	CHL	C3D-C4D-ND	2.79	114.75	110.24
25	AA	614	LUT	C40-C33-C34	-2.79	119.01	122.92
23	AD	308	CHL	CMB-C2B-C1B	2.79	129.62	125.37
24	AB	611	CLA	C3A-C2A-C1A	2.79	105.52	101.34
24	9	612	CLA	O2D-CGD-CBD	2.79	116.22	111.27
25	AA	615	LUT	C40-C33-C34	-2.79	119.02	122.92
23	V	608	CHL	C1C-C2C-C3C	-2.79	104.90	107.11
23	AA	617	CHL	CAA-C2A-C1A	2.79	121.10	111.97
24	0	604	CLA	CHB-C4A-NA	2.79	128.36	124.51
23	V	607	CHL	CMD-C2D-C3D	-2.79	121.21	127.61
24	AQ	612	CLA	C3B-C4B-NB	-2.79	107.93	110.52
24	AR	609	CLA	CHB-C4A-NA	2.78	128.36	124.51
23	AC	608	CHL	CMB-C2B-C1B	2.78	129.61	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AB	611	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
24	AU	613	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
23	V	601	CHL	C1C-C2C-C3C	-2.78	104.91	107.11
24	AK	612	CLA	C3B-C4B-NB	-2.78	107.93	110.52
23	AH	606	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
24	P	509	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
23	v	308	CHL	CHB-C1B-NB	-2.78	121.31	124.26
34	AJ	411	SQD	O8-S-C6	2.78	110.17	105.74
23	AQ	609	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
25	AF	611	LUT	C20-C13-C14	-2.78	119.03	122.92
23	AQ	609	CHL	C3D-C4D-ND	2.78	114.73	110.24
24	P	505	CLA	C3B-C4B-NB	-2.78	107.94	110.52
23	V	608	CHL	CMB-C2B-C1B	2.78	129.60	125.37
23	p	607	CHL	C3D-C4D-ND	2.78	114.73	110.24
23	AU	601	CHL	CHB-C4A-NA	2.78	128.35	124.51
24	AN	610	CLA	C3B-C4B-NB	-2.78	107.94	110.52
32	AJ	407	PHO	O1D-CGD-CBD	2.78	129.36	124.74
23	AU	608	CHL	CMD-C2D-C3D	-2.77	121.23	127.61
25	9	616	LUT	C8-C9-C10	2.77	123.19	118.94
23	AN	601	CHL	O1D-CGD-CBD	-2.77	118.81	124.48
23	AR	607	CHL	CMD-C2D-C3D	-2.77	121.24	127.61
23	AA	606	CHL	C3D-C4D-ND	2.77	114.72	110.24
23	AQ	601	CHL	CMB-C2B-C1B	2.77	129.59	125.37
28	p	617	LHG	O8-C23-C24	2.77	120.60	111.91
25	AD	314	LUT	C32-C33-C34	2.77	123.19	118.94
28	AQ	618	LHG	O8-C23-C24	2.77	120.59	111.91
23	AU	605	CHL	C3D-C4D-ND	2.77	114.71	110.24
23	AS	306	CHL	CHD-C1D-ND	-2.77	121.91	124.45
23	9	601	CHL	CHB-C4A-NA	2.77	128.34	124.51
24	AR	610	CLA	C3B-C4B-NB	-2.76	107.95	110.52
23	AQ	606	CHL	C3D-C4D-ND	2.76	114.71	110.24
23	AE	605	CHL	C3D-C4D-ND	2.76	114.71	110.24
23	AB	607	CHL	CHC-C4B-NB	-2.76	121.33	124.26
23	9	607	CHL	O1D-CGD-CBD	-2.76	118.83	124.48
24	AE	602	CLA	C3B-C4B-NB	-2.76	107.95	110.52
23	0	617	CHL	CHB-C4A-NA	2.76	128.33	124.51
23	AU	607	CHL	C3D-C4D-ND	2.76	114.70	110.24
23	AU	606	CHL	O2A-CGA-CBA	2.76	120.57	111.91
24	AS	313	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	AH	601	CHL	C5-C3-C2	2.76	126.70	121.12
23	AD	307	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
23	AQ	605	CHL	C1C-C2C-C3C	-2.76	104.92	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	610	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	AE	613	LUT	C40-C33-C34	-2.76	119.06	122.92
24	AQ	611	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	V	605	CHL	C3D-C4D-ND	2.76	114.70	110.24
23	AA	617	CHL	C4D-CHA-C1A	-2.76	117.89	121.25
23	AN	608	CHL	C4-C3-C5	2.76	119.91	115.27
24	v	303	CLA	C3B-C4B-NB	-2.76	107.96	110.52
23	AF	605	CHL	C3B-C4B-NB	2.76	113.07	110.52
24	AK	603	CLA	O2D-CGD-CBD	2.76	116.17	111.27
28	V	615	LHG	O8-C23-C24	2.76	120.56	111.91
23	AD	302	CHL	CMB-C2B-C1B	2.76	129.56	125.37
24	AS	313	CLA	C3B-C4B-NB	-2.75	107.96	110.52
24	AF	610	CLA	CHA-C1A-NA	-2.75	120.09	126.40
27	q	617	XAT	C40-C33-C32	-2.75	113.74	118.08
27	AR	616	XAT	C40-C33-C32	-2.75	113.74	118.08
23	AH	606	CHL	CBA-CAA-C2A	-2.75	105.74	113.86
35	AO	102	DGD	CDB-CCB-CBB	-2.75	100.45	114.42
23	9	606	CHL	CMB-C2B-C1B	2.75	129.56	125.37
23	AQ	607	CHL	C3D-C4D-ND	2.75	114.69	110.24
27	q	617	XAT	C25-C24-C23	-2.75	107.31	112.75
24	v	305	CLA	C1-C2-C3	-2.75	122.30	126.75
23	AB	606	CHL	C3D-C4D-ND	2.75	114.69	110.24
29	AK	619	BCR	C33-C5-C6	-2.75	121.44	124.53
23	V	607	CHL	C4-C3-C5	2.75	119.89	115.27
24	AF	603	CLA	C3B-C4B-NB	-2.75	107.97	110.52
23	V	607	CHL	C4D-CHA-C1A	-2.75	117.90	121.25
25	AD	314	LUT	C12-C13-C14	2.75	123.16	118.94
23	AA	608	CHL	O1D-CGD-CBD	-2.75	118.86	124.48
24	q	608	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	9	607	CHL	C3D-C4D-ND	2.75	114.68	110.24
23	AE	617	CHL	C4D-CHA-C1A	-2.75	117.91	121.25
23	AU	601	CHL	C1-O2A-CGA	2.75	123.65	116.44
23	AH	607	CHL	O2A-C1-C2	2.75	115.85	108.64
24	AL	504	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
24	AU	611	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
29	AK	621	BCR	C33-C5-C6	-2.75	121.44	124.53
23	V	601	CHL	O1D-CGD-CBD	-2.75	118.87	124.48
26	AR	615	NEX	C28-C29-C30	2.74	123.15	118.94
23	AH	608	CHL	CMB-C2B-C1B	2.74	129.55	125.37
23	v	308	CHL	CHB-C4A-NA	2.74	128.31	124.51
23	AU	607	CHL	O2A-C1-C2	2.74	115.84	108.64
23	AA	601	CHL	CHB-C4A-NA	2.74	128.30	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	9	609	CHL	C1-C2-C3	-2.74	121.30	126.04
24	AR	601	CLA	C3B-C4B-NB	-2.74	107.97	110.52
23	AH	601	CHL	CHB-C4A-NA	2.74	128.30	124.51
23	AD	301	CHL	O1D-CGD-CBD	-2.74	118.88	124.48
32	J	405	PHO	O1D-CGD-CBD	2.74	129.30	124.74
24	O	603	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	AF	601	CHL	C1C-C2C-C3C	-2.74	104.94	107.11
23	V	605	CHL	CHB-C1B-NB	-2.74	121.36	124.26
32	AJ	408	PHO	C1C-C2C-C3C	-2.74	106.33	108.61
37	Q	405	PL9	C7-C8-C9	-2.74	122.23	126.79
23	AN	605	CHL	C3D-C4D-ND	2.74	114.67	110.24
24	AK	605	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
24	0	610	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	AN	601	CHL	C1C-C2C-C3C	-2.74	104.94	107.11
23	p	601	CHL	CMB-C2B-C1B	2.74	129.54	125.37
29	f	101	BCR	C33-C5-C6	-2.74	121.45	124.53
23	9	605	CHL	CMD-C2D-C3D	-2.74	121.32	127.61
23	AH	605	CHL	C3D-C4D-ND	2.73	114.66	110.24
25	AR	614	LUT	C39-C29-C28	2.73	122.39	118.08
23	AQ	608	CHL	C3D-C4D-ND	2.73	114.66	110.24
35	j	102	DGD	CDB-CCB-CBB	-2.73	100.55	114.42
24	0	602	CLA	C3B-C4B-NB	-2.73	107.98	110.52
23	AD	317	CHL	C2A-C3A-C4A	-2.73	97.45	101.87
24	P	501	CLA	CHB-C4A-NA	2.73	128.29	124.51
24	q	610	CLA	C3B-C4B-NB	-2.73	107.98	110.52
23	AF	607	CHL	CMB-C2B-C1B	2.73	129.53	125.37
24	AA	612	CLA	CHB-C4A-NA	2.73	128.29	124.51
37	AM	405	PL9	C7-C8-C9	-2.73	122.25	126.79
23	AB	607	CHL	CMD-C2D-C3D	-2.73	121.33	127.61
23	AH	607	CHL	C3D-C4D-ND	2.73	114.66	110.24
25	V	613	LUT	C19-C9-C8	2.73	122.38	118.08
23	AD	301	CHL	C4-C3-C5	2.73	119.86	115.27
23	q	613	CHL	C4A-NA-C1A	2.73	107.93	106.71
23	V	608	CHL	C4-C3-C5	2.73	119.86	115.27
25	0	614	LUT	C32-C33-C34	2.73	123.13	118.94
23	AB	605	CHL	CMB-C2B-C1B	2.73	129.52	125.37
24	AH	602	CLA	CHB-C4A-NA	2.73	128.28	124.51
23	AC	605	CHL	CHB-C4A-NA	2.73	128.28	124.51
23	0	605	CHL	C3D-C4D-ND	2.73	114.65	110.24
24	AS	310	CLA	C1-C2-C3	-2.73	121.33	126.04
23	AH	601	CHL	C1-O2A-CGA	2.72	123.59	116.44
29	j	101	BCR	C27-C26-C25	2.72	126.69	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AA	608	CHL	C1C-C2C-C3C	-2.72	104.95	107.11
24	v	305	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	AN	607	CHL	C1D-ND-C4D	-2.72	104.40	106.33
24	AK	610	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
24	AF	609	CLA	CMB-C2B-C1B	-2.72	121.22	125.37
23	AF	606	CHL	CMB-C2B-C1B	2.72	128.59	125.81
24	AD	310	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
24	AH	611	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
23	AA	617	CHL	C2A-C3A-C4A	-2.72	97.47	101.87
24	O	609	CLA	C3B-C4B-NB	-2.72	107.99	110.52
24	AK	614	CLA	C3B-C4B-NB	-2.72	107.99	110.52
35	J	413	DGD	O5D-C6D-C5D	-2.72	104.01	109.05
23	q	607	CHL	CMB-C2B-C1B	2.72	129.51	125.37
23	p	605	CHL	C3D-C4D-ND	2.72	114.64	110.24
23	AD	308	CHL	C6-C7-C8	-2.72	107.12	115.92
23	V	608	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
35	AL	518	DGD	CDB-CCB-CBB	-2.72	100.61	114.42
23	AD	301	CHL	C1-C2-C3	-2.72	121.34	126.04
24	AU	602	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	AC	608	CHL	C11-C12-C13	-2.72	107.13	115.92
26	AU	616	NEX	C28-C29-C30	2.72	123.11	118.94
23	p	605	CHL	C1C-C2C-C3C	-2.72	104.96	107.11
24	v	305	CLA	C3B-C4B-NB	-2.72	107.99	110.52
24	p	604	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
23	AU	601	CHL	C5-C3-C2	2.72	126.62	121.12
25	AS	316	LUT	C39-C29-C28	2.72	122.36	118.08
24	AK	609	CLA	CAA-CBA-CGA	-2.72	105.31	113.25
23	q	606	CHL	C3D-C4D-ND	2.72	114.63	110.24
23	p	608	CHL	C3D-C4D-ND	2.72	114.63	110.24
23	AF	607	CHL	C4A-NA-C1A	2.72	107.93	106.71
24	AH	603	CLA	O2D-CGD-CBD	2.72	116.09	111.27
25	q	614	LUT	C39-C29-C28	2.72	122.36	118.08
24	q	612	CLA	CED-O2D-CGD	-2.72	109.80	115.94
24	AQ	612	CLA	CMB-C2B-C1B	-2.72	121.23	125.37
24	0	611	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
23	v	307	CHL	CHB-C4A-NA	2.71	128.27	124.51
24	AL	502	CLA	CHB-C4A-NA	2.71	128.27	124.51
24	AR	601	CLA	CHB-C4A-NA	2.71	128.27	124.51
23	AD	301	CHL	CHB-C4A-NA	2.71	128.26	124.51
24	J	407	CLA	CHB-C4A-NA	2.71	128.26	124.51
24	AU	603	CLA	O2D-CGD-CBD	2.71	116.09	111.27
23	AC	605	CHL	CAA-C2A-C1A	2.71	120.86	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	404	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
24	AH	610	CLA	CAA-CBA-CGA	-2.71	105.34	113.25
23	AC	601	CHL	CMB-C2B-C1B	2.71	128.57	125.81
24	AJ	409	CLA	CHB-C4A-NA	2.71	128.26	124.51
27	AB	613	XAT	C19-C9-C8	-2.71	113.81	118.08
24	AR	612	CLA	O2A-C1-C2	-2.71	101.53	108.64
29	AL	516	BCR	C15-C14-C13	-2.70	123.45	127.31
24	AD	310	CLA	CHB-C4A-NA	2.70	128.25	124.51
24	AA	612	CLA	C3B-C4B-NB	-2.70	108.01	110.52
29	F	101	BCR	C33-C5-C6	-2.70	121.49	124.53
23	AE	607	CHL	C1-C2-C3	-2.70	121.37	126.04
23	AA	617	CHL	CAA-CBA-CGA	-2.70	105.33	112.51
23	0	606	CHL	C4-C3-C5	2.70	119.82	115.27
24	AL	504	CLA	CGD-CBD-CAD	2.70	119.49	110.73
24	AF	603	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	9	605	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
23	AE	601	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
24	AS	305	CLA	CHB-C4A-NA	2.70	128.25	124.51
24	O	612	CLA	C3B-C4B-NB	-2.70	108.01	110.52
27	AR	616	XAT	C25-C24-C23	-2.70	107.41	112.75
29	k	101	BCR	C15-C14-C13	-2.70	123.46	127.31
24	J	403	CLA	C3B-C4B-NB	-2.70	108.01	110.52
34	o	101	SQD	O48-C23-C24	2.70	120.38	111.91
23	AC	608	CHL	CMD-C2D-C3D	-2.70	121.41	127.61
24	P	507	CLA	CHB-C4A-NA	2.70	128.24	124.51
24	AR	612	CLA	CHB-C4A-NA	2.70	128.24	124.51
23	0	601	CHL	C3D-C4D-ND	2.70	114.60	110.24
23	AN	617	CHL	CHB-C4A-NA	2.70	128.24	124.51
28	AN	616	LHG	O8-C23-C24	2.69	120.36	111.91
25	AE	614	LUT	C20-C13-C14	-2.69	119.15	122.92
24	O	615	CLA	C3B-C4B-NB	-2.69	108.02	110.52
23	AH	608	CHL	C3D-C4D-ND	2.69	114.60	110.24
23	AN	607	CHL	C4-C3-C5	2.69	119.80	115.27
24	AH	610	CLA	C1-C2-C3	-2.69	121.38	126.04
24	AS	309	CLA	C3B-C4B-NB	-2.69	108.02	110.52
24	AU	610	CLA	CAA-CBA-CGA	-2.69	105.38	113.25
23	9	605	CHL	CAA-C2A-C1A	2.69	120.80	111.97
24	AM	404	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	AS	305	CLA	C3B-C4B-NB	-2.69	108.02	110.52
35	AJ	401	DGD	CDB-CCB-CBB	-2.69	100.76	114.42
23	p	608	CHL	CMD-C2D-C3D	-2.69	121.42	127.61
24	O	607	CLA	CAA-CBA-CGA	-2.69	105.39	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	v	306	CHL	CMB-C2B-C1B	2.69	129.47	125.37
23	AR	606	CHL	C3D-C4D-ND	2.69	114.59	110.24
24	0	613	CLA	C3B-C4B-NB	-2.69	108.02	110.52
33	Q	407	LMG	O6-C1-O1	-2.69	103.61	109.97
35	P	516	DGD	CDB-CCB-CBB	-2.69	100.77	114.42
25	0	615	LUT	C12-C13-C14	2.69	123.07	118.94
23	V	616	CHL	CAA-C2A-C1A	2.69	120.79	111.97
24	AE	604	CLA	C3B-C4B-NB	-2.69	108.02	110.52
24	AM	404	CLA	C3B-C4B-NB	-2.69	108.02	110.52
23	AN	607	CHL	CMD-C2D-C3D	-2.69	121.43	127.61
23	AE	617	CHL	CAA-C2A-C1A	2.69	120.78	111.97
29	AO	101	BCR	C27-C26-C25	2.69	126.63	122.73
24	AK	611	CLA	CHB-C4A-NA	2.69	128.23	124.51
35	AJ	401	DGD	O5D-C6D-C5D	-2.69	104.08	109.05
24	V	609	CLA	CHB-C4A-NA	2.69	128.22	124.51
29	P	514	BCR	C15-C14-C13	-2.69	123.48	127.31
24	q	601	CLA	C3B-C4B-NB	-2.68	108.03	110.52
23	AQ	605	CHL	C3D-C4D-ND	2.68	114.58	110.24
23	V	605	CHL	CHB-C4A-NA	2.68	128.22	124.51
28	P	517	LHG	O8-C23-C24	2.68	120.33	111.91
23	AN	607	CHL	OMC-CMC-C2C	-2.68	119.62	125.69
35	J	413	DGD	CDB-CCB-CBB	-2.68	100.80	114.42
24	AD	312	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
24	AH	602	CLA	C1-C2-C3	-2.68	121.41	126.04
23	V	606	CHL	CMB-C2B-C1B	2.68	129.45	125.37
24	O	616	CLA	C3B-C4B-NB	-2.68	108.03	110.52
23	AF	605	CHL	CHC-C4B-NB	-2.68	121.42	124.26
24	AS	309	CLA	CHB-C4A-NA	2.68	128.22	124.51
24	AB	609	CLA	CHD-C1D-ND	-2.68	121.99	124.45
23	AU	608	CHL	C3D-C4D-ND	2.68	114.57	110.24
35	AL	517	DGD	CDB-CCB-CBB	-2.68	100.83	114.42
24	AA	602	CLA	CAA-CBA-CGA	-2.68	105.43	113.25
23	0	606	CHL	CMB-C2B-C1B	2.68	129.45	125.37
24	P	506	CLA	C1-C2-C3	-2.68	121.41	126.04
34	AP	101	SQD	O48-C23-C24	2.68	120.31	111.91
23	AD	302	CHL	C1C-C2C-C3C	-2.68	104.99	107.11
28	AD	316	LHG	O8-C23-C24	2.68	120.31	111.91
23	AU	601	CHL	C2A-C1A-CHA	-2.68	119.18	123.86
29	O	619	BCR	C33-C5-C6	-2.68	121.52	124.53
24	AR	604	CLA	CHB-C4A-NA	2.68	128.21	124.51
25	AN	614	LUT	C39-C29-C28	2.67	122.29	118.08
24	AL	504	CLA	C3B-C4B-NB	-2.67	108.03	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	613	CLA	CHB-C4A-NA	2.67	128.21	124.51
24	V	612	CLA	C3B-C4B-NB	-2.67	108.03	110.52
23	AN	605	CHL	CMB-C2B-C1B	2.67	129.44	125.37
33	AM	407	LMG	O6-C1-O1	-2.67	103.64	109.97
24	O	608	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
23	AD	306	CHL	C6-C5-C3	-2.67	110.25	114.62
25	9	616	LUT	C39-C29-C28	2.67	122.29	118.08
24	v	309	CLA	CHB-C4A-NA	2.67	128.21	124.51
24	AH	611	CLA	CHB-C4A-NA	2.67	128.21	124.51
23	AD	317	CHL	CHB-C1B-NB	-2.67	121.43	124.26
24	AL	507	CLA	C1-C2-C3	-2.67	121.42	126.04
24	P	502	CLA	C3B-C4B-NB	-2.67	108.04	110.52
23	p	606	CHL	C3D-C4D-ND	2.67	114.56	110.24
23	AH	601	CHL	O2A-CGA-CBA	2.67	120.28	111.91
25	AC	615	LUT	C39-C29-C28	2.67	122.28	118.08
25	v	316	LUT	C39-C29-C28	2.67	122.28	118.08
24	AF	604	CLA	C3B-C4B-NB	-2.67	108.04	110.52
23	AN	606	CHL	C1C-C2C-C3C	-2.67	105.00	107.11
33	O	620	LMG	O6-C1-O1	-2.67	103.66	109.97
24	AJ	405	CLA	C3B-C4B-NB	-2.67	108.04	110.52
24	AL	508	CLA	CHB-C4A-NA	2.67	128.20	124.51
28	AH	616	LHG	O8-C23-C24	2.67	120.27	111.91
23	AC	606	CHL	CMB-C2B-C1B	2.67	129.43	125.37
23	v	308	CHL	CMB-C2B-C1B	2.67	129.43	125.37
23	AQ	606	CHL	CMD-C2D-C3D	-2.66	121.48	127.61
24	O	601	CLA	C3B-C4B-NB	-2.66	108.04	110.52
23	V	607	CHL	O2A-CGA-CBA	2.66	120.27	111.91
33	AK	622	LMG	O6-C1-O1	-2.66	103.67	109.97
25	p	615	LUT	C15-C35-C34	2.66	128.93	123.47
24	P	505	CLA	CHB-C4A-NA	2.66	128.19	124.51
24	AN	612	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	0	607	CHL	O1D-CGD-CBD	-2.66	119.04	124.48
23	AQ	608	CHL	C4-C3-C5	2.66	119.75	115.27
23	q	607	CHL	C4A-NA-C1A	2.66	107.90	106.71
23	p	605	CHL	CAA-CBA-CGA	-2.66	105.47	113.25
23	q	605	CHL	OMC-CMC-C2C	-2.66	119.67	125.69
24	O	610	CLA	CHB-C1B-NB	2.66	127.07	124.26
24	9	614	CLA	C3B-C4B-NB	-2.66	108.05	110.52
23	AA	601	CHL	C1C-C2C-C3C	-2.66	105.00	107.11
24	AJ	404	CLA	C3B-C4B-NB	-2.66	108.05	110.52
28	AU	617	LHG	O8-C23-C24	2.66	120.25	111.91
24	AC	613	CLA	C3B-C4B-NB	-2.66	108.05	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AM	403	CLA	C3B-C4B-NB	-2.66	108.05	110.52
29	P	515	BCR	C27-C26-C25	2.66	126.59	122.73
29	k	101	BCR	C27-C26-C25	2.66	126.59	122.73
29	AB	612	BCR	C33-C5-C6	-2.66	121.55	124.53
24	AU	611	CLA	C3B-C4B-NB	-2.66	108.05	110.52
23	9	605	CHL	C3D-C4D-ND	2.66	114.53	110.24
28	O	622	LHG	O8-C23-C24	2.66	120.24	111.91
23	AN	606	CHL	CMB-C2B-C1B	2.66	129.41	125.37
24	AR	604	CLA	C3B-C4B-NB	-2.65	108.05	110.52
28	0	616	LHG	O8-C23-C24	2.65	120.24	111.91
24	AD	305	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	AD	309	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	AD	306	CHL	C4-C3-C5	2.65	119.73	115.27
23	AA	601	CHL	CMD-C2D-C3D	-2.65	121.51	127.61
25	0	614	LUT	C12-C13-C14	2.65	123.01	118.94
29	AV	101	BCR	C33-C5-C6	-2.65	121.55	124.53
24	AQ	614	CLA	O1D-CGD-CBD	2.65	129.91	124.48
24	Q	403	CLA	C3B-C4B-NB	-2.65	108.06	110.52
23	V	606	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
24	AE	611	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	AN	612	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
25	AE	613	LUT	C20-C13-C14	-2.65	119.21	122.92
23	AE	617	CHL	C3B-C4B-NB	2.65	112.97	110.52
32	J	406	PHO	C1C-C2C-C3C	-2.65	106.41	108.61
24	AU	602	CLA	C1-C2-C3	-2.65	121.47	126.04
24	K	101	CLA	C3B-C4B-NB	-2.65	108.06	110.52
23	v	307	CHL	C3D-C4D-ND	2.64	114.52	110.24
24	0	604	CLA	C3B-C4B-NB	-2.64	108.06	110.52
24	AA	613	CLA	C3B-C4B-NB	-2.64	108.06	110.52
23	0	607	CHL	C2C-C1C-CHC	-2.64	119.27	125.72
23	AS	307	CHL	C1-C2-C3	-2.64	121.47	126.04
38	F	102	HEM	C3B-C2B-C1B	2.64	108.45	106.49
24	0	609	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	v	302	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
24	AL	506	CLA	CHB-C4A-NA	2.64	128.16	124.51
24	AK	603	CLA	C3B-C4B-NB	-2.64	108.06	110.52
23	AS	306	CHL	C3C-C4C-CHD	-2.64	119.39	125.23
24	AN	604	CLA	C3B-C4B-NB	-2.64	108.07	110.52
23	AD	301	CHL	O2A-CGA-CBA	2.64	120.19	111.91
23	9	609	CHL	C2A-C3A-C4A	-2.64	97.61	101.87
25	v	316	LUT	C32-C33-C34	2.64	122.99	118.94
24	AB	604	CLA	C3B-C4B-NB	-2.64	108.07	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	0	608	CHL	C2A-C1A-CHA	2.64	128.47	123.86
24	AD	311	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
37	AM	405	PL9	C22-C23-C24	-2.64	121.31	127.66
23	AB	605	CHL	CHC-C4B-NB	-2.64	121.46	124.26
24	AK	613	CLA	O2D-CGD-CBD	2.64	115.95	111.27
24	AH	611	CLA	C3B-C4B-NB	-2.64	108.07	110.52
29	k	101	BCR	C33-C5-C6	-2.64	121.57	124.53
23	AU	601	CHL	O2A-CGA-CBA	2.64	120.18	111.91
28	AK	623	LHG	O8-C23-C24	2.64	120.18	111.91
23	AU	601	CHL	CMB-C2B-C1B	2.63	129.38	125.37
24	AD	303	CLA	C3B-C4B-NB	-2.63	108.07	110.52
24	AR	609	CLA	C3B-C4B-NB	-2.63	108.07	110.52
23	AN	605	CHL	CAA-C2A-C1A	2.63	120.61	111.97
23	AR	605	CHL	CMD-C2D-C3D	-2.63	121.56	127.61
24	AA	604	CLA	C3B-C4B-NB	-2.63	108.07	110.52
24	V	602	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	AN	607	CHL	C4D-CHA-C1A	-2.63	118.05	121.25
23	v	302	CHL	C3D-C4D-ND	2.63	114.50	110.24
23	p	606	CHL	CMD-C2D-C3D	-2.63	121.56	127.61
24	AA	604	CLA	O2D-CGD-CBD	2.63	115.94	111.27
23	AE	607	CHL	C3D-C4D-ND	2.63	114.49	110.24
29	P	515	BCR	C33-C5-C6	-2.63	121.58	124.53
23	AC	608	CHL	C6-C5-C3	-2.63	106.56	113.45
24	AF	602	CLA	CHC-C1C-NC	2.63	128.19	124.20
23	p	601	CHL	C16-C15-C13	-2.63	107.42	115.92
23	AB	605	CHL	CHD-C4C-C3C	-2.63	120.98	124.84
29	AF	612	BCR	C27-C26-C25	2.63	126.55	122.73
23	p	606	CHL	CHB-C4A-NA	2.63	128.15	124.51
24	AE	612	CLA	C3B-C4B-NB	-2.63	108.08	110.52
24	AL	512	CLA	C3B-C4B-NB	-2.63	108.08	110.52
23	AN	607	CHL	C3D-C4D-ND	2.63	114.49	110.24
23	AN	606	CHL	O2A-CGA-CBA	2.63	120.15	111.91
24	AQ	610	CLA	CHB-C4A-NA	2.63	128.14	124.51
24	Q	404	CLA	C3B-C4B-NB	-2.62	108.08	110.52
37	Q	405	PL9	C22-C23-C24	-2.62	121.34	127.66
23	AS	308	CHL	CAC-C3C-C4C	2.62	128.44	125.27
24	AN	609	CLA	CHB-C4A-NA	2.62	128.14	124.51
24	AD	313	CLA	CHB-C4A-NA	2.62	128.14	124.51
23	9	607	CHL	C4-C3-C5	2.62	119.68	115.27
24	V	611	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
29	O	618	BCR	C15-C16-C17	-2.62	118.10	123.47
23	AA	606	CHL	CHB-C4A-NA	2.62	128.14	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	602	CLA	CHB-C4A-NA	2.62	128.14	124.51
23	AE	605	CHL	CHB-C1B-NB	-2.62	121.48	124.26
23	p	601	CHL	C1C-C2C-C3C	-2.62	105.03	107.11
29	AI	101	BCR	C33-C5-C6	-2.62	121.59	124.53
24	AL	503	CLA	C3B-C4B-NB	-2.62	108.08	110.52
24	AU	613	CLA	C3B-C4B-NB	-2.62	108.08	110.52
24	q	612	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	AN	612	CLA	C1-C2-C3	-2.62	121.51	126.04
23	AQ	601	CHL	C1C-C2C-C3C	-2.62	105.04	107.11
23	0	601	CHL	CMD-C2D-C3D	-2.62	121.59	127.61
24	p	602	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	AB	602	CLA	CED-O2D-CGD	-2.62	110.02	115.94
23	AS	302	CHL	C1C-C2C-C3C	-2.62	105.04	107.11
23	AH	601	CHL	CMB-C2B-C1B	2.62	129.35	125.37
25	AA	615	LUT	C35-C15-C14	2.62	128.83	123.47
24	v	309	CLA	C3B-C4B-NB	-2.62	108.09	110.52
23	9	606	CHL	CBA-CAA-C2A	-2.62	106.14	113.86
24	P	503	CLA	C3B-C4B-NB	-2.61	108.09	110.52
26	AC	616	NEX	C28-C29-C30	2.61	122.95	118.94
23	AF	607	CHL	C3D-C4D-ND	2.61	114.46	110.24
24	O	603	CLA	C3B-C4B-NB	-2.61	108.09	110.52
23	AU	601	CHL	C6-C5-C3	-2.61	106.61	113.45
24	AM	403	CLA	CHB-C4A-NA	2.61	128.12	124.51
35	J	411	DGD	C3G-C2G-C1G	-2.61	105.61	111.79
23	V	607	CHL	CAA-C2A-C1A	2.61	120.53	111.97
24	AU	612	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
23	AE	616	CHL	CAA-CBA-CGA	-2.61	105.58	112.51
35	AJ	412	DGD	C3G-C2G-C1G	-2.61	105.62	111.79
23	AC	605	CHL	C3D-C4D-ND	2.61	114.46	110.24
23	9	607	CHL	O2A-CGA-CBA	2.61	120.09	111.91
23	p	608	CHL	C4-C3-C5	2.61	119.66	115.27
23	AS	302	CHL	C3D-C4D-ND	2.61	114.46	110.24
23	AD	307	CHL	CHB-C4A-NA	2.61	128.12	124.51
23	AF	605	CHL	C1D-ND-C4D	-2.61	104.48	106.33
24	AD	312	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	V	601	CHL	C6-C7-C8	-2.61	107.50	115.92
23	q	613	CHL	O2D-CGD-O1D	-2.60	118.75	123.84
23	V	605	CHL	CMB-C2B-C1B	2.60	129.34	125.37
29	AK	620	BCR	C15-C16-C17	-2.60	118.14	123.47
23	AN	601	CHL	C6-C7-C8	-2.60	107.50	115.92
23	AR	606	CHL	CMD-C2D-C3D	-2.60	121.62	127.61
23	0	617	CHL	O2A-CGA-CBA	2.60	122.39	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	0	617	CHL	CAC-C3C-C4C	2.60	128.19	124.81
23	AR	606	CHL	O2A-CGA-O1A	-2.60	117.03	123.59
24	AQ	604	CLA	C3B-C4B-NB	-2.60	108.10	110.52
24	AL	514	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
25	AC	615	LUT	C8-C9-C10	2.60	122.93	118.94
23	AU	601	CHL	CMD-C2D-C3D	-2.60	121.64	127.61
24	K	101	CLA	CHB-C4A-NA	2.60	128.10	124.51
25	9	615	LUT	C8-C9-C10	2.60	122.93	118.94
24	AU	611	CLA	CHB-C4A-NA	2.60	128.10	124.51
23	v	308	CHL	CMD-C2D-C3D	-2.60	121.64	127.61
23	AH	601	CHL	CMD-C2D-C3D	-2.60	121.64	127.61
23	AU	605	CHL	CMD-C2D-C3D	-2.60	121.64	127.61
23	AE	601	CHL	CHB-C4A-NA	2.59	128.10	124.51
24	AE	602	CLA	CHB-C4A-NA	2.59	128.10	124.51
23	AD	307	CHL	O1D-CGD-CBD	-2.59	119.18	124.48
28	q	616	LHG	O8-C23-C24	2.59	120.04	111.91
24	P	512	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
24	p	602	CLA	C3B-C4B-NB	-2.59	108.11	110.52
24	AF	604	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	AE	616	CHL	O2D-CGD-O1D	-2.59	118.78	123.84
29	AK	621	BCR	C24-C23-C22	-2.59	122.32	126.23
24	AB	610	CLA	CGD-CBD-CAD	2.59	119.12	110.73
23	V	601	CHL	CMD-C2D-C3D	-2.59	121.66	127.61
24	AL	512	CLA	CHB-C4A-NA	2.59	128.09	124.51
24	AC	613	CLA	CAA-C2A-C1A	2.59	120.45	111.97
23	AD	307	CHL	C3D-C4D-ND	2.59	114.42	110.24
35	P	516	DGD	O5D-C6D-C5D	-2.59	104.26	109.05
24	Q	403	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	AA	601	CHL	C3D-C4D-ND	2.59	114.42	110.24
28	AD	316	LHG	C11-C10-C9	-2.59	101.30	114.42
23	AH	601	CHL	C4-C3-C2	-2.59	117.05	123.68
23	AN	607	CHL	C2A-C3A-C4A	-2.59	97.69	101.87
23	AA	605	CHL	C4D-CHA-C1A	-2.59	118.10	121.25
23	AD	301	CHL	C1C-C2C-C3C	-2.58	105.06	107.11
24	AR	604	CLA	O2D-CGD-CBD	2.58	115.86	111.27
24	q	609	CLA	CHB-C4A-NA	2.58	128.09	124.51
35	AL	517	DGD	O5D-C6D-C5D	-2.58	104.27	109.05
29	AK	620	BCR	C27-C26-C25	2.58	126.48	122.73
24	AD	313	CLA	C3B-C4B-NB	-2.58	108.12	110.52
23	V	607	CHL	CAA-CBA-CGA	2.58	120.80	113.25
24	p	604	CLA	C3B-C4B-NB	-2.58	108.12	110.52
24	AK	605	CLA	C3B-C4B-NB	-2.58	108.12	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	AM	401	SQD	O48-C23-C24	2.58	120.00	111.91
24	P	511	CLA	CHB-C4A-NA	2.58	128.08	124.51
24	V	611	CLA	C3B-C4B-NB	-2.58	108.12	110.52
23	9	609	CHL	C1C-C2C-C3C	-2.58	105.07	107.11
23	AN	601	CHL	CMD-C2D-C3D	-2.58	121.69	127.61
24	AR	617	CLA	C1D-ND-C4D	2.57	108.16	106.33
24	q	604	CLA	CHB-C4A-NA	2.57	128.07	124.51
23	v	307	CHL	C1C-C2C-C3C	-2.57	105.07	107.11
23	AH	608	CHL	C11-C12-C13	-2.57	107.60	115.92
23	q	606	CHL	CHB-C4A-NA	2.57	128.07	124.51
28	0	616	LHG	C11-C10-C9	-2.57	101.37	114.42
24	AD	310	CLA	C3B-C4B-NB	-2.57	108.13	110.52
24	p	618	CLA	C2D-C1D-ND	-2.57	108.21	110.10
24	p	612	CLA	C3B-C4B-NB	-2.57	108.13	110.52
23	AE	601	CHL	CMD-C2D-C3D	-2.57	121.70	127.61
23	V	606	CHL	O2A-CGA-CBA	2.57	119.97	111.91
23	AC	606	CHL	CHB-C4A-NA	2.57	128.06	124.51
24	P	512	CLA	CAA-C2A-C1A	2.57	120.39	111.97
23	AU	607	CHL	O2A-CGA-CBA	2.57	119.97	111.91
23	V	608	CHL	C1-C2-C3	-2.57	121.60	126.04
23	AB	605	CHL	C3D-C4D-ND	2.57	114.39	110.24
24	AA	609	CLA	CHB-C4A-NA	2.57	128.06	124.51
24	AK	606	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	q	614	LUT	C32-C33-C34	2.57	122.88	118.94
23	AH	607	CHL	O2A-CGA-CBA	2.57	119.96	111.91
25	v	315	LUT	C32-C33-C34	2.57	122.88	118.94
23	p	609	CHL	OMC-CMC-C2C	-2.57	119.89	125.69
23	AH	601	CHL	C2A-C1A-CHA	-2.57	119.37	123.86
24	O	608	CLA	CHD-C1D-ND	-2.56	122.10	124.45
23	0	617	CHL	C1D-ND-C4D	-2.56	104.51	106.33
34	Q	402	SQD	O48-C23-C24	2.56	119.95	111.91
24	AL	513	CLA	CHB-C4A-NA	2.56	128.06	124.51
24	O	605	CLA	C3B-C4B-NB	-2.56	108.14	110.52
24	AR	608	CLA	CMA-C3A-C2A	-2.56	110.12	116.10
29	O	625	BCR	C15-C16-C17	-2.56	118.22	123.47
24	AD	305	CLA	C3B-C4B-NB	-2.56	108.14	110.52
24	AA	602	CLA	C1-C2-C3	-2.56	121.61	126.04
29	O	619	BCR	C24-C23-C22	-2.56	122.36	126.23
25	AD	315	LUT	C32-C33-C34	2.56	122.87	118.94
25	AH	614	LUT	C39-C29-C28	2.56	122.11	118.08
25	AU	614	LUT	C39-C29-C28	2.56	122.11	118.08
24	AH	604	CLA	CHB-C4A-NA	2.56	128.05	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	9	609	CHL	CMD-C2D-C3D	-2.56	121.73	127.61
23	AR	607	CHL	C6-C5-C3	-2.56	110.44	114.62
23	AQ	609	CHL	C1-C2-C3	-2.56	121.62	126.04
24	AE	611	CLA	C3B-C4B-NB	-2.56	108.14	110.52
24	O	607	CLA	C3B-C4B-NB	-2.56	108.14	110.52
24	AH	604	CLA	C3B-C4B-NB	-2.56	108.14	110.52
24	AF	602	CLA	CAA-C2A-C3A	-2.55	110.14	116.10
24	AQ	613	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	AS	310	CLA	C3B-C4B-NB	-2.55	108.14	110.52
23	AH	601	CHL	C6-C5-C3	-2.55	106.76	113.45
23	V	607	CHL	C1D-ND-C4D	-2.55	104.52	106.33
24	AU	604	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	AA	601	CHL	C4D-CHA-C1A	-2.55	118.14	121.25
29	AK	602	BCR	C24-C23-C22	-2.55	122.38	126.23
24	AN	610	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	AD	306	CHL	O2A-CGA-CBA	2.55	119.91	111.91
23	AE	605	CHL	CAA-CBA-CGA	-2.55	105.81	113.25
23	AD	317	CHL	O2A-CGA-CBA	2.55	122.22	114.03
25	V	613	LUT	C39-C29-C28	2.55	122.09	118.08
24	AK	607	CLA	C3B-C4B-NB	-2.55	108.15	110.52
24	AD	303	CLA	CHB-C4A-NA	2.55	128.03	124.51
24	AC	610	CLA	CHB-C1B-NB	2.55	126.95	124.26
23	p	606	CHL	CAA-C2A-C1A	2.55	120.32	111.97
24	9	604	CLA	C3B-C4B-NB	-2.55	108.15	110.52
24	v	305	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
24	AL	505	CLA	CHB-C4A-NA	2.55	128.03	124.51
25	AH	615	LUT	C12-C13-C14	2.55	122.85	118.94
24	AS	310	CLA	CHB-C4A-NA	2.55	128.03	124.51
24	AD	303	CLA	C1-C2-C3	-2.55	121.64	126.04
27	9	618	XAT	C40-C33-C32	-2.55	114.07	118.08
24	AU	604	CLA	C3B-C4B-NB	-2.54	108.15	110.52
23	AE	605	CHL	CMB-C2B-C1B	2.54	129.25	125.37
24	0	612	CLA	CHB-C4A-NA	2.54	128.03	124.51
24	O	602	CLA	CHB-C4A-NA	2.54	128.03	124.51
24	AQ	604	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
24	AC	613	CLA	CHB-C4A-NA	2.54	128.03	124.51
24	AE	608	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	AH	605	CHL	CAA-CBA-CGA	-2.54	105.83	113.25
24	AB	611	CLA	CHB-C4A-NA	2.54	128.03	124.51
24	AS	303	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	AR	607	CHL	CMB-C2B-C1B	2.54	129.24	125.37
24	O	604	CLA	CHB-C4A-NA	2.54	128.02	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AN	605	CHL	CMD-C2D-C3D	-2.54	121.78	127.61
23	AU	601	CHL	O2A-C1-C2	2.54	115.31	108.64
24	AE	604	CLA	O2D-CGD-CBD	2.54	115.78	111.27
23	AD	317	CHL	C3D-C4D-ND	2.54	114.34	110.24
25	V	613	LUT	C15-C35-C34	2.54	128.67	123.47
25	AH	614	LUT	C32-C33-C34	2.54	122.83	118.94
24	V	609	CLA	C3B-C4B-NB	-2.54	108.16	110.52
24	AL	514	CLA	CAA-C2A-C1A	2.53	120.28	111.97
23	q	606	CHL	C2C-C1C-NC	2.53	114.61	110.44
24	O	611	CLA	C3B-C4B-NB	-2.53	108.17	110.52
23	9	601	CHL	CMD-C2D-C3D	-2.53	121.79	127.61
23	AQ	609	CHL	OMC-CMC-C2C	-2.53	119.96	125.69
23	0	607	CHL	C2C-C3C-C4C	-2.53	103.47	106.95
23	0	606	CHL	O2A-CGA-CBA	2.53	119.85	111.91
23	V	605	CHL	O2D-CGD-O1D	-2.53	118.89	123.84
29	AJ	410	BCR	C24-C23-C22	-2.53	122.41	126.23
23	AH	605	CHL	CMD-C2D-C3D	-2.53	121.79	127.61
24	p	613	CLA	CHC-C4B-NB	2.53	126.94	124.26
23	q	605	CHL	CMD-C2D-C3D	-2.53	121.80	127.61
25	p	614	LUT	C39-C29-C28	2.53	122.06	118.08
29	O	617	BCR	C11-C10-C9	-2.53	123.70	127.31
23	0	617	CHL	O2D-CGD-O1D	-2.53	118.89	123.84
23	AD	301	CHL	CMD-C2D-C3D	-2.53	121.80	127.61
24	AK	609	CLA	C3B-C4B-NB	-2.53	108.17	110.52
28	AK	624	LHG	O8-C23-C24	2.53	119.84	111.91
24	v	303	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	AS	315	LUT	C32-C33-C34	2.53	122.82	118.94
23	AU	608	CHL	C11-C12-C13	-2.53	107.75	115.92
23	AS	308	CHL	C2C-C3C-C4C	-2.53	103.48	106.95
23	AU	601	CHL	C4-C3-C2	-2.53	117.20	123.68
24	J	404	CLA	C3B-C4B-NB	-2.53	108.17	110.52
24	AN	612	CLA	CAA-CBA-CGA	-2.53	105.87	113.25
24	9	611	CLA	CHB-C4A-NA	2.53	128.00	124.51
25	AU	615	LUT	C12-C13-C14	2.52	122.81	118.94
28	AK	624	LHG	C11-C10-C9	-2.52	101.61	114.42
25	V	614	LUT	C32-C33-C34	2.52	122.81	118.94
24	v	314	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	AA	605	CHL	OMC-CMC-C2C	-2.52	119.98	125.69
23	AQ	606	CHL	C4D-CHA-C1A	-2.52	118.18	121.25
34	M	101	SQD	O48-C23-C24	2.52	119.82	111.91
24	AB	604	CLA	CHB-C4A-NA	2.52	128.00	124.51
24	0	612	CLA	C3B-C4B-NB	-2.52	108.17	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	O	609	CLA	CHB-C4A-NA	2.52	128.00	124.51
28	O	623	LHG	C11-C10-C9	-2.52	101.63	114.42
23	v	307	CHL	O2D-CGD-O1D	-2.52	118.91	123.84
24	AH	612	CLA	C3B-C4B-NB	-2.52	108.18	110.52
34	m	101	SQD	O48-C23-C24	2.52	119.82	111.91
37	AM	405	PL9	C27-C28-C29	-2.52	121.59	127.66
24	0	613	CLA	CHB-C4A-NA	2.52	128.00	124.51
24	AH	613	CLA	C3B-C4B-NB	-2.52	108.18	110.52
25	AC	614	LUT	C32-C33-C34	2.52	122.80	118.94
24	AU	612	CLA	CHB-C4A-NA	2.52	127.99	124.51
24	AF	609	CLA	CMA-C3A-C2A	-2.52	107.15	114.44
23	q	605	CHL	O2A-CGA-O1A	-2.52	117.24	123.59
23	0	607	CHL	C4D-CHA-C1A	-2.52	118.19	121.25
23	AC	601	CHL	CMD-C2D-C3D	-2.52	121.83	127.61
28	p	617	LHG	C11-C10-C9	-2.52	101.66	114.42
23	AR	605	CHL	O2A-CGA-O1A	-2.51	117.25	123.59
23	v	306	CHL	CHB-C4A-NA	2.51	127.99	124.51
24	AS	313	CLA	C1-C2-C3	-2.51	121.69	126.04
24	AB	610	CLA	CHB-C4A-NA	2.51	127.99	124.51
34	AJ	411	SQD	O48-C23-C24	2.51	119.80	111.91
28	O	623	LHG	O8-C23-C24	2.51	119.79	111.91
23	p	606	CHL	C4D-CHA-C1A	-2.51	118.19	121.25
34	J	410	SQD	O48-C23-C24	2.51	119.79	111.91
25	0	615	LUT	C32-C33-C34	2.51	122.80	118.94
23	AQ	609	CHL	CHB-C4A-NA	2.51	127.98	124.51
28	O	622	LHG	C11-C10-C9	-2.51	101.68	114.42
29	O	625	BCR	C15-C14-C13	-2.51	123.73	127.31
24	v	311	CLA	CHB-C1B-NB	2.51	126.92	124.26
24	AK	605	CLA	CHB-C4A-NA	2.51	127.98	124.51
29	J	408	BCR	C24-C23-C22	-2.51	122.44	126.23
24	AS	314	CLA	CHB-C4A-NA	2.51	127.98	124.51
24	O	607	CLA	O2D-CGD-CBD	2.51	115.73	111.27
23	AU	605	CHL	CAA-CBA-CGA	-2.51	105.92	113.25
24	AF	604	CLA	O1D-CGD-CBD	2.51	129.62	124.48
24	V	603	CLA	CHB-C1B-NB	2.51	126.91	124.26
24	AA	610	CLA	CHB-C4A-NA	2.51	127.98	124.51
24	AF	609	CLA	CHB-C4A-NA	2.51	127.98	124.51
24	AQ	602	CLA	CHB-C4A-NA	2.51	127.98	124.51
32	AJ	407	PHO	C1C-C2C-C3C	-2.51	106.53	108.61
23	AB	607	CHL	C1C-C2C-C3C	-2.51	105.12	107.11
24	P	502	CLA	CED-O2D-CGD	2.51	121.61	115.94
24	O	606	CLA	C3C-C4C-NC	-2.51	107.76	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AS	311	CLA	CHB-C1B-NB	2.51	126.91	124.26
25	0	614	LUT	C39-C29-C28	2.50	122.02	118.08
24	AK	609	CLA	O2D-CGD-CBD	2.50	115.72	111.27
23	q	607	CHL	C3D-C4D-ND	2.50	114.29	110.24
24	Q	401	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	AD	305	CLA	O2D-CGD-CBD	2.50	115.72	111.27
24	AJ	404	CLA	O2D-CGD-CBD	2.50	115.72	111.27
23	AR	607	CHL	CHC-C4B-NB	-2.50	121.61	124.26
25	AU	614	LUT	C32-C33-C34	2.50	122.78	118.94
23	v	302	CHL	C1D-ND-C4D	-2.50	104.56	106.33
23	V	607	CHL	C3D-C4D-ND	2.50	114.28	110.24
24	p	613	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	AA	605	CHL	CMD-C2D-C3D	-2.50	121.86	127.61
24	AB	603	CLA	CHB-C1B-NB	2.50	126.90	124.26
23	V	601	CHL	O2A-CGA-CBA	2.50	119.75	111.91
28	AK	623	LHG	C11-C10-C9	-2.50	101.73	114.42
29	O	618	BCR	C27-C26-C25	2.50	126.36	122.73
24	AF	609	CLA	CHD-C1D-ND	-2.50	122.16	124.45
25	9	616	LUT	C32-C33-C34	2.50	122.78	118.94
28	W	201	LHG	O8-C23-C24	2.50	119.75	111.91
24	AU	612	CLA	C3B-C4B-NB	-2.50	108.20	110.52
24	AH	612	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	q	605	CHL	C6-C7-C8	-2.50	107.84	115.92
37	Q	405	PL9	C27-C28-C29	-2.50	121.65	127.66
25	p	614	LUT	C32-C33-C34	2.50	122.77	118.94
23	AN	617	CHL	OMC-CMC-C2C	-2.50	120.04	125.69
29	AV	101	BCR	C24-C23-C22	-2.50	122.46	126.23
24	AK	616	CLA	CHB-C4A-NA	2.50	127.96	124.51
28	AU	617	LHG	C11-C10-C9	-2.50	101.75	114.42
23	p	609	CHL	C1-C2-C3	-2.50	121.73	126.04
24	p	604	CLA	C1-C2-C3	-2.50	122.71	126.75
23	p	601	CHL	C1-C2-C3	-2.49	121.73	126.04
24	AF	609	CLA	C3C-C4C-NC	-2.49	107.77	110.57
23	AB	608	CHL	CAD-CBD-CHA	-2.49	102.33	105.14
23	V	616	CHL	CBA-CAA-C2A	2.49	121.23	113.86
23	0	607	CHL	C3D-C4D-ND	2.49	114.27	110.24
28	O	621	LHG	C11-C10-C9	-2.49	101.77	114.42
24	AD	312	CLA	C3B-C4B-NB	-2.49	108.20	110.52
23	q	607	CHL	OMC-CMC-C2C	-2.49	120.05	125.69
23	AF	605	CHL	CMD-C2D-C3D	-2.49	121.88	127.61
24	9	604	CLA	CHB-C4A-NA	2.49	127.96	124.51
24	AC	609	CLA	CHB-C4A-NA	2.49	127.96	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AE	605	CHL	C1C-C2C-C3C	-2.49	105.14	107.11
29	P	514	BCR	C27-C26-C25	2.49	126.35	122.73
24	AN	613	CLA	C3B-C4B-NB	-2.49	108.20	110.52
23	AH	607	CHL	CHB-C4A-NA	2.49	127.96	124.51
23	AA	606	CHL	O2A-CGA-CBA	2.49	119.72	111.91
23	AC	605	CHL	C1C-C2C-C3C	-2.49	105.14	107.11
24	v	313	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	AK	612	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	P	508	CLA	C3B-C4B-NB	-2.49	108.21	110.52
28	w	201	LHG	C11-C10-C9	-2.49	101.79	114.42
23	0	607	CHL	CAC-C3C-C4C	2.49	128.28	125.27
25	v	316	LUT	C12-C13-C14	2.49	122.76	118.94
24	AF	614	CLA	C2D-C1D-ND	-2.49	108.27	110.10
28	AM	406	LHG	C11-C10-C9	-2.49	101.79	114.42
23	9	607	CHL	CMD-C2D-C3D	-2.49	121.89	127.61
24	AC	602	CLA	CHB-C4A-NA	2.49	127.95	124.51
25	AF	611	LUT	C32-C33-C34	2.49	122.76	118.94
24	P	504	CLA	C3B-C4B-NB	-2.49	108.21	110.52
28	AH	616	LHG	C11-C10-C9	-2.49	101.80	114.42
28	V	615	LHG	C11-C10-C9	-2.49	101.80	114.42
24	AK	611	CLA	C3B-C4B-NB	-2.49	108.21	110.52
25	AQ	615	LUT	C39-C29-C28	2.49	121.99	118.08
23	AB	607	CHL	C3B-C4B-NB	2.48	112.82	110.52
24	AN	613	CLA	CAA-CBA-CGA	-2.48	105.99	113.25
23	V	608	CHL	CHB-C4A-NA	2.48	127.95	124.51
23	p	609	CHL	CMD-C2D-C3D	-2.48	121.90	127.61
24	AR	617	CLA	CHA-C4D-ND	2.48	137.69	132.50
28	Q	406	LHG	C11-C10-C9	-2.48	101.82	114.42
25	9	615	LUT	C39-C29-C28	2.48	121.99	118.08
28	w	201	LHG	O8-C23-C24	2.48	119.70	111.91
23	AB	606	CHL	CMD-C2D-C3D	-2.48	121.90	127.61
23	AF	601	CHL	CMD-C2D-C3D	-2.48	121.90	127.61
24	AR	608	CLA	CMA-C3A-C4A	-2.48	105.10	111.77
23	AA	601	CHL	OMC-CMC-C2C	-2.48	120.07	125.69
24	AK	604	CLA	C3A-C2A-C1A	2.48	105.06	101.34
25	AA	614	LUT	C8-C9-C10	2.48	122.75	118.94
25	AQ	615	LUT	C32-C33-C34	2.48	122.75	118.94
25	v	315	LUT	C39-C29-C28	2.48	121.98	118.08
26	9	617	NEX	C28-C29-C30	2.48	122.75	118.94
28	W	201	LHG	C11-C10-C9	-2.48	101.84	114.42
23	AD	307	CHL	C4D-CHA-C1A	-2.48	118.23	121.25
24	v	313	CLA	C3B-C4B-NB	-2.48	108.22	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AA	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
24	0	603	CLA	C2D-C1D-ND	-2.48	108.28	110.10
25	AC	615	LUT	C32-C33-C34	2.48	122.74	118.94
23	p	607	CHL	CMD-C2D-C3D	-2.47	121.92	127.61
28	v	301	LHG	C20-C19-C18	-2.47	101.86	114.42
23	v	306	CHL	C3A-C4A-CHB	-2.47	117.49	124.01
28	Q	406	LHG	O8-C23-C24	2.47	119.67	111.91
29	AK	619	BCR	C11-C10-C9	-2.47	123.78	127.31
26	AU	616	NEX	C19-C9-C10	-2.47	119.46	122.92
23	AU	607	CHL	CHB-C4A-NA	2.47	127.93	124.51
28	AN	616	LHG	C11-C10-C9	-2.47	101.88	114.42
23	AE	607	CHL	O2A-CGA-CBA	2.47	119.66	111.91
32	J	406	PHO	CMB-C2B-C3B	2.47	129.30	124.68
24	J	403	CLA	CGD-CBD-CAD	2.47	118.74	110.73
23	v	306	CHL	CMD-C2D-C3D	-2.47	121.93	127.61
29	AL	516	BCR	C27-C26-C25	2.47	126.32	122.73
24	AR	617	CLA	CHD-C1D-C2D	2.47	130.66	125.48
23	V	607	CHL	C2C-C1C-CHC	-2.47	119.69	125.72
23	AE	605	CHL	CMD-C2D-C3D	-2.47	121.93	127.61
24	J	404	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	O	616	CLA	CHB-C4A-NA	2.47	127.93	124.51
35	j	102	DGD	O5D-C6D-C5D	-2.47	104.48	109.05
25	AS	315	LUT	C39-C29-C28	2.47	121.97	118.08
25	AE	613	LUT	C8-C9-C10	2.47	122.73	118.94
23	AE	607	CHL	CAA-C2A-C1A	2.47	120.06	111.97
25	9	615	LUT	C32-C33-C34	2.47	122.73	118.94
25	V	613	LUT	C12-C13-C14	2.47	122.73	118.94
28	AS	301	LHG	C20-C19-C18	-2.47	101.90	114.42
23	AN	601	CHL	O2A-CGA-CBA	2.47	119.65	111.91
24	O	603	CLA	CHB-C4A-NA	2.47	127.92	124.51
24	q	610	CLA	CHB-C4A-NA	2.47	127.92	124.51
26	p	616	NEX	C28-C29-C30	2.47	122.72	118.94
24	AK	610	CLA	CAA-CBA-CGA	-2.47	106.05	113.25
24	p	612	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
24	O	614	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	q	606	CHL	CMD-C2D-C3D	-2.46	121.95	127.61
23	9	601	CHL	C1C-C2C-C3C	-2.46	105.16	107.11
23	AB	601	CHL	C1C-C2C-C3C	-2.46	105.16	107.11
24	AN	612	CLA	C3B-C4B-NB	-2.46	108.23	110.52
24	AK	604	CLA	C1-C2-C3	-2.46	121.78	126.04
29	AO	101	BCR	C15-C14-C13	-2.46	123.80	127.31
32	AJ	408	PHO	CMB-C2B-C3B	2.46	129.28	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	0	606	CHL	C1D-ND-C4D	-2.46	104.59	106.33
23	AQ	607	CHL	CMD-C2D-C3D	-2.46	121.95	127.61
23	V	605	CHL	CAA-C2A-C1A	2.46	120.04	111.97
23	0	617	CHL	C3D-C4D-ND	2.46	114.22	110.24
28	AQ	618	LHG	C11-C10-C9	-2.46	101.94	114.42
24	AR	612	CLA	CGD-CBD-CAD	2.46	118.70	110.73
24	0	610	CLA	C3B-C4B-NB	-2.46	108.23	110.52
25	AE	613	LUT	C39-C29-C28	2.46	121.95	118.08
23	v	307	CHL	CMD-C2D-C3D	-2.46	121.96	127.61
32	J	405	PHO	C1C-C2C-C3C	-2.46	106.57	108.61
24	AL	505	CLA	C3B-C4B-NB	-2.46	108.23	110.52
23	AH	601	CHL	O2A-C1-C2	2.46	115.09	108.64
24	AE	604	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	0	605	CHL	CMD-C2D-C3D	-2.46	121.97	127.61
24	q	602	CLA	CHB-C4A-NA	2.45	127.91	124.51
24	AF	610	CLA	CAA-CBA-CGA	2.45	119.02	112.51
24	AQ	612	CLA	CHB-C1B-NB	2.45	126.86	124.26
29	J	408	BCR	C27-C26-C25	2.45	126.29	122.73
24	AL	509	CLA	C3B-C4B-NB	-2.45	108.24	110.52
24	AN	602	CLA	C3B-C4B-NB	-2.45	108.24	110.52
26	AR	615	NEX	C10-C11-C12	2.45	130.87	123.22
23	V	607	CHL	CAC-C3C-C4C	2.45	128.24	125.27
23	0	617	CHL	CHB-C1B-NB	-2.45	121.66	124.26
23	AB	607	CHL	C3D-C4D-ND	2.45	114.20	110.24
37	AM	405	PL9	C20-C19-C21	2.45	119.39	115.27
24	v	311	CLA	CHB-C4A-NA	2.45	127.90	124.51
29	AB	612	BCR	C11-C10-C9	-2.45	123.81	127.31
28	AM	406	LHG	O8-C23-C24	2.45	119.60	111.91
24	AE	612	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	p	604	CLA	CHB-C4A-NA	2.45	127.90	124.51
33	Q	407	LMG	O1-C7-C8	-2.45	104.99	110.90
24	9	610	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	AN	613	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	AQ	607	CHL	C11-C10-C8	-2.45	108.01	115.92
23	AE	605	CHL	O2A-CGA-CBA	2.45	119.59	111.91
24	AQ	613	CLA	C3B-C4B-NB	-2.45	108.24	110.52
23	AR	613	CHL	C1D-ND-C4D	-2.45	104.60	106.33
25	AS	316	LUT	C32-C33-C34	2.45	122.70	118.94
26	AS	317	NEX	C19-C9-C8	-2.45	113.26	118.93
24	O	608	CLA	CHB-C4A-NA	2.45	127.90	124.51
28	P	517	LHG	C11-C10-C9	-2.45	102.00	114.42
23	AQ	601	CHL	CMD-C2D-C3D	-2.45	121.99	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AN	604	CLA	CHB-C4A-NA	2.44	127.89	124.51
24	AJ	406	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	AC	606	CHL	C4D-CHA-C1A	-2.44	118.28	121.25
23	q	613	CHL	CMD-C2D-C3D	-2.44	122.00	127.61
24	O	601	CLA	C2A-C1A-CHA	2.44	128.13	123.86
23	AN	606	CHL	C11-C10-C8	-2.44	108.03	115.92
24	q	601	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
37	Q	405	PL9	C20-C19-C21	2.44	119.38	115.27
23	v	308	CHL	C2A-C1A-CHA	-2.44	119.59	123.85
29	AJ	410	BCR	C33-C5-C6	-2.44	121.79	124.53
23	AQ	606	CHL	CAA-C2A-C1A	2.44	119.97	111.97
25	AA	615	LUT	C20-C13-C14	-2.44	119.51	122.92
33	AM	407	LMG	O1-C7-C8	-2.44	105.01	110.90
29	AB	612	BCR	C27-C26-C25	2.44	126.27	122.73
24	AJ	409	CLA	C3B-C4B-NB	-2.44	108.25	110.52
38	f	102	HEM	CAA-CBA-CGA	-2.44	108.36	113.60
28	AM	406	LHG	C20-C19-C18	-2.44	102.05	114.42
23	p	605	CHL	CMD-C2D-C3D	-2.44	122.01	127.61
24	AA	603	CLA	CHB-C4A-NA	2.44	127.88	124.51
24	P	504	CLA	CHB-C4A-NA	2.44	127.88	124.51
35	j	102	DGD	C3G-C2G-C1G	-2.44	106.02	111.79
28	Q	406	LHG	C20-C19-C18	-2.44	102.06	114.42
23	AC	608	CHL	O2A-CGA-CBA	2.44	119.55	111.91
24	AD	310	CLA	C1-C2-C3	-2.44	121.83	126.04
24	AE	612	CLA	O1D-CGD-CBD	2.44	129.47	124.48
24	AQ	614	CLA	CHB-C4A-NA	2.43	127.88	124.51
33	O	620	LMG	C40-C39-C38	-2.43	102.07	114.42
24	AJ	405	CLA	CHB-C4A-NA	2.43	127.88	124.51
32	AJ	408	PHO	O1D-CGD-CBD	2.43	128.79	124.74
24	AK	616	CLA	C3B-C4B-NB	-2.43	108.26	110.52
24	0	609	CLA	C1-C2-C3	-2.43	121.83	126.04
23	AB	601	CHL	CMD-C2D-C3D	-2.43	122.02	127.61
29	O	618	BCR	C15-C14-C13	-2.43	123.84	127.31
29	P	513	BCR	C27-C26-C25	2.43	126.26	122.73
25	AN	615	LUT	C32-C33-C34	2.43	122.67	118.94
24	AR	610	CLA	CHB-C4A-NA	2.43	127.88	124.51
23	AU	607	CHL	C1C-C2C-C3C	-2.43	105.18	107.11
24	AK	609	CLA	CHB-C4A-NA	2.43	127.88	124.51
24	V	612	CLA	CAA-CBA-CGA	-2.43	106.15	113.25
23	AH	607	CHL	C1C-C2C-C3C	-2.43	105.19	107.11
24	AK	604	CLA	C3B-C4B-NB	-2.43	108.26	110.52
24	O	607	CLA	CHB-C4A-NA	2.43	127.87	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	AK	622	LMG	C40-C39-C38	-2.43	102.09	114.42
23	AB	605	CHL	CMD-C2D-C3D	-2.43	122.03	127.61
28	AN	616	LHG	C20-C19-C18	-2.43	102.10	114.42
23	AN	605	CHL	CHB-C4A-NA	2.43	127.87	124.51
24	AB	611	CLA	C3B-C4B-NB	-2.43	108.26	110.52
29	AL	515	BCR	C27-C26-C25	2.43	126.25	122.73
23	AN	605	CHL	C4D-CHA-C1A	-2.43	118.30	121.25
24	P	508	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	0	606	CHL	CED-O2D-CGD	2.43	121.42	115.94
23	AR	606	CHL	C1D-ND-C4D	-2.43	104.61	106.33
28	V	615	LHG	C20-C19-C18	-2.43	102.11	114.42
29	J	408	BCR	C33-C5-C6	-2.42	121.81	124.53
24	p	613	CLA	CAC-C3C-C4C	2.42	127.96	124.81
25	AR	614	LUT	C12-C13-C14	2.42	122.66	118.94
24	AS	311	CLA	CHB-C4A-NA	2.42	127.86	124.51
24	P	512	CLA	C2A-C1A-CHA	2.42	128.10	123.86
25	AU	614	LUT	C12-C13-C14	2.42	122.66	118.94
23	AU	607	CHL	CMD-C2D-C3D	-2.42	122.04	127.61
25	AR	614	LUT	C32-C33-C34	2.42	122.66	118.94
29	AI	101	BCR	C24-C23-C22	-2.42	122.58	126.23
33	J	409	LMG	C40-C39-C38	-2.42	102.13	114.42
23	p	601	CHL	CMD-C2D-C3D	-2.42	122.04	127.61
33	AL	501	LMG	C40-C39-C38	-2.42	102.14	114.42
24	AU	603	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
24	O	602	CLA	C3B-C4B-NB	-2.42	108.27	110.52
24	AK	606	CLA	C3B-C4B-NB	-2.42	108.27	110.52
23	9	601	CHL	CMB-C2B-C1B	2.42	128.28	125.81
29	AK	620	BCR	C33-C5-C6	-2.42	121.81	124.53
23	0	601	CHL	C1D-ND-C4D	-2.42	104.62	106.33
25	AA	614	LUT	C39-C29-C28	2.42	121.89	118.08
23	q	606	CHL	C4-C3-C5	2.42	119.34	115.27
25	AD	314	LUT	C39-C29-C28	2.42	121.88	118.08
29	AK	620	BCR	C15-C14-C13	-2.42	123.86	127.31
25	AH	615	LUT	C32-C33-C34	2.42	122.65	118.94
24	AD	311	CLA	CHB-C4A-NA	2.41	127.85	124.51
24	AK	603	CLA	C2A-C1A-CHA	2.41	128.08	123.86
24	AL	514	CLA	C2A-C1A-CHA	2.41	128.08	123.86
24	Q	404	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	AC	608	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
23	AH	605	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
24	9	612	CLA	CHB-C4A-NA	2.41	127.85	124.51
28	AL	519	LHG	C11-C10-C9	-2.41	102.17	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AK	607	CLA	CHB-C4A-NA	2.41	127.85	124.51
24	P	511	CLA	C1-C2-C3	-2.41	121.87	126.04
23	p	608	CHL	OMC-CMC-C2C	-2.41	120.23	125.69
23	p	607	CHL	C11-C10-C8	-2.41	108.13	115.92
24	AN	603	CLA	CHB-C1B-NB	2.41	126.81	124.26
28	q	616	LHG	C11-C10-C9	-2.41	102.19	114.42
23	AR	606	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
23	AR	607	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
23	V	607	CHL	CMB-C2B-C1B	2.41	128.27	125.81
29	AO	101	BCR	C11-C10-C9	-2.41	123.87	127.31
23	AD	302	CHL	C6-C5-C3	-2.41	107.14	113.45
23	AS	308	CHL	C2C-C1C-CHC	-2.41	119.84	125.72
24	AU	609	CLA	CGD-CBD-CAD	2.41	118.53	110.73
23	AH	607	CHL	CMD-C2D-C3D	-2.41	122.08	127.61
33	AL	520	LMG	O6-C1-O1	-2.41	104.27	109.97
24	AQ	604	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	v	302	CHL	CMD-C2D-C3D	-2.41	122.08	127.61
25	AH	614	LUT	C12-C13-C14	2.41	122.63	118.94
24	P	502	CLA	CHB-C4A-NA	2.41	127.84	124.51
24	9	611	CLA	CHB-C1B-NB	2.41	126.80	124.26
33	O	624	LMG	O1-C7-C8	-2.41	105.09	110.90
24	AN	602	CLA	CHB-C4A-NA	2.41	127.84	124.51
24	AK	603	CLA	CBA-CAA-C2A	2.40	120.96	113.86
24	O	611	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
24	O	604	CLA	C1-C2-C3	-2.40	121.89	126.04
24	AH	603	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
24	AN	611	CLA	CHB-C4A-NA	2.40	127.84	124.51
23	0	607	CHL	CAA-CBA-CGA	-2.40	106.13	112.51
24	V	610	CLA	CHB-C4A-NA	2.40	127.83	124.51
24	AK	613	CLA	C3B-C4B-NB	-2.40	108.29	110.52
24	AL	513	CLA	C1-C2-C3	-2.40	121.89	126.04
23	V	607	CHL	C2C-C3C-C4C	-2.40	103.65	106.95
24	O	604	CLA	C3B-C4B-NB	-2.40	108.29	110.52
24	AL	514	CLA	C1B-NB-C4B	2.40	108.04	106.33
24	AH	612	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
24	AE	609	CLA	CHB-C4A-NA	2.40	127.83	124.51
24	AQ	604	CLA	C1-C2-C3	-2.40	122.87	126.75
24	AL	509	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
32	J	405	PHO	CMB-C2B-C3B	2.40	129.17	124.68
24	P	508	CLA	CMB-C2B-C1B	-2.40	121.72	125.37
29	O	618	BCR	C33-C5-C6	-2.40	121.84	124.53
25	AC	614	LUT	C39-C29-C28	2.40	121.85	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AA	613	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	AQ	605	CHL	CMD-C2D-C3D	-2.39	122.11	127.61
23	AE	617	CHL	CAC-C3C-C4C	2.39	127.92	124.81
24	q	602	CLA	C1-C2-C3	-2.39	121.90	126.04
24	J	407	CLA	C3B-C4B-NB	-2.39	108.30	110.52
24	AH	610	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	AF	604	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
23	0	608	CHL	C4D-C3D-CAD	2.39	110.92	108.10
24	AS	303	CLA	C1-C2-C3	-2.39	121.91	126.04
23	AQ	607	CHL	O2A-CGA-CBA	2.39	119.42	111.91
24	AL	509	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	AL	512	CLA	CAA-CBA-CGA	-2.39	106.26	113.25
35	AO	102	DGD	C3G-C2G-C1G	-2.39	106.13	111.79
24	V	611	CLA	CHB-C4A-NA	2.39	127.82	124.51
29	F	101	BCR	C27-C26-C25	2.39	126.20	122.73
23	AU	605	CHL	C1C-C2C-C3C	-2.39	105.22	107.11
24	AM	404	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	AD	302	CHL	CMD-C2D-C3D	-2.39	122.12	127.61
23	AC	606	CHL	CAC-C3C-C4C	2.39	127.91	124.81
28	AQ	618	LHG	C20-C19-C18	-2.39	102.30	114.42
24	AR	602	CLA	C1-C2-C3	-2.39	121.91	126.04
24	AK	608	CLA	CHB-C4A-NA	2.39	127.81	124.51
24	v	310	CLA	CAA-CBA-CGA	-2.39	106.28	113.25
23	q	607	CHL	O2A-CGA-CBA	2.39	119.40	111.91
23	9	609	CHL	C3D-C4D-ND	2.39	114.10	110.24
24	O	614	CLA	C3B-C4B-NB	-2.39	108.30	110.52
24	AE	603	CLA	CHB-C4A-NA	2.39	127.81	124.51
24	AC	604	CLA	C3B-C4B-NB	-2.39	108.30	110.52
25	AU	615	LUT	C32-C33-C34	2.39	122.60	118.94
24	AR	611	CLA	CHB-C4A-NA	2.39	127.81	124.51
23	AS	302	CHL	C1D-ND-C4D	-2.39	104.64	106.33
25	AE	614	LUT	C35-C15-C14	2.39	128.36	123.47
32	J	405	PHO	C1-C2-C3	-2.39	121.92	126.04
23	AB	608	CHL	CHC-C4B-NB	-2.39	121.73	124.26
24	AC	611	CLA	CHB-C4A-NA	2.38	127.81	124.51
33	P	518	LMG	O6-C1-O1	-2.38	104.33	109.97
23	AH	608	CHL	C1-O2A-CGA	2.38	122.70	116.44
29	AO	101	BCR	C2-C1-C6	2.38	114.15	110.48
23	AD	317	CHL	O2D-CGD-O1D	-2.38	119.18	123.84
23	AN	608	CHL	C4A-NA-C1A	2.38	107.78	106.71
23	0	606	CHL	CHC-C4B-NB	-2.38	121.73	124.26
24	q	601	CLA	CHB-C1B-NB	2.38	126.78	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	AS	317	NEX	C28-C29-C30	2.38	122.60	118.94
23	AS	302	CHL	CMD-C2D-C3D	-2.38	122.13	127.61
24	AC	612	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	q	605	CHL	C1C-C2C-C3C	-2.38	105.22	107.11
33	AK	622	LMG	C38-C37-C36	-2.38	102.33	114.42
29	f	101	BCR	C27-C26-C25	2.38	126.19	122.73
33	AK	601	LMG	O1-C7-C8	-2.38	105.16	110.90
23	9	609	CHL	O1D-CGD-CBD	-2.38	119.61	124.48
29	AJ	410	BCR	C27-C26-C25	2.38	126.19	122.73
24	q	603	CLA	CHB-C1B-NB	2.38	126.78	124.26
23	AN	607	CHL	C11-C12-C13	-2.38	108.23	115.92
23	AH	606	CHL	C1C-C2C-C3C	-2.38	105.23	107.11
24	AL	503	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	AQ	606	CHL	OMC-CMC-C2C	-2.38	120.31	125.69
25	AQ	615	LUT	C12-C13-C14	2.38	122.59	118.94
24	AA	604	CLA	CHB-C4A-NA	2.38	127.80	124.51
28	p	617	LHG	C20-C19-C18	-2.38	102.37	114.42
33	O	620	LMG	C38-C37-C36	-2.38	102.37	114.42
23	9	609	CHL	C6-C5-C3	-2.37	107.23	113.45
23	AS	307	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
25	q	614	LUT	C12-C13-C14	2.37	122.58	118.94
23	9	608	CHL	C2C-C1C-NC	2.37	114.35	110.44
25	AQ	616	LUT	C39-C29-C28	2.37	121.82	118.08
23	AR	606	CHL	C4-C3-C5	2.37	119.26	115.27
28	O	623	LHG	C20-C19-C18	-2.37	102.38	114.42
24	AK	603	CLA	CAA-C2A-C1A	2.37	119.75	111.97
24	AS	305	CLA	O2D-CGD-CBD	2.37	115.48	111.27
24	AF	609	CLA	CHB-C1B-NB	2.37	126.77	124.26
24	q	601	CLA	CBA-CAA-C2A	-2.37	106.86	113.86
24	P	506	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	AJ	404	CLA	CHD-C1D-ND	-2.37	122.28	124.45
33	AL	520	LMG	C40-C39-C38	-2.37	102.39	114.42
24	AR	603	CLA	CHB-C1B-NB	2.37	126.77	124.26
23	AA	606	CHL	CAA-CBA-CGA	-2.37	106.33	113.25
24	AH	602	CLA	C3B-C4B-NB	-2.37	108.32	110.52
28	AK	624	LHG	C20-C19-C18	-2.37	102.39	114.42
24	v	310	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	AA	615	LUT	C31-C30-C29	2.37	130.69	127.31
23	AC	606	CHL	O2A-CGA-CBA	2.37	121.64	114.03
23	AN	606	CHL	CMD-C2D-C3D	-2.37	122.17	127.61
33	P	518	LMG	C40-C39-C38	-2.37	102.40	114.42
33	P	518	LMG	C38-C37-C36	-2.37	102.40	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AU	606	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
33	AK	601	LMG	C40-C39-C38	-2.37	102.41	114.42
23	AS	307	CHL	C1-O2A-CGA	2.37	122.66	116.44
24	AQ	614	CLA	CGD-CBD-CAD	2.37	118.40	110.73
25	AA	615	LUT	C39-C29-C28	2.37	121.81	118.08
23	AE	617	CHL	CHB-C1B-C2B	-2.37	120.55	127.24
23	AC	607	CHL	OMC-CMC-C2C	-2.37	118.76	125.27
33	AL	501	LMG	C38-C37-C36	-2.37	102.41	114.42
24	K	101	CLA	CAA-CBA-CGA	-2.37	106.34	113.25
23	AB	608	CHL	OMC-CMC-C2C	-2.37	120.34	125.69
33	AL	520	LMG	C38-C37-C36	-2.37	102.41	114.42
23	AN	601	CHL	C1-C2-C3	-2.37	121.95	126.04
33	J	409	LMG	C38-C37-C36	-2.37	102.42	114.42
24	q	608	CLA	O1D-CGD-CBD	2.37	129.32	124.48
24	O	612	CLA	CHB-C4A-NA	2.36	127.78	124.51
33	O	624	LMG	C40-C39-C38	-2.36	102.42	114.42
38	F	102	HEM	C2A-C1A-NA	-2.36	107.50	110.15
24	O	608	CLA	CAA-CBA-CGA	-2.36	106.35	113.25
23	q	606	CHL	O2A-CGA-O1A	-2.36	117.63	123.59
32	AJ	407	PHO	CMB-C2B-C3B	2.36	129.10	124.68
24	AK	610	CLA	CHB-C4A-NA	2.36	127.78	124.51
28	AH	616	LHG	C20-C19-C18	-2.36	102.44	114.42
23	AE	616	CHL	OMC-CMC-C2C	-2.36	120.35	125.69
29	j	101	BCR	C15-C14-C13	-2.36	123.94	127.31
23	0	617	CHL	CMB-C2B-C1B	2.36	128.96	125.37
24	O	601	CLA	CBA-CAA-C2A	2.36	120.83	113.86
23	V	601	CHL	C1-C2-C3	-2.36	121.96	126.04
24	O	610	CLA	C1-C2-C3	-2.36	121.96	126.04
23	AN	606	CHL	C4-C3-C2	-2.36	117.63	123.68
24	O	605	CLA	CHD-C1D-ND	-2.36	122.29	124.45
28	v	301	LHG	C11-C10-C9	-2.36	102.45	114.42
23	V	607	CHL	C11-C12-C13	-2.36	108.30	115.92
23	0	606	CHL	C1C-C2C-C3C	-2.36	105.24	107.11
24	AS	311	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
23	9	607	CHL	C1-C2-C3	-2.36	121.97	126.04
28	O	621	LHG	C27-C26-C25	-2.36	102.47	114.42
29	AL	516	BCR	C33-C5-C6	-2.36	121.88	124.53
23	AC	605	CHL	O2A-CGA-CBA	2.36	121.60	114.03
23	AA	605	CHL	C1C-C2C-C3C	-2.36	105.25	107.11
29	AV	101	BCR	C27-C26-C25	2.35	126.15	122.73
23	AB	606	CHL	C2C-C1C-NC	2.35	114.31	110.44
24	AQ	610	CLA	CAA-CBA-CGA	-2.35	106.38	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AF	606	CHL	C1B-NB-C4B	-2.35	104.66	106.33
23	AF	605	CHL	C3C-C4C-CHD	-2.35	120.07	125.22
28	AU	617	LHG	C20-C19-C18	-2.35	102.49	114.42
24	AD	304	CLA	CHB-C4A-NA	2.35	127.76	124.51
28	AS	301	LHG	C11-C10-C9	-2.35	102.49	114.42
25	AU	615	LUT	C39-C29-C28	2.35	121.78	118.08
24	AK	614	CLA	CHB-C4A-NA	2.35	127.76	124.51
24	q	611	CLA	CHB-C4A-NA	2.35	127.76	124.51
24	AL	507	CLA	CHB-C4A-NA	2.35	127.76	124.51
24	AN	603	CLA	CHB-C4A-NA	2.35	127.76	124.51
28	O	621	LHG	C20-C19-C18	-2.35	102.50	114.42
29	O	625	BCR	C11-C10-C9	-2.35	123.96	127.31
23	AU	608	CHL	C1-O2A-CGA	2.35	122.60	116.44
23	9	605	CHL	O2A-CGA-CBA	2.35	121.57	114.03
23	V	606	CHL	C11-C10-C8	-2.35	108.33	115.92
23	AE	607	CHL	C4D-CHA-C1A	-2.35	118.39	121.25
24	AH	613	CLA	CHB-C4A-NA	2.35	127.76	124.51
23	AQ	609	CHL	CED-O2D-CGD	2.35	121.24	115.94
24	v	303	CLA	C1-C2-C3	-2.35	121.99	126.04
26	q	615	NEX	C28-C29-C30	2.34	122.54	118.94
24	P	509	CLA	CHB-C4A-NA	2.34	127.75	124.51
28	AL	519	LHG	C20-C19-C18	-2.34	102.53	114.42
24	V	603	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	v	313	CLA	CAA-CBA-CGA	-2.34	106.41	113.25
24	Q	403	CLA	CMB-C2B-C1B	-2.34	121.80	125.37
29	AK	602	BCR	C15-C14-C13	-2.34	123.97	127.31
23	AN	608	CHL	CHD-C1D-C2D	2.34	130.39	125.48
23	AQ	609	CHL	C1C-C2C-C3C	-2.34	105.25	107.11
23	9	605	CHL	C4D-CHA-C1A	-2.34	118.40	121.25
25	AE	614	LUT	C31-C30-C29	2.34	130.65	127.31
23	q	613	CHL	C1C-C2C-C3C	-2.34	105.26	107.11
23	q	606	CHL	C1D-ND-C4D	-2.34	104.67	106.33
24	AK	618	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	AN	603	CLA	CHD-C1D-ND	-2.34	122.30	124.45
35	AL	517	DGD	C3G-C2G-C1G	-2.34	106.25	111.79
28	P	517	LHG	C20-C19-C18	-2.34	102.54	114.42
25	AS	316	LUT	C11-C10-C9	2.34	130.65	127.31
24	P	512	CLA	C1B-NB-C4B	2.34	108.00	106.33
23	AB	605	CHL	C2C-C3C-C4C	-2.34	103.74	106.95
23	AD	317	CHL	CHB-C4A-NA	2.34	127.75	124.51
24	AR	602	CLA	CHB-C4A-NA	2.34	127.75	124.51
29	AI	101	BCR	C27-C26-C25	2.34	126.13	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	O	605	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	AR	608	CLA	CAA-C2A-C3A	-2.34	110.64	116.10
24	AU	609	CLA	CAA-CBA-CGA	-2.34	106.42	113.25
25	AE	614	LUT	C32-C33-C34	2.34	122.53	118.94
25	AH	615	LUT	C39-C29-C28	2.33	121.75	118.08
23	AB	607	CHL	OMC-CMC-C2C	-2.33	120.41	125.69
24	AK	608	CLA	CHD-C1D-ND	-2.33	122.31	124.45
25	V	614	LUT	C12-C13-C14	2.33	122.52	118.94
33	O	624	LMG	C38-C37-C36	-2.33	102.58	114.42
23	AC	608	CHL	O1D-CGD-CBD	-2.33	119.71	124.48
23	9	606	CHL	OMC-CMC-C2C	-2.33	120.42	125.69
35	P	516	DGD	C3G-C2G-C1G	-2.33	106.28	111.79
23	AC	605	CHL	C4D-CHA-C1A	-2.33	118.41	121.25
24	O	601	CLA	CAA-C2A-C1A	2.33	119.61	111.97
28	q	616	LHG	C20-C19-C18	-2.33	102.60	114.42
23	AR	605	CHL	C4D-CHA-C1A	-2.33	118.41	121.25
23	V	606	CHL	C4-C3-C2	-2.33	117.70	123.68
23	0	601	CHL	CHB-C4A-NA	2.33	127.73	124.51
23	AB	608	CHL	C4A-NA-C1A	2.33	107.75	106.71
23	AC	606	CHL	O2D-CGD-O1D	-2.33	119.28	123.84
33	AK	601	LMG	C38-C37-C36	-2.33	102.60	114.42
24	AC	604	CLA	CHB-C4A-NA	2.33	127.73	124.51
24	AL	510	CLA	CHB-C4A-NA	2.33	127.73	124.51
29	F	101	BCR	C24-C23-C22	-2.33	122.72	126.23
23	AD	308	CHL	C4-C3-C5	2.33	119.19	115.27
25	0	614	LUT	C8-C9-C10	2.33	122.51	118.94
38	F	102	HEM	CHC-C1C-NC	2.33	126.95	124.44
24	AC	612	CLA	C3B-C4B-NB	-2.33	108.36	110.52
24	p	612	CLA	CHB-C4A-NA	2.32	127.73	124.51
23	p	606	CHL	OMC-CMC-C2C	-2.32	120.43	125.69
23	AB	607	CHL	CAC-C3C-C4C	2.32	127.83	124.81
23	AF	605	CHL	C4A-NA-C1A	2.32	107.75	106.71
26	AQ	617	NEX	C28-C29-C30	2.32	122.51	118.94
23	0	605	CHL	C1C-C2C-C3C	-2.32	105.27	107.11
23	AC	607	CHL	C2C-C1C-NC	2.32	114.27	110.44
23	AB	605	CHL	CAC-C3C-C4C	2.32	128.08	125.27
24	AK	607	CLA	CHD-C1D-ND	-2.32	122.32	124.45
23	AE	605	CHL	C4-C3-C5	2.32	119.18	115.27
23	V	616	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
24	AC	610	CLA	CHB-C4A-NA	2.32	127.72	124.51
29	k	101	BCR	C11-C10-C9	-2.32	124.00	127.31
24	AS	304	CLA	CHB-C4A-NA	2.32	127.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AQ	601	CHL	C11-C12-C13	-2.32	108.42	115.92
23	AS	302	CHL	O2A-CGA-O1A	-2.32	117.52	123.30
32	J	406	PHO	O1D-CGD-CBD	2.32	128.60	124.74
29	f	101	BCR	C24-C23-C22	-2.32	122.73	126.23
25	p	614	LUT	C12-C13-C14	2.32	122.50	118.94
24	AJ	406	CLA	C1-C2-C3	-2.32	123.00	126.75
23	AA	608	CHL	C6-C7-C8	-2.32	108.43	115.92
23	v	306	CHL	CHB-C1B-NB	-2.32	121.80	124.26
23	AR	607	CHL	C4-C3-C5	2.32	119.17	115.27
23	AD	306	CHL	CMD-C2D-C3D	-2.32	122.28	127.61
24	AK	615	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
24	AB	611	CLA	C2A-C1A-CHA	2.32	127.91	123.86
24	0	602	CLA	O1D-CGD-CBD	2.32	129.22	124.48
28	W	201	LHG	C20-C19-C18	-2.32	102.67	114.42
24	AF	614	CLA	C3A-C2A-C1A	2.32	104.81	101.34
28	AM	406	LHG	C18-C17-C16	-2.32	102.67	114.42
24	AC	602	CLA	C3B-C4B-NB	-2.31	108.37	110.52
24	AK	612	CLA	CHB-C1B-NB	2.31	126.71	124.26
25	AQ	616	LUT	C12-C13-C14	2.31	122.49	118.94
24	q	612	CLA	C3B-C4B-NB	-2.31	108.37	110.52
24	AM	403	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
29	O	619	BCR	C15-C16-C17	-2.31	118.74	123.47
26	v	317	NEX	C28-C29-C30	2.31	122.49	118.94
23	q	607	CHL	C1C-C2C-C3C	-2.31	105.28	107.11
29	AL	515	BCR	C15-C16-C17	-2.31	118.74	123.47
23	p	609	CHL	C1C-C2C-C3C	-2.31	105.28	107.11
28	Q	406	LHG	C18-C17-C16	-2.31	102.69	114.42
24	AH	609	CLA	CGD-CBD-CAD	2.31	118.22	110.73
23	AS	308	CHL	CED-O2D-CGD	2.31	121.16	115.94
24	O	613	CLA	CHB-C4A-NA	2.31	127.70	124.51
29	AJ	410	BCR	C15-C16-C17	-2.31	118.75	123.47
24	O	610	CLA	CHB-C4A-NA	2.31	127.70	124.51
23	AN	608	CHL	CHC-C1C-NC	-2.31	120.70	124.20
23	p	607	CHL	O2A-CGA-CBA	2.31	119.15	111.91
23	AR	607	CHL	O2A-CGA-CBA	2.31	119.15	111.91
23	p	608	CHL	CED-O2D-CGD	2.31	121.15	115.94
24	AU	609	CLA	O2D-CGD-CBD	2.31	115.37	111.27
24	AQ	602	CLA	C3B-C4B-NB	-2.31	108.38	110.52
24	v	304	CLA	CHB-C4A-NA	2.31	127.70	124.51
25	AE	613	LUT	C7-C8-C9	-2.31	122.75	126.23
24	AE	602	CLA	CHD-C1D-ND	-2.30	122.34	124.45
29	AJ	410	BCR	C15-C14-C13	-2.30	124.02	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AQ	611	CLA	C1-C2-C3	-2.30	122.06	126.04
28	v	301	LHG	C18-C17-C16	-2.30	102.73	114.42
23	AD	307	CHL	C1C-C2C-C3C	-2.30	105.29	107.11
23	v	308	CHL	C2C-C1C-CHC	-2.30	120.15	125.67
23	AE	607	CHL	C6-C7-C8	-2.30	108.47	115.92
33	O	620	LMG	O1-C7-C8	-2.30	105.34	110.90
23	AD	317	CHL	C1D-ND-C4D	-2.30	104.70	106.33
24	AU	609	CLA	C1-C2-C3	-2.30	122.06	126.04
24	AU	610	CLA	CHB-C4A-NA	2.30	127.70	124.51
29	AL	516	BCR	C7-C8-C9	-2.30	122.76	126.23
28	w	201	LHG	C20-C19-C18	-2.30	102.74	114.42
24	AQ	612	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
24	AD	310	CLA	O1D-CGD-CBD	2.30	129.19	124.48
29	AK	602	BCR	C15-C16-C17	-2.30	118.76	123.47
24	AK	610	CLA	CHD-C1D-ND	-2.30	122.34	124.45
23	AR	607	CHL	C4D-CHA-C1A	-2.30	118.45	121.25
24	9	614	CLA	CHB-C4A-NA	2.30	127.69	124.51
24	q	608	CLA	CHB-C4A-NA	2.30	127.69	124.51
24	P	510	CLA	CHB-C4A-NA	2.30	127.69	124.51
24	AU	603	CLA	CHB-C1B-NB	2.30	126.69	124.26
33	AK	622	LMG	O1-C7-C8	-2.30	105.36	110.90
24	9	602	CLA	C1-C2-C3	-2.30	122.07	126.04
24	AQ	603	CLA	CHB-C1B-NB	2.30	126.69	124.26
24	V	610	CLA	CHB-C1B-NB	2.30	126.69	124.26
24	AL	511	CLA	CHB-C4A-NA	2.30	127.69	124.51
29	P	514	BCR	C7-C8-C9	-2.30	122.77	126.23
23	AH	607	CHL	C4-C3-C2	-2.29	117.79	123.68
23	V	606	CHL	CMD-C2D-C3D	-2.29	122.33	127.61
24	P	512	CLA	CMB-C2B-C1B	-2.29	123.47	125.81
23	AU	607	CHL	C4-C3-C2	-2.29	117.79	123.68
29	AO	101	BCR	C15-C16-C17	-2.29	118.78	123.47
24	AR	612	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
25	p	615	LUT	C39-C29-C28	2.29	121.69	118.08
24	AH	609	CLA	CHB-C4A-NA	2.29	127.68	124.51
23	AQ	601	CHL	C16-C15-C13	-2.29	108.51	115.92
28	AS	301	LHG	C18-C17-C16	-2.29	102.79	114.42
24	AK	615	CLA	CHB-C4A-NA	2.29	127.68	124.51
24	J	403	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
24	AB	609	CLA	CHB-C4A-NA	2.29	127.68	124.51
29	P	514	BCR	C33-C5-C6	-2.29	121.96	124.53
29	AL	516	BCR	C11-C10-C9	-2.29	124.05	127.31
23	V	606	CHL	CED-O2D-CGD	2.29	121.11	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	AI	101	BCR	C15-C16-C17	-2.29	118.79	123.47
24	v	312	CLA	CHB-C4A-NA	2.29	127.67	124.51
24	AC	613	CLA	CBA-CAA-C2A	2.28	120.61	113.86
24	Q	401	CLA	C1-C2-C3	-2.28	123.06	126.75
24	AC	612	CLA	C2D-C1D-ND	-2.28	108.42	110.10
23	AE	601	CHL	C4D-CHA-C1A	-2.28	118.47	121.25
23	0	601	CHL	O2A-CGA-O1A	-2.28	117.83	123.59
24	9	613	CLA	CAC-C3C-C4C	2.28	127.77	124.81
25	AN	614	LUT	C12-C13-C14	2.28	122.44	118.94
23	AD	306	CHL	CED-O2D-CGD	2.28	121.10	115.94
24	O	608	CLA	CHC-C1C-NC	2.28	127.67	124.20
24	O	613	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
26	AC	616	NEX	C19-C9-C10	-2.28	119.73	122.92
24	AE	610	CLA	CHB-C1B-NB	2.28	126.67	124.26
23	v	302	CHL	O2A-CGA-O1A	-2.28	117.61	123.30
24	AB	611	CLA	O2A-CGA-O1A	-2.28	117.61	123.30
24	AF	609	CLA	CAC-C3C-C2C	-2.28	123.63	127.53
24	AH	609	CLA	CHB-C1B-NB	2.28	126.67	124.26
24	AJ	404	CLA	C3A-C2A-C1A	2.28	104.75	101.34
25	V	614	LUT	C39-C29-C28	2.28	121.67	118.08
25	9	616	LUT	C12-C13-C14	2.28	122.44	118.94
25	AQ	616	LUT	C32-C33-C34	2.28	122.44	118.94
24	AL	512	CLA	C1-C2-C3	-2.28	122.11	126.04
24	AA	611	CLA	CHB-C4A-NA	2.28	127.66	124.51
23	AQ	608	CHL	O2A-CGA-CBA	2.28	119.05	111.91
24	O	606	CLA	CHB-C1B-NB	2.28	126.67	124.26
24	AK	614	CLA	CAA-CBA-CGA	-2.28	106.60	113.25
25	AN	615	LUT	C39-C29-C28	2.28	121.66	118.08
23	0	606	CHL	CMD-C2D-C3D	-2.27	122.38	127.61
24	AD	304	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
24	AE	609	CLA	CHB-C1B-NB	2.27	126.67	124.26
25	v	315	LUT	C12-C13-C14	2.27	122.43	118.94
24	q	610	CLA	O1D-CGD-CBD	2.27	129.14	124.48
24	O	612	CLA	CAA-CBA-CGA	-2.27	106.61	113.25
23	AA	606	CHL	C7-C6-C5	-2.27	107.18	113.36
24	AU	610	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
23	AN	617	CHL	CAA-C2A-C1A	2.27	119.42	111.97
23	AE	617	CHL	CAA-CBA-CGA	-2.27	106.48	112.51
23	AB	607	CHL	CED-O2D-CGD	2.27	121.08	115.94
38	f	102	HEM	CAD-CBD-CGD	-2.27	108.72	113.60
24	V	603	CLA	O2D-CGD-CBD	2.27	115.30	111.27
25	AD	314	LUT	C31-C30-C29	2.27	130.55	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AE	606	CHL	CAA-CBA-CGA	-2.27	106.48	112.51
23	AR	607	CHL	C3D-C4D-ND	2.27	113.91	110.24
24	9	610	CLA	CAA-CBA-CGA	-2.27	106.62	113.25
23	9	609	CHL	C4D-CHA-C1A	-2.27	118.49	121.25
23	9	608	CHL	OMC-CMC-C2C	-2.27	119.03	125.27
24	AL	514	CLA	CMB-C2B-C1B	-2.27	123.50	125.81
38	f	102	HEM	C3B-C2B-C1B	2.27	108.17	106.49
24	AE	603	CLA	O2D-CGD-CBD	2.27	115.30	111.27
23	AN	617	CHL	CMB-C2B-C1B	2.27	128.82	125.37
24	AB	609	CLA	CHB-C1B-NB	2.27	126.66	124.26
28	V	615	LHG	C27-C26-C25	-2.27	102.92	114.42
29	J	408	BCR	C15-C16-C17	-2.27	118.83	123.47
29	P	514	BCR	C11-C10-C9	-2.27	124.08	127.31
23	p	607	CHL	C6-C5-C3	-2.27	107.52	113.45
23	AN	608	CHL	C2D-C1D-ND	2.26	111.77	110.10
29	AK	602	BCR	C11-C10-C9	-2.26	124.08	127.31
25	AN	614	LUT	C32-C33-C34	2.26	122.42	118.94
28	AN	616	LHG	C27-C26-C25	-2.26	102.93	114.42
24	AH	603	CLA	CHB-C1B-NB	2.26	126.65	124.26
23	AR	605	CHL	C6-C7-C8	-2.26	108.61	115.92
24	9	613	CLA	C2D-C1D-ND	-2.26	108.44	110.10
23	AB	608	CHL	C1D-ND-C4D	-2.26	104.73	106.33
24	P	503	CLA	CHB-C4A-NA	2.26	127.64	124.51
24	AK	606	CLA	C1-C2-C3	-2.26	122.14	126.04
24	AL	504	CLA	CHB-C4A-NA	2.26	127.63	124.51
25	V	613	LUT	C32-C33-C34	2.26	122.40	118.94
33	O	624	LMG	O3-C3-C2	-2.26	105.14	110.35
24	AR	612	CLA	C3B-C4B-NB	-2.25	108.42	110.52
23	V	605	CHL	OMC-CMC-C2C	-2.25	120.59	125.69
23	AE	605	CHL	CHB-C1B-C2B	-2.25	120.87	127.24
33	J	409	LMG	O3-C3-C2	-2.25	105.14	110.35
29	P	513	BCR	C15-C16-C17	-2.25	118.86	123.47
24	V	603	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
24	AF	609	CLA	CBD-CHA-C1A	2.25	131.15	128.50
23	AS	302	CHL	O2A-CGA-CBA	2.25	121.26	114.03
24	AN	603	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
23	q	613	CHL	CHC-C4B-NB	-2.25	121.88	124.26
29	AV	101	BCR	C15-C16-C17	-2.25	118.87	123.47
24	AU	602	CLA	C3B-C4B-NB	-2.25	108.43	110.52
29	J	408	BCR	C15-C14-C13	-2.25	124.10	127.31
24	AD	304	CLA	O2D-CGD-CBD	2.25	115.26	111.27
23	v	307	CHL	C4D-CHA-C1A	-2.25	118.51	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AK	608	CLA	CHB-C1B-NB	2.25	126.64	124.26
24	AU	611	CLA	C1-C2-C3	-2.25	122.16	126.04
24	P	501	CLA	O2D-CGD-CBD	2.25	115.26	111.27
23	AR	605	CHL	CAA-CBA-CGA	-2.25	106.69	113.25
23	p	608	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
24	AH	609	CLA	CAA-CBA-CGA	-2.24	106.69	113.25
25	AS	316	LUT	C12-C13-C14	2.24	122.38	118.94
23	AC	608	CHL	CAA-C2A-C1A	2.24	119.33	111.97
24	q	603	CLA	CHB-C4A-NA	2.24	127.61	124.51
28	AL	519	LHG	O8-C23-C24	2.24	118.95	111.91
24	AR	601	CLA	CHB-C1B-NB	2.24	126.63	124.26
25	AC	615	LUT	C12-C13-C14	2.24	122.38	118.94
24	O	606	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
25	AA	615	LUT	C11-C10-C9	2.24	130.51	127.31
24	AK	611	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
23	v	302	CHL	O2A-CGA-CBA	2.24	121.22	114.03
33	Q	407	LMG	O3-C3-C2	-2.24	105.17	110.35
29	AK	621	BCR	C27-C26-C25	2.24	125.98	122.73
24	9	613	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
24	AC	613	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
23	V	616	CHL	CMB-C2B-C1B	2.24	128.78	125.37
24	AQ	610	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
32	AJ	407	PHO	C1-C2-C3	-2.24	122.18	126.04
24	AU	609	CLA	CHB-C4A-NA	2.24	127.60	124.51
29	AK	621	BCR	C15-C16-C17	-2.23	118.90	123.47
24	AQ	603	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
23	v	306	CHL	C2C-C1C-NC	2.23	114.12	110.44
23	AH	608	CHL	O2A-CGA-CBA	2.23	118.92	111.91
28	O	623	LHG	C18-C17-C16	-2.23	103.09	114.42
24	AS	312	CLA	CHB-C4A-NA	2.23	127.60	124.51
24	AJ	409	CLA	C1-C2-C3	-2.23	122.18	126.04
24	p	603	CLA	CHB-C1B-NB	2.23	126.62	124.26
33	AK	601	LMG	O3-C3-C2	-2.23	105.19	110.35
25	AS	315	LUT	C12-C13-C14	2.23	122.36	118.94
25	V	613	LUT	C31-C30-C29	2.23	130.49	127.31
24	AR	601	CLA	CBA-CAA-C2A	-2.23	107.28	113.86
24	AK	613	CLA	C3A-C2A-C1A	2.23	104.68	101.34
28	AK	624	LHG	C18-C17-C16	-2.23	103.11	114.42
33	AL	501	LMG	O3-C3-C2	-2.23	105.19	110.35
23	9	607	CHL	C1C-C2C-C3C	-2.23	105.34	107.11
24	AA	602	CLA	O2D-CGD-CBD	2.23	115.23	111.27
24	AC	612	CLA	O1D-CGD-CBD	2.23	129.04	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	p	611	CLA	CHB-C4A-NA	2.23	127.59	124.51
38	F	102	HEM	CAD-CBD-CGD	-2.23	108.81	113.60
29	j	101	BCR	C15-C16-C17	-2.23	118.91	123.47
25	AR	614	LUT	C8-C9-C10	2.23	122.36	118.94
23	AS	307	CHL	CMD-C2D-C3D	-2.23	122.49	127.61
24	9	614	CLA	CHD-C1D-ND	-2.23	122.41	124.45
28	q	616	LHG	C18-C17-C16	-2.23	103.13	114.42
24	p	618	CLA	C2A-C1A-CHA	2.23	127.75	123.86
24	AB	602	CLA	CAA-C2A-C1A	2.22	119.27	111.97
23	AE	605	CHL	CED-O2D-CGD	2.22	120.97	115.94
29	j	101	BCR	C11-C10-C9	-2.22	124.14	127.31
23	q	607	CHL	C1-C2-C3	-2.22	122.20	126.04
33	AM	407	LMG	O3-C3-C2	-2.22	105.21	110.35
28	p	617	LHG	C27-C26-C25	-2.22	103.14	114.42
24	9	604	CLA	O2D-CGD-CBD	2.22	115.22	111.27
24	AK	613	CLA	CMB-C2B-C1B	-2.22	121.98	125.37
23	AC	605	CHL	OMC-CMC-C2C	-2.22	120.66	125.69
23	AC	606	CHL	OMC-CMC-C2C	-2.22	120.66	125.69
24	AU	609	CLA	CHB-C1B-NB	2.22	126.61	124.26
24	AE	610	CLA	CHB-C4A-NA	2.22	127.58	124.51
24	K	101	CLA	C1-C2-C3	-2.22	122.20	126.04
24	0	603	CLA	C3B-C4B-NB	-2.22	108.45	110.52
24	AC	613	CLA	CHA-C1A-NA	-2.22	121.31	126.40
24	AF	614	CLA	CHC-C4B-NB	2.22	126.61	124.26
24	AF	609	CLA	C3B-C4B-NB	-2.22	108.46	110.52
24	p	603	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
23	AF	607	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
23	q	606	CHL	CED-O2D-CGD	2.22	120.95	115.94
33	AK	622	LMG	O3-C3-C2	-2.22	105.22	110.35
24	q	601	CLA	O1D-CGD-CBD	2.22	129.02	124.48
23	q	613	CHL	C1D-ND-C4D	-2.22	104.76	106.33
25	AA	615	LUT	C11-C12-C13	2.22	132.64	126.42
24	AA	611	CLA	CHB-C1B-NB	2.22	126.60	124.26
28	W	201	LHG	C27-C26-C25	-2.22	103.17	114.42
24	v	311	CLA	CHD-C1D-ND	-2.22	122.42	124.45
24	O	611	CLA	C3A-C2A-C1A	2.22	104.66	101.34
23	AB	607	CHL	C4D-CHA-C1A	-2.22	118.55	121.25
24	AQ	603	CLA	O2D-CGD-CBD	2.22	115.21	111.27
24	0	611	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	AS	302	CHL	CAA-C2A-C1A	2.22	119.24	111.97
25	AN	614	LUT	C19-C9-C8	2.22	121.57	118.08
23	AD	307	CHL	CAA-CBA-CGA	-2.22	106.63	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AF	602	CLA	C2A-C1A-CHA	2.22	127.72	123.85
25	p	615	LUT	C12-C13-C14	2.22	122.34	118.94
24	AS	313	CLA	CAA-CBA-CGA	-2.21	106.78	113.25
29	AK	602	BCR	C27-C26-C25	2.21	125.95	122.73
24	AH	609	CLA	C1-C2-C3	-2.21	122.22	126.04
24	O	615	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
24	AN	603	CLA	O2D-CGD-CBD	2.21	115.20	111.27
23	AA	607	CHL	CAA-CBA-CGA	-2.21	106.63	112.51
23	AR	605	CHL	C2C-C1C-NC	2.21	114.08	110.44
28	AQ	618	LHG	C27-C26-C25	-2.21	103.19	114.42
24	AR	610	CLA	O1D-CGD-CBD	2.21	129.01	124.48
24	O	613	CLA	CHB-C1B-NB	2.21	126.60	124.26
24	AH	609	CLA	O2D-CGD-CBD	2.21	115.20	111.27
24	AA	612	CLA	CAA-C2A-C1A	2.21	119.22	111.97
23	AA	617	CHL	CHB-C1B-C2B	-2.21	120.99	127.24
23	q	607	CHL	C4D-CHA-C1A	-2.21	118.56	121.25
24	V	611	CLA	CHB-C1B-NB	2.21	126.60	124.26
28	AD	316	LHG	C27-C26-C25	-2.21	103.20	114.42
28	w	201	LHG	C27-C26-C25	-2.21	103.21	114.42
24	AN	611	CLA	CHB-C1B-NB	2.21	126.60	124.26
24	O	609	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
24	AH	610	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
24	q	612	CLA	CAA-CBA-CGA	-2.21	106.80	113.25
23	9	606	CHL	C2A-C1A-CHA	-2.21	120.00	123.86
25	AA	615	LUT	C15-C14-C13	2.21	130.46	127.31
23	AF	607	CHL	CED-O2D-CGD	2.21	120.93	115.94
29	O	619	BCR	C27-C26-C25	2.21	125.94	122.73
23	AE	605	CHL	C1-C2-C3	-2.21	122.22	126.04
23	AN	607	CHL	C1-O2A-CGA	2.21	122.24	116.44
23	p	608	CHL	O2A-CGA-CBA	2.21	118.83	111.91
24	AC	612	CLA	CMA-C3A-C2A	-2.21	110.95	116.10
28	0	616	LHG	C27-C26-C25	-2.21	103.22	114.42
24	AD	309	CLA	C1-C2-C3	-2.21	122.23	126.04
24	O	612	CLA	C1-C2-C3	-2.21	122.23	126.04
24	AC	602	CLA	C1-C2-C3	-2.20	122.23	126.04
24	AB	602	CLA	C3B-C4B-NB	-2.20	108.47	110.52
24	AR	608	CLA	CHB-C1B-NB	2.20	126.59	124.26
28	AK	623	LHG	C27-C26-C25	-2.20	103.24	114.42
24	O	606	CLA	C3B-C4B-NB	-2.20	108.47	110.52
24	P	503	CLA	CGD-CBD-CAD	2.20	117.87	110.73
23	AA	608	CHL	O2A-CGA-O1A	-2.20	118.03	123.59
24	0	603	CLA	O2A-CGA-O1A	-2.20	118.03	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	O	620	LMG	O2-C2-C1	-2.20	104.70	110.05
35	AL	518	DGD	C3G-C2G-C1G	-2.20	106.59	111.79
23	AN	606	CHL	CED-O2D-CGD	2.20	120.91	115.94
23	AU	608	CHL	O2A-CGA-CBA	2.20	118.81	111.91
26	AA	616	NEX	C10-C11-C12	2.20	130.08	123.22
24	AK	615	CLA	CHB-C1B-NB	2.20	126.58	124.26
24	AK	617	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
24	O	615	CLA	CHB-C4A-NA	2.20	127.55	124.51
28	AQ	618	LHG	C18-C17-C16	-2.20	103.27	114.42
24	p	610	CLA	CAA-C2A-C1A	2.20	119.05	111.86
28	AL	519	LHG	C18-C17-C16	-2.20	103.27	114.42
24	AK	611	CLA	O2D-CGD-CBD	2.20	115.17	111.27
33	O	620	LMG	O3-C3-C2	-2.20	105.27	110.35
23	AQ	601	CHL	OMC-CMC-C2C	-2.20	120.72	125.69
33	P	518	LMG	O3-C3-C2	-2.20	105.27	110.35
24	P	508	CLA	O2D-CGD-CBD	2.19	115.17	111.27
28	p	617	LHG	C18-C17-C16	-2.19	103.28	114.42
23	v	308	CHL	CED-O2D-CGD	2.19	120.90	115.94
29	P	515	BCR	C38-C26-C25	-2.19	122.06	124.53
29	J	408	BCR	C11-C10-C9	-2.19	124.18	127.31
23	AE	616	CHL	O2A-CGA-CBA	2.19	121.08	114.03
23	AR	606	CHL	CHB-C4A-NA	2.19	127.54	124.51
35	AL	517	DGD	CAB-C9B-C8B	-2.19	103.29	114.42
24	AL	509	CLA	O2D-CGD-CBD	2.19	115.16	111.27
28	P	517	LHG	C18-C17-C16	-2.19	103.30	114.42
26	AE	615	NEX	C10-C11-C12	2.19	130.05	123.22
29	k	101	BCR	C38-C26-C25	-2.19	122.07	124.53
29	AI	101	BCR	C15-C14-C13	-2.19	124.19	127.31
25	AC	614	LUT	C8-C9-C10	2.19	122.30	118.94
24	AN	609	CLA	CHB-C1B-NB	2.19	126.57	124.26
24	AD	303	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	P	511	CLA	CHB-C1B-NB	2.19	126.57	124.26
28	O	622	LHG	C27-C26-C25	-2.19	103.32	114.42
24	AS	314	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	V	603	CLA	CHD-C1D-ND	-2.19	122.44	124.45
35	P	516	DGD	CAB-C9B-C8B	-2.19	103.33	114.42
23	AD	317	CHL	CMB-C2B-C1B	2.19	128.70	125.37
33	AL	520	LMG	O3-C3-C2	-2.18	105.30	110.35
29	AB	612	BCR	C24-C23-C22	-2.18	122.93	126.23
23	0	606	CHL	C4A-NA-C1A	2.18	107.69	106.71
24	V	611	CLA	O1D-CGD-CBD	2.18	128.95	124.48
24	p	603	CLA	O2D-CGD-CBD	2.18	115.15	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AQ	612	CLA	C2D-C1D-ND	-2.18	108.50	110.10
24	AK	617	CLA	CHB-C4A-NA	2.18	127.53	124.51
33	AK	622	LMG	O2-C2-C1	-2.18	104.74	110.05
24	p	618	CLA	CHA-C4D-ND	2.18	137.06	132.50
28	AU	617	LHG	C18-C17-C16	-2.18	103.34	114.42
24	AK	614	CLA	C1-C2-C3	-2.18	122.27	126.04
38	f	102	HEM	C3D-C4D-ND	-2.18	107.74	110.17
24	P	504	CLA	CAA-CBA-CGA	-2.18	106.88	113.25
37	Q	405	PL9	C37-C38-C39	-2.18	122.41	127.66
24	AS	313	CLA	C2D-C1D-ND	-2.18	108.50	110.10
32	AJ	408	PHO	C1-C2-C3	-2.18	122.27	126.04
28	AH	616	LHG	C18-C17-C16	-2.18	103.36	114.42
24	AE	608	CLA	C1-C2-C3	-2.18	123.22	126.75
23	0	605	CHL	CAA-C2A-C1A	2.18	119.12	111.97
24	AC	613	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
35	AO	102	DGD	O5D-C6D-C5D	-2.18	105.02	109.05
24	AN	604	CLA	CAA-C2A-C3A	-2.18	111.02	116.10
23	V	607	CHL	C1-O2A-CGA	2.18	122.16	116.44
24	AR	603	CLA	CHB-C4A-NA	2.18	127.52	124.51
29	j	101	BCR	C38-C26-C25	-2.18	122.08	124.53
23	AA	606	CHL	CMD-C2D-C3D	-2.18	122.61	127.61
24	AK	618	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
24	AF	603	CLA	CHB-C4A-NA	2.18	127.52	124.51
28	AU	617	LHG	C27-C26-C25	-2.18	103.38	114.42
23	V	616	CHL	CAA-C2A-C3A	2.18	118.73	112.78
23	AA	601	CHL	CAA-C2A-C1A	2.17	119.10	111.97
24	AK	604	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	AH	606	CHL	O2A-CGA-O1A	-2.17	118.11	123.59
24	AA	603	CLA	O2D-CGD-CBD	2.17	115.12	111.27
23	AC	608	CHL	C4D-CHA-C1A	-2.17	118.61	121.25
23	AA	617	CHL	O2A-CGA-CBA	2.17	121.00	114.03
24	AK	617	CLA	CHB-C1B-NB	2.17	126.55	124.26
24	v	314	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
23	AS	307	CHL	OMC-CMC-C2C	-2.17	120.78	125.69
23	AH	606	CHL	O2D-CGD-O1D	-2.17	119.60	123.84
24	AK	603	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
23	AC	605	CHL	C2A-C3A-C4A	-2.17	98.37	101.87
24	AF	603	CLA	CHB-C1B-NB	2.17	126.55	124.26
23	AN	606	CHL	C4D-CHA-C1A	-2.17	118.61	121.25
28	AH	616	LHG	C27-C26-C25	-2.17	103.42	114.42
24	O	615	CLA	CHB-C1B-NB	2.17	126.55	124.26
38	F	102	HEM	CHB-C1B-NB	2.17	127.05	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	v	307	CHL	CBC-CAC-C3C	-2.17	106.46	112.43
24	P	504	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
23	AD	308	CHL	C4D-CHA-C1A	-2.17	118.61	121.25
24	AQ	604	CLA	O2D-CGD-CBD	2.16	115.11	111.27
24	AH	611	CLA	C1-C2-C3	-2.16	122.30	126.04
24	AE	604	CLA	O2A-CGA-O1A	-2.16	117.91	123.30
35	AL	518	DGD	CBB-CAB-C9B	-2.16	103.44	114.42
23	AA	608	CHL	OMC-CMC-C2C	-2.16	120.80	125.69
24	q	601	CLA	C2D-C1D-ND	-2.16	108.51	110.10
24	AE	603	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
24	AD	312	CLA	O1D-CGD-CBD	2.16	128.91	124.48
24	AU	613	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	AE	616	CHL	CHB-C1B-NB	-2.16	121.97	124.26
23	V	616	CHL	OBD-CAD-C3D	-2.16	123.32	128.52
25	AD	314	LUT	C8-C9-C10	2.16	122.26	118.94
24	AB	603	CLA	CHB-C4A-NA	2.16	127.50	124.51
28	O	621	LHG	C18-C17-C16	-2.16	103.46	114.42
24	AS	311	CLA	O1D-CGD-CBD	2.16	128.91	124.48
24	AR	617	CLA	O1A-CGA-CBA	2.16	130.02	123.08
23	9	606	CHL	C4D-CHA-C1A	-2.16	118.62	121.25
24	O	616	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	p	602	CLA	C1-C2-C3	-2.16	122.31	126.04
37	AM	405	PL9	C37-C38-C39	-2.16	122.46	127.66
28	v	301	LHG	C27-C26-C25	-2.16	103.46	114.42
25	p	615	LUT	C32-C33-C34	2.16	122.25	118.94
23	AQ	607	CHL	CAA-CBA-CGA	-2.16	106.94	113.25
25	AN	615	LUT	C12-C13-C14	2.16	122.25	118.94
23	p	606	CHL	O2A-CGA-O1A	-2.16	118.14	123.59
23	p	609	CHL	O2A-CGA-CBA	2.16	118.68	111.91
28	AL	519	LHG	C27-C26-C25	-2.16	103.47	114.42
24	9	603	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
29	AO	101	BCR	C33-C5-C6	-2.16	122.11	124.53
24	AF	614	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
24	AL	513	CLA	CHB-C1B-NB	2.16	126.54	124.26
24	O	605	CLA	C2D-C1D-ND	-2.16	108.52	110.10
23	AU	605	CHL	O2D-CGD-O1D	-2.16	119.62	123.84
24	O	610	CLA	C2D-C1D-ND	-2.15	108.52	110.10
24	O	602	CLA	CHD-C1D-ND	-2.15	122.47	124.45
24	AJ	404	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
24	AL	506	CLA	O1D-CGD-CBD	2.15	128.89	124.48
24	AC	613	CLA	C2A-C1A-CHA	2.15	127.62	123.86
24	p	611	CLA	CHB-C1B-NB	2.15	126.54	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AK	614	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
24	AS	312	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
23	V	608	CHL	O2A-CGA-CBA	2.15	118.66	111.91
29	P	515	BCR	C11-C10-C9	-2.15	124.24	127.31
29	AJ	410	BCR	C11-C10-C9	-2.15	124.24	127.31
23	AR	613	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
23	AA	617	CHL	CMB-C2B-C1B	2.15	128.65	125.37
23	p	607	CHL	CAA-CBA-CGA	-2.15	106.96	113.25
28	O	623	LHG	C27-C26-C25	-2.15	103.50	114.42
24	9	602	CLA	CAA-CBA-CGA	-2.15	106.97	113.25
38	F	102	HEM	C4C-NC-C1C	2.15	107.45	105.35
29	O	625	BCR	C8-C7-C6	-2.15	121.16	127.20
25	AE	614	LUT	C19-C9-C8	2.15	121.47	118.08
24	AR	603	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
28	P	517	LHG	C27-C26-C25	-2.15	103.51	114.42
23	AR	607	CHL	C1-C2-C3	-2.15	122.33	126.04
28	AS	301	LHG	C27-C26-C25	-2.15	103.51	114.42
24	AF	602	CLA	CHB-C1B-NB	2.15	126.53	124.26
24	AC	603	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
24	AK	615	CLA	O1D-CGD-CBD	2.15	128.88	124.48
23	v	302	CHL	CAA-C2A-C1A	2.15	119.01	111.97
24	P	506	CLA	CHB-C1B-NB	2.15	126.53	124.26
23	AN	605	CHL	CAA-CBA-CGA	-2.14	106.98	113.25
24	AN	610	CLA	CAA-C2A-C3A	-2.14	111.09	116.10
23	AU	606	CHL	CAA-C2A-C3A	-2.14	106.91	112.78
23	0	605	CHL	O2A-CGA-CBA	2.14	120.92	114.03
23	AD	307	CHL	OMC-CMC-C2C	-2.14	120.84	125.69
24	J	403	CLA	C3A-C2A-C1A	2.14	104.55	101.34
33	O	624	LMG	O2-C2-C1	-2.14	104.84	110.05
24	AQ	610	CLA	CGD-CBD-CAD	2.14	117.68	110.73
24	O	607	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
24	AK	609	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
25	AQ	616	LUT	C7-C8-C9	-2.14	123.00	126.23
23	AU	601	CHL	O2D-CGD-O1D	-2.14	119.65	123.84
29	AL	516	BCR	C24-C23-C22	-2.14	123.00	126.23
29	O	625	BCR	C27-C26-C25	2.14	125.84	122.73
23	AD	307	CHL	CAA-C2A-C1A	2.14	118.99	111.97
33	AK	601	LMG	O2-C2-C1	-2.14	104.84	110.05
29	AK	602	BCR	C8-C7-C6	-2.14	121.19	127.20
24	AM	403	CLA	CHD-C1D-ND	-2.14	122.49	124.45
24	AA	603	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
24	O	613	CLA	O1D-CGD-CBD	2.14	128.86	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	505	CLA	O1D-CGD-CBD	2.14	128.86	124.48
24	q	612	CLA	CHC-C4B-NB	2.14	126.52	124.26
24	AK	612	CLA	C1-C2-C3	-2.14	122.34	126.04
24	AA	609	CLA	C1-C2-C3	-2.14	123.29	126.75
23	AA	608	CHL	C3B-C4B-NB	2.14	112.50	110.52
24	v	312	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
23	q	613	CHL	C4D-CHA-C1A	-2.14	118.65	121.25
24	AD	312	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
29	AV	101	BCR	C15-C14-C13	-2.14	124.26	127.31
24	AJ	404	CLA	CHB-C1B-NB	2.14	126.52	124.26
24	V	602	CLA	C3B-C4B-NB	-2.14	108.53	110.52
33	O	624	LMG	O1-C1-C2	-2.14	104.97	108.30
23	0	601	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
23	AQ	607	CHL	C6-C5-C3	-2.14	107.85	113.45
33	AM	407	LMG	O1-C1-C2	-2.14	104.97	108.30
24	O	612	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
24	J	403	CLA	CHD-C1D-ND	-2.13	122.49	124.45
35	j	102	DGD	CBB-CAB-C9B	-2.13	103.59	114.42
23	AR	607	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
23	AE	601	CHL	CAA-C2A-C1A	2.13	118.97	111.97
25	q	614	LUT	C31-C30-C29	2.13	130.36	127.31
25	AS	316	LUT	C3-C4-C5	2.13	116.11	111.85
24	AS	311	CLA	CHD-C1D-ND	-2.13	122.49	124.45
24	AA	613	CLA	O1D-CGD-CBD	2.13	128.85	124.48
24	AF	609	CLA	CMB-C2B-C3B	2.13	131.75	126.59
24	AC	603	CLA	CHB-C4A-NA	2.13	127.46	124.51
23	p	607	CHL	CHB-C1B-C2B	-2.13	121.22	127.24
33	Q	407	LMG	O2-C2-C1	-2.13	104.87	110.05
24	0	612	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
24	q	602	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
28	w	201	LHG	C18-C17-C16	-2.13	103.61	114.42
23	v	307	CHL	OMC-CMC-C2C	-2.13	120.87	125.69
23	p	607	CHL	C1C-C2C-C3C	-2.13	105.42	107.11
28	AK	624	LHG	C27-C26-C25	-2.13	103.61	114.42
24	AS	303	CLA	C2D-C1D-ND	-2.13	108.53	110.10
38	f	102	HEM	C1B-NB-C4B	2.13	107.27	105.07
23	AQ	609	CHL	C6-C7-C8	-2.13	109.04	115.92
23	AF	606	CHL	CED-O2D-CGD	2.13	120.75	115.94
28	W	201	LHG	C18-C17-C16	-2.13	103.62	114.42
23	0	617	CHL	OMC-CMC-C2C	-2.13	120.88	125.69
24	AD	313	CLA	CED-O2D-CGD	-2.13	111.12	115.94
35	AO	102	DGD	CBB-CAB-C9B	-2.13	103.62	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	q	603	CLA	CMB-C2B-C1B	-2.13	122.13	125.37
24	9	603	CLA	CHB-C4A-NA	2.13	127.45	124.51
24	v	313	CLA	C1-C2-C3	-2.13	122.36	126.04
24	AA	611	CLA	O2A-CGA-O1A	-2.13	118.00	123.30
24	AM	404	CLA	CHB-C1B-NB	2.13	126.51	124.26
28	V	615	LHG	C18-C17-C16	-2.13	103.64	114.42
23	AE	616	CHL	CHB-C1B-C2B	-2.13	121.23	127.24
23	AC	601	CHL	CHC-C4B-C3B	-2.13	120.88	130.47
37	AM	405	PL9	O1-C4-C3	-2.12	118.38	120.72
28	AN	616	LHG	C18-C17-C16	-2.12	103.64	114.42
24	q	612	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
23	AE	616	CHL	C3D-C4D-ND	2.12	113.67	110.24
33	AL	520	LMG	O2-C2-C1	-2.12	104.89	110.05
35	AL	517	DGD	C5B-C4B-C3B	-2.12	103.65	114.42
24	V	602	CLA	CHD-C1D-ND	-2.12	122.50	124.45
25	AQ	616	LUT	C8-C9-C10	2.12	122.20	118.94
23	q	606	CHL	CAA-C2A-C1A	2.12	118.92	111.97
33	AM	407	LMG	O2-C2-C1	-2.12	104.89	110.05
24	AL	503	CLA	O2D-CGD-CBD	2.12	115.03	111.27
24	0	611	CLA	CHB-C1B-NB	2.12	126.50	124.26
23	AC	606	CHL	C4D-C3D-CAD	2.12	110.59	108.10
23	AR	607	CHL	OMC-CMC-C2C	-2.12	120.90	125.69
23	AS	307	CHL	CBC-CAC-C3C	-2.12	106.59	112.43
23	9	607	CHL	OMC-CMC-C2C	-2.12	120.90	125.69
24	9	610	CLA	C1-C2-C3	-2.12	122.38	126.04
24	AQ	613	CLA	C1-C2-C3	-2.12	122.38	126.04
24	AE	608	CLA	CAA-CBA-CGA	-2.12	107.06	113.25
24	O	601	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
24	O	613	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	AD	302	CHL	CHC-C4B-NB	-2.12	122.02	124.26
23	q	607	CHL	CHC-C4B-NB	-2.12	122.02	124.26
24	AA	603	CLA	CHB-C1B-NB	2.12	126.50	124.26
24	AQ	611	CLA	CHB-C1B-NB	2.12	126.50	124.26
23	AC	608	CHL	CHB-C4A-NA	2.12	127.44	124.51
24	AK	604	CLA	O2D-CGD-CBD	2.12	115.03	111.27
23	V	606	CHL	C4D-CHA-C1A	-2.12	118.67	121.25
23	AF	608	CHL	C1D-ND-C4D	-2.12	104.83	106.33
24	q	612	CLA	C1-C2-C3	-2.12	122.38	126.04
26	q	615	NEX	C10-C11-C12	2.12	129.82	123.22
23	9	608	CHL	CAA-CBA-CGA	-2.12	106.89	112.51
23	AR	613	CHL	CMD-C2D-C3D	-2.11	122.75	127.61
29	F	101	BCR	C16-C15-C14	-2.11	119.14	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AF	602	CLA	C1D-ND-C4D	2.11	107.84	106.33
24	p	612	CLA	CHB-C1B-NB	2.11	126.50	124.26
23	9	609	CHL	C6-C7-C8	-2.11	109.09	115.92
23	p	609	CHL	C6-C7-C8	-2.11	109.09	115.92
23	AQ	609	CHL	C4-C3-C5	2.11	118.83	115.27
33	P	518	LMG	O2-C2-C1	-2.11	104.91	110.05
35	P	516	DGD	C5B-C4B-C3B	-2.11	103.70	114.42
35	AJ	412	DGD	CBB-CAB-C9B	-2.11	103.70	114.42
24	AL	505	CLA	CED-O2D-CGD	2.11	120.72	115.94
35	AL	518	DGD	CAB-C9B-C8B	-2.11	103.70	114.42
35	AL	517	DGD	CBB-CAB-C9B	-2.11	103.71	114.42
35	AJ	412	DGD	C3D-C4D-C5D	-2.11	106.47	110.24
37	Q	405	PL9	O1-C4-C3	-2.11	118.39	120.72
29	O	625	BCR	C24-C23-C22	-2.11	123.05	126.23
24	Q	403	CLA	CHD-C1D-ND	-2.11	122.51	124.45
24	AF	610	CLA	C3B-C4B-NB	-2.11	108.56	110.52
36	J	412	BCT	O3-C-O1	-2.11	114.07	119.55
24	AE	603	CLA	CHB-C1B-NB	2.11	126.49	124.26
24	O	602	CLA	C3A-C2A-C1A	2.11	104.50	101.34
35	AJ	412	DGD	CAB-C9B-C8B	-2.11	103.72	114.42
24	AL	514	CLA	CMB-C2B-C3B	2.11	129.73	124.52
23	p	606	CHL	CBB-CAB-C3B	-2.11	117.13	127.62
23	V	607	CHL	CHC-C4B-C3B	-2.11	120.95	130.47
23	AU	607	CHL	C11-C10-C8	-2.11	109.11	115.92
23	V	607	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
24	P	512	CLA	CMB-C2B-C3B	2.11	129.73	124.52
32	J	406	PHO	C1-C2-C3	-2.11	122.40	126.04
29	AF	612	BCR	C15-C14-C13	-2.11	124.31	127.31
24	AK	608	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
24	AQ	610	CLA	CHB-C1B-NB	2.10	126.48	124.26
23	p	601	CHL	OMC-CMC-C2C	-2.10	120.93	125.69
23	AA	608	CHL	C3D-C4D-ND	2.10	113.64	110.24
35	J	411	DGD	CBB-CAB-C9B	-2.10	103.75	114.42
35	J	411	DGD	C3D-C4D-C5D	-2.10	106.49	110.24
24	AL	508	CLA	O2D-CGD-CBD	2.10	115.00	111.27
24	O	615	CLA	CHD-C1D-ND	-2.10	122.52	124.45
24	AK	607	CLA	C2D-C1D-ND	-2.10	108.56	110.10
23	AS	306	CHL	C2C-C1C-NC	2.10	113.90	110.44
23	V	605	CHL	CBA-CAA-C2A	2.10	120.07	113.86
24	AN	612	CLA	CMB-C2B-C3B	2.10	131.68	126.59
23	AQ	606	CHL	CAA-CBA-CGA	-2.10	107.11	113.25
28	AD	316	LHG	C18-C17-C16	-2.10	103.76	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	P	516	DGD	CBB-CAB-C9B	-2.10	103.76	114.42
37	AM	405	PL9	O2-C1-C6	2.10	124.23	120.59
29	f	101	BCR	C16-C15-C14	-2.10	119.17	123.47
23	V	607	CHL	C4A-NA-C1A	2.10	107.65	106.71
35	J	413	DGD	CBB-CAB-C9B	-2.10	103.77	114.42
23	p	609	CHL	C4-C3-C5	2.10	118.80	115.27
24	P	505	CLA	CHC-C4B-NB	2.10	126.48	124.26
35	J	411	DGD	CAB-C9B-C8B	-2.10	103.77	114.42
24	P	501	CLA	CHB-C1B-NB	2.10	126.48	124.26
29	AK	619	BCR	C7-C8-C9	-2.10	123.07	126.23
24	AC	609	CLA	CAA-CBA-CGA	-2.10	107.13	113.25
23	AD	317	CHL	CMD-C2D-C3D	-2.10	122.79	127.61
24	AK	615	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
29	P	513	BCR	C24-C23-C22	-2.10	123.07	126.23
24	AK	614	CLA	CHC-C4B-NB	2.10	126.47	124.26
24	V	612	CLA	CHB-C4A-NA	2.09	127.41	124.51
24	AN	602	CLA	C1-C2-C3	-2.09	122.42	126.04
33	AK	601	LMG	O1-C1-C2	-2.09	105.03	108.30
24	AC	613	CLA	CHB-C1B-NB	2.09	126.47	124.26
24	AN	613	CLA	CMB-C2B-C1B	-2.09	122.18	125.37
23	v	302	CHL	OMC-CMC-C2C	-2.09	120.95	125.69
24	0	603	CLA	O2D-CGD-CBD	2.09	114.99	111.27
24	AK	603	CLA	CHA-C1A-NA	-2.09	121.61	126.40
23	p	609	CHL	CAA-C2A-C3A	-2.09	107.05	112.78
23	AS	302	CHL	CHC-C4B-C3B	-2.09	121.03	130.47
23	AS	307	CHL	O2A-CGA-O1A	-2.09	118.31	123.59
24	9	613	CLA	C3B-C4B-NB	-2.09	108.57	110.52
23	AE	617	CHL	C1D-ND-C4D	-2.09	104.85	106.33
24	AN	611	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
24	AE	609	CLA	CHD-C1D-ND	-2.09	122.53	124.45
24	AN	612	CLA	CHB-C1B-NB	2.09	126.47	124.26
24	9	613	CLA	O1D-CGD-CBD	2.09	128.76	124.48
23	AN	607	CHL	CHC-C4B-NB	-2.09	122.04	124.26
35	AJ	401	DGD	CBB-CAB-C9B	-2.09	103.81	114.42
24	O	604	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
25	0	614	LUT	C31-C30-C29	2.09	130.29	127.31
24	P	507	CLA	O2D-CGD-CBD	2.09	114.98	111.27
24	AF	604	CLA	CGD-CBD-CAD	2.09	117.50	110.73
24	AE	610	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
23	v	302	CHL	CHC-C4B-C3B	-2.09	121.05	130.47
24	q	608	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
23	AB	606	CHL	CHB-C4A-NA	2.09	127.40	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	J	407	CLA	C1-C2-C3	-2.09	122.43	126.04
24	AE	611	CLA	CAA-C2A-C1A	2.09	118.81	111.97
23	q	606	CHL	O2D-CGD-O1D	-2.09	119.76	123.84
23	AH	607	CHL	C11-C10-C8	-2.09	109.17	115.92
24	V	610	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
23	v	306	CHL	CHB-C1B-C2B	-2.09	121.34	127.24
23	AN	605	CHL	C1C-C2C-C3C	-2.09	105.46	107.11
23	AH	608	CHL	CED-O2D-CGD	2.09	120.65	115.94
23	AD	302	CHL	O2D-CGD-O1D	-2.08	119.76	123.84
25	v	316	LUT	C31-C30-C29	2.08	130.28	127.31
24	AL	502	CLA	O2D-CGD-CBD	2.08	114.97	111.27
24	p	611	CLA	CHD-C1D-ND	-2.08	122.54	124.45
24	q	602	CLA	CHB-C1B-NB	2.08	126.46	124.26
24	AS	304	CLA	CHB-C1B-NB	2.08	126.46	124.26
23	AQ	608	CHL	CED-O2D-CGD	2.08	120.65	115.94
23	AH	601	CHL	O2D-CGD-O1D	-2.08	119.77	123.84
24	AQ	614	CLA	CHB-C1B-NB	2.08	126.46	124.26
24	AU	611	CLA	CHB-C1B-NB	2.08	126.46	124.26
33	Q	407	LMG	O1-C1-C2	-2.08	105.05	108.30
24	AU	604	CLA	O2D-CGD-CBD	2.08	114.97	111.27
24	0	612	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
24	0	612	CLA	O1D-CGD-CBD	2.08	128.74	124.48
23	AN	608	CHL	O2A-CGA-CBA	2.08	118.44	111.91
37	Q	405	PL9	O2-C1-C6	2.08	124.19	120.59
33	O	620	LMG	O1-C1-C2	-2.08	105.06	108.30
23	AA	606	CHL	OMC-CMC-C2C	-2.08	120.98	125.69
28	q	616	LHG	C27-C26-C25	-2.08	103.87	114.42
24	AR	617	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	AD	309	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
23	AN	605	CHL	OMC-CMC-C2C	-2.08	120.99	125.69
23	9	601	CHL	CHC-C4B-C3B	-2.08	121.09	130.47
23	AE	606	CHL	CBC-CAC-C3C	-2.08	106.70	112.43
24	AH	613	CLA	CMA-C3A-C4A	2.08	117.36	111.77
24	AQ	611	CLA	C2A-C1A-CHA	2.08	127.49	123.86
33	AK	622	LMG	O1-C1-C2	-2.08	105.06	108.30
24	AA	610	CLA	CHB-C1B-NB	2.08	126.45	124.26
24	AL	506	CLA	CHC-C4B-NB	2.08	126.45	124.26
24	AL	507	CLA	CHB-C1B-NB	2.08	126.45	124.26
29	AL	515	BCR	C24-C23-C22	-2.08	123.10	126.23
24	AL	502	CLA	CHB-C1B-NB	2.08	126.45	124.26
23	AF	607	CHL	C1D-ND-C4D	-2.07	104.86	106.33
24	AF	603	CLA	CHD-C1D-ND	-2.07	122.55	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	O	606	CLA	CMB-C2B-C1B	-2.07	122.21	125.37
24	0	602	CLA	C1-C2-C3	-2.07	122.46	126.04
24	9	603	CLA	C1-C2-C3	-2.07	122.46	126.04
23	9	609	CHL	O2A-CGA-CBA	2.07	118.41	111.91
24	O	611	CLA	CMB-C2B-C3B	2.07	131.61	126.59
26	AS	317	NEX	C10-C11-C12	2.07	129.68	123.22
24	9	602	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	AD	302	CHL	CED-O2D-CGD	2.07	120.62	115.94
24	AE	611	CLA	CHB-C1B-NB	2.07	126.45	124.26
29	O	619	BCR	C15-C14-C13	-2.07	124.35	127.31
38	F	102	HEM	C4A-NA-C1A	2.07	107.38	105.35
24	AK	610	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
24	O	601	CLA	CHA-C1A-NA	-2.07	121.66	126.40
24	AU	610	CLA	CHB-C1B-NB	2.07	126.45	124.26
24	AF	603	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
24	AQ	612	CLA	CMB-C2B-C3B	2.07	131.60	126.59
23	AA	605	CHL	C4D-C3D-CAD	2.07	110.53	108.10
23	AC	608	CHL	C2A-C3A-C4A	-2.07	98.53	101.87
24	Q	403	CLA	CMB-C2B-C3B	2.07	131.60	126.59
23	AE	607	CHL	C4D-C3D-CAD	2.07	110.53	108.10
24	AD	304	CLA	CHC-C4B-NB	2.07	126.44	124.26
24	q	618	CLA	C3B-C4B-NB	-2.07	108.60	110.52
24	AH	603	CLA	CHB-C4A-NA	2.07	127.37	124.51
25	AN	614	LUT	C31-C30-C29	2.07	130.26	127.31
24	p	612	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
24	AS	310	CLA	CAA-CBA-CGA	-2.06	107.22	113.25
24	AE	604	CLA	CHB-C1B-NB	2.06	126.44	124.26
24	v	304	CLA	CHB-C1B-NB	2.06	126.44	124.26
24	AE	604	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
24	AL	511	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
24	AR	617	CLA	C2B-C1B-NB	-2.06	108.85	110.23
23	AD	308	CHL	C1-C2-C3	-2.06	122.48	126.04
24	AQ	610	CLA	CMB-C2B-C3B	2.06	131.58	126.59
24	q	611	CLA	CHB-C1B-NB	2.06	126.44	124.26
24	AA	602	CLA	CHD-C1D-ND	-2.06	122.56	124.45
24	AS	311	CLA	CAA-CBA-CGA	-2.06	107.23	113.25
29	AO	101	BCR	C38-C26-C25	-2.06	122.21	124.53
24	Q	404	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	AJ	406	CLA	CHB-C1B-NB	2.06	126.44	124.26
25	AA	614	LUT	C32-C33-C34	2.06	122.10	118.94
37	Q	405	PL9	C31-C32-C33	-2.06	105.11	111.88
23	AR	613	CHL	O1D-CGD-CBD	-2.06	120.27	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AD	301	CHL	CAA-CBA-CGA	-2.06	107.23	113.25
24	AM	403	CLA	CMB-C2B-C3B	2.06	131.57	126.59
23	0	607	CHL	CAA-C2A-C1A	2.06	118.72	111.97
23	0	601	CHL	C6-C5-C3	-2.06	108.06	113.45
24	AF	610	CLA	CHA-C4D-ND	2.06	136.81	132.50
24	v	311	CLA	CGD-CBD-CAD	2.06	117.40	110.73
24	AR	601	CLA	O1D-CGD-CBD	2.06	128.69	124.48
23	0	607	CHL	C4D-C3D-CAD	2.06	110.52	108.10
24	AU	610	CLA	O1D-CGD-CBD	2.06	128.69	124.48
23	AU	601	CHL	CED-O2D-CGD	2.06	120.59	115.94
23	AN	606	CHL	OMC-CMC-C2C	-2.06	121.04	125.69
23	V	601	CHL	C1-O2A-CGA	2.06	121.84	116.44
23	V	606	CHL	C1-O2A-CGA	2.06	121.84	116.44
24	q	601	CLA	C3A-C2A-C1A	2.06	104.42	101.34
23	AA	617	CHL	OMC-CMC-C2C	-2.06	121.04	125.69
23	AD	301	CHL	C4D-CHA-C1A	-2.06	118.75	121.25
24	q	618	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
24	AF	614	CLA	C3B-C4B-NB	-2.05	108.61	110.52
24	AU	613	CLA	CHB-C1B-NB	2.05	126.43	124.26
23	AH	606	CHL	CAA-C2A-C1A	2.05	118.70	111.97
23	AE	617	CHL	C2A-C3A-C4A	-2.05	98.55	101.87
25	v	315	LUT	C31-C30-C29	2.05	130.24	127.31
24	AF	614	CLA	CHA-C4D-ND	2.05	136.79	132.50
24	AC	603	CLA	CHB-C1B-NB	2.05	126.43	124.26
23	q	607	CHL	C1D-ND-C4D	-2.05	104.88	106.33
23	AH	605	CHL	O2D-CGD-O1D	-2.05	119.83	123.84
23	AB	606	CHL	CAA-C2A-C1A	2.05	118.70	111.97
23	AB	605	CHL	O2A-CGA-CBA	2.05	120.62	114.03
23	AU	608	CHL	CHB-C1B-C2B	-2.05	121.44	127.24
23	AN	601	CHL	C1-O2A-CGA	2.05	121.82	116.44
28	Q	406	LHG	C27-C26-C25	-2.05	104.02	114.42
24	AQ	604	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
25	AE	613	LUT	C32-C33-C34	2.05	122.09	118.94
24	P	508	CLA	CMB-C2B-C3B	2.05	131.55	126.59
24	AA	613	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
29	O	617	BCR	C7-C8-C9	-2.05	123.14	126.23
29	F	101	BCR	C7-C8-C9	-2.05	123.14	126.23
23	AN	607	CHL	C4-C3-C2	-2.05	118.42	123.68
23	AN	605	CHL	CED-O2D-CGD	2.05	120.57	115.94
23	AS	302	CHL	OMC-CMC-C2C	-2.05	121.06	125.69
24	AK	604	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
24	V	604	CLA	CHD-C1D-ND	-2.05	122.57	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AU	602	CLA	CHD-C1D-ND	-2.05	122.57	124.45
24	v	314	CLA	CAA-CBA-CGA	-2.05	107.27	113.25
37	AM	405	PL9	C31-C32-C33	-2.05	105.15	111.88
26	AE	615	NEX	C31-C30-C29	2.05	130.23	127.31
23	0	605	CHL	O2D-CGD-O1D	-2.05	119.84	123.84
24	P	510	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
23	AU	608	CHL	CED-O2D-CGD	2.04	120.56	115.94
23	AF	606	CHL	CBD-CHA-C1A	-2.04	126.09	128.50
23	AA	607	CHL	CBC-CAC-C3C	-2.04	106.80	112.43
24	AR	602	CLA	CHB-C1B-NB	2.04	126.42	124.26
23	V	605	CHL	O2A-CGA-O1A	-2.04	118.44	123.59
23	AQ	608	CHL	C1C-C2C-C3C	-2.04	105.49	107.11
24	AJ	409	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
24	AM	404	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
24	AM	403	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
23	AB	601	CHL	O2D-CGD-O1D	-2.04	119.45	124.09
23	AC	606	CHL	CHB-C1B-C2B	-2.04	121.47	127.24
24	AL	503	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	AM	404	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
29	O	617	BCR	C27-C26-C25	2.04	125.69	122.73
28	AM	406	LHG	C27-C26-C25	-2.04	104.06	114.42
37	AM	405	PL9	C12-C13-C14	-2.04	122.75	127.66
24	AL	504	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	AA	617	CHL	C3D-C4D-ND	2.04	113.54	110.24
37	AM	405	PL9	O2-C1-C2	-2.04	117.11	121.78
37	Q	405	PL9	C12-C13-C14	-2.04	122.75	127.66
24	AE	612	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
23	9	606	CHL	CHB-C4A-NA	2.04	127.33	124.51
24	p	612	CLA	O2D-CGD-CBD	2.04	114.89	111.27
23	p	601	CHL	C2A-C1A-CHA	-2.04	120.29	123.86
23	9	607	CHL	CAA-C2A-C1A	2.04	118.66	111.97
24	AC	610	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
24	AK	604	CLA	CMB-C2B-C3B	2.04	131.52	126.59
24	AD	304	CLA	CHB-C1B-NB	2.04	126.41	124.26
23	AF	608	CHL	CMD-C2D-C3D	-2.04	122.93	127.61
23	p	608	CHL	C7-C6-C5	-2.04	107.83	113.36
24	q	608	CLA	C2D-C1D-ND	-2.04	108.60	110.10
24	AK	606	CLA	CAA-CBA-CGA	-2.04	107.30	113.25
24	AS	305	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
29	AV	101	BCR	C37-C22-C21	-2.04	120.07	122.92
23	AA	606	CHL	CED-O2D-CGD	2.04	120.54	115.94
37	AM	405	PL9	C36-C34-C33	-2.04	117.00	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	J	411	DGD	O2D-C2D-C1D	-2.04	105.10	110.05
23	AE	607	CHL	C11-C12-C13	-2.04	106.39	115.98
23	AN	617	CHL	CBA-CAA-C2A	2.04	119.87	113.86
24	AM	404	CLA	CHD-C1D-ND	-2.03	122.58	124.45
23	AF	605	CHL	OBD-CAD-C3D	-2.03	125.38	128.74
24	AU	602	CLA	CAA-CBA-CGA	-2.03	107.31	113.25
24	AK	617	CLA	CHD-C1D-ND	-2.03	122.58	124.45
25	v	316	LUT	C11-C10-C9	2.03	130.21	127.31
35	AJ	412	DGD	O2D-C2D-C1D	-2.03	105.11	110.05
24	AL	505	CLA	CAA-CBA-CGA	-2.03	107.31	113.25
25	AS	315	LUT	C31-C30-C29	2.03	130.21	127.31
23	AF	601	CHL	C2A-C1A-CHA	-2.03	120.31	123.86
24	AQ	603	CLA	CHB-C4A-NA	2.03	127.32	124.51
24	AB	603	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
24	v	303	CLA	CHD-C1D-ND	-2.03	122.59	124.45
23	AN	605	CHL	O2A-CGA-O1A	-2.03	118.47	123.59
23	AN	608	CHL	C6-C7-C8	-2.03	109.35	115.92
23	AQ	609	CHL	O2A-CGA-CBA	2.03	118.28	111.91
23	AA	601	CHL	CHC-C4B-NB	-2.03	122.11	124.26
25	AR	614	LUT	C31-C30-C29	2.03	130.21	127.31
23	AH	601	CHL	CED-O2D-CGD	2.03	120.53	115.94
23	q	605	CHL	CAA-C2A-C1A	2.03	118.63	111.97
23	AQ	607	CHL	CHB-C1B-C2B	-2.03	121.50	127.24
24	AU	613	CLA	O1D-CGD-CBD	2.03	128.64	124.48
23	AU	607	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
24	V	602	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
24	AL	507	CLA	CHD-C1D-ND	-2.03	122.59	124.45
29	AB	612	BCR	C8-C7-C6	-2.03	121.51	127.20
23	AB	608	CHL	C1C-C2C-C3C	-2.03	105.50	107.11
23	AF	608	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
35	j	102	DGD	CAB-C9B-C8B	-2.03	104.14	114.42
23	AQ	608	CHL	C6-C5-C3	-2.03	108.14	113.45
24	AR	611	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
24	AL	509	CLA	CMB-C2B-C3B	2.03	131.49	126.59
23	AF	606	CHL	O2D-CGD-O1D	-2.03	119.88	123.84
23	AQ	606	CHL	C1C-C2C-C3C	-2.03	105.51	107.11
35	AL	518	DGD	O3E-C3E-C2E	-2.03	105.67	110.35
23	AQ	606	CHL	O2A-CGA-O1A	-2.03	118.48	123.59
24	AF	602	CLA	CHD-C1D-C2D	2.02	129.73	125.48
23	AS	307	CHL	C6-C7-C8	-2.02	109.37	115.92
24	AA	610	CLA	CHD-C1D-ND	-2.02	122.59	124.45
35	j	102	DGD	O3E-C3E-C2E	-2.02	105.67	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	AF	612	BCR	C8-C7-C6	-2.02	121.52	127.20
24	AB	602	CLA	C2A-C1A-CHA	2.02	127.40	123.86
24	9	603	CLA	CHB-C1B-NB	2.02	126.40	124.26
37	Q	405	PL9	O2-C1-C2	-2.02	117.14	121.78
23	AH	606	CHL	CHB-C1B-C2B	-2.02	121.52	127.24
23	AA	601	CHL	O2A-CGA-CBA	2.02	120.53	114.03
24	9	611	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
24	AH	612	CLA	O1D-CGD-CBD	2.02	128.62	124.48
25	AS	316	LUT	C31-C30-C29	2.02	130.20	127.31
29	AK	621	BCR	C15-C14-C13	-2.02	124.42	127.31
23	AH	608	CHL	C4-C3-C2	-2.02	118.49	123.68
24	AK	611	CLA	CGD-CBD-CAD	2.02	117.28	110.73
24	AK	606	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	AF	601	CHL	O2D-CGD-O1D	-2.02	119.50	124.09
23	p	601	CHL	C1-O2A-CGA	2.02	121.74	116.44
23	0	607	CHL	CBC-CAC-C3C	-2.02	108.64	113.82
25	AS	316	LUT	C4-C5-C6	2.02	125.35	120.85
29	O	618	BCR	C8-C7-C6	-2.02	121.53	127.20
24	AK	604	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
23	AB	606	CHL	CAA-CBA-CGA	-2.02	107.15	112.51
23	AN	606	CHL	C1-O2A-CGA	2.02	121.74	116.44
24	AS	313	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
37	Q	405	PL9	C36-C34-C33	-2.02	117.04	121.12
24	AH	611	CLA	CHB-C1B-NB	2.02	126.39	124.26
23	AA	608	CHL	C1-O2A-CGA	2.02	121.73	116.44
24	AE	611	CLA	CBA-CAA-C2A	2.02	119.81	113.86
24	Q	403	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
32	AJ	407	PHO	O2A-CGA-O1A	-2.02	118.51	123.59
24	AL	504	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
24	AB	611	CLA	O1A-CGA-CBA	2.01	129.55	123.08
23	AC	607	CHL	CAA-CBA-CGA	-2.01	107.16	112.51
35	AO	102	DGD	CAB-C9B-C8B	-2.01	104.20	114.42
24	AQ	610	CLA	O2D-CGD-CBD	2.01	114.85	111.27
23	AF	607	CHL	CHC-C4B-NB	-2.01	122.12	124.26
23	V	608	CHL	C6-C7-C8	-2.01	109.41	115.92
27	AF	613	XAT	C25-C24-C23	-2.01	108.77	112.75
24	AU	603	CLA	CHB-C4A-NA	2.01	127.30	124.51
24	AF	602	CLA	CHA-C1A-NA	-2.01	121.79	126.40
23	p	608	CHL	C6-C5-C3	-2.01	108.18	113.45
24	AJ	405	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	V	607	CHL	CBC-CAC-C3C	-2.01	108.66	113.82
24	O	614	CLA	CGD-CBD-CAD	2.01	117.25	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	v	312	CLA	CHB-C1B-NB	2.01	126.39	124.26
29	AK	602	BCR	C33-C5-C6	-2.01	122.27	124.53
27	AF	613	XAT	C5-C4-C3	-2.01	108.77	112.75
23	AQ	606	CHL	CBB-CAB-C3B	-2.01	117.62	127.62
29	AI	101	BCR	C37-C22-C21	-2.01	120.11	122.92
24	O	614	CLA	CHC-C4B-NB	2.01	126.39	124.26
29	O	619	BCR	C8-C7-C6	-2.01	121.56	127.20
25	V	614	LUT	C8-C9-C10	2.01	122.03	118.94
23	AB	601	CHL	C2A-C1A-CHA	-2.01	120.34	123.86
23	v	302	CHL	CAA-CBA-CGA	2.01	117.84	112.51
24	V	609	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
35	AL	518	DGD	O5D-C6D-C5D	-2.01	105.33	109.05
24	J	407	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
23	0	601	CHL	C11-C12-C13	-2.01	109.42	115.92
25	9	616	LUT	C31-C30-C29	2.01	130.18	127.31
24	P	506	CLA	CHD-C1D-ND	-2.01	122.61	124.45
24	O	616	CLA	O2D-CGD-CBD	2.01	114.83	111.27
24	9	614	CLA	CHB-C1B-NB	2.01	126.38	124.26
24	AR	611	CLA	CHB-C1B-NB	2.01	126.38	124.26
24	AQ	613	CLA	O1D-CGD-CBD	2.01	128.59	124.48
23	AH	607	CHL	C4D-CHA-C1A	-2.01	118.81	121.25
24	P	503	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
24	AC	603	CLA	C1-C2-C3	-2.01	122.57	126.04
24	P	511	CLA	O2D-CGD-CBD	2.01	114.83	111.27
35	J	411	DGD	O6E-C1E-O5D	-2.01	105.22	109.97
29	f	101	BCR	C7-C8-C9	-2.01	123.20	126.23
24	AL	502	CLA	O1D-CGD-CBD	2.01	128.59	124.48
35	P	516	DGD	O3E-C3E-C2E	-2.01	105.71	110.35
24	AL	508	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
23	AR	613	CHL	OMC-CMC-C2C	-2.00	121.15	125.69
24	v	310	CLA	CHB-C1B-NB	2.00	126.38	124.26
24	J	404	CLA	CHD-C1D-ND	-2.00	122.61	124.45
23	AU	607	CHL	OMC-CMC-C2C	-2.00	121.16	125.69
24	AN	602	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
23	AH	605	CHL	C4D-CHA-C1A	-2.00	118.81	121.25
24	p	618	CLA	C3A-C2A-C1A	2.00	104.34	101.34
24	AK	618	CLA	O2D-CGD-CBD	2.00	114.83	111.27
23	AD	308	CHL	O2A-CGA-CBA	2.00	118.19	111.91
24	AJ	409	CLA	CHD-C1D-ND	-2.00	122.61	124.45
23	AU	605	CHL	C4D-CHA-C1A	-2.00	118.81	121.25
23	AQ	601	CHL	C2A-C1A-CHA	-2.00	120.36	123.86
24	q	611	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	V	607	CHL	C4-C3-C2	-2.00	118.55	123.68
24	AJ	404	CLA	C3C-C4C-NC	-2.00	108.33	110.57

There are no chirality outliers.

All (4813) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	9	601	CHL	C3A-C2A-CAA-CBA
23	9	605	CHL	C1A-C2A-CAA-CBA
23	9	605	CHL	C3A-C2A-CAA-CBA
23	9	605	CHL	CBD-CGD-O2D-CED
23	9	606	CHL	C2B-C3B-CAB-CBB
23	9	606	CHL	C4B-C3B-CAB-CBB
23	9	606	CHL	C1C-C2C-CMC-OMC
23	9	607	CHL	C1A-C2A-CAA-CBA
23	9	608	CHL	C3A-C2A-CAA-CBA
23	9	608	CHL	C1C-C2C-CMC-OMC
23	9	608	CHL	C3C-C2C-CMC-OMC
23	0	601	CHL	C3A-C2A-CAA-CBA
23	0	605	CHL	C1A-C2A-CAA-CBA
23	0	605	CHL	C3A-C2A-CAA-CBA
23	0	606	CHL	C1A-C2A-CAA-CBA
23	0	606	CHL	C3A-C2A-CAA-CBA
23	0	606	CHL	CBD-CGD-O2D-CED
23	0	607	CHL	C1A-C2A-CAA-CBA
23	0	607	CHL	C3A-C2A-CAA-CBA
23	0	617	CHL	C2A-CAA-CBA-CGA
23	0	617	CHL	CBD-CGD-O2D-CED
23	AA	601	CHL	C1A-C2A-CAA-CBA
23	AA	601	CHL	C1C-C2C-CMC-OMC
23	AA	601	CHL	C3C-C2C-CMC-OMC
23	AA	605	CHL	C3A-C2A-CAA-CBA
23	AA	605	CHL	C1C-C2C-CMC-OMC
23	AA	605	CHL	C3C-C2C-CMC-OMC
23	AA	607	CHL	C1A-C2A-CAA-CBA
23	AA	607	CHL	C3A-C2A-CAA-CBA
23	AA	607	CHL	C2B-C3B-CAB-CBB
23	AA	607	CHL	C4B-C3B-CAB-CBB
23	AA	607	CHL	C1C-C2C-CMC-OMC
23	AA	607	CHL	C3C-C2C-CMC-OMC
23	AA	608	CHL	C3C-C2C-CMC-OMC
23	AA	617	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	AA	617	CHL	CBD-CGD-O2D-CED
23	AB	605	CHL	C1A-C2A-CAA-CBA
23	AB	605	CHL	C3A-C2A-CAA-CBA
23	AB	606	CHL	C1A-C2A-CAA-CBA
23	AB	606	CHL	C3A-C2A-CAA-CBA
23	AB	607	CHL	C1A-C2A-CAA-CBA
23	AB	607	CHL	C3A-C2A-CAA-CBA
23	AB	607	CHL	C1C-C2C-CMC-OMC
23	AB	607	CHL	C3C-C2C-CMC-OMC
23	AB	608	CHL	C3A-C2A-CAA-CBA
23	AB	608	CHL	C2A-CAA-CBA-CGA
23	AB	608	CHL	C3C-C2C-CMC-OMC
23	AC	601	CHL	C3A-C2A-CAA-CBA
23	AC	601	CHL	C2A-CAA-CBA-CGA
23	AC	601	CHL	CBD-CGD-O2D-CED
23	AC	605	CHL	C1A-C2A-CAA-CBA
23	AC	605	CHL	C3A-C2A-CAA-CBA
23	AC	605	CHL	CBD-CGD-O2D-CED
23	AC	606	CHL	C4B-C3B-CAB-CBB
23	AC	607	CHL	C3A-C2A-CAA-CBA
23	AC	607	CHL	C1C-C2C-CMC-OMC
23	AC	607	CHL	C3C-C2C-CMC-OMC
23	AD	301	CHL	C1A-C2A-CAA-CBA
23	AD	301	CHL	C2A-CAA-CBA-CGA
23	AD	302	CHL	C1A-C2A-CAA-CBA
23	AD	302	CHL	C3A-C2A-CAA-CBA
23	AD	306	CHL	C1A-C2A-CAA-CBA
23	AD	306	CHL	C3A-C2A-CAA-CBA
23	AD	306	CHL	CBD-CGD-O2D-CED
23	AD	307	CHL	C1A-C2A-CAA-CBA
23	AD	307	CHL	C3A-C2A-CAA-CBA
23	AD	307	CHL	CHA-CBD-CGD-O1D
23	AD	307	CHL	CHA-CBD-CGD-O2D
23	AD	317	CHL	C2A-CAA-CBA-CGA
23	AD	317	CHL	CBD-CGD-O2D-CED
23	AE	601	CHL	C1A-C2A-CAA-CBA
23	AE	601	CHL	C3A-C2A-CAA-CBA
23	AE	601	CHL	CHA-CBD-CGD-O1D
23	AE	601	CHL	CHA-CBD-CGD-O2D
23	AE	606	CHL	C1A-C2A-CAA-CBA
23	AE	606	CHL	C3A-C2A-CAA-CBA
23	AE	606	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	AE	606	CHL	C4B-C3B-CAB-CBB
23	AE	606	CHL	C1C-C2C-CMC-OMC
23	AE	606	CHL	C3C-C2C-CMC-OMC
23	AE	616	CHL	C1A-C2A-CAA-CBA
23	AE	616	CHL	CBD-CGD-O2D-CED
23	AE	617	CHL	C1A-C2A-CAA-CBA
23	AE	617	CHL	C3A-C2A-CAA-CBA
23	AF	606	CHL	CBD-CGD-O2D-CED
23	AF	607	CHL	C1A-C2A-CAA-CBA
23	AF	607	CHL	C3A-C2A-CAA-CBA
23	AF	607	CHL	C1C-C2C-CMC-OMC
23	AF	607	CHL	C3C-C2C-CMC-OMC
23	AF	608	CHL	C3C-C2C-CMC-OMC
23	V	601	CHL	CHA-CBD-CGD-O1D
23	V	601	CHL	CHA-CBD-CGD-O2D
23	V	605	CHL	C1A-C2A-CAA-CBA
23	V	605	CHL	C3A-C2A-CAA-CBA
23	V	605	CHL	C1C-C2C-CMC-OMC
23	V	606	CHL	CBD-CGD-O2D-CED
23	V	606	CHL	C6-C7-C8-C9
23	V	607	CHL	C1A-C2A-CAA-CBA
23	V	616	CHL	C3A-C2A-CAA-CBA
23	V	616	CHL	C3C-C2C-CMC-OMC
23	p	601	CHL	C3C-C2C-CMC-OMC
23	p	601	CHL	C2-C3-C5-C6
23	p	601	CHL	C4-C3-C5-C6
23	p	605	CHL	C3A-C2A-CAA-CBA
23	p	605	CHL	CBD-CGD-O2D-CED
23	p	606	CHL	C1A-C2A-CAA-CBA
23	p	606	CHL	C3A-C2A-CAA-CBA
23	p	606	CHL	C4B-C3B-CAB-CBB
23	p	606	CHL	C1C-C2C-CMC-OMC
23	p	606	CHL	C3C-C2C-CMC-OMC
23	p	606	CHL	CBD-CGD-O2D-CED
23	p	607	CHL	C2B-C3B-CAB-CBB
23	p	607	CHL	C4B-C3B-CAB-CBB
23	p	608	CHL	C3C-C2C-CMC-OMC
23	p	609	CHL	C3C-C2C-CMC-OMC
23	q	605	CHL	C1A-C2A-CAA-CBA
23	q	605	CHL	C1C-C2C-CMC-OMC
23	q	605	CHL	C3C-C2C-CMC-OMC
23	q	605	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	q	606	CHL	C2A-CAA-CBA-CGA
23	q	606	CHL	C1C-C2C-CMC-OMC
23	q	606	CHL	C3C-C2C-CMC-OMC
23	q	607	CHL	C1A-C2A-CAA-CBA
23	q	607	CHL	C3A-C2A-CAA-CBA
23	q	607	CHL	C3C-C2C-CMC-OMC
23	q	607	CHL	C2-C3-C5-C6
23	q	613	CHL	CAD-CBD-CGD-O1D
23	q	613	CHL	CAD-CBD-CGD-O2D
23	v	306	CHL	C1C-C2C-CMC-OMC
23	v	306	CHL	C3C-C2C-CMC-OMC
23	v	307	CHL	C1A-C2A-CAA-CBA
23	v	307	CHL	C3A-C2A-CAA-CBA
23	v	307	CHL	C3C-C2C-CMC-OMC
23	AH	601	CHL	C6-C7-C8-C9
23	AH	605	CHL	C1A-C2A-CAA-CBA
23	AH	605	CHL	C3A-C2A-CAA-CBA
23	AH	606	CHL	CBD-CGD-O2D-CED
23	AH	607	CHL	C6-C7-C8-C9
23	AH	608	CHL	C1C-C2C-CMC-OMC
23	AH	608	CHL	C3C-C2C-CMC-OMC
23	AN	601	CHL	CHA-CBD-CGD-O1D
23	AN	601	CHL	CHA-CBD-CGD-O2D
23	AN	601	CHL	C4-C3-C5-C6
23	AN	605	CHL	C1A-C2A-CAA-CBA
23	AN	605	CHL	C3A-C2A-CAA-CBA
23	AN	605	CHL	C1C-C2C-CMC-OMC
23	AN	606	CHL	CBD-CGD-O2D-CED
23	AN	606	CHL	C6-C7-C8-C9
23	AN	607	CHL	C1A-C2A-CAA-CBA
23	AN	607	CHL	C3A-C2A-CAA-CBA
23	AN	607	CHL	C1C-C2C-CMC-OMC
23	AN	607	CHL	C3C-C2C-CMC-OMC
23	AN	607	CHL	C2-C3-C5-C6
23	AN	607	CHL	C4-C3-C5-C6
23	AN	608	CHL	C2B-C3B-CAB-CBB
23	AN	608	CHL	C4B-C3B-CAB-CBB
23	AN	617	CHL	C3A-C2A-CAA-CBA
23	AQ	601	CHL	C3C-C2C-CMC-OMC
23	AQ	601	CHL	CBD-CGD-O2D-CED
23	AQ	601	CHL	C6-C7-C8-C9
23	AQ	605	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	AQ	605	CHL	CBD-CGD-O2D-CED
23	AQ	606	CHL	C1A-C2A-CAA-CBA
23	AQ	606	CHL	C3A-C2A-CAA-CBA
23	AQ	606	CHL	C2B-C3B-CAB-CBB
23	AQ	606	CHL	C4B-C3B-CAB-CBB
23	AQ	606	CHL	C1C-C2C-CMC-OMC
23	AQ	606	CHL	C3C-C2C-CMC-OMC
23	AQ	606	CHL	CBD-CGD-O2D-CED
23	AQ	607	CHL	C1A-C2A-CAA-CBA
23	AQ	608	CHL	C1C-C2C-CMC-OMC
23	AQ	608	CHL	C3C-C2C-CMC-OMC
23	AR	605	CHL	C1A-C2A-CAA-CBA
23	AR	605	CHL	C3A-C2A-CAA-CBA
23	AR	605	CHL	C1C-C2C-CMC-OMC
23	AR	605	CHL	C3C-C2C-CMC-OMC
23	AR	605	CHL	CBD-CGD-O2D-CED
23	AR	607	CHL	C1A-C2A-CAA-CBA
23	AR	607	CHL	C3A-C2A-CAA-CBA
23	AR	613	CHL	CHA-CBD-CGD-O1D
23	AS	306	CHL	C1C-C2C-CMC-OMC
23	AS	306	CHL	C3C-C2C-CMC-OMC
23	AS	307	CHL	C3C-C2C-CMC-OMC
23	AS	308	CHL	C3A-C2A-CAA-CBA
23	AU	601	CHL	C6-C7-C8-C9
23	AU	605	CHL	C1A-C2A-CAA-CBA
23	AU	605	CHL	C3A-C2A-CAA-CBA
23	AU	606	CHL	CBD-CGD-O2D-CED
23	AU	607	CHL	C6-C7-C8-C9
23	AU	608	CHL	C1C-C2C-CMC-OMC
23	AU	608	CHL	C3C-C2C-CMC-OMC
24	9	603	CLA	C4B-C3B-CAB-CBB
24	9	604	CLA	C1A-C2A-CAA-CBA
24	9	604	CLA	C3A-C2A-CAA-CBA
24	9	613	CLA	CBD-CGD-O2D-CED
24	0	602	CLA	C3A-C2A-CAA-CBA
24	0	604	CLA	C1A-C2A-CAA-CBA
24	0	604	CLA	C3A-C2A-CAA-CBA
24	0	604	CLA	CBD-CGD-O2D-CED
24	0	604	CLA	O1D-CGD-O2D-CED
24	0	609	CLA	C2-C3-C5-C6
24	0	609	CLA	C4-C3-C5-C6
24	0	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	0	610	CLA	CHA-CBD-CGD-O1D
24	0	610	CLA	CHA-CBD-CGD-O2D
24	0	612	CLA	CBD-CGD-O2D-CED
24	0	613	CLA	C1A-C2A-CAA-CBA
24	0	613	CLA	C3A-C2A-CAA-CBA
24	0	613	CLA	CBD-CGD-O2D-CED
24	AA	602	CLA	CBD-CGD-O2D-CED
24	AA	604	CLA	C3A-C2A-CAA-CBA
24	AA	610	CLA	C3A-C2A-CAA-CBA
24	AA	611	CLA	CBD-CGD-O2D-CED
24	AA	612	CLA	C1A-C2A-CAA-CBA
24	AA	612	CLA	C3A-C2A-CAA-CBA
24	AA	612	CLA	CBD-CGD-O2D-CED
24	AA	613	CLA	CBD-CGD-O2D-CED
24	AB	603	CLA	CBD-CGD-O2D-CED
24	AB	604	CLA	C1A-C2A-CAA-CBA
24	AB	604	CLA	C3A-C2A-CAA-CBA
24	AB	604	CLA	CBD-CGD-O2D-CED
24	AB	609	CLA	CHA-CBD-CGD-O1D
24	AB	609	CLA	CHA-CBD-CGD-O2D
24	AB	609	CLA	CBD-CGD-O2D-CED
24	AB	611	CLA	CBD-CGD-O2D-CED
24	AC	602	CLA	CBD-CGD-O2D-CED
24	AC	603	CLA	C4B-C3B-CAB-CBB
24	AC	604	CLA	C1A-C2A-CAA-CBA
24	AC	604	CLA	C3A-C2A-CAA-CBA
24	AC	604	CLA	CBD-CGD-O2D-CED
24	AC	610	CLA	C1A-C2A-CAA-CBA
24	AC	612	CLA	CBD-CGD-O2D-CED
24	AC	613	CLA	C1A-C2A-CAA-CBA
24	AD	303	CLA	C1A-C2A-CAA-CBA
24	AD	303	CLA	C3A-C2A-CAA-CBA
24	AD	305	CLA	C3A-C2A-CAA-CBA
24	AD	305	CLA	CBD-CGD-O2D-CED
24	AD	310	CLA	C1A-C2A-CAA-CBA
24	AD	310	CLA	CHA-CBD-CGD-O1D
24	AD	313	CLA	C1A-C2A-CAA-CBA
24	AD	313	CLA	C3A-C2A-CAA-CBA
24	AD	313	CLA	CBD-CGD-O2D-CED
24	AE	602	CLA	C3A-C2A-CAA-CBA
24	AE	602	CLA	CBD-CGD-O2D-CED
24	AE	604	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	AE	609	CLA	C3A-C2A-CAA-CBA
24	AE	609	CLA	CHA-CBD-CGD-O1D
24	AE	611	CLA	C1A-C2A-CAA-CBA
24	AE	611	CLA	C3A-C2A-CAA-CBA
24	AE	611	CLA	CBD-CGD-O2D-CED
24	AE	612	CLA	C1A-C2A-CAA-CBA
24	AE	612	CLA	CBD-CGD-O2D-CED
24	AF	604	CLA	C1A-C2A-CAA-CBA
24	AF	604	CLA	C3A-C2A-CAA-CBA
24	AF	609	CLA	CHA-CBD-CGD-O1D
24	AF	609	CLA	CHA-CBD-CGD-O2D
24	AF	609	CLA	CBD-CGD-O2D-CED
24	AF	614	CLA	C1A-C2A-CAA-CBA
24	AF	614	CLA	C3A-C2A-CAA-CBA
24	J	403	CLA	CAD-CBD-CGD-O1D
24	O	603	CLA	CBD-CGD-O2D-CED
24	O	604	CLA	C3A-C2A-CAA-CBA
24	O	605	CLA	C1A-C2A-CAA-CBA
24	O	605	CLA	C3A-C2A-CAA-CBA
24	O	605	CLA	CBD-CGD-O2D-CED
24	O	607	CLA	C1A-C2A-CAA-CBA
24	O	607	CLA	C3A-C2A-CAA-CBA
24	O	607	CLA	C2-C3-C5-C6
24	O	607	CLA	C4-C3-C5-C6
24	O	608	CLA	C1A-C2A-CAA-CBA
24	O	608	CLA	CBD-CGD-O2D-CED
24	O	609	CLA	C1A-C2A-CAA-CBA
24	O	609	CLA	C3A-C2A-CAA-CBA
24	O	609	CLA	CHA-CBD-CGD-O1D
24	O	609	CLA	CHA-CBD-CGD-O2D
24	O	609	CLA	CAD-CBD-CGD-O1D
24	O	609	CLA	CBD-CGD-O2D-CED
24	O	611	CLA	C1A-C2A-CAA-CBA
24	O	611	CLA	C3A-C2A-CAA-CBA
24	O	612	CLA	C3A-C2A-CAA-CBA
24	O	613	CLA	CBD-CGD-O2D-CED
24	O	613	CLA	C4-C3-C5-C6
24	O	614	CLA	C1A-C2A-CAA-CBA
24	O	614	CLA	C3A-C2A-CAA-CBA
24	O	614	CLA	C2-C3-C5-C6
24	O	614	CLA	C4-C3-C5-C6
24	P	501	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	P	501	CLA	CHA-CBD-CGD-O1D
24	P	501	CLA	CHA-CBD-CGD-O2D
24	P	501	CLA	CBD-CGD-O2D-CED
24	P	501	CLA	C14-C13-C15-C16
24	P	502	CLA	C1A-C2A-CAA-CBA
24	P	502	CLA	C3A-C2A-CAA-CBA
24	P	502	CLA	CBD-CGD-O2D-CED
24	P	503	CLA	C1A-C2A-CAA-CBA
24	P	503	CLA	C3A-C2A-CAA-CBA
24	P	503	CLA	CBD-CGD-O2D-CED
24	P	503	CLA	C2-C3-C5-C6
24	P	503	CLA	C4-C3-C5-C6
24	P	503	CLA	C11-C10-C8-C9
24	P	504	CLA	C1A-C2A-CAA-CBA
24	P	504	CLA	C3A-C2A-CAA-CBA
24	P	504	CLA	CBD-CGD-O2D-CED
24	P	505	CLA	C1A-C2A-CAA-CBA
24	P	505	CLA	CHA-CBD-CGD-O1D
24	P	505	CLA	CHA-CBD-CGD-O2D
24	P	505	CLA	CBD-CGD-O2D-CED
24	P	506	CLA	CBD-CGD-O2D-CED
24	P	507	CLA	CBD-CGD-O2D-CED
24	P	507	CLA	C2-C3-C5-C6
24	P	507	CLA	C4-C3-C5-C6
24	P	508	CLA	C1A-C2A-CAA-CBA
24	P	508	CLA	C3A-C2A-CAA-CBA
24	P	508	CLA	CBD-CGD-O2D-CED
24	P	508	CLA	C4-C3-C5-C6
24	P	509	CLA	CHA-CBD-CGD-O1D
24	P	509	CLA	CHA-CBD-CGD-O2D
24	P	509	CLA	CBD-CGD-O2D-CED
24	P	512	CLA	C1A-C2A-CAA-CBA
24	Q	403	CLA	C2-C3-C5-C6
24	Q	403	CLA	C4-C3-C5-C6
24	Q	404	CLA	CBD-CGD-O2D-CED
24	V	602	CLA	C1A-C2A-CAA-CBA
24	V	602	CLA	CBA-CGA-O2A-C1
24	V	602	CLA	O1A-CGA-O2A-C1
24	V	609	CLA	C3A-C2A-CAA-CBA
24	V	610	CLA	CHA-CBD-CGD-O2D
24	V	612	CLA	C1A-C2A-CAA-CBA
24	V	612	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	K	101	CLA	C2A-CAA-CBA-CGA
24	p	604	CLA	C1A-C2A-CAA-CBA
24	p	604	CLA	C3A-C2A-CAA-CBA
24	p	604	CLA	CBD-CGD-O2D-CED
24	p	610	CLA	CHA-C1A-C2A-CAA
24	p	613	CLA	CBD-CGD-O2D-CED
24	p	618	CLA	CBD-CGD-O2D-CED
24	q	601	CLA	CHA-CBD-CGD-O1D
24	q	601	CLA	CHA-CBD-CGD-O2D
24	q	601	CLA	CBD-CGD-O2D-CED
24	q	604	CLA	C1A-C2A-CAA-CBA
24	q	608	CLA	C1A-C2A-CAA-CBA
24	q	608	CLA	C3A-C2A-CAA-CBA
24	q	608	CLA	CBD-CGD-O2D-CED
24	q	609	CLA	C2B-C3B-CAB-CBB
24	q	609	CLA	C4B-C3B-CAB-CBB
24	q	610	CLA	C1A-C2A-CAA-CBA
24	q	610	CLA	C3A-C2A-CAA-CBA
24	q	610	CLA	CBD-CGD-O2D-CED
24	q	611	CLA	CBD-CGD-O2D-CED
24	q	618	CLA	C1A-C2A-CAA-CBA
24	q	618	CLA	C3A-C2A-CAA-CBA
24	q	618	CLA	CBD-CGD-O2D-CED
24	v	303	CLA	C1A-C2A-CAA-CBA
24	v	303	CLA	C3A-C2A-CAA-CBA
24	v	303	CLA	C11-C10-C8-C9
24	v	304	CLA	CBD-CGD-O2D-CED
24	v	305	CLA	C1A-C2A-CAA-CBA
24	v	305	CLA	CBD-CGD-O2D-CED
24	v	309	CLA	C1A-C2A-CAA-CBA
24	v	309	CLA	C3A-C2A-CAA-CBA
24	v	311	CLA	C3A-C2A-CAA-CBA
24	v	311	CLA	C2A-CAA-CBA-CGA
24	v	311	CLA	C2-C1-O2A-CGA
24	v	311	CLA	CBD-CGD-O2D-CED
24	v	311	CLA	O1D-CGD-O2D-CED
24	v	313	CLA	C1A-C2A-CAA-CBA
24	v	314	CLA	CBD-CGD-O2D-CED
24	v	314	CLA	O1D-CGD-O2D-CED
24	AH	604	CLA	C1A-C2A-CAA-CBA
24	AH	604	CLA	C3A-C2A-CAA-CBA
24	AH	604	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	AH	609	CLA	CBD-CGD-O2D-CED
24	AH	610	CLA	C3A-C2A-CAA-CBA
24	AH	610	CLA	CBD-CGD-O2D-CED
24	AH	610	CLA	C2-C3-C5-C6
24	AH	610	CLA	C4-C3-C5-C6
24	AH	612	CLA	C1A-C2A-CAA-CBA
24	AJ	404	CLA	CBD-CGD-O2D-CED
24	AK	604	CLA	CBD-CGD-O2D-CED
24	AK	605	CLA	CBD-CGD-O2D-CED
24	AK	606	CLA	C3A-C2A-CAA-CBA
24	AK	606	CLA	C6-C7-C8-C9
24	AK	607	CLA	C1A-C2A-CAA-CBA
24	AK	607	CLA	C3A-C2A-CAA-CBA
24	AK	609	CLA	C1A-C2A-CAA-CBA
24	AK	609	CLA	C3A-C2A-CAA-CBA
24	AK	609	CLA	C2-C3-C5-C6
24	AK	609	CLA	C4-C3-C5-C6
24	AK	610	CLA	C1A-C2A-CAA-CBA
24	AK	610	CLA	CBD-CGD-O2D-CED
24	AK	611	CLA	C1A-C2A-CAA-CBA
24	AK	611	CLA	C3A-C2A-CAA-CBA
24	AK	611	CLA	CHA-CBD-CGD-O1D
24	AK	611	CLA	CHA-CBD-CGD-O2D
24	AK	611	CLA	CBD-CGD-O2D-CED
24	AK	613	CLA	C1A-C2A-CAA-CBA
24	AK	613	CLA	C3A-C2A-CAA-CBA
24	AK	614	CLA	C3A-C2A-CAA-CBA
24	AK	615	CLA	C4-C3-C5-C6
24	AK	616	CLA	C1A-C2A-CAA-CBA
24	AK	616	CLA	C3A-C2A-CAA-CBA
24	AK	616	CLA	C2-C3-C5-C6
24	AK	616	CLA	C4-C3-C5-C6
24	AL	502	CLA	C3A-C2A-CAA-CBA
24	AL	502	CLA	CHA-CBD-CGD-O1D
24	AL	502	CLA	CHA-CBD-CGD-O2D
24	AL	502	CLA	CBD-CGD-O2D-CED
24	AL	503	CLA	C1A-C2A-CAA-CBA
24	AL	503	CLA	C3A-C2A-CAA-CBA
24	AL	503	CLA	CBD-CGD-O2D-CED
24	AL	504	CLA	C1A-C2A-CAA-CBA
24	AL	504	CLA	CBD-CGD-O2D-CED
24	AL	504	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	AL	504	CLA	C4-C3-C5-C6
24	AL	504	CLA	C11-C10-C8-C9
24	AL	505	CLA	C1A-C2A-CAA-CBA
24	AL	505	CLA	C3A-C2A-CAA-CBA
24	AL	505	CLA	CBD-CGD-O2D-CED
24	AL	506	CLA	C1A-C2A-CAA-CBA
24	AL	506	CLA	CHA-CBD-CGD-O1D
24	AL	506	CLA	CHA-CBD-CGD-O2D
24	AL	506	CLA	CBD-CGD-O2D-CED
24	AL	508	CLA	CBD-CGD-O2D-CED
24	AL	508	CLA	C2-C3-C5-C6
24	AL	508	CLA	C4-C3-C5-C6
24	AL	509	CLA	C1A-C2A-CAA-CBA
24	AL	509	CLA	C3A-C2A-CAA-CBA
24	AL	509	CLA	CBD-CGD-O2D-CED
24	AL	509	CLA	C4-C3-C5-C6
24	AL	510	CLA	CHA-CBD-CGD-O1D
24	AL	510	CLA	CHA-CBD-CGD-O2D
24	AL	510	CLA	CBD-CGD-O2D-CED
24	AL	510	CLA	C6-C7-C8-C9
24	AL	512	CLA	C2A-CAA-CBA-CGA
24	AL	514	CLA	C1A-C2A-CAA-CBA
24	AM	403	CLA	C2-C3-C5-C6
24	AM	403	CLA	C4-C3-C5-C6
24	AM	404	CLA	O1A-CGA-O2A-C1
24	AM	404	CLA	CBD-CGD-O2D-CED
24	AN	602	CLA	C1A-C2A-CAA-CBA
24	AN	602	CLA	CBA-CGA-O2A-C1
24	AN	602	CLA	O1A-CGA-O2A-C1
24	AN	609	CLA	C3A-C2A-CAA-CBA
24	AN	613	CLA	C1A-C2A-CAA-CBA
24	AN	613	CLA	C3A-C2A-CAA-CBA
24	AN	613	CLA	CBD-CGD-O2D-CED
24	AQ	604	CLA	C1A-C2A-CAA-CBA
24	AQ	604	CLA	C3A-C2A-CAA-CBA
24	AQ	604	CLA	CBD-CGD-O2D-CED
24	AQ	610	CLA	C1A-C2A-CAA-CBA
24	AQ	610	CLA	C3A-C2A-CAA-CBA
24	AQ	610	CLA	CBA-CGA-O2A-C1
24	AQ	610	CLA	O1A-CGA-O2A-C1
24	AQ	610	CLA	CBD-CGD-O2D-CED
24	AQ	611	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	AQ	611	CLA	C2-C3-C5-C6
24	AQ	611	CLA	C4-C3-C5-C6
24	AQ	613	CLA	CBD-CGD-O2D-CED
24	AQ	614	CLA	CBD-CGD-O2D-CED
24	AQ	614	CLA	O1D-CGD-O2D-CED
24	AR	601	CLA	CBD-CGD-O2D-CED
24	AR	604	CLA	C1A-C2A-CAA-CBA
24	AR	609	CLA	C2B-C3B-CAB-CBB
24	AR	609	CLA	C4B-C3B-CAB-CBB
24	AR	610	CLA	C3A-C2A-CAA-CBA
24	AR	610	CLA	CBD-CGD-O2D-CED
24	AR	611	CLA	CBD-CGD-O2D-CED
24	AR	612	CLA	C1A-C2A-CAA-CBA
24	AR	612	CLA	C3A-C2A-CAA-CBA
24	AR	617	CLA	C1A-C2A-CAA-CBA
24	AR	617	CLA	C3A-C2A-CAA-CBA
24	AS	303	CLA	C1A-C2A-CAA-CBA
24	AS	303	CLA	C3A-C2A-CAA-CBA
24	AS	304	CLA	CBD-CGD-O2D-CED
24	AS	305	CLA	C1A-C2A-CAA-CBA
24	AS	305	CLA	CBD-CGD-O2D-CED
24	AS	309	CLA	C1A-C2A-CAA-CBA
24	AS	309	CLA	C3A-C2A-CAA-CBA
24	AS	311	CLA	C3A-C2A-CAA-CBA
24	AS	311	CLA	C2A-CAA-CBA-CGA
24	AS	311	CLA	C2-C1-O2A-CGA
24	AS	311	CLA	CBD-CGD-O2D-CED
24	AS	311	CLA	O1D-CGD-O2D-CED
24	AS	313	CLA	C1A-C2A-CAA-CBA
24	AS	314	CLA	CBD-CGD-O2D-CED
24	AS	314	CLA	O1D-CGD-O2D-CED
24	AU	604	CLA	C1A-C2A-CAA-CBA
24	AU	604	CLA	C3A-C2A-CAA-CBA
24	AU	604	CLA	CBD-CGD-O2D-CED
24	AU	609	CLA	CBD-CGD-O2D-CED
24	AU	610	CLA	C3A-C2A-CAA-CBA
24	AU	610	CLA	C2-C3-C5-C6
24	AU	610	CLA	C4-C3-C5-C6
24	AU	612	CLA	C1A-C2A-CAA-CBA
24	AU	613	CLA	CBD-CGD-O2D-CED
25	AF	611	LUT	C7-C8-C9-C10
25	AF	611	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
25	V	613	LUT	C7-C8-C9-C19
25	v	315	LUT	C7-C8-C9-C19
25	AN	614	LUT	C7-C8-C9-C19
25	AS	316	LUT	C7-C8-C9-C19
26	9	617	NEX	C13-C14-C15-C35
26	9	617	NEX	O24-C26-C27-C28
26	9	617	NEX	C32-C33-C34-C35
26	9	617	NEX	C40-C33-C34-C35
26	AA	616	NEX	C7-C8-C9-C10
26	AA	616	NEX	C11-C10-C9-C8
26	AA	616	NEX	C11-C10-C9-C19
26	AA	616	NEX	C9-C10-C11-C12
26	AA	616	NEX	C10-C11-C12-C13
26	AA	616	NEX	C11-C12-C13-C14
26	AA	616	NEX	C11-C12-C13-C20
26	AA	616	NEX	C12-C13-C14-C15
26	AA	616	NEX	C20-C13-C14-C15
26	AA	616	NEX	O24-C26-C27-C28
26	AA	616	NEX	C32-C33-C34-C35
26	AA	616	NEX	C40-C33-C34-C35
26	AC	616	NEX	C13-C14-C15-C35
26	AC	616	NEX	O24-C26-C27-C28
26	AC	616	NEX	C32-C33-C34-C35
26	AC	616	NEX	C40-C33-C34-C35
26	AE	615	NEX	C7-C8-C9-C10
26	AE	615	NEX	C11-C10-C9-C8
26	AE	615	NEX	C11-C10-C9-C19
26	AE	615	NEX	C9-C10-C11-C12
26	AE	615	NEX	C10-C11-C12-C13
26	AE	615	NEX	C20-C13-C14-C15
26	AE	615	NEX	O24-C26-C27-C28
26	AE	615	NEX	C31-C32-C33-C34
26	AE	615	NEX	C31-C32-C33-C40
26	p	616	NEX	C11-C10-C9-C8
26	p	616	NEX	C11-C10-C9-C19
26	p	616	NEX	C10-C11-C12-C13
26	p	616	NEX	C11-C12-C13-C14
26	p	616	NEX	C11-C12-C13-C20
26	p	616	NEX	C13-C14-C15-C35
26	p	616	NEX	O24-C26-C27-C28
26	p	616	NEX	C32-C33-C34-C35
26	p	616	NEX	C40-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
26	q	615	NEX	C11-C10-C9-C8
26	q	615	NEX	C11-C10-C9-C19
26	q	615	NEX	C10-C11-C12-C13
26	q	615	NEX	C20-C13-C14-C15
26	q	615	NEX	C27-C28-C29-C30
26	q	615	NEX	C27-C28-C29-C39
26	q	615	NEX	C32-C33-C34-C35
26	q	615	NEX	C40-C33-C34-C35
26	v	317	NEX	C7-C8-C9-C10
26	v	317	NEX	C10-C11-C12-C13
26	v	317	NEX	C13-C14-C15-C35
26	v	317	NEX	C27-C28-C29-C30
26	v	317	NEX	C27-C28-C29-C39
26	v	317	NEX	C31-C32-C33-C34
26	v	317	NEX	C31-C32-C33-C40
26	v	317	NEX	C32-C33-C34-C35
26	v	317	NEX	C40-C33-C34-C35
26	AQ	617	NEX	C11-C10-C9-C8
26	AQ	617	NEX	C11-C10-C9-C19
26	AQ	617	NEX	C10-C11-C12-C13
26	AQ	617	NEX	C11-C12-C13-C14
26	AQ	617	NEX	C11-C12-C13-C20
26	AQ	617	NEX	O24-C26-C27-C28
26	AQ	617	NEX	C32-C33-C34-C35
26	AQ	617	NEX	C40-C33-C34-C35
26	AR	615	NEX	C11-C10-C9-C8
26	AR	615	NEX	C11-C10-C9-C19
26	AR	615	NEX	C27-C28-C29-C30
26	AR	615	NEX	C27-C28-C29-C39
26	AR	615	NEX	C32-C33-C34-C35
26	AR	615	NEX	C40-C33-C34-C35
26	AR	615	NEX	C33-C34-C35-C15
26	AS	317	NEX	C7-C8-C9-C10
26	AS	317	NEX	C10-C11-C12-C13
26	AS	317	NEX	C13-C14-C15-C35
26	AS	317	NEX	C27-C28-C29-C30
26	AS	317	NEX	C27-C28-C29-C39
26	AS	317	NEX	C31-C32-C33-C34
26	AS	317	NEX	C31-C32-C33-C40
26	AS	317	NEX	C32-C33-C34-C35
26	AS	317	NEX	C40-C33-C34-C35
26	AU	616	NEX	O24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
26	AU	616	NEX	C32-C33-C34-C35
26	AU	616	NEX	C40-C33-C34-C35
27	9	618	XAT	O4-C6-C7-C8
27	9	618	XAT	C6-C7-C8-C9
27	9	618	XAT	C11-C10-C9-C8
27	9	618	XAT	C10-C11-C12-C13
27	9	618	XAT	C12-C13-C14-C15
27	9	618	XAT	C27-C28-C29-C30
27	9	618	XAT	C39-C29-C30-C31
27	AB	613	XAT	O4-C6-C7-C8
27	AB	613	XAT	C7-C8-C9-C19
27	AB	613	XAT	C11-C10-C9-C19
27	AB	613	XAT	C20-C13-C14-C15
27	AB	613	XAT	C14-C15-C35-C34
27	AB	613	XAT	O24-C26-C27-C28
27	AB	613	XAT	C27-C28-C29-C39
27	AB	613	XAT	C39-C29-C30-C31
27	AB	613	XAT	C30-C31-C32-C33
27	AB	613	XAT	C31-C32-C33-C34
27	AB	613	XAT	C40-C33-C34-C35
27	AF	613	XAT	O4-C6-C7-C8
27	AF	613	XAT	C7-C8-C9-C19
27	AF	613	XAT	C11-C10-C9-C19
27	AF	613	XAT	C10-C11-C12-C13
27	AF	613	XAT	C11-C12-C13-C14
27	AF	613	XAT	C20-C13-C14-C15
27	AF	613	XAT	C14-C15-C35-C34
27	AF	613	XAT	O24-C26-C27-C28
27	AF	613	XAT	C39-C29-C30-C31
27	AF	613	XAT	C31-C32-C33-C34
27	AF	613	XAT	C31-C32-C33-C40
27	q	617	XAT	O4-C6-C7-C8
27	q	617	XAT	C7-C8-C9-C19
27	q	617	XAT	C11-C10-C9-C8
27	q	617	XAT	C11-C10-C9-C19
27	q	617	XAT	C10-C11-C12-C13
27	q	617	XAT	C12-C13-C14-C15
27	q	617	XAT	O24-C26-C27-C28
27	q	617	XAT	C26-C27-C28-C29
27	q	617	XAT	C27-C28-C29-C30
27	q	617	XAT	C27-C28-C29-C39
27	q	617	XAT	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
27	q	617	XAT	C31-C32-C33-C40
27	AR	616	XAT	O4-C6-C7-C8
27	AR	616	XAT	C7-C8-C9-C19
27	AR	616	XAT	C11-C10-C9-C8
27	AR	616	XAT	C11-C10-C9-C19
27	AR	616	XAT	C10-C11-C12-C13
27	AR	616	XAT	C12-C13-C14-C15
27	AR	616	XAT	O24-C26-C27-C28
27	AR	616	XAT	C26-C27-C28-C29
27	AR	616	XAT	C27-C28-C29-C30
27	AR	616	XAT	C27-C28-C29-C39
27	AR	616	XAT	C28-C29-C30-C31
27	AR	616	XAT	C31-C32-C33-C40
27	AR	616	XAT	C32-C33-C34-C35
28	O	621	LHG	C1-C2-C3-O3
28	O	621	LHG	O2-C2-C3-O3
28	O	621	LHG	C3-O3-P-O4
28	O	621	LHG	C3-O3-P-O5
28	O	621	LHG	C4-O6-P-O5
28	O	621	LHG	O10-C23-O8-C6
28	O	621	LHG	C24-C23-O8-C6
28	O	622	LHG	C4-O6-P-O5
28	O	623	LHG	O1-C1-C2-O2
28	O	623	LHG	O1-C1-C2-C3
28	O	623	LHG	C3-O3-P-O5
28	O	623	LHG	C4-O6-P-O4
28	P	517	LHG	C3-O3-P-O5
28	Q	406	LHG	C4-O6-P-O4
28	q	616	LHG	C2-C3-O3-P
28	q	616	LHG	C3-O3-P-O4
28	q	616	LHG	C3-O3-P-O6
28	v	301	LHG	O1-C1-C2-C3
28	v	301	LHG	C3-O3-P-O4
28	W	201	LHG	C3-O3-P-O4
28	W	201	LHG	C3-O3-P-O5
28	AH	616	LHG	C3-O3-P-O4
28	AK	623	LHG	C4-O6-P-O5
28	AK	624	LHG	O1-C1-C2-C3
28	AK	624	LHG	C3-O3-P-O5
28	AK	624	LHG	C4-O6-P-O4
28	AL	519	LHG	C3-O3-P-O5
28	AM	406	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
28	AQ	618	LHG	C1-C2-C3-O3
28	AQ	618	LHG	C3-O3-P-O4
28	AQ	618	LHG	C3-O3-P-O5
28	AS	301	LHG	O1-C1-C2-C3
28	AS	301	LHG	C3-O3-P-O4
28	w	201	LHG	C3-O3-P-O4
28	w	201	LHG	C3-O3-P-O5
28	AU	617	LHG	C3-O3-P-O4
29	AB	612	BCR	C1-C6-C7-C8
29	AB	612	BCR	C6-C7-C8-C9
29	AB	612	BCR	C7-C8-C9-C10
29	AB	612	BCR	C7-C8-C9-C34
29	AB	612	BCR	C18-C19-C20-C21
29	AB	612	BCR	C22-C23-C24-C25
29	AF	612	BCR	C6-C7-C8-C9
29	AF	612	BCR	C7-C8-C9-C10
29	AF	612	BCR	C7-C8-C9-C34
29	AF	612	BCR	C37-C22-C23-C24
29	AF	612	BCR	C22-C23-C24-C25
29	O	617	BCR	C21-C22-C23-C24
29	O	617	BCR	C37-C22-C23-C24
29	O	617	BCR	C22-C23-C24-C25
29	O	618	BCR	C7-C8-C9-C10
29	O	618	BCR	C7-C8-C9-C34
29	O	625	BCR	C1-C6-C7-C8
29	O	625	BCR	C6-C7-C8-C9
29	O	625	BCR	C7-C8-C9-C34
29	O	625	BCR	C11-C12-C13-C14
29	O	625	BCR	C11-C12-C13-C35
29	O	625	BCR	C21-C22-C23-C24
29	O	625	BCR	C37-C22-C23-C24
29	P	515	BCR	C1-C6-C7-C8
29	P	515	BCR	C7-C8-C9-C34
29	F	101	BCR	C7-C8-C9-C10
29	F	101	BCR	C7-C8-C9-C34
29	j	101	BCR	C7-C8-C9-C10
29	j	101	BCR	C7-C8-C9-C34
29	AI	101	BCR	C1-C6-C7-C8
29	AI	101	BCR	C7-C8-C9-C10
29	AI	101	BCR	C7-C8-C9-C34
29	AI	101	BCR	C21-C22-C23-C24
29	AI	101	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
29	AK	602	BCR	C1-C6-C7-C8
29	AK	602	BCR	C6-C7-C8-C9
29	AK	602	BCR	C7-C8-C9-C34
29	AK	602	BCR	C11-C12-C13-C14
29	AK	602	BCR	C11-C12-C13-C35
29	AK	602	BCR	C21-C22-C23-C24
29	AK	619	BCR	C21-C22-C23-C24
29	AK	619	BCR	C37-C22-C23-C24
29	AK	619	BCR	C22-C23-C24-C25
29	AK	620	BCR	C7-C8-C9-C10
29	AK	620	BCR	C7-C8-C9-C34
29	f	101	BCR	C7-C8-C9-C10
29	f	101	BCR	C7-C8-C9-C34
29	AO	101	BCR	C7-C8-C9-C34
29	k	101	BCR	C1-C6-C7-C8
29	k	101	BCR	C7-C8-C9-C34
29	AV	101	BCR	C1-C6-C7-C8
29	AV	101	BCR	C7-C8-C9-C10
29	AV	101	BCR	C7-C8-C9-C34
29	AV	101	BCR	C21-C22-C23-C24
29	AV	101	BCR	C37-C22-C23-C24
32	J	406	PHO	C1A-C2A-CAA-CBA
32	AJ	408	PHO	CHA-CBD-CGD-O2D
33	J	409	LMG	C2-C1-O1-C7
33	J	409	LMG	O6-C1-O1-C7
33	AL	501	LMG	C2-C1-O1-C7
33	AL	501	LMG	O6-C1-O1-C7
34	J	410	SQD	O6-C44-C45-O47
34	J	410	SQD	O47-C45-C46-O48
34	Q	402	SQD	C8-C7-O47-C45
34	Q	402	SQD	O5-C5-C6-S
34	o	101	SQD	C2-C1-O6-C44
34	o	101	SQD	O5-C1-O6-C44
34	o	101	SQD	O49-C7-O47-C45
34	o	101	SQD	C8-C7-O47-C45
34	M	101	SQD	O5-C1-O6-C44
34	M	101	SQD	C8-C7-O47-C45
34	AJ	411	SQD	O6-C44-C45-O47
34	AJ	411	SQD	O47-C45-C46-O48
34	AM	401	SQD	C8-C7-O47-C45
34	AM	401	SQD	O5-C5-C6-S
34	AP	101	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
34	AP	101	SQD	O5-C1-O6-C44
34	AP	101	SQD	O49-C7-O47-C45
34	AP	101	SQD	C8-C7-O47-C45
34	m	101	SQD	O5-C1-O6-C44
34	m	101	SQD	C8-C7-O47-C45
35	J	413	DGD	C2B-C1B-O2G-C2G
35	J	413	DGD	C2D-C1D-O3G-C3G
35	J	413	DGD	O6D-C1D-O3G-C3G
35	AJ	401	DGD	C2B-C1B-O2G-C2G
35	AJ	401	DGD	C2D-C1D-O3G-C3G
35	AJ	401	DGD	O6D-C1D-O3G-C3G
35	AL	518	DGD	C2D-C1D-O3G-C3G
35	AL	518	DGD	O6D-C1D-O3G-C3G
35	AL	518	DGD	C2E-C1E-O5D-C6D
35	AL	518	DGD	O6E-C1E-O5D-C6D
23	AC	601	CHL	C2C-C3C-CAC-CBC
23	9	601	CHL	O1D-CGD-O2D-CED
23	9	605	CHL	O1D-CGD-O2D-CED
23	AC	601	CHL	O1D-CGD-O2D-CED
23	AC	605	CHL	O1D-CGD-O2D-CED
23	AD	317	CHL	O1D-CGD-O2D-CED
23	V	616	CHL	O1D-CGD-O2D-CED
23	p	606	CHL	O1D-CGD-O2D-CED
23	q	605	CHL	O1D-CGD-O2D-CED
23	q	613	CHL	O1D-CGD-O2D-CED
23	AH	605	CHL	O1D-CGD-O2D-CED
23	AH	606	CHL	O1D-CGD-O2D-CED
23	AN	617	CHL	O1D-CGD-O2D-CED
23	AQ	601	CHL	O1D-CGD-O2D-CED
23	AQ	605	CHL	O1D-CGD-O2D-CED
23	AQ	606	CHL	O1D-CGD-O2D-CED
23	AU	605	CHL	O1D-CGD-O2D-CED
23	AU	606	CHL	O1D-CGD-O2D-CED
24	0	603	CLA	O1D-CGD-O2D-CED
24	AA	613	CLA	O1D-CGD-O2D-CED
24	AC	612	CLA	O1D-CGD-O2D-CED
24	AE	612	CLA	O1D-CGD-O2D-CED
24	J	403	CLA	O1D-CGD-O2D-CED
24	O	605	CLA	O1D-CGD-O2D-CED
24	O	608	CLA	O1D-CGD-O2D-CED
24	P	510	CLA	O1D-CGD-O2D-CED
24	p	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	p	612	CLA	O1D-CGD-O2D-CED
24	p	613	CLA	O1D-CGD-O2D-CED
24	p	618	CLA	O1D-CGD-O2D-CED
24	q	608	CLA	O1D-CGD-O2D-CED
24	AJ	404	CLA	O1D-CGD-O2D-CED
24	AK	607	CLA	O1D-CGD-O2D-CED
24	AK	610	CLA	O1D-CGD-O2D-CED
24	AK	611	CLA	O1D-CGD-O2D-CED
24	AL	504	CLA	O1D-CGD-O2D-CED
24	AL	505	CLA	O1D-CGD-O2D-CED
24	AL	511	CLA	O1D-CGD-O2D-CED
24	AN	612	CLA	O1D-CGD-O2D-CED
24	AQ	604	CLA	O1D-CGD-O2D-CED
24	AQ	613	CLA	O1D-CGD-O2D-CED
24	AS	305	CLA	O1D-CGD-O2D-CED
24	AH	609	CLA	C10-C11-C12-C13
24	AU	609	CLA	C10-C11-C12-C13
23	0	617	CHL	O1D-CGD-O2D-CED
23	AA	606	CHL	O1D-CGD-O2D-CED
23	AA	617	CHL	O1D-CGD-O2D-CED
23	AB	606	CHL	O1D-CGD-O2D-CED
23	AE	605	CHL	O1D-CGD-O2D-CED
23	AE	616	CHL	O1D-CGD-O2D-CED
23	V	606	CHL	O1D-CGD-O2D-CED
23	p	605	CHL	O1D-CGD-O2D-CED
23	q	606	CHL	O1D-CGD-O2D-CED
23	AH	607	CHL	O1D-CGD-O2D-CED
23	AR	605	CHL	O1D-CGD-O2D-CED
23	AR	606	CHL	O1D-CGD-O2D-CED
23	AU	607	CHL	O1D-CGD-O2D-CED
24	9	613	CLA	O1D-CGD-O2D-CED
24	0	602	CLA	O1D-CGD-O2D-CED
24	AA	612	CLA	O1D-CGD-O2D-CED
24	AB	609	CLA	O1D-CGD-O2D-CED
24	AE	611	CLA	O1D-CGD-O2D-CED
24	AF	609	CLA	O1D-CGD-O2D-CED
24	AF	614	CLA	O1D-CGD-O2D-CED
24	O	603	CLA	O1D-CGD-O2D-CED
24	P	502	CLA	O1D-CGD-O2D-CED
24	P	508	CLA	O1D-CGD-O2D-CED
24	V	612	CLA	O1D-CGD-O2D-CED
24	q	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	q	611	CLA	O1D-CGD-O2D-CED
24	v	305	CLA	O1D-CGD-O2D-CED
24	AK	605	CLA	O1D-CGD-O2D-CED
24	AL	507	CLA	O1D-CGD-O2D-CED
24	AL	510	CLA	O1D-CGD-O2D-CED
24	AN	611	CLA	O1D-CGD-O2D-CED
24	AR	610	CLA	O1D-CGD-O2D-CED
24	AR	611	CLA	O1D-CGD-O2D-CED
23	9	601	CHL	CBD-CGD-O2D-CED
23	0	601	CHL	CBD-CGD-O2D-CED
23	AA	605	CHL	CBD-CGD-O2D-CED
23	AA	606	CHL	CBD-CGD-O2D-CED
23	AA	607	CHL	CBD-CGD-O2D-CED
23	AB	606	CHL	CBD-CGD-O2D-CED
23	AD	302	CHL	CBD-CGD-O2D-CED
23	AE	605	CHL	CBD-CGD-O2D-CED
23	AE	606	CHL	CBD-CGD-O2D-CED
23	AE	617	CHL	CBD-CGD-O2D-CED
23	V	607	CHL	CBD-CGD-O2D-CED
23	V	616	CHL	CBD-CGD-O2D-CED
23	p	601	CHL	CBD-CGD-O2D-CED
23	p	607	CHL	CBD-CGD-O2D-CED
23	q	606	CHL	CBD-CGD-O2D-CED
23	q	613	CHL	CBD-CGD-O2D-CED
23	AH	605	CHL	CBD-CGD-O2D-CED
23	AH	607	CHL	CBD-CGD-O2D-CED
23	AN	607	CHL	CBD-CGD-O2D-CED
23	AN	617	CHL	CBD-CGD-O2D-CED
23	AQ	607	CHL	CBD-CGD-O2D-CED
23	AR	606	CHL	CBD-CGD-O2D-CED
23	AR	607	CHL	CBD-CGD-O2D-CED
23	AR	613	CHL	CBD-CGD-O2D-CED
23	AU	605	CHL	CBD-CGD-O2D-CED
23	AU	607	CHL	CBD-CGD-O2D-CED
24	9	602	CLA	CBD-CGD-O2D-CED
24	9	604	CLA	CBD-CGD-O2D-CED
24	0	602	CLA	CBD-CGD-O2D-CED
24	0	603	CLA	CBD-CGD-O2D-CED
24	AA	604	CLA	CBD-CGD-O2D-CED
24	AB	610	CLA	CBD-CGD-O2D-CED
24	AD	303	CLA	CBD-CGD-O2D-CED
24	AD	304	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	AD	311	CLA	CBD-CGD-O2D-CED
24	AE	610	CLA	CBD-CGD-O2D-CED
24	AF	610	CLA	CBD-CGD-O2D-CED
24	AF	614	CLA	CBD-CGD-O2D-CED
24	J	403	CLA	CBD-CGD-O2D-CED
24	O	602	CLA	CBD-CGD-O2D-CED
24	O	610	CLA	CBD-CGD-O2D-CED
24	O	611	CLA	CBD-CGD-O2D-CED
24	O	616	CLA	CBD-CGD-O2D-CED
24	P	510	CLA	CBD-CGD-O2D-CED
24	V	610	CLA	CBD-CGD-O2D-CED
24	V	612	CLA	CBD-CGD-O2D-CED
24	p	602	CLA	CBD-CGD-O2D-CED
24	p	610	CLA	CBD-CGD-O2D-CED
24	p	612	CLA	CBD-CGD-O2D-CED
24	v	312	CLA	CBD-CGD-O2D-CED
24	AH	602	CLA	CBD-CGD-O2D-CED
24	AK	607	CLA	CBD-CGD-O2D-CED
24	AK	612	CLA	CBD-CGD-O2D-CED
24	AK	613	CLA	CBD-CGD-O2D-CED
24	AK	615	CLA	CBD-CGD-O2D-CED
24	AK	618	CLA	CBD-CGD-O2D-CED
24	AL	507	CLA	CBD-CGD-O2D-CED
24	AL	511	CLA	CBD-CGD-O2D-CED
24	AN	611	CLA	CBD-CGD-O2D-CED
24	AN	612	CLA	CBD-CGD-O2D-CED
24	AQ	602	CLA	CBD-CGD-O2D-CED
24	AS	312	CLA	CBD-CGD-O2D-CED
24	AU	602	CLA	CBD-CGD-O2D-CED
24	AU	610	CLA	CBD-CGD-O2D-CED
24	AU	611	CLA	CBD-CGD-O2D-CED
24	P	510	CLA	O1A-CGA-O2A-C1
24	Q	404	CLA	O1A-CGA-O2A-C1
24	p	610	CLA	O1A-CGA-O2A-C1
24	q	610	CLA	O1A-CGA-O2A-C1
24	AL	511	CLA	O1A-CGA-O2A-C1
24	AR	610	CLA	O1A-CGA-O2A-C1
33	P	518	LMG	O10-C28-O8-C9
33	AL	520	LMG	O10-C28-O8-C9
23	AC	601	CHL	C4C-C3C-CAC-CBC
23	AA	605	CHL	O1D-CGD-O2D-CED
23	p	601	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	p	607	CHL	O1D-CGD-O2D-CED
23	AN	606	CHL	O1D-CGD-O2D-CED
23	AQ	607	CHL	O1D-CGD-O2D-CED
24	9	604	CLA	O1D-CGD-O2D-CED
24	AB	604	CLA	O1D-CGD-O2D-CED
24	AB	610	CLA	O1D-CGD-O2D-CED
24	AD	303	CLA	O1D-CGD-O2D-CED
24	AD	304	CLA	O1D-CGD-O2D-CED
24	P	501	CLA	O1D-CGD-O2D-CED
24	P	509	CLA	O1D-CGD-O2D-CED
24	V	610	CLA	O1D-CGD-O2D-CED
24	q	601	CLA	O1D-CGD-O2D-CED
24	AL	509	CLA	O1D-CGD-O2D-CED
23	0	606	CHL	O1D-CGD-O2D-CED
23	AD	306	CHL	O1D-CGD-O2D-CED
23	AE	617	CHL	O1D-CGD-O2D-CED
24	AA	611	CLA	O1D-CGD-O2D-CED
24	AB	611	CLA	O1D-CGD-O2D-CED
24	AC	602	CLA	O1D-CGD-O2D-CED
24	AD	305	CLA	O1D-CGD-O2D-CED
24	AE	610	CLA	O1D-CGD-O2D-CED
24	AF	610	CLA	O1D-CGD-O2D-CED
24	O	602	CLA	O1D-CGD-O2D-CED
24	P	503	CLA	O1D-CGD-O2D-CED
24	P	504	CLA	O1D-CGD-O2D-CED
24	P	505	CLA	O1D-CGD-O2D-CED
24	P	506	CLA	O1D-CGD-O2D-CED
24	P	507	CLA	O1D-CGD-O2D-CED
24	Q	404	CLA	O1D-CGD-O2D-CED
24	q	618	CLA	O1D-CGD-O2D-CED
24	AK	604	CLA	O1D-CGD-O2D-CED
24	AL	502	CLA	O1D-CGD-O2D-CED
24	AL	503	CLA	O1D-CGD-O2D-CED
24	AL	506	CLA	O1D-CGD-O2D-CED
24	AU	604	CLA	O1D-CGD-O2D-CED
24	AU	609	CLA	O1D-CGD-O2D-CED
24	AU	613	CLA	O1D-CGD-O2D-CED
24	p	610	CLA	CBA-CGA-O2A-C1
24	q	610	CLA	CBA-CGA-O2A-C1
24	AR	610	CLA	CBA-CGA-O2A-C1
33	P	518	LMG	C29-C28-O8-C9
33	AL	520	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
23	0	607	CHL	CBD-CGD-O2D-CED
23	AC	606	CHL	CBD-CGD-O2D-CED
23	AC	607	CHL	CBD-CGD-O2D-CED
23	V	605	CHL	CBD-CGD-O2D-CED
23	AH	601	CHL	CBD-CGD-O2D-CED
23	AQ	609	CHL	CBD-CGD-O2D-CED
23	AU	601	CHL	CBD-CGD-O2D-CED
24	9	603	CLA	CBD-CGD-O2D-CED
24	0	611	CLA	CBD-CGD-O2D-CED
24	AA	603	CLA	CBD-CGD-O2D-CED
24	AC	603	CLA	CBD-CGD-O2D-CED
24	AD	310	CLA	CBD-CGD-O2D-CED
24	AE	603	CLA	CBD-CGD-O2D-CED
24	AE	604	CLA	CBD-CGD-O2D-CED
24	AF	603	CLA	CBD-CGD-O2D-CED
24	O	607	CLA	CBD-CGD-O2D-CED
24	V	602	CLA	CBD-CGD-O2D-CED
24	p	603	CLA	CBD-CGD-O2D-CED
24	AH	611	CLA	CBD-CGD-O2D-CED
24	AK	609	CLA	CBD-CGD-O2D-CED
24	AN	602	CLA	CBD-CGD-O2D-CED
24	AQ	603	CLA	CBD-CGD-O2D-CED
24	AU	612	CLA	CBD-CGD-O2D-CED
23	AH	608	CHL	O1A-CGA-O2A-C1
23	AU	608	CHL	O1A-CGA-O2A-C1
24	O	601	CLA	O1A-CGA-O2A-C1
24	O	616	CLA	O1A-CGA-O2A-C1
24	P	506	CLA	O1A-CGA-O2A-C1
24	Q	401	CLA	O1A-CGA-O2A-C1
24	v	311	CLA	O1A-CGA-O2A-C1
24	AH	613	CLA	O1A-CGA-O2A-C1
24	AJ	406	CLA	O1A-CGA-O2A-C1
24	AK	603	CLA	O1A-CGA-O2A-C1
24	AK	618	CLA	O1A-CGA-O2A-C1
24	AL	507	CLA	O1A-CGA-O2A-C1
24	AS	311	CLA	O1A-CGA-O2A-C1
24	AU	613	CLA	O1A-CGA-O2A-C1
32	J	405	PHO	O1A-CGA-O2A-C1
32	AJ	407	PHO	O1A-CGA-O2A-C1
35	J	413	DGD	O1A-C1A-O1G-C1G
35	AJ	401	DGD	O1A-C1A-O1G-C1G
24	0	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	AB	603	CLA	O1D-CGD-O2D-CED
24	AD	313	CLA	O1D-CGD-O2D-CED
24	v	304	CLA	O1D-CGD-O2D-CED
24	AH	604	CLA	O1D-CGD-O2D-CED
24	AH	609	CLA	O1D-CGD-O2D-CED
24	AH	610	CLA	O1D-CGD-O2D-CED
24	AL	508	CLA	O1D-CGD-O2D-CED
24	AM	404	CLA	O1D-CGD-O2D-CED
24	AR	601	CLA	O1D-CGD-O2D-CED
24	AS	304	CLA	O1D-CGD-O2D-CED
24	AA	602	CLA	O1D-CGD-O2D-CED
24	AE	602	CLA	O1D-CGD-O2D-CED
24	O	609	CLA	O1D-CGD-O2D-CED
24	O	613	CLA	O1D-CGD-O2D-CED
24	AQ	610	CLA	O1D-CGD-O2D-CED
24	P	511	CLA	CBD-CGD-O2D-CED
24	V	603	CLA	CBD-CGD-O2D-CED
24	AH	612	CLA	CBD-CGD-O2D-CED
24	AL	513	CLA	CBD-CGD-O2D-CED
24	0	612	CLA	O1D-CGD-O2D-CED
24	AC	604	CLA	O1D-CGD-O2D-CED
24	AK	615	CLA	O1D-CGD-O2D-CED
28	AL	519	LHG	O9-C7-O7-C5
34	Q	402	SQD	O49-C7-O47-C45
34	M	101	SQD	O49-C7-O47-C45
34	AM	401	SQD	O49-C7-O47-C45
34	m	101	SQD	O49-C7-O47-C45
23	AF	606	CHL	O1D-CGD-O2D-CED
23	q	605	CHL	C3-C5-C6-C7
23	AR	605	CHL	C3-C5-C6-C7
24	AA	603	CLA	C3-C5-C6-C7
24	O	605	CLA	C3-C5-C6-C7
24	O	607	CLA	C3-C5-C6-C7
24	O	616	CLA	C3-C5-C6-C7
24	V	609	CLA	C3-C5-C6-C7
24	V	610	CLA	C3-C5-C6-C7
24	v	311	CLA	C3-C5-C6-C7
24	AK	607	CLA	C3-C5-C6-C7
24	AK	609	CLA	C3-C5-C6-C7
24	AK	618	CLA	C3-C5-C6-C7
24	AN	609	CLA	C3-C5-C6-C7
24	AN	611	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	AQ	610	CLA	C3-C5-C6-C7
24	AR	603	CLA	C3-C5-C6-C7
24	AR	612	CLA	C3-C5-C6-C7
24	AS	311	CLA	C3-C5-C6-C7
23	9	609	CHL	CBA-CGA-O2A-C1
23	AC	608	CHL	CBA-CGA-O2A-C1
23	V	608	CHL	CBA-CGA-O2A-C1
23	p	601	CHL	CBA-CGA-O2A-C1
23	AN	608	CHL	CBA-CGA-O2A-C1
24	AA	603	CLA	CBA-CGA-O2A-C1
24	O	601	CLA	CBA-CGA-O2A-C1
24	O	604	CLA	CBA-CGA-O2A-C1
24	O	610	CLA	CBA-CGA-O2A-C1
24	O	616	CLA	CBA-CGA-O2A-C1
24	P	510	CLA	CBA-CGA-O2A-C1
24	Q	404	CLA	CBA-CGA-O2A-C1
24	AK	603	CLA	CBA-CGA-O2A-C1
24	AK	606	CLA	CBA-CGA-O2A-C1
24	AK	618	CLA	CBA-CGA-O2A-C1
24	AL	511	CLA	CBA-CGA-O2A-C1
24	AM	404	CLA	CBA-CGA-O2A-C1
24	AU	613	CLA	CBA-CGA-O2A-C1
35	J	413	DGD	C2A-C1A-O1G-C1G
35	AJ	401	DGD	C2A-C1A-O1G-C1G
28	AL	519	LHG	C8-C7-O7-C5
23	AR	613	CHL	O1D-CGD-O2D-CED
24	AN	613	CLA	O1D-CGD-O2D-CED
24	AN	603	CLA	CBD-CGD-O2D-CED
24	AQ	611	CLA	O1A-CGA-O2A-C1
23	0	601	CHL	C2C-C3C-CAC-CBC
23	AR	607	CHL	C3-C5-C6-C7
23	V	607	CHL	C4-C3-C5-C6
23	AH	608	CHL	C4-C3-C5-C6
23	AU	608	CHL	C4-C3-C5-C6
23	V	607	CHL	C2-C3-C5-C6
23	AH	608	CHL	C2-C3-C5-C6
23	AU	608	CHL	C2-C3-C5-C6
24	P	508	CLA	C2-C3-C5-C6
24	AK	615	CLA	C2-C3-C5-C6
24	AL	509	CLA	C2-C3-C5-C6
23	9	608	CHL	CBD-CGD-O2D-CED
23	q	607	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	9	607	CHL	C2A-CAA-CBA-CGA
23	9	608	CHL	C2A-CAA-CBA-CGA
23	0	605	CHL	C2A-CAA-CBA-CGA
23	0	606	CHL	C2A-CAA-CBA-CGA
23	AA	606	CHL	C2A-CAA-CBA-CGA
23	AC	607	CHL	C2A-CAA-CBA-CGA
23	AD	306	CHL	C2A-CAA-CBA-CGA
23	AE	605	CHL	C2A-CAA-CBA-CGA
23	V	606	CHL	C2A-CAA-CBA-CGA
23	V	607	CHL	C2A-CAA-CBA-CGA
23	p	607	CHL	C2A-CAA-CBA-CGA
23	AH	607	CHL	C2A-CAA-CBA-CGA
23	AN	606	CHL	C2A-CAA-CBA-CGA
23	AQ	607	CHL	C2A-CAA-CBA-CGA
23	AR	606	CHL	C2A-CAA-CBA-CGA
23	AU	607	CHL	C2A-CAA-CBA-CGA
24	9	604	CLA	C2A-CAA-CBA-CGA
24	9	611	CLA	C2A-CAA-CBA-CGA
24	AA	610	CLA	C2A-CAA-CBA-CGA
24	AA	613	CLA	C2A-CAA-CBA-CGA
24	AC	604	CLA	C2A-CAA-CBA-CGA
24	AC	610	CLA	C2A-CAA-CBA-CGA
24	AD	305	CLA	C2A-CAA-CBA-CGA
24	AE	609	CLA	C2A-CAA-CBA-CGA
24	AE	612	CLA	C2A-CAA-CBA-CGA
24	AF	610	CLA	C2A-CAA-CBA-CGA
24	J	403	CLA	C2A-CAA-CBA-CGA
24	J	407	CLA	C2A-CAA-CBA-CGA
24	O	606	CLA	C2A-CAA-CBA-CGA
24	O	607	CLA	C2A-CAA-CBA-CGA
24	P	504	CLA	C2A-CAA-CBA-CGA
24	P	505	CLA	C2A-CAA-CBA-CGA
24	Q	404	CLA	C2A-CAA-CBA-CGA
24	p	618	CLA	C2A-CAA-CBA-CGA
24	q	610	CLA	C2A-CAA-CBA-CGA
24	v	303	CLA	C2A-CAA-CBA-CGA
24	AH	604	CLA	C2A-CAA-CBA-CGA
24	AJ	404	CLA	C2A-CAA-CBA-CGA
24	AJ	409	CLA	C2A-CAA-CBA-CGA
24	AK	609	CLA	C2A-CAA-CBA-CGA
24	AL	502	CLA	C2A-CAA-CBA-CGA
24	AL	505	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	AL	506	CLA	C2A-CAA-CBA-CGA
24	AM	404	CLA	C2A-CAA-CBA-CGA
24	AQ	613	CLA	C2A-CAA-CBA-CGA
24	AR	610	CLA	C2A-CAA-CBA-CGA
24	AS	303	CLA	C2A-CAA-CBA-CGA
24	AU	604	CLA	C2A-CAA-CBA-CGA
24	V	612	CLA	O1A-CGA-O2A-C1
24	AK	610	CLA	O1A-CGA-O2A-C1
23	AD	302	CHL	O1D-CGD-O2D-CED
24	9	613	CLA	C3-C5-C6-C7
24	P	503	CLA	C3-C5-C6-C7
24	p	610	CLA	C3-C5-C6-C7
24	q	603	CLA	C3-C5-C6-C7
24	AH	602	CLA	C3-C5-C6-C7
24	AL	504	CLA	C3-C5-C6-C7
24	AU	602	CLA	C3-C5-C6-C7
32	J	405	PHO	C3-C5-C6-C7
32	J	406	PHO	C3-C5-C6-C7
32	AJ	407	PHO	C3-C5-C6-C7
23	AE	607	CHL	CBA-CGA-O2A-C1
23	V	607	CHL	CBA-CGA-O2A-C1
23	p	609	CHL	CBA-CGA-O2A-C1
23	AH	608	CHL	CBA-CGA-O2A-C1
23	AN	607	CHL	CBA-CGA-O2A-C1
23	AQ	609	CHL	CBA-CGA-O2A-C1
23	AU	608	CHL	CBA-CGA-O2A-C1
24	9	613	CLA	CBA-CGA-O2A-C1
24	AD	303	CLA	CBA-CGA-O2A-C1
24	AE	603	CLA	CBA-CGA-O2A-C1
24	P	501	CLA	CBA-CGA-O2A-C1
24	P	506	CLA	CBA-CGA-O2A-C1
24	P	512	CLA	CBA-CGA-O2A-C1
24	Q	401	CLA	CBA-CGA-O2A-C1
24	V	612	CLA	CBA-CGA-O2A-C1
24	q	609	CLA	CBA-CGA-O2A-C1
24	v	311	CLA	CBA-CGA-O2A-C1
24	AH	613	CLA	CBA-CGA-O2A-C1
24	AJ	406	CLA	CBA-CGA-O2A-C1
24	AK	612	CLA	CBA-CGA-O2A-C1
24	AK	616	CLA	CBA-CGA-O2A-C1
24	AL	507	CLA	CBA-CGA-O2A-C1
24	AL	514	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	AN	613	CLA	CBA-CGA-O2A-C1
24	AQ	611	CLA	CBA-CGA-O2A-C1
24	AS	303	CLA	CBA-CGA-O2A-C1
24	AS	311	CLA	CBA-CGA-O2A-C1
32	J	405	PHO	CBA-CGA-O2A-C1
32	AJ	407	PHO	CBA-CGA-O2A-C1
23	AE	606	CHL	O1D-CGD-O2D-CED
24	O	611	CLA	O1D-CGD-O2D-CED
24	v	312	CLA	O1D-CGD-O2D-CED
24	AS	312	CLA	O1D-CGD-O2D-CED
24	AA	604	CLA	O1D-CGD-O2D-CED
24	AU	610	CLA	O1D-CGD-O2D-CED
28	P	517	LHG	O9-C7-O7-C5
35	AJ	412	DGD	O1B-C1B-O2G-C2G
35	P	516	DGD	C4E-C5E-C6E-O5E
35	AL	517	DGD	C4E-C5E-C6E-O5E
23	9	609	CHL	O1A-CGA-O2A-C1
23	AE	607	CHL	O1A-CGA-O2A-C1
23	V	607	CHL	O1A-CGA-O2A-C1
23	p	601	CHL	O1A-CGA-O2A-C1
23	p	609	CHL	O1A-CGA-O2A-C1
23	AN	607	CHL	O1A-CGA-O2A-C1
23	AN	608	CHL	O1A-CGA-O2A-C1
23	AQ	601	CHL	O1A-CGA-O2A-C1
23	AQ	609	CHL	O1A-CGA-O2A-C1
24	0	602	CLA	O1A-CGA-O2A-C1
24	AA	603	CLA	O1A-CGA-O2A-C1
24	AD	304	CLA	O1A-CGA-O2A-C1
24	O	604	CLA	O1A-CGA-O2A-C1
24	P	501	CLA	O1A-CGA-O2A-C1
24	P	512	CLA	O1A-CGA-O2A-C1
24	q	609	CLA	O1A-CGA-O2A-C1
24	v	303	CLA	O1A-CGA-O2A-C1
24	AK	606	CLA	O1A-CGA-O2A-C1
24	AL	502	CLA	O1A-CGA-O2A-C1
24	AL	514	CLA	O1A-CGA-O2A-C1
24	AR	609	CLA	O1A-CGA-O2A-C1
24	AS	303	CLA	O1A-CGA-O2A-C1
24	O	610	CLA	O1D-CGD-O2D-CED
24	O	616	CLA	O1D-CGD-O2D-CED
26	q	615	NEX	C13-C14-C15-C35
26	v	317	NEX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	AR	615	NEX	C9-C10-C11-C12
26	AS	317	NEX	C9-C10-C11-C12
26	AU	616	NEX	C13-C14-C15-C35
27	9	618	XAT	C29-C30-C31-C32
27	AB	613	XAT	C33-C34-C35-C15
29	AB	612	BCR	C19-C20-C21-C22
35	J	411	DGD	O6E-C5E-C6E-O5E
23	AS	308	CHL	CBD-CGD-O2D-CED
24	q	604	CLA	CBD-CGD-O2D-CED
24	AK	603	CLA	CBD-CGD-O2D-CED
24	AR	604	CLA	CBD-CGD-O2D-CED
32	J	406	PHO	CBD-CGD-O2D-CED
23	AN	607	CHL	O1D-CGD-O2D-CED
24	p	602	CLA	O1D-CGD-O2D-CED
24	AH	602	CLA	O1D-CGD-O2D-CED
24	AQ	602	CLA	O1D-CGD-O2D-CED
28	P	517	LHG	O2-C2-C3-O3
28	AK	623	LHG	O2-C2-C3-O3
28	AL	519	LHG	O2-C2-C3-O3
28	AQ	618	LHG	O2-C2-C3-O3
24	9	603	CLA	C3-C5-C6-C7
24	AC	603	CLA	C3-C5-C6-C7
24	AH	609	CLA	C3-C5-C6-C7
32	AJ	408	PHO	C3-C5-C6-C7
35	AO	102	DGD	C4D-C5D-C6D-O5D
23	AD	308	CHL	CBA-CGA-O2A-C1
23	AQ	601	CHL	CBA-CGA-O2A-C1
24	0	602	CLA	CBA-CGA-O2A-C1
24	0	603	CLA	CBA-CGA-O2A-C1
24	AA	609	CLA	CBA-CGA-O2A-C1
24	O	614	CLA	CBA-CGA-O2A-C1
24	V	603	CLA	CBA-CGA-O2A-C1
24	v	303	CLA	CBA-CGA-O2A-C1
24	AK	610	CLA	CBA-CGA-O2A-C1
24	AL	502	CLA	CBA-CGA-O2A-C1
24	AL	512	CLA	CBA-CGA-O2A-C1
24	AN	603	CLA	CBA-CGA-O2A-C1
35	AL	518	DGD	C2A-C1A-O1G-C1G
23	AC	608	CHL	O1A-CGA-O2A-C1
23	AD	308	CHL	O1A-CGA-O2A-C1
23	V	608	CHL	O1A-CGA-O2A-C1
24	0	603	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	O	608	CLA	O1A-CGA-O2A-C1
24	O	610	CLA	O1A-CGA-O2A-C1
24	AK	612	CLA	O1A-CGA-O2A-C1
24	AN	613	CLA	O1A-CGA-O2A-C1
33	Q	407	LMG	O6-C5-C6-O5
33	AM	407	LMG	O6-C5-C6-O5
35	AO	102	DGD	O6E-C5E-C6E-O5E
23	0	601	CHL	O1D-CGD-O2D-CED
24	AK	613	CLA	O1D-CGD-O2D-CED
24	AU	602	CLA	O1D-CGD-O2D-CED
28	P	517	LHG	C8-C7-O7-C5
23	AA	608	CHL	C1A-C2A-CAA-CBA
23	AH	608	CHL	CBD-CGD-O2D-CED
23	AN	605	CHL	CBD-CGD-O2D-CED
24	0	610	CLA	CBD-CGD-O2D-CED
32	AJ	408	PHO	CBD-CGD-O2D-CED
35	AJ	412	DGD	O6E-C5E-C6E-O5E
24	AD	303	CLA	O1A-CGA-O2A-C1
24	AK	612	CLA	O1D-CGD-O2D-CED
24	AU	611	CLA	O1D-CGD-O2D-CED
24	P	506	CLA	C3-C5-C6-C7
24	AK	615	CLA	C3-C5-C6-C7
24	AD	304	CLA	CBA-CGA-O2A-C1
24	AE	608	CLA	CBA-CGA-O2A-C1
24	O	608	CLA	CBA-CGA-O2A-C1
24	AR	609	CLA	CBA-CGA-O2A-C1
24	AD	311	CLA	O1D-CGD-O2D-CED
35	J	411	DGD	O1B-C1B-O2G-C2G
28	Q	406	LHG	C28-C29-C30-C31
28	AM	406	LHG	C28-C29-C30-C31
24	9	613	CLA	O1A-CGA-O2A-C1
24	O	614	CLA	O1A-CGA-O2A-C1
24	V	603	CLA	O1A-CGA-O2A-C1
24	AK	616	CLA	O1A-CGA-O2A-C1
24	AL	512	CLA	O1A-CGA-O2A-C1
28	O	621	LHG	C30-C31-C32-C33
23	AU	601	CHL	C5-C6-C7-C8
23	V	601	CHL	C4-C3-C5-C6
23	AQ	601	CHL	C4-C3-C5-C6
24	O	602	CLA	C4-C3-C5-C6
24	O	603	CLA	C4-C3-C5-C6
24	O	605	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	AK	604	CLA	C4-C3-C5-C6
24	AK	605	CLA	C4-C3-C5-C6
24	AK	607	CLA	C4-C3-C5-C6
23	V	601	CHL	C2-C3-C5-C6
23	AN	601	CHL	C2-C3-C5-C6
23	AQ	601	CHL	C2-C3-C5-C6
24	O	602	CLA	C2-C3-C5-C6
24	O	603	CLA	C2-C3-C5-C6
24	O	605	CLA	C2-C3-C5-C6
24	O	613	CLA	C2-C3-C5-C6
24	AK	604	CLA	C2-C3-C5-C6
24	AK	605	CLA	C2-C3-C5-C6
24	AK	607	CLA	C2-C3-C5-C6
23	AA	607	CHL	C2A-CAA-CBA-CGA
23	AB	605	CHL	C2A-CAA-CBA-CGA
23	AB	606	CHL	C2A-CAA-CBA-CGA
23	AE	606	CHL	C2A-CAA-CBA-CGA
23	p	605	CHL	C2A-CAA-CBA-CGA
23	AQ	605	CHL	C2A-CAA-CBA-CGA
23	AS	307	CHL	C2A-CAA-CBA-CGA
24	0	602	CLA	C2A-CAA-CBA-CGA
24	AF	614	CLA	C2A-CAA-CBA-CGA
24	P	510	CLA	C2A-CAA-CBA-CGA
24	AL	511	CLA	C2A-CAA-CBA-CGA
23	AA	607	CHL	O1D-CGD-O2D-CED
24	AK	618	CLA	O1D-CGD-O2D-CED
34	AJ	411	SQD	C17-C18-C19-C20
35	P	516	DGD	O6E-C5E-C6E-O5E
35	AL	517	DGD	O6E-C5E-C6E-O5E
24	AA	609	CLA	O1A-CGA-O2A-C1
24	AE	603	CLA	O1A-CGA-O2A-C1
34	AM	401	SQD	O5-C1-O6-C44
28	AQ	618	LHG	C28-C29-C30-C31
24	P	508	CLA	C3-C5-C6-C7
24	AC	603	CLA	CBA-CGA-O2A-C1
24	q	611	CLA	CBA-CGA-O2A-C1
24	v	314	CLA	CBA-CGA-O2A-C1
24	AJ	409	CLA	CBA-CGA-O2A-C1
24	AM	403	CLA	CBA-CGA-O2A-C1
24	AQ	613	CLA	CBA-CGA-O2A-C1
24	AR	611	CLA	CBA-CGA-O2A-C1
24	AS	314	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	p	617	LHG	C28-C29-C30-C31
34	J	410	SQD	C17-C18-C19-C20
24	p	610	CLA	O1D-CGD-O2D-CED
23	0	601	CHL	C4C-C3C-CAC-CBC
23	V	607	CHL	O1D-CGD-O2D-CED
23	AR	607	CHL	O1D-CGD-O2D-CED
24	9	602	CLA	O1D-CGD-O2D-CED
24	0	611	CLA	O1D-CGD-O2D-CED
24	AH	611	CLA	O1D-CGD-O2D-CED
24	AE	608	CLA	O1A-CGA-O2A-C1
24	AN	603	CLA	O1A-CGA-O2A-C1
35	J	411	DGD	C4E-C5E-C6E-O5E
35	AJ	412	DGD	C4E-C5E-C6E-O5E
23	V	605	CHL	O1D-CGD-O2D-CED
24	AF	603	CLA	O1D-CGD-O2D-CED
24	O	607	CLA	O1D-CGD-O2D-CED
24	p	603	CLA	O1D-CGD-O2D-CED
24	AK	609	CLA	O1D-CGD-O2D-CED
24	AQ	603	CLA	O1D-CGD-O2D-CED
24	AU	612	CLA	O1D-CGD-O2D-CED
24	Q	403	CLA	CBD-CGD-O2D-CED
23	AA	608	CHL	C2A-CAA-CBA-CGA
35	J	413	DGD	O6E-C5E-C6E-O5E
35	AJ	401	DGD	O6E-C5E-C6E-O5E
24	v	314	CLA	O1A-CGA-O2A-C1
24	AQ	613	CLA	O1A-CGA-O2A-C1
24	AS	314	CLA	O1A-CGA-O2A-C1
24	AE	603	CLA	C3-C5-C6-C7
24	O	613	CLA	C3-C5-C6-C7
24	AL	509	CLA	C3-C5-C6-C7
24	AN	612	CLA	C3-C5-C6-C7
24	AU	609	CLA	C3-C5-C6-C7
24	AE	604	CLA	O1D-CGD-O2D-CED
23	V	601	CHL	CBA-CGA-O2A-C1
23	AH	601	CHL	CBA-CGA-O2A-C1
23	AN	601	CHL	CBA-CGA-O2A-C1
23	AU	601	CHL	CBA-CGA-O2A-C1
24	9	602	CLA	CBA-CGA-O2A-C1
24	9	603	CLA	CBA-CGA-O2A-C1
24	AC	602	CLA	CBA-CGA-O2A-C1
24	AD	313	CLA	CBA-CGA-O2A-C1
24	J	407	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	P	505	CLA	CBA-CGA-O2A-C1
24	Q	403	CLA	CBA-CGA-O2A-C1
24	K	101	CLA	CBA-CGA-O2A-C1
24	p	603	CLA	CBA-CGA-O2A-C1
24	q	601	CLA	CBA-CGA-O2A-C1
24	v	305	CLA	CBA-CGA-O2A-C1
24	v	310	CLA	CBA-CGA-O2A-C1
24	v	313	CLA	CBA-CGA-O2A-C1
24	AH	602	CLA	CBA-CGA-O2A-C1
24	AH	609	CLA	CBA-CGA-O2A-C1
24	AL	506	CLA	CBA-CGA-O2A-C1
24	AQ	603	CLA	CBA-CGA-O2A-C1
24	AR	601	CLA	CBA-CGA-O2A-C1
24	AS	310	CLA	CBA-CGA-O2A-C1
24	AU	602	CLA	CBA-CGA-O2A-C1
24	AU	609	CLA	CBA-CGA-O2A-C1
32	J	406	PHO	CBA-CGA-O2A-C1
32	AJ	408	PHO	CBA-CGA-O2A-C1
34	J	410	SQD	C24-C23-O48-C46
34	M	101	SQD	C24-C23-O48-C46
34	AJ	411	SQD	C24-C23-O48-C46
34	m	101	SQD	C24-C23-O48-C46
26	p	616	NEX	C29-C30-C31-C32
26	AR	615	NEX	C13-C14-C15-C35
26	AU	616	NEX	C9-C10-C11-C12
23	AH	601	CHL	C5-C6-C7-C8
23	AQ	608	CHL	C13-C15-C16-C17
23	AU	601	CHL	C8-C10-C11-C12
24	AK	608	CLA	C8-C10-C11-C12
24	AK	618	CLA	C5-C6-C7-C8
23	AD	302	CHL	C5-C6-C7-C8
23	AH	601	CHL	C8-C10-C11-C12
23	AN	606	CHL	C13-C15-C16-C17
24	9	602	CLA	C5-C6-C7-C8
24	O	607	CLA	C13-C15-C16-C17
24	O	610	CLA	C15-C16-C17-C18
24	O	611	CLA	C8-C10-C11-C12
24	O	616	CLA	C5-C6-C7-C8
24	P	507	CLA	C13-C15-C16-C17
24	v	311	CLA	C5-C6-C7-C8
24	AK	609	CLA	C13-C15-C16-C17
24	AK	613	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	AL	508	CLA	C13-C15-C16-C17
24	AS	311	CLA	C5-C6-C7-C8
28	O	622	LHG	O2-C2-C3-O3
28	AQ	618	LHG	C23-C24-C25-C26
23	AH	601	CHL	O1A-CGA-O2A-C1
23	AN	601	CHL	O1A-CGA-O2A-C1
23	AU	601	CHL	O1A-CGA-O2A-C1
23	0	601	CHL	C11-C10-C8-C9
23	0	601	CHL	C14-C13-C15-C16
23	AA	606	CHL	C6-C7-C8-C9
23	AD	302	CHL	C11-C10-C8-C9
23	AE	605	CHL	C6-C7-C8-C9
23	V	601	CHL	C6-C7-C8-C9
23	V	607	CHL	C11-C10-C8-C9
23	V	607	CHL	C14-C13-C15-C16
23	p	601	CHL	C6-C7-C8-C9
23	p	607	CHL	C6-C7-C8-C9
23	p	608	CHL	C14-C13-C15-C16
23	AH	607	CHL	C11-C12-C13-C14
23	AH	608	CHL	C11-C10-C8-C9
23	AH	608	CHL	C14-C13-C15-C16
23	AN	601	CHL	C6-C7-C8-C9
23	AN	607	CHL	C11-C10-C8-C9
23	AN	607	CHL	C14-C13-C15-C16
23	AQ	607	CHL	C6-C7-C8-C9
23	AQ	607	CHL	C11-C12-C13-C14
23	AQ	608	CHL	C14-C13-C15-C16
23	AU	608	CHL	C11-C10-C8-C9
23	AU	608	CHL	C14-C13-C15-C16
24	9	602	CLA	C11-C10-C8-C9
24	0	602	CLA	C11-C10-C8-C9
24	AD	303	CLA	C11-C10-C8-C9
24	O	603	CLA	C14-C13-C15-C16
24	O	604	CLA	C6-C7-C8-C9
24	O	615	CLA	C11-C10-C8-C9
24	P	506	CLA	C14-C13-C15-C16
24	P	507	CLA	C11-C10-C8-C9
24	P	509	CLA	C6-C7-C8-C9
24	P	512	CLA	C14-C13-C15-C16
24	Q	403	CLA	C6-C7-C8-C9
24	V	609	CLA	C6-C7-C8-C9
24	p	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	p	603	CLA	C6-C7-C8-C9
24	q	609	CLA	C6-C7-C8-C9
24	q	612	CLA	C6-C7-C8-C9
24	AH	602	CLA	C11-C10-C8-C9
24	AH	602	CLA	C14-C13-C15-C16
24	AH	610	CLA	C11-C10-C8-C9
24	AK	605	CLA	C14-C13-C15-C16
24	AK	617	CLA	C11-C10-C8-C9
24	AL	502	CLA	C14-C13-C15-C16
24	AL	507	CLA	C14-C13-C15-C16
24	AL	508	CLA	C11-C10-C8-C9
24	AL	514	CLA	C14-C13-C15-C16
24	AM	403	CLA	C6-C7-C8-C9
24	AN	609	CLA	C6-C7-C8-C9
24	AQ	602	CLA	C11-C10-C8-C9
24	AQ	603	CLA	C6-C7-C8-C9
24	AQ	611	CLA	C11-C10-C8-C9
24	AR	609	CLA	C6-C7-C8-C9
24	AR	612	CLA	C11-C10-C8-C9
24	AS	303	CLA	C11-C10-C8-C9
24	AU	602	CLA	C14-C13-C15-C16
24	AU	610	CLA	C11-C10-C8-C9
32	J	405	PHO	C14-C13-C15-C16
32	J	406	PHO	C6-C7-C8-C9
32	AJ	407	PHO	C14-C13-C15-C16
32	AJ	408	PHO	C6-C7-C8-C9
23	AC	606	CHL	O1D-CGD-O2D-CED
23	AQ	609	CHL	O1D-CGD-O2D-CED
24	9	603	CLA	O1D-CGD-O2D-CED
24	V	602	CLA	O1D-CGD-O2D-CED
23	AD	307	CHL	C2A-CAA-CBA-CGA
23	AE	601	CHL	C2A-CAA-CBA-CGA
23	AE	616	CHL	C2A-CAA-CBA-CGA
23	V	608	CHL	C2A-CAA-CBA-CGA
23	AS	308	CHL	C2A-CAA-CBA-CGA
24	0	604	CLA	C2A-CAA-CBA-CGA
24	O	605	CLA	C2A-CAA-CBA-CGA
24	O	614	CLA	C2A-CAA-CBA-CGA
24	AH	613	CLA	C2A-CAA-CBA-CGA
24	AK	616	CLA	C2A-CAA-CBA-CGA
25	9	615	LUT	C7-C8-C9-C19
25	AC	614	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
25	v	316	LUT	C7-C8-C9-C19
25	AH	614	LUT	C7-C8-C9-C19
25	AS	315	LUT	C7-C8-C9-C19
26	AE	615	NEX	C11-C12-C13-C20
26	q	615	NEX	C11-C12-C13-C20
26	q	615	NEX	C31-C32-C33-C40
26	AQ	617	NEX	C27-C28-C29-C39
26	AQ	617	NEX	C31-C32-C33-C40
26	AR	615	NEX	C11-C12-C13-C20
27	AB	613	XAT	C11-C12-C13-C20
27	AF	613	XAT	C11-C12-C13-C20
27	AF	613	XAT	C27-C28-C29-C39
27	q	617	XAT	C11-C12-C13-C20
27	AR	616	XAT	C11-C12-C13-C20
29	AB	612	BCR	C37-C22-C23-C24
29	AK	602	BCR	C37-C22-C23-C24
25	9	615	LUT	C7-C8-C9-C10
25	AC	614	LUT	C7-C8-C9-C10
26	q	615	NEX	C11-C12-C13-C14
26	AR	615	NEX	C11-C12-C13-C14
28	O	621	LHG	O9-C7-O7-C5
28	O	623	LHG	C23-C24-C25-C26
28	p	617	LHG	C23-C24-C25-C26
23	V	601	CHL	O1A-CGA-O2A-C1
24	AD	313	CLA	O1A-CGA-O2A-C1
24	K	101	CLA	O1A-CGA-O2A-C1
24	p	603	CLA	O1A-CGA-O2A-C1
24	v	305	CLA	O1A-CGA-O2A-C1
24	AH	602	CLA	O1A-CGA-O2A-C1
32	J	406	PHO	O1A-CGA-O2A-C1
32	AJ	408	PHO	O1A-CGA-O2A-C1
23	0	601	CHL	C5-C6-C7-C8
23	AA	608	CHL	C8-C10-C11-C12
23	V	608	CHL	C8-C10-C11-C12
23	AH	608	CHL	C15-C16-C17-C18
23	AQ	608	CHL	C15-C16-C17-C18
24	AD	309	CLA	C10-C11-C12-C13
24	O	609	CLA	C5-C6-C7-C8
24	O	613	CLA	C8-C10-C11-C12
24	O	615	CLA	C8-C10-C11-C12
24	O	616	CLA	C15-C16-C17-C18
24	P	510	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	V	603	CLA	C15-C16-C17-C18
24	AH	611	CLA	C5-C6-C7-C8
24	AK	607	CLA	C8-C10-C11-C12
24	AK	614	CLA	C10-C11-C12-C13
24	AK	615	CLA	C8-C10-C11-C12
24	AL	506	CLA	C5-C6-C7-C8
24	AL	511	CLA	C13-C15-C16-C17
24	AM	403	CLA	C15-C16-C17-C18
24	AN	603	CLA	C15-C16-C17-C18
23	AU	601	CHL	O1D-CGD-O2D-CED
24	AA	603	CLA	O1D-CGD-O2D-CED
24	AD	310	CLA	O1D-CGD-O2D-CED
24	AL	507	CLA	C3-C5-C6-C7
24	AS	313	CLA	C3-C5-C6-C7
23	AS	307	CHL	C8-C10-C11-C12
24	O	612	CLA	CBA-CGA-O2A-C1
23	AC	608	CHL	C8-C10-C11-C12
23	AD	308	CHL	C8-C10-C11-C12
23	AD	308	CHL	C10-C11-C12-C13
23	V	608	CHL	C5-C6-C7-C8
23	p	608	CHL	C13-C15-C16-C17
23	p	608	CHL	C15-C16-C17-C18
23	p	609	CHL	C8-C10-C11-C12
23	AQ	609	CHL	C8-C10-C11-C12
23	AR	605	CHL	C8-C10-C11-C12
23	AU	608	CHL	C15-C16-C17-C18
24	0	602	CLA	C10-C11-C12-C13
24	0	603	CLA	C5-C6-C7-C8
24	O	606	CLA	C8-C10-C11-C12
24	O	612	CLA	C10-C11-C12-C13
24	P	506	CLA	C15-C16-C17-C18
24	P	512	CLA	C15-C16-C17-C18
24	AL	507	CLA	C15-C16-C17-C18
24	AL	514	CLA	C15-C16-C17-C18
32	AJ	407	PHO	C13-C15-C16-C17
28	O	622	LHG	C23-C24-C25-C26
28	AK	623	LHG	C23-C24-C25-C26
28	AK	624	LHG	C23-C24-C25-C26
34	o	101	SQD	C23-C24-C25-C26
35	j	102	DGD	C1A-C2A-C3A-C4A
23	9	609	CHL	C8-C10-C11-C12
23	AE	607	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	p	601	CHL	C13-C15-C16-C17
23	p	607	CHL	C5-C6-C7-C8
23	p	607	CHL	C15-C16-C17-C18
23	AN	608	CHL	C5-C6-C7-C8
23	AN	608	CHL	C8-C10-C11-C12
23	AQ	601	CHL	C13-C15-C16-C17
23	AQ	607	CHL	C15-C16-C17-C18
24	0	609	CLA	C10-C11-C12-C13
24	O	605	CLA	C8-C10-C11-C12
24	O	608	CLA	C5-C6-C7-C8
24	O	608	CLA	C8-C10-C11-C12
24	O	614	CLA	C8-C10-C11-C12
24	P	505	CLA	C5-C6-C7-C8
24	P	505	CLA	C15-C16-C17-C18
24	Q	403	CLA	C15-C16-C17-C18
24	Q	404	CLA	C15-C16-C17-C18
24	V	602	CLA	C5-C6-C7-C8
24	V	602	CLA	C15-C16-C17-C18
24	p	602	CLA	C8-C10-C11-C12
24	p	610	CLA	C15-C16-C17-C18
24	AK	605	CLA	C15-C16-C17-C18
24	AK	610	CLA	C5-C6-C7-C8
24	AK	616	CLA	C8-C10-C11-C12
24	AK	617	CLA	C8-C10-C11-C12
24	AL	506	CLA	C15-C16-C17-C18
24	AM	404	CLA	C15-C16-C17-C18
24	AN	602	CLA	C5-C6-C7-C8
24	AQ	610	CLA	C15-C16-C17-C18
24	AR	612	CLA	C10-C11-C12-C13
24	AU	611	CLA	C5-C6-C7-C8
32	J	405	PHO	C13-C15-C16-C17
28	O	621	LHG	O1-C1-C2-O2
24	AU	602	CLA	O1A-CGA-O2A-C1
34	J	410	SQD	O10-C23-O48-C46
28	P	517	LHG	C23-C24-C25-C26
34	M	101	SQD	C23-C24-C25-C26
34	AP	101	SQD	C23-C24-C25-C26
34	m	101	SQD	C23-C24-C25-C26
35	AO	102	DGD	C1A-C2A-C3A-C4A
24	v	303	CLA	CBD-CGD-O2D-CED
23	AH	601	CHL	O1D-CGD-O2D-CED
23	AA	606	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	AE	605	CHL	C5-C6-C7-C8
23	V	607	CHL	C15-C16-C17-C18
23	AH	607	CHL	C15-C16-C17-C18
23	AN	607	CHL	C15-C16-C17-C18
23	AQ	607	CHL	C5-C6-C7-C8
24	0	610	CLA	C5-C6-C7-C8
24	AC	602	CLA	C8-C10-C11-C12
24	O	603	CLA	C15-C16-C17-C18
24	P	503	CLA	C15-C16-C17-C18
24	v	310	CLA	C5-C6-C7-C8
24	AK	604	CLA	C5-C6-C7-C8
24	AK	611	CLA	C5-C6-C7-C8
24	AL	504	CLA	C15-C16-C17-C18
24	AN	602	CLA	C15-C16-C17-C18
24	AK	614	CLA	CBA-CGA-O2A-C1
38	f	102	HEM	C1A-C2A-CAA-CBA
23	V	606	CHL	C13-C15-C16-C17
23	AR	605	CHL	C15-C16-C17-C18
23	AU	607	CHL	C15-C16-C17-C18
24	q	609	CLA	C15-C16-C17-C18
24	AH	611	CLA	C10-C11-C12-C13
24	AL	512	CLA	C5-C6-C7-C8
24	AU	611	CLA	C10-C11-C12-C13
24	AC	603	CLA	O1D-CGD-O2D-CED
28	V	615	LHG	C23-C24-C25-C26
28	v	301	LHG	C23-C24-C25-C26
28	AL	519	LHG	C23-C24-C25-C26
28	AN	616	LHG	C23-C24-C25-C26
28	AS	301	LHG	C23-C24-C25-C26
33	O	620	LMG	C28-C29-C30-C31
33	AK	622	LMG	C28-C29-C30-C31
23	9	606	CHL	CBD-CGD-O2D-CED
24	AS	303	CLA	CBD-CGD-O2D-CED
23	9	607	CHL	C13-C15-C16-C17
23	AD	301	CHL	C13-C15-C16-C17
28	AN	616	LHG	C28-C29-C30-C31
24	AD	310	CLA	C5-C6-C7-C8
24	O	602	CLA	C5-C6-C7-C8
24	AK	610	CLA	C8-C10-C11-C12
24	AQ	602	CLA	C8-C10-C11-C12
23	V	608	CHL	C11-C10-C8-C7
23	q	605	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	AN	607	CHL	C12-C13-C15-C16
23	AN	608	CHL	C11-C10-C8-C7
23	AR	605	CHL	C11-C10-C8-C7
24	AD	303	CLA	C11-C10-C8-C7
24	O	616	CLA	C12-C13-C15-C16
24	P	501	CLA	C12-C13-C15-C16
24	p	602	CLA	C11-C10-C8-C7
24	AL	502	CLA	C12-C13-C15-C16
24	AQ	610	CLA	C11-C10-C8-C7
32	J	406	PHO	C11-C10-C8-C7
32	AJ	408	PHO	C11-C10-C8-C7
24	9	602	CLA	O1A-CGA-O2A-C1
24	J	407	CLA	O1A-CGA-O2A-C1
24	v	310	CLA	O1A-CGA-O2A-C1
24	v	313	CLA	O1A-CGA-O2A-C1
24	AH	609	CLA	O1A-CGA-O2A-C1
24	AL	506	CLA	O1A-CGA-O2A-C1
24	AQ	603	CLA	O1A-CGA-O2A-C1
24	AR	601	CLA	O1A-CGA-O2A-C1
24	AU	609	CLA	O1A-CGA-O2A-C1
34	M	101	SQD	O10-C23-O48-C46
35	AL	518	DGD	O1A-C1A-O1G-C1G
26	q	615	NEX	C9-C10-C11-C12
26	q	615	NEX	C33-C34-C35-C15
26	AQ	617	NEX	C13-C14-C15-C35
27	AB	613	XAT	C29-C30-C31-C32
27	AF	613	XAT	C33-C34-C35-C15
27	q	617	XAT	C29-C30-C31-C32
27	AR	616	XAT	C29-C30-C31-C32
29	O	625	BCR	C19-C20-C21-C22
24	AR	602	CLA	CBA-CGA-O2A-C1
23	AD	308	CHL	C2A-CAA-CBA-CGA
23	v	307	CHL	C2A-CAA-CBA-CGA
23	AH	606	CHL	C2A-CAA-CBA-CGA
23	AN	608	CHL	C2A-CAA-CBA-CGA
23	AS	302	CHL	C2A-CAA-CBA-CGA
24	9	602	CLA	C2A-CAA-CBA-CGA
24	9	613	CLA	C2A-CAA-CBA-CGA
24	AA	604	CLA	C2A-CAA-CBA-CGA
24	AC	611	CLA	C2A-CAA-CBA-CGA
24	AD	304	CLA	C2A-CAA-CBA-CGA
24	O	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	P	501	CLA	C2A-CAA-CBA-CGA
24	AH	609	CLA	C2A-CAA-CBA-CGA
24	AK	606	CLA	C2A-CAA-CBA-CGA
24	AK	607	CLA	C2A-CAA-CBA-CGA
24	AU	602	CLA	C2A-CAA-CBA-CGA
24	AU	609	CLA	C2A-CAA-CBA-CGA
24	AE	603	CLA	O1D-CGD-O2D-CED
24	AH	612	CLA	O1D-CGD-O2D-CED
24	AL	513	CLA	O1D-CGD-O2D-CED
24	AN	602	CLA	O1D-CGD-O2D-CED
23	0	601	CHL	C13-C15-C16-C17
24	O	601	CLA	C10-C11-C12-C13
24	AK	603	CLA	C10-C11-C12-C13
24	AK	612	CLA	C15-C16-C17-C18
24	AL	514	CLA	C8-C10-C11-C12
28	V	615	LHG	C28-C29-C30-C31
29	F	101	BCR	C6-C7-C8-C9
29	f	101	BCR	C6-C7-C8-C9
24	9	603	CLA	O1A-CGA-O2A-C1
24	AC	602	CLA	O1A-CGA-O2A-C1
24	Q	403	CLA	O1A-CGA-O2A-C1
24	q	601	CLA	O1A-CGA-O2A-C1
28	AL	519	LHG	O10-C23-O8-C6
34	AJ	411	SQD	O10-C23-O48-C46
34	m	101	SQD	O10-C23-O48-C46
35	J	411	DGD	O1A-C1A-O1G-C1G
35	AJ	412	DGD	O1A-C1A-O1G-C1G
24	AM	403	CLA	CBD-CGD-O2D-CED
33	P	518	LMG	O6-C1-O1-C7
33	AL	520	LMG	O6-C1-O1-C7
24	P	512	CLA	C13-C15-C16-C17
24	K	101	CLA	C5-C6-C7-C8
24	AK	614	CLA	C15-C16-C17-C18
37	Q	405	PL9	C39-C41-C42-C43
37	AM	405	PL9	C39-C41-C42-C43
28	O	621	LHG	C23-C24-C25-C26
33	J	409	LMG	C10-C11-C12-C13
26	AU	616	NEX	C30-C31-C32-C33
27	AB	613	XAT	C10-C11-C12-C13
29	AF	612	BCR	C18-C19-C20-C21
23	AD	302	CHL	C13-C15-C16-C17
23	V	601	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	p	607	CHL	C10-C11-C12-C13
23	p	608	CHL	C5-C6-C7-C8
23	q	605	CHL	C8-C10-C11-C12
23	AH	601	CHL	C15-C16-C17-C18
23	AQ	601	CHL	C5-C6-C7-C8
23	AQ	601	CHL	C8-C10-C11-C12
23	AQ	609	CHL	C15-C16-C17-C18
23	AU	601	CHL	C15-C16-C17-C18
24	9	602	CLA	C8-C10-C11-C12
24	AA	602	CLA	C5-C6-C7-C8
24	AA	602	CLA	C10-C11-C12-C13
24	AC	602	CLA	C5-C6-C7-C8
24	J	407	CLA	C8-C10-C11-C12
24	O	607	CLA	C8-C10-C11-C12
24	O	608	CLA	C15-C16-C17-C18
24	P	512	CLA	C8-C10-C11-C12
24	V	603	CLA	C13-C15-C16-C17
24	AH	610	CLA	C8-C10-C11-C12
24	AK	609	CLA	C8-C10-C11-C12
24	AK	610	CLA	C15-C16-C17-C18
24	AK	614	CLA	C13-C15-C16-C17
24	AR	603	CLA	C10-C11-C12-C13
24	AR	609	CLA	C15-C16-C17-C18
24	AS	305	CLA	CBA-CGA-O2A-C1
23	AQ	608	CHL	CBD-CGD-O2D-CED
24	P	511	CLA	O1D-CGD-O2D-CED
24	AC	603	CLA	O1A-CGA-O2A-C1
24	P	505	CLA	O1A-CGA-O2A-C1
24	q	611	CLA	O1A-CGA-O2A-C1
24	AJ	409	CLA	O1A-CGA-O2A-C1
24	AM	403	CLA	O1A-CGA-O2A-C1
24	AR	611	CLA	O1A-CGA-O2A-C1
24	AS	310	CLA	O1A-CGA-O2A-C1
34	AJ	411	SQD	C7-C8-C9-C10
33	Q	407	LMG	C4-C5-C6-O5
33	AM	407	LMG	C4-C5-C6-O5
35	AO	102	DGD	C4E-C5E-C6E-O5E
23	AC	607	CHL	O1D-CGD-O2D-CED
23	p	601	CHL	C10-C11-C12-C13
23	AH	607	CHL	C13-C15-C16-C17
23	AQ	607	CHL	C10-C11-C12-C13
23	AU	607	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	O	613	CLA	C10-C11-C12-C13
24	p	603	CLA	C5-C6-C7-C8
24	p	603	CLA	C15-C16-C17-C18
24	q	609	CLA	C5-C6-C7-C8
24	AK	608	CLA	C5-C6-C7-C8
24	AK	616	CLA	C10-C11-C12-C13
24	AL	507	CLA	C5-C6-C7-C8
24	AL	508	CLA	C15-C16-C17-C18
24	AQ	603	CLA	C15-C16-C17-C18
24	V	603	CLA	O1D-CGD-O2D-CED
24	AN	603	CLA	O1D-CGD-O2D-CED
24	O	612	CLA	O1A-CGA-O2A-C1
24	p	610	CLA	C1A-C2A-CAA-CBA
23	V	607	CHL	C13-C15-C16-C17
23	p	601	CHL	C5-C6-C7-C8
23	p	609	CHL	C15-C16-C17-C18
23	AH	608	CHL	C8-C10-C11-C12
23	AN	601	CHL	C8-C10-C11-C12
23	AN	607	CHL	C13-C15-C16-C17
24	O	606	CLA	C5-C6-C7-C8
24	O	614	CLA	C10-C11-C12-C13
24	P	504	CLA	C13-C15-C16-C17
24	P	510	CLA	C15-C16-C17-C18
24	q	603	CLA	C10-C11-C12-C13
24	q	612	CLA	C10-C11-C12-C13
24	AJ	409	CLA	C8-C10-C11-C12
24	AK	608	CLA	C10-C11-C12-C13
24	AL	511	CLA	C15-C16-C17-C18
24	AL	514	CLA	C13-C15-C16-C17
24	AN	603	CLA	C13-C15-C16-C17
24	AQ	603	CLA	C5-C6-C7-C8
24	AQ	610	CLA	C5-C6-C7-C8
24	AQ	611	CLA	C10-C11-C12-C13
24	AU	610	CLA	C8-C10-C11-C12
28	O	621	LHG	C3-O3-P-O6
28	P	517	LHG	C3-O3-P-O6
28	v	301	LHG	C3-O3-P-O6
28	W	201	LHG	C3-O3-P-O6
28	AL	519	LHG	C3-O3-P-O6
28	AQ	618	LHG	C3-O3-P-O6
28	AS	301	LHG	C3-O3-P-O6
28	w	201	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
28	W	201	LHG	C23-C24-C25-C26
23	AD	301	CHL	C3-C5-C6-C7
24	v	313	CLA	C3-C5-C6-C7
24	p	602	CLA	CBA-CGA-O2A-C1
24	q	602	CLA	CBA-CGA-O2A-C1
24	AS	313	CLA	CBA-CGA-O2A-C1
23	p	601	CHL	C8-C10-C11-C12
23	AQ	608	CHL	C5-C6-C7-C8
23	AU	608	CHL	C8-C10-C11-C12
24	AD	304	CLA	C5-C6-C7-C8
24	J	407	CLA	C10-C11-C12-C13
24	O	604	CLA	C8-C10-C11-C12
24	P	506	CLA	C5-C6-C7-C8
24	AJ	409	CLA	C10-C11-C12-C13
24	AK	615	CLA	C10-C11-C12-C13
24	AL	505	CLA	C13-C15-C16-C17
24	AR	609	CLA	C5-C6-C7-C8
33	AL	501	LMG	C10-C11-C12-C13
34	J	410	SQD	C7-C8-C9-C10
28	O	622	LHG	C1-C2-C3-O3
28	P	517	LHG	C1-C2-C3-O3
28	AK	623	LHG	C1-C2-C3-O3
28	AL	519	LHG	C1-C2-C3-O3
23	AN	606	CHL	C4-C3-C5-C6
23	V	601	CHL	C10-C11-C12-C13
24	P	507	CLA	C15-C16-C17-C18
24	q	602	CLA	C10-C11-C12-C13
24	AK	617	CLA	CBD-CGD-O2D-CED
23	0	607	CHL	O1D-CGD-O2D-CED
23	0	607	CHL	C2A-CAA-CBA-CGA
23	p	601	CHL	C2A-CAA-CBA-CGA
23	p	609	CHL	C2A-CAA-CBA-CGA
23	v	302	CHL	C2A-CAA-CBA-CGA
23	AQ	601	CHL	C2A-CAA-CBA-CGA
24	0	611	CLA	C2A-CAA-CBA-CGA
24	AC	613	CLA	C2A-CAA-CBA-CGA
24	AD	303	CLA	C2A-CAA-CBA-CGA
24	AD	311	CLA	C2A-CAA-CBA-CGA
24	AE	604	CLA	C2A-CAA-CBA-CGA
24	AF	604	CLA	C2A-CAA-CBA-CGA
24	J	404	CLA	C2A-CAA-CBA-CGA
24	P	508	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	v	313	CLA	C2A-CAA-CBA-CGA
24	AH	602	CLA	C2A-CAA-CBA-CGA
24	AJ	405	CLA	C2A-CAA-CBA-CGA
24	AL	509	CLA	C2A-CAA-CBA-CGA
24	AQ	611	CLA	C2A-CAA-CBA-CGA
24	AR	612	CLA	C2A-CAA-CBA-CGA
24	AU	613	CLA	C2A-CAA-CBA-CGA
23	0	606	CHL	CBA-CGA-O2A-C1
24	0	609	CLA	CBA-CGA-O2A-C1
24	AD	310	CLA	CBA-CGA-O2A-C1
24	AK	604	CLA	CBA-CGA-O2A-C1
35	J	411	DGD	C2A-C1A-O1G-C1G
35	AJ	412	DGD	C2A-C1A-O1G-C1G
23	AH	601	CHL	C13-C15-C16-C17
24	O	612	CLA	C13-C15-C16-C17
24	O	607	CLA	C5-C6-C7-C8
29	AK	602	BCR	C19-C20-C21-C22
34	Q	402	SQD	C10-C11-C12-C13
28	O	621	LHG	C8-C7-O7-C5
23	0	601	CHL	C10-C11-C12-C13
23	AQ	601	CHL	C10-C11-C12-C13
24	O	612	CLA	C15-C16-C17-C18
24	AK	609	CLA	C5-C6-C7-C8
26	9	617	NEX	C11-C10-C9-C19
26	9	617	NEX	C20-C13-C14-C15
26	AC	616	NEX	C11-C10-C9-C19
26	AC	616	NEX	C20-C13-C14-C15
26	p	616	NEX	C20-C13-C14-C15
26	v	317	NEX	C11-C10-C9-C19
26	AQ	617	NEX	C20-C13-C14-C15
26	AR	615	NEX	C20-C13-C14-C15
26	AS	317	NEX	C20-C13-C14-C15
26	AU	616	NEX	C20-C13-C14-C15
27	9	618	XAT	C40-C33-C34-C35
27	AF	613	XAT	C40-C33-C34-C35
29	AF	612	BCR	C20-C21-C22-C37
29	O	625	BCR	C20-C21-C22-C37
29	P	514	BCR	C20-C21-C22-C37
29	AI	101	BCR	C20-C21-C22-C37
29	AK	602	BCR	C20-C21-C22-C37
29	AL	516	BCR	C20-C21-C22-C37
29	AV	101	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
24	0	610	CLA	C3-C5-C6-C7
24	AN	602	CLA	C3-C5-C6-C7
28	AK	624	LHG	C32-C33-C34-C35
28	AS	301	LHG	C31-C32-C33-C34
33	O	620	LMG	C19-C20-C21-C22
33	AK	601	LMG	C32-C33-C34-C35
33	AK	622	LMG	C19-C20-C21-C22
34	o	101	SQD	C12-C13-C14-C15
34	AJ	411	SQD	C31-C32-C33-C34
34	AM	401	SQD	C10-C11-C12-C13
34	AP	101	SQD	C12-C13-C14-C15
34	m	101	SQD	C9-C10-C11-C12
35	P	516	DGD	C5B-C6B-C7B-C8B
35	AL	517	DGD	C5B-C6B-C7B-C8B
23	AR	605	CHL	C16-C17-C18-C20
24	q	603	CLA	C11-C12-C13-C14
24	AL	512	CLA	C16-C17-C18-C20
24	AR	603	CLA	C11-C12-C13-C14
24	AU	609	CLA	C11-C12-C13-C14
23	q	607	CHL	CBA-CGA-O2A-C1
28	O	623	LHG	C32-C33-C34-C35
28	v	301	LHG	C12-C13-C14-C15
28	v	301	LHG	C31-C32-C33-C34
33	O	624	LMG	C32-C33-C34-C35
34	o	101	SQD	C27-C28-C29-C30
34	M	101	SQD	C9-C10-C11-C12
34	AM	401	SQD	C29-C30-C31-C32
34	AP	101	SQD	C27-C28-C29-C30
35	J	413	DGD	O1B-C1B-O2G-C2G
35	AJ	401	DGD	O1B-C1B-O2G-C2G
23	AN	601	CHL	C10-C11-C12-C13
23	AU	601	CHL	C13-C15-C16-C17
24	p	610	CLA	C5-C6-C7-C8
28	w	201	LHG	C23-C24-C25-C26
23	AU	608	CHL	CBD-CGD-O2D-CED
33	Q	407	LMG	C18-C19-C20-C21
33	AM	407	LMG	C18-C19-C20-C21
34	Q	402	SQD	C29-C30-C31-C32
35	j	102	DGD	CCA-CDA-CEA-CFA
35	AO	102	DGD	CCA-CDA-CEA-CFA
33	O	624	LMG	C30-C31-C32-C33
34	J	410	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
35	j	102	DGD	C5B-C6B-C7B-C8B
38	f	102	HEM	C3D-CAD-CBD-CGD
28	AS	301	LHG	C12-C13-C14-C15
33	AK	601	LMG	C30-C31-C32-C33
34	J	410	SQD	C32-C33-C34-C35
34	AJ	411	SQD	C32-C33-C34-C35
34	m	101	SQD	C11-C12-C13-C14
35	J	413	DGD	CCB-CDB-CEB-CFB
23	9	609	CHL	CBD-CGD-O2D-CED
23	q	607	CHL	O1D-CGD-O2D-CED
26	9	617	NEX	C12-C13-C14-C15
26	AC	616	NEX	C11-C10-C9-C8
26	AC	616	NEX	C12-C13-C14-C15
26	AE	615	NEX	C12-C13-C14-C15
26	p	616	NEX	C12-C13-C14-C15
26	q	615	NEX	C12-C13-C14-C15
26	AQ	617	NEX	C12-C13-C14-C15
26	AR	615	NEX	C12-C13-C14-C15
26	AU	616	NEX	C12-C13-C14-C15
27	AB	613	XAT	C11-C10-C9-C8
27	AB	613	XAT	C12-C13-C14-C15
27	AF	613	XAT	C32-C33-C34-C35
27	q	617	XAT	C32-C33-C34-C35
29	F	101	BCR	C12-C13-C14-C15
29	f	101	BCR	C12-C13-C14-C15
34	J	410	SQD	C2-C1-O6-C44
34	AJ	411	SQD	C2-C1-O6-C44
35	J	411	DGD	C2E-C1E-O5D-C6D
35	AJ	412	DGD	C2E-C1E-O5D-C6D
24	P	511	CLA	CBA-CGA-O2A-C1
24	AK	609	CLA	CBA-CGA-O2A-C1
24	AL	513	CLA	CBA-CGA-O2A-C1
24	AQ	602	CLA	CBA-CGA-O2A-C1
28	p	617	LHG	C25-C26-C27-C28
28	AQ	618	LHG	C11-C10-C9-C8
33	O	620	LMG	C17-C18-C19-C20
33	AK	622	LMG	C17-C18-C19-C20
34	Q	402	SQD	C9-C10-C11-C12
34	M	101	SQD	C11-C12-C13-C14
34	AM	401	SQD	C9-C10-C11-C12
35	AO	102	DGD	CBA-CCA-CDA-CEA
23	AH	608	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	AR	606	CHL	C5-C6-C7-C8
24	O	602	CLA	C15-C16-C17-C18
24	AK	614	CLA	O1A-CGA-O2A-C1
23	AA	608	CHL	C11-C12-C13-C15
23	AE	607	CHL	C11-C12-C13-C15
23	V	608	CHL	C11-C12-C13-C15
23	AN	606	CHL	C16-C17-C18-C20
23	AN	608	CHL	C11-C12-C13-C15
23	AQ	601	CHL	C16-C17-C18-C19
24	AD	303	CLA	C11-C12-C13-C15
24	P	508	CLA	C16-C17-C18-C20
24	K	101	CLA	C16-C17-C18-C20
24	AH	609	CLA	C11-C12-C13-C14
24	AL	509	CLA	C16-C17-C18-C20
23	0	606	CHL	C4-C3-C5-C6
23	AD	306	CHL	C4-C3-C5-C6
23	V	606	CHL	C4-C3-C5-C6
24	AE	603	CLA	C4-C3-C5-C6
24	O	615	CLA	C4-C3-C5-C6
24	P	505	CLA	C4-C3-C5-C6
24	AK	617	CLA	C4-C3-C5-C6
24	AL	506	CLA	C4-C3-C5-C6
28	Q	406	LHG	C29-C30-C31-C32
28	AM	406	LHG	C29-C30-C31-C32
34	J	410	SQD	C11-C12-C13-C14
34	AJ	411	SQD	C11-C12-C13-C14
35	j	102	DGD	CBA-CCA-CDA-CEA
23	AN	606	CHL	C2-C3-C5-C6
24	AE	603	CLA	C2-C3-C5-C6
24	AN	612	CLA	C2-C3-C5-C6
23	9	607	CHL	C6-C7-C8-C9
23	AC	608	CHL	C11-C10-C8-C9
23	V	601	CHL	C11-C10-C8-C9
23	V	608	CHL	C11-C10-C8-C9
23	p	607	CHL	C11-C12-C13-C14
23	q	605	CHL	C11-C10-C8-C9
23	AN	601	CHL	C11-C10-C8-C9
23	AN	608	CHL	C11-C10-C8-C9
23	AR	605	CHL	C11-C10-C8-C9
23	AU	607	CHL	C11-C12-C13-C14
24	AC	602	CLA	C11-C10-C8-C9
24	O	614	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	P	505	CLA	C11-C10-C8-C9
24	P	512	CLA	C11-C12-C13-C14
24	p	603	CLA	C11-C10-C8-C9
24	p	610	CLA	C11-C10-C8-C9
24	AH	602	CLA	C6-C7-C8-C9
24	AK	606	CLA	C14-C13-C15-C16
24	AK	616	CLA	C14-C13-C15-C16
24	AK	618	CLA	C14-C13-C15-C16
24	AL	506	CLA	C11-C10-C8-C9
24	AL	514	CLA	C11-C12-C13-C14
24	AQ	603	CLA	C11-C10-C8-C9
24	AU	602	CLA	C6-C7-C8-C9
24	AU	602	CLA	C11-C10-C8-C9
23	9	608	CHL	O1D-CGD-O2D-CED
24	AK	603	CLA	O1D-CGD-O2D-CED
28	Q	406	LHG	C11-C10-C9-C8
28	p	617	LHG	C11-C10-C9-C8
33	O	620	LMG	C13-C14-C15-C16
33	Q	407	LMG	C33-C34-C35-C36
33	AM	407	LMG	C33-C34-C35-C36
34	o	101	SQD	C25-C26-C27-C28
35	AJ	412	DGD	C4B-C5B-C6B-C7B
35	AL	518	DGD	C4A-C5A-C6A-C7A
23	AU	608	CHL	C13-C15-C16-C17
24	AC	609	CLA	C5-C6-C7-C8
24	AQ	602	CLA	C5-C6-C7-C8
32	AJ	408	PHO	C8-C10-C11-C12
23	AD	302	CHL	C2A-CAA-CBA-CGA
23	AQ	609	CHL	C2A-CAA-CBA-CGA
24	0	603	CLA	C2A-CAA-CBA-CGA
24	AB	610	CLA	C2A-CAA-CBA-CGA
24	AC	602	CLA	C2A-CAA-CBA-CGA
24	O	612	CLA	C2A-CAA-CBA-CGA
24	AR	602	CLA	O1A-CGA-O2A-C1
35	j	102	DGD	C4D-C5D-C6D-O5D
27	9	618	XAT	C7-C8-C9-C19
27	9	618	XAT	C11-C12-C13-C20
28	AM	406	LHG	C11-C10-C9-C8
33	J	409	LMG	C32-C33-C34-C35
33	AK	622	LMG	C13-C14-C15-C16
34	AJ	411	SQD	C33-C34-C35-C36
35	J	411	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
28	O	621	LHG	O1-C1-C2-C3
28	O	622	LHG	O1-C1-C2-C3
28	V	615	LHG	O1-C1-C2-C3
28	q	616	LHG	O1-C1-C2-C3
28	AK	623	LHG	O1-C1-C2-C3
28	AN	616	LHG	O1-C1-C2-C3
27	AB	613	XAT	C11-C12-C13-C14
29	AB	612	BCR	C21-C22-C23-C24
29	O	625	BCR	C7-C8-C9-C10
29	P	515	BCR	C7-C8-C9-C10
29	AK	602	BCR	C7-C8-C9-C10
23	p	601	CHL	C15-C16-C17-C18
23	AN	601	CHL	C13-C15-C16-C17
24	AN	612	CLA	C15-C16-C17-C18
24	AR	602	CLA	C10-C11-C12-C13
28	V	615	LHG	C25-C26-C27-C28
33	AL	501	LMG	C32-C33-C34-C35
34	J	410	SQD	C33-C34-C35-C36
34	AP	101	SQD	C25-C26-C27-C28
32	J	406	PHO	O1D-CGD-O2D-CED
28	P	517	LHG	C13-C14-C15-C16
28	V	615	LHG	C27-C28-C29-C30
28	W	201	LHG	C32-C33-C34-C35
28	AL	519	LHG	C13-C14-C15-C16
28	AN	616	LHG	C27-C28-C29-C30
28	w	201	LHG	C32-C33-C34-C35
33	P	518	LMG	C34-C35-C36-C37
33	AL	520	LMG	C34-C35-C36-C37
35	P	516	DGD	C4B-C5B-C6B-C7B
35	AL	517	DGD	C4B-C5B-C6B-C7B
23	AN	605	CHL	C4B-C3B-CAB-CBB
23	AQ	607	CHL	C4B-C3B-CAB-CBB
24	9	610	CLA	C4B-C3B-CAB-CBB
24	AA	609	CLA	C4B-C3B-CAB-CBB
24	AC	611	CLA	C4B-C3B-CAB-CBB
24	AD	305	CLA	C4B-C3B-CAB-CBB
24	AE	608	CLA	C4B-C3B-CAB-CBB
24	AK	617	CLA	C4B-C3B-CAB-CBB
24	AR	610	CLA	C4B-C3B-CAB-CBB
24	AR	612	CLA	C4B-C3B-CAB-CBB
23	p	601	CHL	C16-C17-C18-C19
23	p	601	CHL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	AQ	601	CHL	C16-C17-C18-C20
23	AU	607	CHL	C16-C17-C18-C19
24	0	602	CLA	C11-C12-C13-C14
24	0	602	CLA	C11-C12-C13-C15
34	J	410	SQD	O5-C1-O6-C44
34	AJ	411	SQD	O5-C1-O6-C44
35	J	411	DGD	O6E-C1E-O5D-C6D
35	AJ	412	DGD	O6E-C1E-O5D-C6D
23	9	607	CHL	C5-C6-C7-C8
23	AA	608	CHL	C5-C6-C7-C8
23	AQ	607	CHL	C13-C15-C16-C17
24	O	605	CLA	C15-C16-C17-C18
24	O	606	CLA	C10-C11-C12-C13
24	V	602	CLA	C13-C15-C16-C17
32	J	406	PHO	C8-C10-C11-C12
28	AN	616	LHG	C25-C26-C27-C28
28	AQ	618	LHG	C25-C26-C27-C28
34	J	410	SQD	C13-C14-C15-C16
34	Q	402	SQD	C25-C26-C27-C28
35	AL	518	DGD	C6B-C7B-C8B-C9B
24	AC	602	CLA	C2C-C3C-CAC-CBC
28	O	622	LHG	C27-C28-C29-C30
28	AK	623	LHG	C27-C28-C29-C30
34	AJ	411	SQD	C13-C14-C15-C16
34	AM	401	SQD	C25-C26-C27-C28
35	AO	102	DGD	C5B-C6B-C7B-C8B
24	O	607	CLA	C10-C11-C12-C13
24	O	613	CLA	C13-C15-C16-C17
24	P	508	CLA	C13-C15-C16-C17
24	AK	604	CLA	C15-C16-C17-C18
24	AK	607	CLA	C15-C16-C17-C18
24	AK	615	CLA	C13-C15-C16-C17
24	AL	511	CLA	C10-C11-C12-C13
24	AN	602	CLA	C13-C15-C16-C17
24	q	602	CLA	O1A-CGA-O2A-C1
24	AK	604	CLA	O1A-CGA-O2A-C1
28	V	615	LHG	C18-C19-C20-C21
28	AK	624	LHG	C27-C28-C29-C30
28	AL	519	LHG	C27-C28-C29-C30
28	AN	616	LHG	C18-C19-C20-C21
35	J	411	DGD	C2A-C3A-C4A-C5A
24	AL	512	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	AD	312	CLA	CBA-CGA-O2A-C1
28	O	621	LHG	C29-C30-C31-C32
28	O	623	LHG	C27-C28-C29-C30
28	v	301	LHG	C24-C25-C26-C27
28	v	301	LHG	C26-C27-C28-C29
35	j	102	DGD	C9A-CAA-CBA-CCA
24	q	604	CLA	O1D-CGD-O2D-CED
24	AR	604	CLA	O1D-CGD-O2D-CED
23	p	601	CHL	C3A-C2A-CAA-CBA
23	q	605	CHL	C3A-C2A-CAA-CBA
24	0	610	CLA	C3A-C2A-CAA-CBA
24	AC	613	CLA	C3A-C2A-CAA-CBA
24	AD	310	CLA	C3A-C2A-CAA-CBA
24	O	608	CLA	C3A-C2A-CAA-CBA
24	P	512	CLA	C3A-C2A-CAA-CBA
24	p	618	CLA	C3A-C2A-CAA-CBA
24	q	604	CLA	C3A-C2A-CAA-CBA
24	v	305	CLA	C3A-C2A-CAA-CBA
24	AL	504	CLA	C3A-C2A-CAA-CBA
24	AL	514	CLA	C3A-C2A-CAA-CBA
24	AR	604	CLA	C3A-C2A-CAA-CBA
24	AS	305	CLA	C3A-C2A-CAA-CBA
23	V	601	CHL	C13-C15-C16-C17
23	p	607	CHL	C13-C15-C16-C17
24	AL	513	CLA	C10-C11-C12-C13
28	O	622	LHG	C32-C33-C34-C35
28	AS	301	LHG	C26-C27-C28-C29
34	J	410	SQD	C25-C26-C27-C28
34	AJ	411	SQD	C16-C17-C18-C19
35	J	411	DGD	C6A-C7A-C8A-C9A
35	AJ	412	DGD	C2A-C3A-C4A-C5A
24	p	602	CLA	O1A-CGA-O2A-C1
23	V	601	CHL	C16-C17-C18-C19
23	p	607	CHL	C16-C17-C18-C19
23	AR	605	CHL	C16-C17-C18-C19
24	AD	303	CLA	C11-C12-C13-C14
24	q	603	CLA	C11-C12-C13-C15
24	AR	603	CLA	C11-C12-C13-C15
24	V	609	CLA	C15-C16-C17-C18
24	AN	609	CLA	C15-C16-C17-C18
28	AK	623	LHG	C32-C33-C34-C35
28	AS	301	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
35	AJ	412	DGD	C6A-C7A-C8A-C9A
23	AS	308	CHL	O1D-CGD-O2D-CED
33	Q	407	LMG	O1-C7-C8-C9
33	AM	407	LMG	O1-C7-C8-C9
34	o	101	SQD	C44-C45-C46-O48
28	O	623	LHG	C29-C30-C31-C32
33	Q	407	LMG	C14-C15-C16-C17
33	AM	407	LMG	C14-C15-C16-C17
34	J	410	SQD	C16-C17-C18-C19
35	AO	102	DGD	C9A-CAA-CBA-CCA
26	AU	616	NEX	C14-C15-C35-C34
29	O	625	BCR	C14-C15-C16-C17
29	AK	602	BCR	C14-C15-C16-C17
23	9	609	CHL	C3-C5-C6-C7
33	AL	520	LMG	C18-C19-C20-C21
24	AS	305	CLA	O1A-CGA-O2A-C1
24	AK	609	CLA	C10-C11-C12-C13
23	AH	601	CHL	C4-C3-C5-C6
24	0	603	CLA	C4-C3-C5-C6
24	J	404	CLA	CBA-CGA-O2A-C1
24	O	607	CLA	CBA-CGA-O2A-C1
24	AJ	405	CLA	CBA-CGA-O2A-C1
23	0	606	CHL	C2-C3-C5-C6
23	AD	306	CHL	C2-C3-C5-C6
23	V	606	CHL	C2-C3-C5-C6
24	0	603	CLA	C2-C3-C5-C6
24	P	505	CLA	C2-C3-C5-C6
24	p	612	CLA	C2-C3-C5-C6
34	AJ	411	SQD	C25-C26-C27-C28
23	q	607	CHL	C2A-CAA-CBA-CGA
24	AE	608	CLA	C2A-CAA-CBA-CGA
24	AK	614	CLA	C2A-CAA-CBA-CGA
28	O	622	LHG	O1-C1-C2-O2
28	v	301	LHG	O1-C1-C2-O2
28	AK	624	LHG	O1-C1-C2-O2
28	AN	616	LHG	O1-C1-C2-O2
28	AS	301	LHG	O1-C1-C2-O2
33	O	620	LMG	C30-C31-C32-C33
33	P	518	LMG	C18-C19-C20-C21
33	AK	622	LMG	C30-C31-C32-C33
35	AL	518	DGD	C3B-C4B-C5B-C6B
23	q	605	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	0	609	CLA	O1A-CGA-O2A-C1
24	AD	310	CLA	O1A-CGA-O2A-C1
23	AH	607	CHL	C16-C17-C18-C19
23	AN	601	CHL	C16-C17-C18-C19
23	AQ	607	CHL	C16-C17-C18-C19
24	K	101	CLA	C16-C17-C18-C19
24	AU	609	CLA	C11-C12-C13-C15
34	J	410	SQD	C11-C10-C9-C8
23	9	608	CHL	C2B-C3B-CAB-CBB
23	AC	606	CHL	C2B-C3B-CAB-CBB
23	AC	607	CHL	C2B-C3B-CAB-CBB
23	p	606	CHL	C2B-C3B-CAB-CBB
23	AN	605	CHL	C2B-C3B-CAB-CBB
23	AQ	607	CHL	C2B-C3B-CAB-CBB
24	9	603	CLA	C2B-C3B-CAB-CBB
24	9	610	CLA	C2B-C3B-CAB-CBB
24	9	612	CLA	C2B-C3B-CAB-CBB
24	AA	609	CLA	C2B-C3B-CAB-CBB
24	AC	603	CLA	C2B-C3B-CAB-CBB
24	AC	611	CLA	C2B-C3B-CAB-CBB
24	AD	305	CLA	C2B-C3B-CAB-CBB
24	AE	608	CLA	C2B-C3B-CAB-CBB
24	AF	614	CLA	C2B-C3B-CAB-CBB
24	AK	617	CLA	C2B-C3B-CAB-CBB
24	AR	610	CLA	C2B-C3B-CAB-CBB
24	AR	612	CLA	C2B-C3B-CAB-CBB
23	AN	607	CHL	C5-C6-C7-C8
24	AL	509	CLA	C13-C15-C16-C17
24	0	603	CLA	C2C-C3C-CAC-CBC
28	AK	624	LHG	C29-C30-C31-C32
35	AJ	401	DGD	CCB-CDB-CEB-CFB
23	0	606	CHL	O1A-CGA-O2A-C1
23	q	607	CHL	O1A-CGA-O2A-C1
24	AK	609	CLA	O1A-CGA-O2A-C1
24	AS	313	CLA	O1A-CGA-O2A-C1
23	9	609	CHL	C10-C11-C12-C13
38	F	102	HEM	C1A-C2A-CAA-CBA
28	P	517	LHG	C27-C28-C29-C30
35	J	411	DGD	C7A-C8A-C9A-CAA
35	J	411	DGD	CCA-CDA-CEA-CFA
35	AJ	412	DGD	CCA-CDA-CEA-CFA
28	O	621	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
33	O	620	LMG	C33-C34-C35-C36
33	AK	622	LMG	C33-C34-C35-C36
33	AL	501	LMG	C17-C18-C19-C20
33	AM	407	LMG	C32-C33-C34-C35
35	J	411	DGD	C6B-C7B-C8B-C9B
23	V	607	CHL	C5-C6-C7-C8
24	P	510	CLA	C10-C11-C12-C13
24	O	607	CLA	O1A-CGA-O2A-C1
24	P	511	CLA	O1A-CGA-O2A-C1
24	AL	513	CLA	O1A-CGA-O2A-C1
28	O	622	LHG	C30-C31-C32-C33
28	O	623	LHG	C9-C10-C11-C12
28	AK	623	LHG	C30-C31-C32-C33
33	J	409	LMG	C17-C18-C19-C20
33	Q	407	LMG	C32-C33-C34-C35
35	AJ	412	DGD	C7A-C8A-C9A-CAA
35	AJ	412	DGD	C6B-C7B-C8B-C9B
24	AQ	611	CLA	C11-C12-C13-C14
28	O	623	LHG	C7-C8-C9-C10
28	AK	624	LHG	C7-C8-C9-C10
24	K	101	CLA	C3-C5-C6-C7
25	9	616	LUT	C1-C6-C7-C8
25	AC	615	LUT	C1-C6-C7-C8
25	V	614	LUT	C1-C6-C7-C8
25	V	614	LUT	C5-C6-C7-C8
25	AN	615	LUT	C1-C6-C7-C8
25	AN	615	LUT	C5-C6-C7-C8
29	AB	612	BCR	C5-C6-C7-C8
29	AF	612	BCR	C1-C6-C7-C8
29	AF	612	BCR	C5-C6-C7-C8
29	J	408	BCR	C23-C24-C25-C30
29	O	617	BCR	C1-C6-C7-C8
29	O	617	BCR	C5-C6-C7-C8
29	O	619	BCR	C1-C6-C7-C8
29	O	619	BCR	C5-C6-C7-C8
29	O	625	BCR	C5-C6-C7-C8
29	P	513	BCR	C1-C6-C7-C8
29	P	513	BCR	C5-C6-C7-C8
29	P	515	BCR	C5-C6-C7-C8
29	P	515	BCR	C23-C24-C25-C26
29	P	515	BCR	C23-C24-C25-C30
29	F	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	F	101	BCR	C5-C6-C7-C8
29	j	101	BCR	C23-C24-C25-C26
29	j	101	BCR	C23-C24-C25-C30
29	AI	101	BCR	C5-C6-C7-C8
29	AJ	410	BCR	C23-C24-C25-C30
29	AK	602	BCR	C5-C6-C7-C8
29	AK	619	BCR	C1-C6-C7-C8
29	AK	619	BCR	C5-C6-C7-C8
29	AK	621	BCR	C1-C6-C7-C8
29	AK	621	BCR	C5-C6-C7-C8
29	AL	515	BCR	C1-C6-C7-C8
29	AL	515	BCR	C5-C6-C7-C8
29	f	101	BCR	C1-C6-C7-C8
29	f	101	BCR	C5-C6-C7-C8
29	AO	101	BCR	C23-C24-C25-C26
29	AO	101	BCR	C23-C24-C25-C30
29	k	101	BCR	C5-C6-C7-C8
29	k	101	BCR	C23-C24-C25-C26
29	k	101	BCR	C23-C24-C25-C30
29	AV	101	BCR	C5-C6-C7-C8
28	AK	624	LHG	C9-C10-C11-C12
33	O	620	LMG	C32-C33-C34-C35
32	AJ	408	PHO	O1D-CGD-O2D-CED
23	AR	607	CHL	CBA-CGA-O2A-C1
23	AC	608	CHL	C10-C11-C12-C13
23	AD	302	CHL	C10-C11-C12-C13
23	V	606	CHL	C10-C11-C12-C13
23	AQ	601	CHL	C15-C16-C17-C18
23	AQ	609	CHL	C5-C6-C7-C8
24	AD	303	CLA	C10-C11-C12-C13
24	P	506	CLA	C13-C15-C16-C17
24	P	511	CLA	C10-C11-C12-C13
24	AK	612	CLA	C13-C15-C16-C17
24	AL	507	CLA	C13-C15-C16-C17
24	p	618	CLA	O2A-C1-C2-C3
24	AQ	602	CLA	O1A-CGA-O2A-C1
23	AC	608	CHL	C14-C13-C15-C16
33	AK	622	LMG	C32-C33-C34-C35
23	AE	607	CHL	C10-C11-C12-C13
23	p	609	CHL	C5-C6-C7-C8
23	AH	608	CHL	C5-C6-C7-C8
23	AU	608	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	O	614	CLA	C13-C15-C16-C17
24	q	603	CLA	C5-C6-C7-C8
24	AK	616	CLA	C13-C15-C16-C17
24	AK	618	CLA	C15-C16-C17-C18
33	O	624	LMG	C35-C36-C37-C38
23	9	607	CHL	C4-C3-C5-C6
23	AU	601	CHL	C4-C3-C5-C6
24	O	606	CLA	C4-C3-C5-C6
24	p	612	CLA	C4-C3-C5-C6
24	AN	612	CLA	C4-C3-C5-C6
23	9	607	CHL	C2-C3-C5-C6
23	9	609	CHL	C11-C10-C8-C7
23	AC	608	CHL	C11-C10-C8-C7
23	V	607	CHL	C12-C13-C15-C16
23	p	607	CHL	C11-C12-C13-C15
23	p	608	CHL	C12-C13-C15-C16
23	AH	607	CHL	C11-C12-C13-C15
23	AH	608	CHL	C12-C13-C15-C16
23	AQ	601	CHL	C12-C13-C15-C16
23	AQ	607	CHL	C11-C12-C13-C15
23	AR	607	CHL	C2-C3-C5-C6
23	AU	607	CHL	C11-C12-C13-C15
23	AU	608	CHL	C12-C13-C15-C16
24	9	602	CLA	C11-C10-C8-C7
24	AA	603	CLA	C2-C3-C5-C6
24	AD	303	CLA	C6-C7-C8-C10
24	P	502	CLA	C12-C13-C15-C16
24	P	503	CLA	C11-C10-C8-C7
24	P	505	CLA	C11-C10-C8-C7
24	P	506	CLA	C11-C12-C13-C15
24	P	506	CLA	C12-C13-C15-C16
24	p	603	CLA	C11-C10-C8-C7
24	AH	603	CLA	C2-C3-C5-C6
24	AK	618	CLA	C12-C13-C15-C16
24	AL	503	CLA	C12-C13-C15-C16
24	AL	504	CLA	C11-C10-C8-C7
24	AL	506	CLA	C2-C3-C5-C6
24	AL	506	CLA	C11-C10-C8-C7
24	AL	507	CLA	C11-C12-C13-C15
24	AL	507	CLA	C12-C13-C15-C16
24	AL	513	CLA	C6-C7-C8-C10
24	AQ	602	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	AQ	603	CLA	C11-C10-C8-C7
24	AU	603	CLA	C2-C3-C5-C6
23	AA	606	CHL	C3-C5-C6-C7
23	AC	608	CHL	C3-C5-C6-C7
24	AD	310	CLA	C3-C5-C6-C7
24	AD	312	CLA	O1A-CGA-O2A-C1
24	J	404	CLA	O1A-CGA-O2A-C1
24	AJ	405	CLA	O1A-CGA-O2A-C1
24	O	610	CLA	C13-C15-C16-C17
29	AF	612	BCR	C19-C20-C21-C22
23	AA	608	CHL	C11-C12-C13-C14
23	AE	607	CHL	C11-C12-C13-C14
24	P	508	CLA	C16-C17-C18-C19
24	AH	609	CLA	C11-C12-C13-C15
24	AL	509	CLA	C16-C17-C18-C19
35	AL	518	DGD	O1B-C1B-O2G-C2G
23	AA	608	CHL	CBA-CGA-O2A-C1
23	AD	306	CHL	CBA-CGA-O2A-C1
24	0	613	CLA	CBA-CGA-O2A-C1
24	AN	612	CLA	CBA-CGA-O2A-C1
33	J	409	LMG	C29-C28-O8-C9
33	AL	501	LMG	C29-C28-O8-C9
28	AQ	618	LHG	C24-C25-C26-C27
35	AJ	412	DGD	C3B-C4B-C5B-C6B
23	0	601	CHL	C2A-CAA-CBA-CGA
23	AA	601	CHL	C2A-CAA-CBA-CGA
24	AA	609	CLA	C2A-CAA-CBA-CGA
24	AD	310	CLA	C2A-CAA-CBA-CGA
24	V	603	CLA	C2A-CAA-CBA-CGA
24	q	618	CLA	C2A-CAA-CBA-CGA
24	AK	608	CLA	C2A-CAA-CBA-CGA
24	AK	618	CLA	C2A-CAA-CBA-CGA
24	AL	507	CLA	C2A-CAA-CBA-CGA
24	AS	313	CLA	C2A-CAA-CBA-CGA
24	AS	314	CLA	C2A-CAA-CBA-CGA
24	AU	612	CLA	C2A-CAA-CBA-CGA
23	V	601	CHL	C15-C16-C17-C18
23	q	606	CHL	C5-C6-C7-C8
24	0	609	CLA	C5-C6-C7-C8
24	O	606	CLA	C13-C15-C16-C17
24	P	507	CLA	C10-C11-C12-C13
24	AL	508	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	AK	601	LMG	C35-C36-C37-C38
35	J	411	DGD	C3B-C4B-C5B-C6B
23	AN	605	CHL	O1D-CGD-O2D-CED
35	P	516	DGD	C5A-C6A-C7A-C8A
24	0	610	CLA	O1D-CGD-O2D-CED
23	AN	601	CHL	C15-C16-C17-C18
24	p	602	CLA	C5-C6-C7-C8
24	AS	310	CLA	C5-C6-C7-C8
28	p	617	LHG	C33-C34-C35-C36
28	AK	624	LHG	C31-C32-C33-C34
28	AQ	618	LHG	C33-C34-C35-C36
33	AK	622	LMG	C18-C19-C20-C21
34	AM	401	SQD	C11-C12-C13-C14
35	J	413	DGD	C8B-C9B-CAB-CBB
23	AD	302	CHL	C3-C5-C6-C7
24	P	505	CLA	C3-C5-C6-C7
24	AL	506	CLA	C3-C5-C6-C7
28	v	301	LHG	C27-C28-C29-C30
28	AS	301	LHG	C27-C28-C29-C30
33	O	620	LMG	C18-C19-C20-C21
34	AM	401	SQD	C11-C10-C9-C8
35	AL	517	DGD	C5A-C6A-C7A-C8A
29	j	101	BCR	C6-C7-C8-C9
24	0	610	CLA	CBA-CGA-O2A-C1
28	w	201	LHG	C24-C23-O8-C6
23	AE	607	CHL	C5-C6-C7-C8
23	AN	601	CHL	C5-C6-C7-C8
24	AA	603	CLA	C5-C6-C7-C8
34	J	410	SQD	C9-C10-C11-C12
35	AO	102	DGD	C2B-C3B-C4B-C5B
33	O	620	LMG	C11-C10-O7-C8
33	AK	622	LMG	C11-C10-O7-C8
35	J	411	DGD	C2B-C1B-O2G-C2G
35	AJ	412	DGD	C2B-C1B-O2G-C2G
28	v	301	LHG	C13-C14-C15-C16
34	Q	402	SQD	C11-C10-C9-C8
23	AA	608	CHL	C10-C11-C12-C13
23	V	601	CHL	C5-C6-C7-C8
23	AN	606	CHL	C10-C11-C12-C13
24	AR	603	CLA	C5-C6-C7-C8
24	0	613	CLA	O1A-CGA-O2A-C1
28	O	623	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
23	AH	601	CHL	C3-C5-C6-C7
34	J	410	SQD	C28-C29-C30-C31
34	Q	402	SQD	C11-C12-C13-C14
23	9	606	CHL	O1D-CGD-O2D-CED
28	q	616	LHG	O7-C5-C6-O8
28	v	301	LHG	O7-C5-C6-O8
28	AS	301	LHG	O7-C5-C6-O8
34	o	101	SQD	O47-C45-C46-O48
34	AP	101	SQD	O47-C45-C46-O48
28	O	621	LHG	C14-C15-C16-C17
23	AN	608	CHL	C11-C12-C13-C14
23	V	607	CHL	C8-C10-C11-C12
24	AK	606	CLA	C8-C10-C11-C12
24	AK	608	CLA	C13-C15-C16-C17
23	AR	607	CHL	C4-C3-C5-C6
24	AA	603	CLA	C4-C3-C5-C6
24	AM	404	CLA	C4-C3-C5-C6
24	O	615	CLA	C2-C3-C5-C6
24	AK	617	CLA	C2-C3-C5-C6
23	p	609	CHL	C11-C10-C8-C9
23	AQ	601	CHL	C14-C13-C15-C16
23	AQ	609	CHL	C11-C10-C8-C9
24	0	602	CLA	C6-C7-C8-C9
24	O	605	CLA	C14-C13-C15-C16
24	O	616	CLA	C14-C13-C15-C16
24	P	501	CLA	C11-C10-C8-C9
24	P	502	CLA	C14-C13-C15-C16
24	P	506	CLA	C11-C12-C13-C14
24	P	511	CLA	C6-C7-C8-C9
24	Q	404	CLA	C6-C7-C8-C9
24	V	603	CLA	C11-C10-C8-C9
24	q	602	CLA	C11-C10-C8-C9
24	AH	602	CLA	C11-C12-C13-C14
24	AK	608	CLA	C11-C12-C13-C14
24	AL	502	CLA	C11-C10-C8-C9
24	AL	503	CLA	C14-C13-C15-C16
24	AL	507	CLA	C11-C12-C13-C14
24	AL	513	CLA	C6-C7-C8-C9
24	AM	404	CLA	C6-C7-C8-C9
24	AN	603	CLA	C11-C10-C8-C9
24	AQ	610	CLA	C11-C10-C8-C9
24	AR	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	AU	602	CLA	C11-C12-C13-C14
23	AC	608	CHL	CBD-CGD-O2D-CED
28	AS	301	LHG	C13-C14-C15-C16
33	P	518	LMG	C32-C33-C34-C35
34	AJ	411	SQD	C28-C29-C30-C31
23	V	601	CHL	C2A-CAA-CBA-CGA
23	AH	601	CHL	C2A-CAA-CBA-CGA
23	AN	601	CHL	C2A-CAA-CBA-CGA
23	AR	605	CHL	C2A-CAA-CBA-CGA
23	AU	601	CHL	C2A-CAA-CBA-CGA
24	O	602	CLA	C2A-CAA-CBA-CGA
24	P	506	CLA	C2A-CAA-CBA-CGA
24	v	314	CLA	C2A-CAA-CBA-CGA
24	AN	603	CLA	C2A-CAA-CBA-CGA
24	AN	612	CLA	C2A-CAA-CBA-CGA
32	J	406	PHO	C2A-CAA-CBA-CGA
32	AJ	408	PHO	C2A-CAA-CBA-CGA
28	AK	624	LHG	C30-C31-C32-C33
35	J	411	DGD	C5A-C6A-C7A-C8A
35	AJ	412	DGD	C5A-C6A-C7A-C8A
25	9	616	LUT	C7-C8-C9-C19
25	AU	614	LUT	C7-C8-C9-C19
24	AL	504	CLA	C5-C6-C7-C8
23	9	601	CHL	C2C-C3C-CAC-CBC
35	AJ	401	DGD	C8B-C9B-CAB-CBB
35	AJ	412	DGD	C5B-C6B-C7B-C8B
29	AO	101	BCR	C7-C8-C9-C10
23	AA	608	CHL	O1A-CGA-O2A-C1
23	AR	607	CHL	O1A-CGA-O2A-C1
23	9	608	CHL	C1A-C2A-CAA-CBA
23	0	601	CHL	C1A-C2A-CAA-CBA
23	AA	605	CHL	C1A-C2A-CAA-CBA
23	AA	617	CHL	C1A-C2A-CAA-CBA
23	AB	608	CHL	C1A-C2A-CAA-CBA
23	AC	601	CHL	C1A-C2A-CAA-CBA
23	AC	607	CHL	C1A-C2A-CAA-CBA
23	AC	608	CHL	C1A-C2A-CAA-CBA
23	AD	308	CHL	C1A-C2A-CAA-CBA
23	AE	607	CHL	C1A-C2A-CAA-CBA
23	V	608	CHL	C1A-C2A-CAA-CBA
23	V	616	CHL	C1A-C2A-CAA-CBA
23	p	601	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	p	605	CHL	C1A-C2A-CAA-CBA
23	p	607	CHL	C1A-C2A-CAA-CBA
23	p	608	CHL	C1A-C2A-CAA-CBA
23	p	609	CHL	C1A-C2A-CAA-CBA
23	AH	608	CHL	C1A-C2A-CAA-CBA
23	AN	608	CHL	C1A-C2A-CAA-CBA
23	AN	617	CHL	C1A-C2A-CAA-CBA
23	AQ	605	CHL	C1A-C2A-CAA-CBA
23	AQ	608	CHL	C1A-C2A-CAA-CBA
23	AQ	609	CHL	C1A-C2A-CAA-CBA
23	AS	308	CHL	C1A-C2A-CAA-CBA
23	AU	608	CHL	C1A-C2A-CAA-CBA
24	9	611	CLA	C1A-C2A-CAA-CBA
24	0	602	CLA	C1A-C2A-CAA-CBA
24	AA	604	CLA	C1A-C2A-CAA-CBA
24	AA	610	CLA	C1A-C2A-CAA-CBA
24	AA	613	CLA	C1A-C2A-CAA-CBA
24	AB	602	CLA	C1A-C2A-CAA-CBA
24	AB	610	CLA	C1A-C2A-CAA-CBA
24	AC	602	CLA	C1A-C2A-CAA-CBA
24	AC	609	CLA	C1A-C2A-CAA-CBA
24	AD	305	CLA	C1A-C2A-CAA-CBA
24	AE	604	CLA	C1A-C2A-CAA-CBA
24	AE	609	CLA	C1A-C2A-CAA-CBA
24	J	404	CLA	C1A-C2A-CAA-CBA
24	O	601	CLA	C1A-C2A-CAA-CBA
24	O	604	CLA	C1A-C2A-CAA-CBA
24	O	612	CLA	C1A-C2A-CAA-CBA
24	P	501	CLA	C1A-C2A-CAA-CBA
24	Q	401	CLA	C1A-C2A-CAA-CBA
24	V	609	CLA	C1A-C2A-CAA-CBA
24	K	101	CLA	C1A-C2A-CAA-CBA
24	p	618	CLA	C1A-C2A-CAA-CBA
24	q	609	CLA	C1A-C2A-CAA-CBA
24	q	612	CLA	C1A-C2A-CAA-CBA
24	v	311	CLA	C1A-C2A-CAA-CBA
24	v	314	CLA	C1A-C2A-CAA-CBA
24	AH	602	CLA	C1A-C2A-CAA-CBA
24	AH	610	CLA	C1A-C2A-CAA-CBA
24	AJ	405	CLA	C1A-C2A-CAA-CBA
24	AJ	406	CLA	C1A-C2A-CAA-CBA
24	AK	603	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	AK	606	CLA	C1A-C2A-CAA-CBA
24	AK	614	CLA	C1A-C2A-CAA-CBA
24	AL	502	CLA	C1A-C2A-CAA-CBA
24	AN	609	CLA	C1A-C2A-CAA-CBA
24	AQ	611	CLA	C1A-C2A-CAA-CBA
24	AR	601	CLA	C1A-C2A-CAA-CBA
24	AR	609	CLA	C1A-C2A-CAA-CBA
24	AR	610	CLA	C1A-C2A-CAA-CBA
24	AS	311	CLA	C1A-C2A-CAA-CBA
24	AS	314	CLA	C1A-C2A-CAA-CBA
24	AU	610	CLA	C1A-C2A-CAA-CBA
23	V	608	CHL	C11-C12-C13-C14
24	AL	512	CLA	C16-C17-C18-C19
28	O	621	LHG	C32-C33-C34-C35
33	O	620	LMG	C34-C35-C36-C37
33	Q	407	LMG	C16-C17-C18-C19
33	AM	407	LMG	C16-C17-C18-C19
35	J	411	DGD	C5B-C6B-C7B-C8B
26	AE	615	NEX	C13-C14-C15-C35
27	AB	613	XAT	C13-C14-C15-C35
27	AF	613	XAT	C13-C14-C15-C35
27	q	617	XAT	C9-C10-C11-C12
24	p	603	CLA	C10-C11-C12-C13
24	AQ	603	CLA	C10-C11-C12-C13
28	O	623	LHG	C4-O6-P-O3
33	AK	622	LMG	C34-C35-C36-C37
33	AL	520	LMG	C32-C33-C34-C35
28	O	622	LHG	C7-C8-C9-C10
28	AK	623	LHG	C7-C8-C9-C10
23	AU	601	CHL	C3-C5-C6-C7
24	V	602	CLA	C3-C5-C6-C7
24	Q	403	CLA	O1D-CGD-O2D-CED
24	P	503	CLA	C5-C6-C7-C8
24	AK	615	CLA	C15-C16-C17-C18
24	q	612	CLA	CBA-CGA-O2A-C1
28	O	621	LHG	O6-C4-C5-C6
28	P	517	LHG	O6-C4-C5-C6
34	AJ	411	SQD	C9-C10-C11-C12
35	J	413	DGD	C4E-C5E-C6E-O5E
34	o	101	SQD	C7-C8-C9-C10
34	AP	101	SQD	C7-C8-C9-C10
34	m	101	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	AK	610	CLA	C13-C15-C16-C17
34	M	101	SQD	C16-C17-C18-C19
23	AE	605	CHL	C3-C5-C6-C7
23	AH	608	CHL	O1D-CGD-O2D-CED
24	Q	404	CLA	C4-C3-C5-C6
24	AH	603	CLA	C4-C3-C5-C6
24	AU	603	CLA	C4-C3-C5-C6
35	AJ	401	DGD	C4E-C5E-C6E-O5E
35	j	102	DGD	C2B-C3B-C4B-C5B
28	O	623	LHG	C30-C31-C32-C33
33	AK	622	LMG	C16-C17-C18-C19
35	AJ	401	DGD	C5B-C6B-C7B-C8B
23	AD	306	CHL	O1A-CGA-O2A-C1
28	O	623	LHG	O2-C2-C3-O3
33	J	409	LMG	C37-C38-C39-C40
34	J	410	SQD	C30-C31-C32-C33
24	O	603	CLA	C13-C15-C16-C17
24	0	613	CLA	C2A-CAA-CBA-CGA
24	P	502	CLA	C2A-CAA-CBA-CGA
24	q	611	CLA	C2A-CAA-CBA-CGA
24	AH	612	CLA	C2A-CAA-CBA-CGA
24	AL	503	CLA	C2A-CAA-CBA-CGA
23	V	606	CHL	C16-C17-C18-C20
24	AM	403	CLA	C3-C5-C6-C7
28	v	301	LHG	C4-C5-C6-O8
28	AS	301	LHG	C4-C5-C6-O8
28	AS	301	LHG	C32-C33-C34-C35
28	w	201	LHG	C4-C5-C6-O8
33	J	409	LMG	C7-C8-C9-O8
33	O	620	LMG	C16-C17-C18-C19
33	O	624	LMG	C7-C8-C9-O8
33	AK	601	LMG	C7-C8-C9-O8
33	AL	501	LMG	C7-C8-C9-O8
34	J	410	SQD	O6-C44-C45-C46
34	AJ	411	SQD	O6-C44-C45-C46
34	AP	101	SQD	C44-C45-C46-O48
35	J	413	DGD	O1G-C1G-C2G-C3G
35	AJ	401	DGD	C7B-C8B-C9B-CAB
35	AJ	401	DGD	O1G-C1G-C2G-C3G
28	AK	624	LHG	C24-C23-O8-C6
28	v	301	LHG	C32-C33-C34-C35
28	AL	519	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	O	620	LMG	C35-C36-C37-C38
33	AL	501	LMG	C37-C38-C39-C40
34	Q	402	SQD	C27-C28-C29-C30
35	J	413	DGD	C5B-C6B-C7B-C8B
26	AC	616	NEX	C14-C15-C35-C34
33	P	518	LMG	C8-C7-O1-C1
33	AL	520	LMG	C8-C7-O1-C1
33	AK	601	LMG	C36-C37-C38-C39
33	AK	622	LMG	C35-C36-C37-C38
33	AL	520	LMG	C17-C18-C19-C20
34	Q	402	SQD	C14-C15-C16-C17
23	9	609	CHL	C14-C13-C15-C16
24	AN	612	CLA	O1A-CGA-O2A-C1
34	AJ	411	SQD	C11-C10-C9-C8
35	J	413	DGD	C7B-C8B-C9B-CAB
24	AA	602	CLA	C3-C5-C6-C7
24	O	613	CLA	C15-C16-C17-C18
33	O	624	LMG	C36-C37-C38-C39
28	q	616	LHG	O1-C1-C2-O2
28	AK	623	LHG	O1-C1-C2-O2
24	q	604	CLA	O2A-C1-C2-C3
34	AJ	411	SQD	C30-C31-C32-C33
34	AM	401	SQD	C27-C28-C29-C30
23	AN	607	CHL	C8-C10-C11-C12
24	O	608	CLA	C13-C15-C16-C17
24	AK	611	CLA	C15-C16-C17-C18
34	Q	402	SQD	C23-C24-C25-C26
34	AM	401	SQD	C14-C15-C16-C17
33	P	518	LMG	C17-C18-C19-C20
24	0	609	CLA	C8-C10-C11-C12
24	AK	605	CLA	C13-C15-C16-C17
24	AK	607	CLA	C10-C11-C12-C13
26	v	317	NEX	C20-C13-C14-C15
23	AA	606	CHL	C4-C3-C5-C6
23	AD	301	CHL	C4-C3-C5-C6
23	p	607	CHL	C4-C3-C5-C6
23	AH	607	CHL	C4-C3-C5-C6
23	AQ	607	CHL	C4-C3-C5-C6
23	AU	607	CHL	C4-C3-C5-C6
24	9	603	CLA	C4-C3-C5-C6
24	AU	611	CLA	C4-C3-C5-C6
28	AK	623	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
23	AH	607	CHL	C2-C3-C5-C6
23	AU	607	CHL	C2-C3-C5-C6
34	AM	401	SQD	C23-C24-C25-C26
24	AR	602	CLA	C11-C12-C13-C15
28	O	623	LHG	C24-C23-O8-C6
34	o	101	SQD	C24-C23-O48-C46
28	O	622	LHG	C28-C29-C30-C31
23	AH	601	CHL	C10-C11-C12-C13
23	AU	601	CHL	C10-C11-C12-C13
24	O	609	CLA	C15-C16-C17-C18
24	AN	603	CLA	C5-C6-C7-C8
34	AJ	411	SQD	C29-C30-C31-C32
33	AL	501	LMG	O6-C5-C6-O5
23	AU	606	CHL	C2A-CAA-CBA-CGA
24	AR	611	CLA	C2A-CAA-CBA-CGA
23	AC	608	CHL	C5-C6-C7-C8
24	J	407	CLA	C2-C1-O2A-CGA
24	Q	401	CLA	C2-C1-O2A-CGA
24	v	314	CLA	C2-C1-O2A-CGA
24	AJ	406	CLA	C2-C1-O2A-CGA
24	AR	609	CLA	C2-C1-O2A-CGA
24	AS	314	CLA	C2-C1-O2A-CGA
33	P	518	LMG	C38-C39-C40-C41
33	AL	520	LMG	C38-C39-C40-C41
33	J	409	LMG	O6-C5-C6-O5
35	j	102	DGD	O6E-C5E-C6E-O5E
24	Q	403	CLA	C3-C5-C6-C7
32	AJ	408	PHO	C5-C6-C7-C8
24	AD	309	CLA	CBA-CGA-O2A-C1
24	AL	503	CLA	CBA-CGA-O2A-C1
28	W	201	LHG	C24-C23-O8-C6
33	Q	407	LMG	C29-C28-O8-C9
34	AP	101	SQD	C24-C23-O48-C46
28	AU	617	LHG	O6-C4-C5-O7
24	V	603	CLA	C5-C6-C7-C8
23	AD	302	CHL	C15-C16-C17-C18
33	J	409	LMG	C19-C20-C21-C22
33	AL	501	LMG	C19-C20-C21-C22
23	AA	606	CHL	C10-C11-C12-C13
26	v	317	NEX	C12-C13-C14-C15
26	AS	317	NEX	C12-C13-C14-C15
27	9	618	XAT	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
27	AF	613	XAT	C28-C29-C30-C31
23	V	606	CHL	CAA-CBA-CGA-O2A
33	J	409	LMG	O7-C8-C9-O8
33	Q	407	LMG	O1-C7-C8-O7
33	AL	501	LMG	O7-C8-C9-O8
34	m	101	SQD	C35-C36-C37-C38
35	P	516	DGD	O6D-C5D-C6D-O5D
35	AL	517	DGD	O6D-C5D-C6D-O5D
32	J	406	PHO	C5-C6-C7-C8
24	0	610	CLA	O1A-CGA-O2A-C1
32	J	406	PHO	CHA-CBD-CGD-O2D
32	AJ	408	PHO	CHA-CBD-CGD-O1D
34	M	101	SQD	C35-C36-C37-C38
23	AE	605	CHL	C4-C3-C5-C6
24	AC	603	CLA	C4-C3-C5-C6
23	AD	308	CHL	C11-C10-C8-C7
23	V	601	CHL	C11-C10-C8-C7
23	V	601	CHL	C11-C12-C13-C15
23	V	606	CHL	C6-C7-C8-C10
23	p	601	CHL	C6-C7-C8-C10
23	p	601	CHL	C12-C13-C15-C16
23	p	607	CHL	C2-C3-C5-C6
23	p	609	CHL	C11-C10-C8-C7
23	AN	601	CHL	C11-C10-C8-C7
23	AN	601	CHL	C11-C12-C13-C15
23	AN	606	CHL	C6-C7-C8-C10
23	AQ	601	CHL	C6-C7-C8-C10
23	AQ	607	CHL	C2-C3-C5-C6
23	AQ	608	CHL	C12-C13-C15-C16
23	AQ	609	CHL	C11-C10-C8-C7
23	AS	307	CHL	C11-C10-C8-C7
24	9	602	CLA	C11-C12-C13-C15
24	9	603	CLA	C2-C3-C5-C6
24	0	602	CLA	C6-C7-C8-C10
24	0	602	CLA	C11-C10-C8-C7
24	AC	603	CLA	C2-C3-C5-C6
24	O	606	CLA	C12-C13-C15-C16
24	P	501	CLA	C11-C10-C8-C7
24	P	507	CLA	C11-C10-C8-C7
24	P	509	CLA	C11-C10-C8-C7
24	P	511	CLA	C6-C7-C8-C10
24	Q	404	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	V	603	CLA	C11-C10-C8-C7
24	V	609	CLA	C12-C13-C15-C16
24	p	610	CLA	C11-C10-C8-C7
24	AH	602	CLA	C11-C12-C13-C15
24	AK	617	CLA	C11-C12-C13-C15
24	AL	502	CLA	C11-C10-C8-C7
24	AL	508	CLA	C11-C10-C8-C7
24	AL	510	CLA	C11-C10-C8-C7
24	AL	511	CLA	C12-C13-C15-C16
24	AM	404	CLA	C6-C7-C8-C10
24	AN	603	CLA	C11-C10-C8-C7
24	AN	609	CLA	C12-C13-C15-C16
24	AN	612	CLA	C6-C7-C8-C10
24	AN	612	CLA	C12-C13-C15-C16
24	AR	609	CLA	C6-C7-C8-C10
24	AU	602	CLA	C6-C7-C8-C10
24	AU	602	CLA	C11-C12-C13-C15
24	AU	612	CLA	C6-C7-C8-C10
23	AN	606	CHL	CAA-CBA-CGA-O2A
23	AD	302	CHL	C14-C13-C15-C16
23	AD	308	CHL	C11-C10-C8-C9
23	p	601	CHL	C14-C13-C15-C16
23	q	605	CHL	C14-C13-C15-C16
23	AR	605	CHL	C14-C13-C15-C16
23	AS	307	CHL	C11-C10-C8-C9
24	AC	602	CLA	C11-C12-C13-C14
24	AD	303	CLA	C6-C7-C8-C9
24	O	606	CLA	C11-C12-C13-C14
24	O	615	CLA	C14-C13-C15-C16
24	V	609	CLA	C14-C13-C15-C16
24	p	602	CLA	C11-C12-C13-C14
24	p	610	CLA	C11-C12-C13-C14
24	q	609	CLA	C11-C10-C8-C9
24	AH	612	CLA	C14-C13-C15-C16
24	AK	607	CLA	C14-C13-C15-C16
24	AK	617	CLA	C11-C12-C13-C14
24	AK	617	CLA	C14-C13-C15-C16
24	AK	618	CLA	C11-C10-C8-C9
24	AN	609	CLA	C14-C13-C15-C16
24	AN	612	CLA	C14-C13-C15-C16
24	AQ	602	CLA	C11-C12-C13-C14
24	AQ	610	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	AQ	613	CLA	C6-C7-C8-C9
24	AU	612	CLA	C14-C13-C15-C16
24	AD	312	CLA	CBD-CGD-O2D-CED
24	9	610	CLA	CBA-CGA-O2A-C1
24	0	612	CLA	CBA-CGA-O2A-C1
24	P	502	CLA	CBA-CGA-O2A-C1
24	p	604	CLA	CBA-CGA-O2A-C1
24	AH	603	CLA	CBA-CGA-O2A-C1
24	AL	509	CLA	CBA-CGA-O2A-C1
24	AU	603	CLA	CBA-CGA-O2A-C1
33	AM	407	LMG	C29-C28-O8-C9
24	O	616	CLA	C2A-CAA-CBA-CGA
24	v	310	CLA	C2A-CAA-CBA-CGA
35	P	516	DGD	C4D-C5D-C6D-O5D
35	AL	517	DGD	C4D-C5D-C6D-O5D
23	0	601	CHL	C15-C16-C17-C18
24	AC	602	CLA	C4C-C3C-CAC-CBC
24	v	303	CLA	O1D-CGD-O2D-CED
25	V	613	LUT	C7-C8-C9-C10
26	AQ	617	NEX	C31-C32-C33-C34
29	k	101	BCR	C7-C8-C9-C10
35	AO	102	DGD	O6D-C5D-C6D-O5D
23	AQ	608	CHL	C3-C5-C6-C7
24	AK	617	CLA	O1D-CGD-O2D-CED
28	O	623	LHG	C1-C2-C3-O3
23	9	609	CHL	C5-C6-C7-C8
24	AQ	611	CLA	C8-C10-C11-C12
28	v	301	LHG	C8-C7-O7-C5
24	AL	504	CLA	CBA-CGA-O2A-C1
24	AQ	604	CLA	CBA-CGA-O2A-C1
28	P	517	LHG	C11-C12-C13-C14
33	AK	601	LMG	C37-C38-C39-C40
24	O	605	CLA	C10-C11-C12-C13
24	AS	303	CLA	O1D-CGD-O2D-CED
23	9	607	CHL	CBD-CGD-O2D-CED
23	9	608	CHL	C4B-C3B-CAB-CBB
23	AC	607	CHL	C4B-C3B-CAB-CBB
23	V	605	CHL	C4B-C3B-CAB-CBB
24	9	612	CLA	C4B-C3B-CAB-CBB
24	0	604	CLA	C4B-C3B-CAB-CBB
24	0	609	CLA	C4B-C3B-CAB-CBB
24	0	613	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	AA	602	CLA	C4B-C3B-CAB-CBB
24	AC	609	CLA	C4B-C3B-CAB-CBB
24	AD	304	CLA	C4B-C3B-CAB-CBB
24	AD	309	CLA	C4B-C3B-CAB-CBB
24	AD	313	CLA	C4B-C3B-CAB-CBB
24	AF	614	CLA	C4B-C3B-CAB-CBB
24	O	615	CLA	C4B-C3B-CAB-CBB
24	P	505	CLA	C4B-C3B-CAB-CBB
24	P	506	CLA	C4B-C3B-CAB-CBB
24	P	507	CLA	C4B-C3B-CAB-CBB
24	Q	401	CLA	C4B-C3B-CAB-CBB
24	q	610	CLA	C4B-C3B-CAB-CBB
24	q	612	CLA	C4B-C3B-CAB-CBB
24	v	314	CLA	C4B-C3B-CAB-CBB
24	AH	609	CLA	C4B-C3B-CAB-CBB
24	AH	613	CLA	C4B-C3B-CAB-CBB
24	AJ	406	CLA	C4B-C3B-CAB-CBB
24	AK	614	CLA	C4B-C3B-CAB-CBB
24	AL	506	CLA	C4B-C3B-CAB-CBB
24	AL	507	CLA	C4B-C3B-CAB-CBB
24	AL	508	CLA	C4B-C3B-CAB-CBB
24	AS	314	CLA	C4B-C3B-CAB-CBB
23	AN	606	CHL	C16-C17-C18-C19
28	AL	519	LHG	O6-C4-C5-C6
24	AM	403	CLA	O1D-CGD-O2D-CED
27	9	618	XAT	C26-C27-C28-C29
23	AR	605	CHL	CBA-CGA-O2A-C1
24	J	403	CLA	CBA-CGA-O2A-C1
24	AE	603	CLA	C5-C6-C7-C8
24	O	601	CLA	C5-C6-C7-C8
24	AH	602	CLA	C13-C15-C16-C17
23	AA	606	CHL	C2-C3-C5-C6
23	AD	301	CHL	C2-C3-C5-C6
23	AH	601	CHL	C2-C3-C5-C6
28	w	201	LHG	C24-C25-C26-C27
24	AK	618	CLA	C13-C15-C16-C17
24	AU	602	CLA	C13-C15-C16-C17
28	AK	624	LHG	O2-C2-C3-O3
23	0	601	CHL	C3-C5-C6-C7
24	AK	603	CLA	C5-C6-C7-C8
24	AQ	604	CLA	C2A-CAA-CBA-CGA
24	AS	312	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	P	517	LHG	C24-C23-O8-C6
28	AL	519	LHG	C24-C23-O8-C6
28	AD	316	LHG	C23-C24-C25-C26
23	AN	608	CHL	C2C-C3C-CAC-CBC
35	AL	518	DGD	C4B-C5B-C6B-C7B
23	9	607	CHL	C3A-C2A-CAA-CBA
23	AA	601	CHL	C3A-C2A-CAA-CBA
23	AD	301	CHL	C3A-C2A-CAA-CBA
23	AE	616	CHL	C3A-C2A-CAA-CBA
23	V	601	CHL	C3A-C2A-CAA-CBA
23	p	607	CHL	C3A-C2A-CAA-CBA
23	AH	601	CHL	C3A-C2A-CAA-CBA
23	AN	601	CHL	C3A-C2A-CAA-CBA
23	AQ	601	CHL	C3A-C2A-CAA-CBA
23	AQ	607	CHL	C3A-C2A-CAA-CBA
23	AU	601	CHL	C3A-C2A-CAA-CBA
24	AA	613	CLA	C3A-C2A-CAA-CBA
24	AB	602	CLA	C3A-C2A-CAA-CBA
24	AC	610	CLA	C3A-C2A-CAA-CBA
24	AE	612	CLA	C3A-C2A-CAA-CBA
24	P	505	CLA	C3A-C2A-CAA-CBA
24	Q	403	CLA	C3A-C2A-CAA-CBA
24	V	602	CLA	C3A-C2A-CAA-CBA
24	v	313	CLA	C3A-C2A-CAA-CBA
24	AH	612	CLA	C3A-C2A-CAA-CBA
24	AK	610	CLA	C3A-C2A-CAA-CBA
24	AL	506	CLA	C3A-C2A-CAA-CBA
24	AM	403	CLA	C3A-C2A-CAA-CBA
24	AN	602	CLA	C3A-C2A-CAA-CBA
24	AS	313	CLA	C3A-C2A-CAA-CBA
24	AU	612	CLA	C3A-C2A-CAA-CBA
24	0	603	CLA	C4C-C3C-CAC-CBC
27	AR	616	XAT	C9-C10-C11-C12
28	W	201	LHG	C24-C25-C26-C27
33	O	624	LMG	C37-C38-C39-C40
35	AL	518	DGD	C8B-C9B-CAB-CBB
28	AK	624	LHG	C13-C14-C15-C16
34	Q	402	SQD	C16-C17-C18-C19
38	F	102	HEM	C3D-CAD-CBD-CGD
24	P	503	CLA	CBA-CGA-O2A-C1
24	P	508	CLA	CBA-CGA-O2A-C1
28	p	617	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
35	AJ	401	DGD	C6A-C7A-C8A-C9A
28	q	616	LHG	C4-C5-C6-O8
28	W	201	LHG	C4-C5-C6-O8
33	P	518	LMG	O1-C7-C8-C9
33	AL	520	LMG	O1-C7-C8-C9
34	J	410	SQD	C44-C45-C46-O48
34	AJ	411	SQD	C19-C20-C21-C22
24	q	612	CLA	O1A-CGA-O2A-C1
34	AM	401	SQD	C16-C17-C18-C19
35	J	413	DGD	C6A-C7A-C8A-C9A
23	V	608	CHL	C2C-C3C-CAC-CBC
28	0	616	LHG	C28-C29-C30-C31
24	AL	513	CLA	C3-C5-C6-C7
34	AP	101	SQD	O10-C23-O48-C46
24	AH	611	CLA	C4-C3-C5-C6
24	AR	602	CLA	C11-C12-C13-C14
23	AE	605	CHL	C2-C3-C5-C6
23	9	606	CHL	C3C-C2C-CMC-OMC
23	9	607	CHL	C3C-C2C-CMC-OMC
23	AA	606	CHL	C3C-C2C-CMC-OMC
23	AE	616	CHL	C3C-C2C-CMC-OMC
23	V	601	CHL	C3C-C2C-CMC-OMC
23	V	605	CHL	C3C-C2C-CMC-OMC
23	AN	605	CHL	C3C-C2C-CMC-OMC
23	AN	606	CHL	C3C-C2C-CMC-OMC
23	AQ	609	CHL	C3C-C2C-CMC-OMC
23	AR	606	CHL	C3C-C2C-CMC-OMC
28	Q	406	LHG	C23-C24-C25-C26
28	AS	301	LHG	C7-C8-C9-C10
34	AM	401	SQD	C31-C32-C33-C34
24	AK	608	CLA	C3-C5-C6-C7
24	AK	616	CLA	C3-C5-C6-C7
23	q	605	CHL	C2A-CAA-CBA-CGA
24	p	604	CLA	C2A-CAA-CBA-CGA
28	O	621	LHG	O6-C4-C5-O7
28	AH	616	LHG	O6-C4-C5-O7
23	q	606	CHL	CBA-CGA-O2A-C1
24	O	602	CLA	CBA-CGA-O2A-C1
24	v	312	CLA	CBA-CGA-O2A-C1
24	AL	503	CLA	O1A-CGA-O2A-C1
34	o	101	SQD	O10-C23-O48-C46
23	AH	601	CHL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	AU	601	CHL	C16-C17-C18-C20
23	p	609	CHL	C13-C15-C16-C17
34	m	101	SQD	C33-C34-C35-C36
23	q	605	CHL	C2B-C3B-CAB-CBB
24	0	613	CLA	C2B-C3B-CAB-CBB
24	AC	609	CLA	C2B-C3B-CAB-CBB
24	AD	304	CLA	C2B-C3B-CAB-CBB
24	AD	309	CLA	C2B-C3B-CAB-CBB
24	O	615	CLA	C2B-C3B-CAB-CBB
24	P	506	CLA	C2B-C3B-CAB-CBB
24	P	507	CLA	C2B-C3B-CAB-CBB
24	q	610	CLA	C2B-C3B-CAB-CBB
24	q	612	CLA	C2B-C3B-CAB-CBB
24	v	314	CLA	C2B-C3B-CAB-CBB
24	AJ	406	CLA	C2B-C3B-CAB-CBB
24	AS	314	CLA	C2B-C3B-CAB-CBB
28	AN	616	LHG	C9-C10-C11-C12
24	AL	504	CLA	C10-C11-C12-C13
24	9	610	CLA	O1A-CGA-O2A-C1
24	p	604	CLA	O1A-CGA-O2A-C1
28	AM	406	LHG	C7-C8-C9-C10
28	AM	406	LHG	C23-C24-C25-C26
24	AB	610	CLA	C2C-C3C-CAC-CBC
34	Q	402	SQD	C31-C32-C33-C34
28	W	201	LHG	O7-C5-C6-O8
28	w	201	LHG	O7-C5-C6-O8
33	O	624	LMG	O7-C8-C9-O8
33	P	518	LMG	O1-C7-C8-O7
33	AK	601	LMG	O7-C8-C9-O8
33	AL	520	LMG	O1-C7-C8-O7
33	AM	407	LMG	O1-C7-C8-O7
35	J	413	DGD	O1G-C1G-C2G-O2G
35	AJ	401	DGD	O1G-C1G-C2G-O2G
28	AD	316	LHG	C28-C29-C30-C31
28	AS	301	LHG	C8-C7-O7-C5
23	AH	607	CHL	C16-C17-C18-C20
24	q	602	CLA	C11-C12-C13-C15
28	O	623	LHG	C13-C14-C15-C16
34	Q	402	SQD	O5-C1-O6-C44
35	AO	102	DGD	O6E-C1E-O5D-C6D
24	9	610	CLA	C5-C6-C7-C8
28	Q	406	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	AM	406	LHG	C1-C2-C3-O3
34	M	101	SQD	C33-C34-C35-C36
23	AD	302	CHL	C2-C1-O2A-CGA
23	V	607	CHL	C2-C1-O2A-CGA
23	p	606	CHL	C2-C1-O2A-CGA
23	AN	605	CHL	C2-C1-O2A-CGA
24	0	603	CLA	C2-C1-O2A-CGA
24	O	604	CLA	C2-C1-O2A-CGA
24	AJ	409	CLA	C2-C1-O2A-CGA
24	AK	606	CLA	C2-C1-O2A-CGA
24	AL	509	CLA	O1A-CGA-O2A-C1
24	9	602	CLA	C11-C12-C13-C14
24	P	502	CLA	C11-C10-C8-C9
24	P	503	CLA	C14-C13-C15-C16
24	P	508	CLA	C14-C13-C15-C16
24	V	609	CLA	C11-C12-C13-C14
24	p	602	CLA	C6-C7-C8-C9
24	AL	503	CLA	C11-C10-C8-C9
24	AL	504	CLA	C14-C13-C15-C16
24	AL	509	CLA	C14-C13-C15-C16
24	AN	602	CLA	C11-C10-C8-C9
24	AN	609	CLA	C11-C12-C13-C14
24	AR	609	CLA	C11-C10-C8-C9
28	AH	616	LHG	C31-C32-C33-C34
23	AQ	609	CHL	C13-C15-C16-C17
24	O	611	CLA	C5-C6-C7-C8
24	P	503	CLA	C10-C11-C12-C13
24	AQ	610	CLA	C10-C11-C12-C13
23	q	607	CHL	C4-C3-C5-C6
32	AJ	408	PHO	C1A-C2A-CAA-CBA
24	0	612	CLA	O1A-CGA-O2A-C1
24	AD	309	CLA	O1A-CGA-O2A-C1
23	V	606	CHL	C16-C17-C18-C19
23	p	607	CHL	C16-C17-C18-C20
23	AH	601	CHL	C16-C17-C18-C19
23	AN	601	CHL	C16-C17-C18-C20
23	AQ	607	CHL	C16-C17-C18-C20
23	AU	601	CHL	C16-C17-C18-C19
24	P	511	CLA	C3-C5-C6-C7
25	0	615	LUT	C1-C6-C7-C8
25	AA	614	LUT	C1-C6-C7-C8
25	AA	615	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	AD	315	LUT	C1-C6-C7-C8
25	AE	613	LUT	C1-C6-C7-C8
25	AE	613	LUT	C5-C6-C7-C8
25	AE	614	LUT	C1-C6-C7-C8
25	p	615	LUT	C1-C6-C7-C8
25	AH	615	LUT	C1-C6-C7-C8
25	AQ	616	LUT	C1-C6-C7-C8
25	AU	615	LUT	C1-C6-C7-C8
29	AB	612	BCR	C23-C24-C25-C26
29	J	408	BCR	C1-C6-C7-C8
29	J	408	BCR	C23-C24-C25-C26
29	O	618	BCR	C1-C6-C7-C8
29	O	618	BCR	C5-C6-C7-C8
29	O	618	BCR	C23-C24-C25-C26
29	O	619	BCR	C23-C24-C25-C30
29	O	625	BCR	C23-C24-C25-C26
29	O	625	BCR	C23-C24-C25-C30
29	P	514	BCR	C5-C6-C7-C8
29	P	514	BCR	C23-C24-C25-C26
29	P	514	BCR	C23-C24-C25-C30
29	AI	101	BCR	C23-C24-C25-C26
29	AJ	410	BCR	C1-C6-C7-C8
29	AJ	410	BCR	C5-C6-C7-C8
29	AJ	410	BCR	C23-C24-C25-C26
29	AK	620	BCR	C1-C6-C7-C8
29	AK	620	BCR	C5-C6-C7-C8
29	AK	620	BCR	C23-C24-C25-C26
29	AK	621	BCR	C23-C24-C25-C26
29	AK	621	BCR	C23-C24-C25-C30
29	AL	516	BCR	C1-C6-C7-C8
29	AL	516	BCR	C5-C6-C7-C8
29	AL	516	BCR	C23-C24-C25-C26
29	AL	516	BCR	C23-C24-C25-C30
24	v	313	CLA	C5-C6-C7-C8
24	AL	506	CLA	C10-C11-C12-C13
24	AM	403	CLA	C13-C15-C16-C17
34	o	101	SQD	C29-C30-C31-C32
34	M	101	SQD	C26-C27-C28-C29
27	9	618	XAT	C31-C32-C33-C40
28	q	616	LHG	C11-C10-C9-C8
34	J	410	SQD	C29-C30-C31-C32
24	P	502	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	9	601	CHL	C1A-C2A-CAA-CBA
25	v	315	LUT	C7-C8-C9-C10
25	AN	614	LUT	C7-C8-C9-C10
26	AE	615	NEX	C11-C12-C13-C14
26	AQ	617	NEX	C27-C28-C29-C30
27	9	618	XAT	C31-C32-C33-C34
24	P	505	CLA	C10-C11-C12-C13
24	Q	403	CLA	C13-C15-C16-C17
33	P	518	LMG	C35-C36-C37-C38
28	Q	406	LHG	C7-C8-C9-C10
26	9	617	NEX	C14-C15-C35-C34
26	AE	615	NEX	C14-C15-C35-C34
34	AP	101	SQD	C29-C30-C31-C32
23	AN	607	CHL	C16-C17-C18-C20
23	AU	607	CHL	C16-C17-C18-C20
24	AQ	611	CLA	C11-C12-C13-C15
34	J	410	SQD	C19-C20-C21-C22
23	q	605	CHL	C10-C11-C12-C13
28	O	622	LHG	C24-C25-C26-C27
28	AL	519	LHG	C29-C30-C31-C32
28	AQ	618	LHG	C27-C28-C29-C30
33	AL	520	LMG	C35-C36-C37-C38
33	AM	407	LMG	C17-C18-C19-C20
23	AR	605	CHL	O1A-CGA-O2A-C1
24	P	503	CLA	O1A-CGA-O2A-C1
28	q	616	LHG	C24-C25-C26-C27
28	AL	519	LHG	C9-C10-C11-C12
33	Q	407	LMG	C17-C18-C19-C20
34	m	101	SQD	C26-C27-C28-C29
23	9	609	CHL	C11-C12-C13-C15
23	AC	608	CHL	C11-C12-C13-C15
23	V	606	CHL	C12-C13-C15-C16
23	p	607	CHL	C6-C7-C8-C10
23	q	605	CHL	C12-C13-C15-C16
23	AH	601	CHL	C6-C7-C8-C10
23	AH	601	CHL	C11-C12-C13-C15
23	AH	607	CHL	C6-C7-C8-C10
23	AH	607	CHL	C12-C13-C15-C16
23	AQ	607	CHL	C12-C13-C15-C16
23	AR	605	CHL	C12-C13-C15-C16
23	AU	601	CHL	C6-C7-C8-C10
23	AU	601	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	AU	607	CHL	C6-C7-C8-C10
23	AU	607	CHL	C12-C13-C15-C16
24	AC	602	CLA	C11-C10-C8-C7
24	AC	602	CLA	C11-C12-C13-C15
24	O	603	CLA	C12-C13-C15-C16
24	O	606	CLA	C2-C3-C5-C6
24	O	612	CLA	C11-C10-C8-C7
24	O	615	CLA	C11-C10-C8-C7
24	O	615	CLA	C11-C12-C13-C15
24	O	615	CLA	C12-C13-C15-C16
24	P	509	CLA	C6-C7-C8-C10
24	P	510	CLA	C12-C13-C15-C16
24	P	512	CLA	C11-C12-C13-C15
24	P	512	CLA	C12-C13-C15-C16
24	V	609	CLA	C11-C10-C8-C7
24	V	609	CLA	C11-C12-C13-C15
24	p	602	CLA	C6-C7-C8-C10
24	p	602	CLA	C11-C12-C13-C15
24	p	610	CLA	C11-C12-C13-C15
24	q	602	CLA	C6-C7-C8-C10
24	q	609	CLA	C6-C7-C8-C10
24	q	609	CLA	C11-C10-C8-C7
24	q	612	CLA	C6-C7-C8-C10
24	AH	602	CLA	C6-C7-C8-C10
24	AH	612	CLA	C6-C7-C8-C10
24	AH	612	CLA	C11-C12-C13-C15
24	AH	612	CLA	C12-C13-C15-C16
24	AK	605	CLA	C12-C13-C15-C16
24	AK	614	CLA	C11-C10-C8-C7
24	AK	617	CLA	C12-C13-C15-C16
24	AL	503	CLA	C11-C10-C8-C7
24	AL	510	CLA	C6-C7-C8-C10
24	AL	514	CLA	C11-C12-C13-C15
24	AL	514	CLA	C12-C13-C15-C16
24	AN	609	CLA	C11-C10-C8-C7
24	AN	609	CLA	C11-C12-C13-C15
24	AQ	602	CLA	C6-C7-C8-C10
24	AQ	602	CLA	C11-C12-C13-C15
24	AQ	610	CLA	C11-C12-C13-C15
24	AQ	613	CLA	C6-C7-C8-C10
24	AR	602	CLA	C6-C7-C8-C10
24	AR	609	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	AU	611	CLA	C2-C3-C5-C6
24	AU	612	CLA	C12-C13-C15-C16
24	AQ	604	CLA	O1A-CGA-O2A-C1
28	AK	623	LHG	C24-C25-C26-C27
26	AC	616	NEX	C9-C10-C11-C12
23	V	601	CHL	C16-C17-C18-C20
35	AJ	401	DGD	C3B-C4B-C5B-C6B
28	V	615	LHG	C9-C10-C11-C12
28	AK	623	LHG	C11-C10-C9-C8
24	AU	603	CLA	O1A-CGA-O2A-C1
28	P	517	LHG	O10-C23-O8-C6
23	AE	617	CHL	C2A-CAA-CBA-CGA
23	AF	608	CHL	C2A-CAA-CBA-CGA
24	q	602	CLA	C2A-CAA-CBA-CGA
24	O	611	CLA	C10-C11-C12-C13
26	AS	317	NEX	C39-C29-C30-C31
26	AU	616	NEX	C11-C10-C9-C19
27	q	617	XAT	C39-C29-C30-C31
27	AR	616	XAT	C39-C29-C30-C31
28	O	622	LHG	C11-C10-C9-C8
29	AB	612	BCR	C20-C21-C22-C37
29	F	101	BCR	C16-C17-C18-C36
29	f	101	BCR	C16-C17-C18-C36
33	P	518	LMG	C28-C29-C30-C31
24	AJ	404	CLA	C3-C5-C6-C7
23	AD	301	CHL	CBA-CGA-O2A-C1
24	AC	602	CLA	C12-C13-C15-C16
23	AE	605	CHL	C8-C10-C11-C12
24	AD	303	CLA	C8-C10-C11-C12
24	O	616	CLA	C13-C15-C16-C17
23	AA	608	CHL	CBD-CGD-O2D-CED
23	9	606	CHL	CAD-CBD-CGD-O2D
23	9	607	CHL	CAD-CBD-CGD-O2D
23	0	601	CHL	CAD-CBD-CGD-O2D
23	AA	605	CHL	CAD-CBD-CGD-O2D
23	AA	607	CHL	CAD-CBD-CGD-O2D
23	AD	302	CHL	CAD-CBD-CGD-O2D
23	AE	606	CHL	CAD-CBD-CGD-O2D
23	p	606	CHL	CAD-CBD-CGD-O2D
23	p	608	CHL	CAD-CBD-CGD-O2D
23	q	606	CHL	CAD-CBD-CGD-O2D
23	v	302	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	AH	606	CHL	CAD-CBD-CGD-O2D
23	AH	608	CHL	CAD-CBD-CGD-O2D
23	AQ	608	CHL	CAD-CBD-CGD-O2D
23	AU	606	CHL	CAD-CBD-CGD-O2D
23	AU	608	CHL	CAD-CBD-CGD-O2D
24	9	613	CLA	CAD-CBD-CGD-O2D
24	AA	603	CLA	CAD-CBD-CGD-O2D
24	AC	602	CLA	CAD-CBD-CGD-O2D
24	AC	612	CLA	CAD-CBD-CGD-O2D
24	AE	603	CLA	CAD-CBD-CGD-O2D
24	J	403	CLA	CAD-CBD-CGD-O2D
24	V	602	CLA	CAD-CBD-CGD-O2D
24	p	602	CLA	CAD-CBD-CGD-O2D
24	AH	609	CLA	CAD-CBD-CGD-O2D
24	AK	613	CLA	CAD-CBD-CGD-O2D
24	AK	616	CLA	CAD-CBD-CGD-O2D
24	AN	602	CLA	CAD-CBD-CGD-O2D
24	AN	603	CLA	CAD-CBD-CGD-O2D
24	AN	612	CLA	CAD-CBD-CGD-O2D
24	AQ	602	CLA	CAD-CBD-CGD-O2D
24	AQ	610	CLA	CAD-CBD-CGD-O2D
24	AQ	611	CLA	CAD-CBD-CGD-O2D
24	AU	609	CLA	CAD-CBD-CGD-O2D
26	AA	616	NEX	C7-C8-C9-C19
26	AE	615	NEX	C7-C8-C9-C19
26	v	317	NEX	C7-C8-C9-C19
26	AS	317	NEX	C7-C8-C9-C19
28	AU	617	LHG	C31-C32-C33-C34
35	J	413	DGD	C3B-C4B-C5B-C6B
23	AH	607	CHL	C10-C11-C12-C13
24	v	303	CLA	C10-C11-C12-C13
24	AQ	613	CLA	C8-C10-C11-C12
28	P	517	LHG	C9-C10-C11-C12
28	AH	616	LHG	C27-C28-C29-C30
28	AN	616	LHG	C17-C18-C19-C20
28	AU	617	LHG	C32-C33-C34-C35
24	AH	611	CLA	CBA-CGA-O2A-C1
33	O	620	LMG	O6-C1-O1-C7
33	AK	622	LMG	O6-C1-O1-C7
23	AU	601	CHL	C2-C3-C5-C6
28	P	517	LHG	C2-C3-O3-P
28	Q	406	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
28	V	615	LHG	C4-C5-C6-O8
28	AL	519	LHG	C2-C3-O3-P
34	AJ	411	SQD	C44-C45-C46-O48
24	J	403	CLA	O1A-CGA-O2A-C1
24	AH	603	CLA	O1A-CGA-O2A-C1
24	AL	504	CLA	O1A-CGA-O2A-C1
23	AU	605	CHL	CAA-CBA-CGA-O2A
24	q	610	CLA	O2A-C1-C2-C3
24	AR	610	CLA	O2A-C1-C2-C3
28	AN	616	LHG	C24-C25-C26-C27
34	AP	101	SQD	C9-C10-C11-C12
24	AD	313	CLA	C2A-CAA-CBA-CGA
24	AK	610	CLA	C2A-CAA-CBA-CGA
23	AU	607	CHL	C10-C11-C12-C13
24	AL	509	CLA	C5-C6-C7-C8
24	AQ	610	CLA	C13-C15-C16-C17
33	AL	520	LMG	C30-C31-C32-C33
34	AM	401	SQD	C18-C19-C20-C21
24	q	602	CLA	C11-C12-C13-C14
28	O	622	LHG	C33-C34-C35-C36
34	Q	402	SQD	C18-C19-C20-C21
23	0	607	CHL	CHA-CBD-CGD-O1D
23	0	607	CHL	CHA-CBD-CGD-O2D
23	V	616	CHL	CHA-CBD-CGD-O1D
23	V	616	CHL	CHA-CBD-CGD-O2D
23	v	307	CHL	CHA-CBD-CGD-O1D
23	v	307	CHL	CHA-CBD-CGD-O2D
23	AN	617	CHL	CHA-CBD-CGD-O1D
23	AN	617	CHL	CHA-CBD-CGD-O2D
23	AR	613	CHL	CHA-CBD-CGD-O2D
24	AA	604	CLA	CHA-CBD-CGD-O1D
24	AD	310	CLA	CHA-CBD-CGD-O2D
24	AD	313	CLA	CHA-CBD-CGD-O1D
24	AE	604	CLA	CHA-CBD-CGD-O1D
24	AE	609	CLA	CHA-CBD-CGD-O2D
24	O	605	CLA	CHA-CBD-CGD-O1D
24	O	610	CLA	CHA-CBD-CGD-O1D
24	O	610	CLA	CHA-CBD-CGD-O2D
24	O	614	CLA	CHA-CBD-CGD-O1D
24	V	610	CLA	CHA-CBD-CGD-O1D
24	p	604	CLA	CHA-CBD-CGD-O1D
24	p	612	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	p	612	CLA	CHA-CBD-CGD-O2D
24	q	604	CLA	CHA-CBD-CGD-O1D
24	v	303	CLA	CHA-CBD-CGD-O1D
24	v	303	CLA	CHA-CBD-CGD-O2D
24	AK	606	CLA	CHA-CBD-CGD-O1D
24	AK	612	CLA	CHA-CBD-CGD-O1D
24	AK	612	CLA	CHA-CBD-CGD-O2D
24	AN	611	CLA	CHA-CBD-CGD-O1D
24	AN	611	CLA	CHA-CBD-CGD-O2D
24	AS	303	CLA	CHA-CBD-CGD-O1D
24	AS	303	CLA	CHA-CBD-CGD-O2D
24	AS	305	CLA	CHA-CBD-CGD-O1D
24	AS	305	CLA	CHA-CBD-CGD-O2D
23	p	608	CHL	C3-C5-C6-C7
23	q	606	CHL	O1A-CGA-O2A-C1
24	O	602	CLA	O1A-CGA-O2A-C1
24	v	312	CLA	O1A-CGA-O2A-C1
24	AS	312	CLA	O1A-CGA-O2A-C1
33	P	518	LMG	C30-C31-C32-C33
35	AO	102	DGD	C2E-C1E-O5D-C6D
28	AK	623	LHG	C33-C34-C35-C36
35	P	516	DGD	O2G-C2G-C3G-O3G
28	O	622	LHG	C29-C30-C31-C32
24	AK	613	CLA	C10-C11-C12-C13
24	P	508	CLA	O1A-CGA-O2A-C1
28	AS	301	LHG	C14-C15-C16-C17
28	AU	617	LHG	C27-C28-C29-C30
23	V	607	CHL	C16-C17-C18-C20
28	W	201	LHG	C30-C31-C32-C33
28	AM	406	LHG	C34-C35-C36-C37
28	w	201	LHG	C30-C31-C32-C33
34	o	101	SQD	C9-C10-C11-C12
24	J	403	CLA	C3-C5-C6-C7
24	0	602	CLA	C8-C10-C11-C12
24	P	510	CLA	C4-C3-C5-C6
28	P	517	LHG	C29-C30-C31-C32
28	AK	623	LHG	C29-C30-C31-C32
34	M	101	SQD	C25-C26-C27-C28
23	AD	301	CHL	O1A-CGA-O2A-C1
33	AL	520	LMG	C28-C29-C30-C31
23	AQ	608	CHL	O1D-CGD-O2D-CED
23	AE	605	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	AN	606	CHL	C5-C6-C7-C8
24	O	604	CLA	C5-C6-C7-C8
24	p	612	CLA	C5-C6-C7-C8
24	AK	606	CLA	C5-C6-C7-C8
23	AH	601	CHL	C11-C12-C13-C14
23	AU	601	CHL	C11-C12-C13-C14
24	O	602	CLA	C14-C13-C15-C16
24	O	609	CLA	C11-C12-C13-C14
24	O	615	CLA	C11-C12-C13-C14
24	V	602	CLA	C14-C13-C15-C16
24	V	609	CLA	C11-C10-C8-C9
24	AN	602	CLA	C14-C13-C15-C16
24	AN	609	CLA	C11-C10-C8-C9
24	AQ	602	CLA	C6-C7-C8-C9
24	p	618	CLA	O1A-CGA-O2A-C1
34	m	101	SQD	C25-C26-C27-C28
35	AL	518	DGD	C6A-C7A-C8A-C9A
24	P	508	CLA	C5-C6-C7-C8
24	AK	613	CLA	C5-C6-C7-C8
34	AM	401	SQD	C5-C6-S-O8
24	O	608	CLA	C2A-CAA-CBA-CGA
34	J	410	SQD	O47-C7-C8-C9
33	O	624	LMG	C39-C40-C41-C42
23	AR	606	CHL	O1A-CGA-O2A-C1
24	AH	611	CLA	O1A-CGA-O2A-C1
26	AC	616	NEX	C31-C32-C33-C40
25	v	316	LUT	C7-C8-C9-C10
25	AS	316	LUT	C7-C8-C9-C10
26	q	615	NEX	C31-C32-C33-C34
29	F	101	BCR	C21-C22-C23-C24
29	f	101	BCR	C21-C22-C23-C24
28	V	615	LHG	C17-C18-C19-C20
35	j	102	DGD	C6A-C7A-C8A-C9A
23	V	601	CHL	C1A-C2A-CAA-CBA
23	AN	601	CHL	C1A-C2A-CAA-CBA
23	AQ	601	CHL	C1A-C2A-CAA-CBA
24	9	610	CLA	C1A-C2A-CAA-CBA
24	Q	403	CLA	C1A-C2A-CAA-CBA
24	AJ	409	CLA	C1A-C2A-CAA-CBA
24	AM	403	CLA	C1A-C2A-CAA-CBA
24	AU	602	CLA	C1A-C2A-CAA-CBA
24	O	613	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	AR	606	CHL	CBA-CGA-O2A-C1
24	p	618	CLA	CBA-CGA-O2A-C1
24	AJ	404	CLA	CBA-CGA-O2A-C1
35	AO	102	DGD	C4B-C5B-C6B-C7B
23	9	609	CHL	O1D-CGD-O2D-CED
28	O	621	LHG	C4-O6-P-O3
28	O	623	LHG	C3-O3-P-O6
28	Q	406	LHG	C3-O3-P-O6
28	AK	624	LHG	C3-O3-P-O6
28	Q	406	LHG	C34-C35-C36-C37
28	0	616	LHG	C23-C24-C25-C26
23	AU	608	CHL	O1D-CGD-O2D-CED
24	AD	304	CLA	C4-C3-C5-C6
24	p	610	CLA	C4-C3-C5-C6
24	AL	511	CLA	C4-C3-C5-C6
24	AL	514	CLA	C3-C5-C6-C7
28	AM	406	LHG	C2-C3-O3-P
24	AM	404	CLA	C2-C3-C5-C6
28	O	621	LHG	C28-C29-C30-C31
23	q	605	CHL	C4B-C3B-CAB-CBB
23	AH	606	CHL	C4B-C3B-CAB-CBB
23	AR	605	CHL	C4B-C3B-CAB-CBB
23	AU	606	CHL	C4B-C3B-CAB-CBB
23	AU	608	CHL	C4B-C3B-CAB-CBB
24	0	611	CLA	C4B-C3B-CAB-CBB
24	AA	610	CLA	C4B-C3B-CAB-CBB
24	AB	610	CLA	C4B-C3B-CAB-CBB
24	AD	311	CLA	C4B-C3B-CAB-CBB
24	AE	609	CLA	C4B-C3B-CAB-CBB
24	AE	610	CLA	C4B-C3B-CAB-CBB
24	K	101	CLA	C4B-C3B-CAB-CBB
24	p	603	CLA	C4B-C3B-CAB-CBB
24	p	611	CLA	C4B-C3B-CAB-CBB
24	AH	603	CLA	C4B-C3B-CAB-CBB
24	AL	512	CLA	C4B-C3B-CAB-CBB
24	AN	603	CLA	C4B-C3B-CAB-CBB
24	AN	610	CLA	C4B-C3B-CAB-CBB
24	AQ	603	CLA	C4B-C3B-CAB-CBB
24	AQ	611	CLA	C4B-C3B-CAB-CBB
24	AS	311	CLA	C4B-C3B-CAB-CBB
28	P	517	LHG	C3-O3-P-O4
28	Q	406	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
28	v	301	LHG	C3-O3-P-O5
28	AL	519	LHG	C3-O3-P-O4
28	AM	406	LHG	C3-O3-P-O4
28	AS	301	LHG	C3-O3-P-O5
38	f	102	HEM	C3A-C2A-CAA-CBA
35	J	411	DGD	O6D-C1D-O3G-C3G
35	AJ	412	DGD	O6D-C1D-O3G-C3G
24	AK	608	CLA	CBA-CGA-O2A-C1
24	AU	611	CLA	CBA-CGA-O2A-C1
28	q	616	LHG	O6-C4-C5-C6
28	AH	616	LHG	O6-C4-C5-C6
28	AU	617	LHG	O6-C4-C5-C6
28	AN	616	LHG	C34-C35-C36-C37
33	AK	601	LMG	C39-C40-C41-C42
23	AH	605	CHL	CAA-CBA-CGA-O2A
34	AJ	411	SQD	O47-C7-C8-C9
28	P	517	LHG	C33-C34-C35-C36
28	AH	616	LHG	C32-C33-C34-C35
28	O	621	LHG	C34-C35-C36-C37
24	0	613	CLA	O2A-C1-C2-C3
35	AO	102	DGD	C6A-C7A-C8A-C9A
23	V	616	CHL	CAD-CBD-CGD-O1D
23	AN	617	CHL	CAD-CBD-CGD-O1D
23	AR	613	CHL	CAD-CBD-CGD-O1D
24	AE	604	CLA	CAD-CBD-CGD-O1D
24	AE	609	CLA	CAD-CBD-CGD-O1D
24	P	501	CLA	CAD-CBD-CGD-O1D
24	P	505	CLA	CAD-CBD-CGD-O1D
24	P	509	CLA	CAD-CBD-CGD-O1D
24	p	612	CLA	CAD-CBD-CGD-O1D
24	AJ	404	CLA	CAD-CBD-CGD-O1D
24	AK	611	CLA	CAD-CBD-CGD-O1D
24	AL	502	CLA	CAD-CBD-CGD-O1D
24	AL	506	CLA	CAD-CBD-CGD-O1D
24	AL	510	CLA	CAD-CBD-CGD-O1D
34	M	101	SQD	O5-C5-C6-S
34	m	101	SQD	O5-C5-C6-S
23	V	606	CHL	C5-C6-C7-C8
24	p	610	CLA	C13-C15-C16-C17
24	AN	609	CLA	C5-C6-C7-C8
24	P	512	CLA	C3-C5-C6-C7
35	AO	102	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
24	O	605	CLA	CBA-CGA-O2A-C1
24	AD	312	CLA	O1D-CGD-O2D-CED
28	AK	624	LHG	C1-C2-C3-O3
28	V	615	LHG	C34-C35-C36-C37
23	AQ	609	CHL	C16-C17-C18-C19
23	AA	617	CHL	C3A-C2A-CAA-CBA
23	AD	302	CHL	C11-C10-C8-C7
23	AE	605	CHL	C6-C7-C8-C10
23	p	607	CHL	C12-C13-C15-C16
23	AH	608	CHL	C11-C10-C8-C7
23	AN	606	CHL	C12-C13-C15-C16
23	AQ	607	CHL	C6-C7-C8-C10
23	AU	608	CHL	C11-C10-C8-C7
24	9	602	CLA	C6-C7-C8-C10
24	AC	602	CLA	C6-C7-C8-C10
24	O	616	CLA	C6-C7-C8-C10
24	P	502	CLA	C11-C10-C8-C7
24	P	507	CLA	C6-C7-C8-C10
24	P	507	CLA	C12-C13-C15-C16
24	P	510	CLA	C11-C10-C8-C7
24	Q	403	CLA	C6-C7-C8-C10
24	Q	403	CLA	C11-C10-C8-C7
24	Q	404	CLA	C11-C12-C13-C15
24	AH	603	CLA	C12-C13-C15-C16
24	AH	611	CLA	C2-C3-C5-C6
24	AK	608	CLA	C12-C13-C15-C16
24	AK	617	CLA	C11-C10-C8-C7
24	AL	508	CLA	C6-C7-C8-C10
24	AL	508	CLA	C12-C13-C15-C16
24	AL	511	CLA	C11-C10-C8-C7
24	AM	403	CLA	C6-C7-C8-C10
24	AM	403	CLA	C11-C10-C8-C7
24	AM	404	CLA	C11-C12-C13-C15
24	AQ	611	CLA	C11-C10-C8-C7
24	AU	603	CLA	C12-C13-C15-C16
24	AU	612	CLA	C11-C12-C13-C15
28	P	517	LHG	O6-C4-C5-O7
28	q	616	LHG	O6-C4-C5-O7
28	AL	519	LHG	O6-C4-C5-O7
24	AK	603	CLA	C13-C15-C16-C17
28	v	301	LHG	C14-C15-C16-C17
28	AM	406	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
26	AC	616	NEX	C29-C30-C31-C32
28	AM	406	LHG	C32-C33-C34-C35
34	AP	101	SQD	C11-C12-C13-C14
24	AK	615	CLA	C5-C6-C7-C8
28	AL	519	LHG	C25-C26-C27-C28
23	AN	607	CHL	C2C-C3C-CAC-CBC
23	p	609	CHL	C16-C17-C18-C19
28	AL	519	LHG	C33-C34-C35-C36
23	AU	607	CHL	CAA-CBA-CGA-O2A
23	9	607	CHL	C1C-C2C-CMC-OMC
23	AA	606	CHL	C1C-C2C-CMC-OMC
23	AA	608	CHL	C1C-C2C-CMC-OMC
23	AB	608	CHL	C1C-C2C-CMC-OMC
23	AE	616	CHL	C1C-C2C-CMC-OMC
23	AF	608	CHL	C1C-C2C-CMC-OMC
23	V	601	CHL	C1C-C2C-CMC-OMC
23	V	616	CHL	C1C-C2C-CMC-OMC
23	p	601	CHL	C1C-C2C-CMC-OMC
23	p	608	CHL	C1C-C2C-CMC-OMC
23	p	609	CHL	C1C-C2C-CMC-OMC
23	q	607	CHL	C1C-C2C-CMC-OMC
23	v	307	CHL	C1C-C2C-CMC-OMC
23	AN	606	CHL	C1C-C2C-CMC-OMC
23	AN	608	CHL	C4C-C3C-CAC-CBC
23	AQ	601	CHL	C1C-C2C-CMC-OMC
23	AQ	609	CHL	C1C-C2C-CMC-OMC
23	AR	606	CHL	C1C-C2C-CMC-OMC
23	AS	307	CHL	C1C-C2C-CMC-OMC
33	J	409	LMG	O1-C7-C8-C9
33	O	624	LMG	C31-C32-C33-C34
33	AL	501	LMG	O1-C7-C8-C9
35	P	516	DGD	C1G-C2G-C3G-O3G
35	AL	517	DGD	C1G-C2G-C3G-O3G
24	O	605	CLA	O1A-CGA-O2A-C1
33	J	409	LMG	O1-C7-C8-O7
33	AL	501	LMG	O1-C7-C8-O7
35	AL	517	DGD	O2G-C2G-C3G-O3G
35	AL	518	DGD	O2G-C2G-C3G-O3G
33	AM	407	LMG	C15-C16-C17-C18
35	AL	518	DGD	CBB-CCB-CDB-CEB
24	AJ	404	CLA	O1A-CGA-O2A-C1
24	AL	505	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	Q	407	LMG	C15-C16-C17-C18
35	AL	518	DGD	C5D-C6D-O5D-C1E
23	9	607	CHL	C8-C10-C11-C12
24	AL	511	CLA	C3-C5-C6-C7
28	V	615	LHG	C30-C31-C32-C33
35	j	102	DGD	C1B-C2B-C3B-C4B
24	AU	611	CLA	O1A-CGA-O2A-C1
23	AC	608	CHL	O1D-CGD-O2D-CED
32	AJ	407	PHO	C15-C16-C17-C18
24	AK	610	CLA	C4-C3-C5-C6
24	AC	602	CLA	C14-C13-C15-C16
24	AL	505	CLA	CBA-CGA-O2A-C1
28	Q	406	LHG	C24-C25-C26-C27
24	AM	403	CLA	CAA-CBA-CGA-O2A
28	P	517	LHG	C25-C26-C27-C28
24	AD	309	CLA	C8-C10-C11-C12
23	p	607	CHL	C14-C13-C15-C16
23	AH	607	CHL	C14-C13-C15-C16
23	AN	606	CHL	C14-C13-C15-C16
23	AU	607	CHL	C14-C13-C15-C16
24	O	612	CLA	C11-C10-C8-C9
24	O	614	CLA	C11-C10-C8-C9
24	P	509	CLA	C11-C10-C8-C9
24	P	510	CLA	C14-C13-C15-C16
24	q	602	CLA	C6-C7-C8-C9
24	AH	612	CLA	C6-C7-C8-C9
24	AH	612	CLA	C11-C12-C13-C14
24	AK	604	CLA	C14-C13-C15-C16
24	AK	614	CLA	C11-C10-C8-C9
24	AK	616	CLA	C11-C10-C8-C9
24	AL	510	CLA	C11-C10-C8-C9
24	AL	511	CLA	C14-C13-C15-C16
24	AQ	611	CLA	C6-C7-C8-C9
24	AR	602	CLA	C6-C7-C8-C9
24	AU	612	CLA	C6-C7-C8-C9
24	AU	612	CLA	C11-C12-C13-C14
24	AK	608	CLA	O1A-CGA-O2A-C1
35	AL	517	DGD	O6D-C1D-O3G-C3G
24	O	601	CLA	C13-C15-C16-C17
28	p	617	LHG	C24-C25-C26-C27
34	o	101	SQD	C11-C12-C13-C14
23	AH	607	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	AH	602	CLA	C8-C10-C11-C12
26	9	617	NEX	C29-C30-C31-C32
28	v	301	LHG	C25-C26-C27-C28
33	AK	622	LMG	C21-C22-C23-C24
23	AA	606	CHL	C8-C10-C11-C12
24	P	502	CLA	C8-C10-C11-C12
24	Q	404	CLA	C10-C11-C12-C13
24	p	610	CLA	C10-C11-C12-C13
28	AS	301	LHG	C25-C26-C27-C28
33	Q	407	LMG	C34-C35-C36-C37
33	AK	601	LMG	C31-C32-C33-C34
28	v	301	LHG	C7-C8-C9-C10
33	O	620	LMG	C21-C22-C23-C24
24	AF	602	CLA	C2C-C3C-CAC-CBC
24	O	601	CLA	CBD-CGD-O2D-CED
23	V	605	CHL	C2B-C3B-CAB-CBB
23	AH	606	CHL	C2B-C3B-CAB-CBB
23	AU	606	CHL	C2B-C3B-CAB-CBB
24	0	603	CLA	C2B-C3B-CAB-CBB
24	0	604	CLA	C2B-C3B-CAB-CBB
24	0	609	CLA	C2B-C3B-CAB-CBB
24	0	611	CLA	C2B-C3B-CAB-CBB
24	AA	602	CLA	C2B-C3B-CAB-CBB
24	AA	612	CLA	C2B-C3B-CAB-CBB
24	AB	610	CLA	C2B-C3B-CAB-CBB
24	AD	311	CLA	C2B-C3B-CAB-CBB
24	AD	313	CLA	C2B-C3B-CAB-CBB
24	AE	610	CLA	C2B-C3B-CAB-CBB
24	P	505	CLA	C2B-C3B-CAB-CBB
24	Q	401	CLA	C2B-C3B-CAB-CBB
24	K	101	CLA	C2B-C3B-CAB-CBB
24	v	303	CLA	C2B-C3B-CAB-CBB
24	AH	603	CLA	C2B-C3B-CAB-CBB
24	AH	609	CLA	C2B-C3B-CAB-CBB
24	AH	613	CLA	C2B-C3B-CAB-CBB
24	AK	614	CLA	C2B-C3B-CAB-CBB
24	AL	506	CLA	C2B-C3B-CAB-CBB
24	AL	507	CLA	C2B-C3B-CAB-CBB
24	AL	508	CLA	C2B-C3B-CAB-CBB
24	AN	609	CLA	C2B-C3B-CAB-CBB
24	AN	610	CLA	C2B-C3B-CAB-CBB
24	AQ	603	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	AS	311	CLA	C2B-C3B-CAB-CBB
24	AU	609	CLA	C2B-C3B-CAB-CBB
24	AU	613	CLA	C2B-C3B-CAB-CBB
28	AQ	618	LHG	C13-C14-C15-C16
24	AL	503	CLA	C8-C10-C11-C12
32	J	405	PHO	C15-C16-C17-C18
27	q	617	XAT	C40-C33-C34-C35
29	P	515	BCR	C20-C21-C22-C37
28	AD	316	LHG	C10-C11-C12-C13
28	p	617	LHG	C34-C35-C36-C37
24	P	510	CLA	C3-C5-C6-C7
23	9	607	CHL	O1D-CGD-O2D-CED
24	AD	312	CLA	C4-C3-C5-C6
24	AS	313	CLA	C4-C3-C5-C6
24	Q	403	CLA	CAA-CBA-CGA-O2A
28	p	617	LHG	C13-C14-C15-C16
24	Q	404	CLA	C2-C3-C5-C6
24	AL	511	CLA	C2-C3-C5-C6
24	AM	404	CLA	C10-C11-C12-C13
28	AN	616	LHG	C30-C31-C32-C33
28	AQ	618	LHG	C34-C35-C36-C37
23	AA	608	CHL	NA-C1A-C2A-CAA
23	V	605	CHL	C1-C2-C3-C4
23	p	606	CHL	C1-C2-C3-C4
23	AH	606	CHL	C1-C2-C3-C4
23	AN	605	CHL	C1-C2-C3-C4
23	AQ	606	CHL	C1-C2-C3-C4
23	AU	606	CHL	C1-C2-C3-C4
24	p	610	CLA	NA-C1A-C2A-CAA
24	q	601	CLA	C1-C2-C3-C4
24	q	611	CLA	C1-C2-C3-C4
24	v	312	CLA	C1-C2-C3-C4
24	v	314	CLA	C1-C2-C3-C4
24	AR	601	CLA	C1-C2-C3-C4
24	AR	611	CLA	C1-C2-C3-C4
24	AS	312	CLA	C1-C2-C3-C4
24	AS	314	CLA	C1-C2-C3-C4
24	O	614	CLA	C3-C5-C6-C7
33	AM	407	LMG	C34-C35-C36-C37
28	P	517	LHG	C6-C5-O7-C7
28	AL	519	LHG	C6-C5-O7-C7
23	p	608	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	0	610	CLA	C2A-CAA-CBA-CGA
24	AA	603	CLA	C2A-CAA-CBA-CGA
24	AB	604	CLA	C2A-CAA-CBA-CGA
24	AD	312	CLA	C2A-CAA-CBA-CGA
24	p	602	CLA	C2A-CAA-CBA-CGA
24	AR	602	CLA	C2A-CAA-CBA-CGA
24	AR	617	CLA	C2A-CAA-CBA-CGA
24	AS	310	CLA	C2A-CAA-CBA-CGA
24	O	604	CLA	C2C-C3C-CAC-CBC
24	AU	602	CLA	C8-C10-C11-C12
23	V	605	CHL	C2-C1-O2A-CGA
23	AH	601	CHL	C2-C1-O2A-CGA
23	AQ	606	CHL	C2-C1-O2A-CGA
23	AU	601	CHL	C2-C1-O2A-CGA
24	0	609	CLA	C2-C1-O2A-CGA
24	AA	609	CLA	C2-C1-O2A-CGA
24	AE	608	CLA	C2-C1-O2A-CGA
24	O	610	CLA	C2-C1-O2A-CGA
24	O	615	CLA	C2-C1-O2A-CGA
24	Q	403	CLA	C2-C1-O2A-CGA
24	q	609	CLA	C2-C1-O2A-CGA
24	AK	612	CLA	C2-C1-O2A-CGA
24	AM	403	CLA	C2-C1-O2A-CGA
35	AL	518	DGD	CCA-CDA-CEA-CFA
24	AL	509	CLA	C8-C10-C11-C12
28	0	616	LHG	C10-C11-C12-C13
28	Q	406	LHG	C27-C28-C29-C30
28	AM	406	LHG	C24-C25-C26-C27
23	AN	607	CHL	C16-C17-C18-C19
24	AR	611	CLA	O2A-C1-C2-C3
25	AC	615	LUT	C5-C6-C7-C8
29	AB	612	BCR	C23-C24-C25-C30
29	J	408	BCR	C5-C6-C7-C8
29	O	618	BCR	C23-C24-C25-C30
29	O	619	BCR	C23-C24-C25-C26
29	P	514	BCR	C1-C6-C7-C8
29	AI	101	BCR	C23-C24-C25-C30
29	AK	602	BCR	C23-C24-C25-C26
29	AK	602	BCR	C23-C24-C25-C30
29	AK	620	BCR	C23-C24-C25-C30
29	AV	101	BCR	C23-C24-C25-C26
29	AV	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
24	P	510	CLA	C2-C3-C5-C6
28	Q	406	LHG	C32-C33-C34-C35
35	J	411	DGD	C1A-C2A-C3A-C4A
24	AL	503	CLA	C16-C17-C18-C20
33	P	518	LMG	C11-C10-O7-C8
33	AL	520	LMG	C11-C10-O7-C8
24	V	602	CLA	C10-C11-C12-C13
26	9	617	NEX	C11-C10-C9-C8
26	AS	317	NEX	C28-C29-C30-C31
27	9	618	XAT	C28-C29-C30-C31
24	AK	604	CLA	CAA-CBA-CGA-O2A
24	AL	508	CLA	C5-C6-C7-C8
34	m	101	SQD	C27-C28-C29-C30
28	P	517	LHG	C4-O6-P-O3
28	Q	406	LHG	C4-O6-P-O3
28	AK	624	LHG	C4-O6-P-O3
28	AL	519	LHG	C4-O6-P-O3
28	AM	406	LHG	C3-O3-P-O6
28	AM	406	LHG	C4-O6-P-O3
28	Q	406	LHG	C30-C31-C32-C33
33	AL	501	LMG	C31-C32-C33-C34
24	P	508	CLA	C8-C10-C11-C12
24	AK	606	CLA	C2C-C3C-CAC-CBC
32	J	406	PHO	CHA-CBD-CGD-O1D
33	J	409	LMG	C33-C34-C35-C36
24	q	609	CLA	C13-C15-C16-C17
28	V	615	LHG	C24-C25-C26-C27
35	AL	518	DGD	C1G-C2G-C3G-O3G
28	AN	616	LHG	C13-C14-C15-C16
34	M	101	SQD	C32-C33-C34-C35
23	0	601	CHL	C12-C13-C15-C16
23	AH	601	CHL	C11-C10-C8-C7
23	AU	601	CHL	C11-C10-C8-C7
24	AD	304	CLA	C2-C3-C5-C6
24	O	609	CLA	C11-C12-C13-C15
24	P	503	CLA	C12-C13-C15-C16
24	q	602	CLA	C11-C10-C8-C7
24	AR	602	CLA	C11-C10-C8-C7
28	AD	316	LHG	C27-C28-C29-C30
28	AM	406	LHG	C27-C28-C29-C30
24	v	303	CLA	C3-C5-C6-C7
23	9	609	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	9	609	CHL	C11-C12-C13-C14
23	AC	608	CHL	C11-C12-C13-C14
23	V	601	CHL	C11-C12-C13-C14
23	V	606	CHL	C14-C13-C15-C16
23	AN	601	CHL	C11-C12-C13-C14
23	AQ	607	CHL	C14-C13-C15-C16
24	9	602	CLA	C6-C7-C8-C9
24	AC	602	CLA	C6-C7-C8-C9
24	O	606	CLA	C14-C13-C15-C16
24	O	616	CLA	C6-C7-C8-C9
24	P	507	CLA	C14-C13-C15-C16
24	P	510	CLA	C11-C10-C8-C9
24	Q	404	CLA	C11-C12-C13-C14
24	AK	609	CLA	C6-C7-C8-C9
24	AK	611	CLA	C11-C12-C13-C14
24	AL	508	CLA	C14-C13-C15-C16
24	AM	404	CLA	C11-C12-C13-C14
24	AN	612	CLA	C6-C7-C8-C9
26	AA	616	NEX	C29-C30-C31-C32
23	V	607	CHL	C16-C17-C18-C19
24	AS	313	CLA	C6-C7-C8-C10
35	J	411	DGD	C4D-C5D-C6D-O5D
35	AJ	412	DGD	C4D-C5D-C6D-O5D
33	AL	501	LMG	C33-C34-C35-C36
35	j	102	DGD	C4B-C5B-C6B-C7B
24	AS	303	CLA	C10-C11-C12-C13
34	m	101	SQD	C32-C33-C34-C35
24	O	606	CLA	C3-C5-C6-C7
24	v	313	CLA	C6-C7-C8-C10
33	AK	601	LMG	C29-C30-C31-C32
34	M	101	SQD	C27-C28-C29-C30
24	AK	607	CLA	CBA-CGA-O2A-C1
24	AQ	602	CLA	C2C-C3C-CAC-CBC
35	AJ	412	DGD	C1A-C2A-C3A-C4A
24	AK	603	CLA	C15-C16-C17-C18
23	9	609	CHL	C12-C13-C15-C16
23	AC	608	CHL	C12-C13-C15-C16
24	9	602	CLA	C12-C13-C15-C16
24	q	611	CLA	O2A-C1-C2-C3
24	P	507	CLA	C5-C6-C7-C8
28	V	615	LHG	O1-C1-C2-O2
24	O	601	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	O	610	CLA	C16-C17-C18-C20
24	AK	603	CLA	C16-C17-C18-C20
23	q	605	CHL	CBA-CGA-O2A-C1
23	AS	307	CHL	CBA-CGA-O2A-C1
34	Q	402	SQD	C24-C23-O48-C46
28	V	615	LHG	C13-C14-C15-C16
33	O	620	LMG	C37-C38-C39-C40
24	AK	607	CLA	O1A-CGA-O2A-C1
28	V	615	LHG	C29-C30-C31-C32
33	AK	622	LMG	C37-C38-C39-C40
24	O	605	CLA	C13-C15-C16-C17
24	AH	603	CLA	C5-C6-C7-C8
24	AU	603	CLA	C5-C6-C7-C8
23	q	605	CHL	O1A-CGA-O2A-C1
24	0	602	CLA	C4B-C3B-CAB-CBB
24	0	603	CLA	C4B-C3B-CAB-CBB
24	AA	611	CLA	C4B-C3B-CAB-CBB
24	AA	612	CLA	C4B-C3B-CAB-CBB
24	J	403	CLA	C4B-C3B-CAB-CBB
24	P	510	CLA	C4B-C3B-CAB-CBB
24	v	303	CLA	C4B-C3B-CAB-CBB
24	v	310	CLA	C4B-C3B-CAB-CBB
24	AJ	404	CLA	C4B-C3B-CAB-CBB
24	AL	510	CLA	C4B-C3B-CAB-CBB
24	AL	511	CLA	C4B-C3B-CAB-CBB
24	AN	609	CLA	C4B-C3B-CAB-CBB
24	AS	303	CLA	C4B-C3B-CAB-CBB
24	AS	305	CLA	C4B-C3B-CAB-CBB
24	AU	603	CLA	C4B-C3B-CAB-CBB
24	AU	609	CLA	C4B-C3B-CAB-CBB
24	AU	610	CLA	C4B-C3B-CAB-CBB
24	AU	613	CLA	C4B-C3B-CAB-CBB
24	0	609	CLA	C2A-CAA-CBA-CGA
24	V	612	CLA	C2A-CAA-CBA-CGA
24	AQ	602	CLA	C2A-CAA-CBA-CGA
23	AC	601	CHL	CAA-CBA-CGA-O1A
24	9	611	CLA	CAA-CBA-CGA-O1A
24	AE	611	CLA	CAA-CBA-CGA-O1A
35	P	516	DGD	O6D-C1D-O3G-C3G
26	q	615	NEX	C29-C30-C31-C32
35	J	413	DGD	C4A-C5A-C6A-C7A
28	O	623	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
34	Q	402	SQD	O10-C23-O48-C46
24	O	601	CLA	C15-C16-C17-C18
24	V	609	CLA	C5-C6-C7-C8
24	AS	313	CLA	C5-C6-C7-C8
23	V	608	CHL	C4C-C3C-CAC-CBC
24	q	618	CLA	CAA-CBA-CGA-O2A
28	0	616	LHG	O6-C4-C5-O7
27	AR	616	XAT	C30-C31-C32-C33
28	AU	617	LHG	C25-C26-C27-C28
24	0	612	CLA	C4-C3-C5-C6
24	V	602	CLA	C4-C3-C5-C6
32	AJ	408	PHO	C4-C3-C5-C6
23	AD	308	CHL	C2C-C3C-CAC-CBC
24	0	612	CLA	C2-C3-C5-C6
24	AD	312	CLA	C2-C3-C5-C6
24	J	404	CLA	C2C-C3C-CAC-CBC
23	9	609	CHL	C2-C1-O2A-CGA
24	AD	304	CLA	C2-C1-O2A-CGA
24	P	504	CLA	C2-C1-O2A-CGA
24	P	511	CLA	C2-C1-O2A-CGA
24	v	312	CLA	C2-C1-O2A-CGA
24	AL	505	CLA	C2-C1-O2A-CGA
24	AQ	611	CLA	C2-C1-O2A-CGA
24	AS	312	CLA	C2-C1-O2A-CGA
28	O	623	LHG	C10-C11-C12-C13
28	AN	616	LHG	C29-C30-C31-C32
23	V	606	CHL	C15-C16-C17-C18
24	P	502	CLA	C16-C17-C18-C20
24	q	618	CLA	CAA-CBA-CGA-O1A
23	AH	605	CHL	C2A-CAA-CBA-CGA
23	AQ	608	CHL	C2A-CAA-CBA-CGA
24	AN	609	CLA	C2A-CAA-CBA-CGA
28	V	615	LHG	O7-C5-C6-O8
35	j	102	DGD	O2G-C1B-C2B-C3B
28	AH	616	LHG	C12-C13-C14-C15
28	V	615	LHG	C5-C4-O6-P
28	AH	616	LHG	C2-C3-O3-P
28	AU	617	LHG	C2-C3-O3-P
23	V	606	CHL	CAA-CBA-CGA-O1A
23	AN	606	CHL	CAA-CBA-CGA-O1A
28	AD	316	LHG	C12-C13-C14-C15
33	J	409	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
23	V	607	CHL	C3A-C2A-CAA-CBA
24	9	611	CLA	C3A-C2A-CAA-CBA
24	O	601	CLA	C3A-C2A-CAA-CBA
24	AK	603	CLA	C3A-C2A-CAA-CBA
23	v	307	CHL	CAA-CBA-CGA-O1A
24	AQ	603	CLA	C16-C17-C18-C20
26	9	617	NEX	C9-C10-C11-C12
26	AU	616	NEX	C29-C30-C31-C32
28	AK	624	LHG	C10-C11-C12-C13
33	AK	622	LMG	C40-C41-C42-C43
34	o	101	SQD	C13-C14-C15-C16
28	O	621	LHG	C11-C12-C13-C14
37	Q	405	PL9	C13-C14-C16-C17
24	O	601	CLA	C11-C12-C13-C14
24	O	601	CLA	C14-C13-C15-C16
24	O	607	CLA	C6-C7-C8-C9
24	O	616	CLA	C11-C10-C8-C9
24	P	505	CLA	C6-C7-C8-C9
24	V	602	CLA	C11-C10-C8-C9
24	q	612	CLA	C11-C10-C8-C9
24	AH	609	CLA	C11-C10-C8-C9
24	AK	603	CLA	C14-C13-C15-C16
24	AL	506	CLA	C6-C7-C8-C9
24	AL	511	CLA	C11-C10-C8-C9
24	AN	611	CLA	C6-C7-C8-C9
38	F	102	HEM	C3A-C2A-CAA-CBA
24	p	603	CLA	C16-C17-C18-C20
24	AK	616	CLA	C16-C17-C18-C20
28	O	623	LHG	C11-C12-C13-C14
24	AK	607	CLA	C13-C15-C16-C17
24	AU	612	CLA	C8-C10-C11-C12
33	O	620	LMG	C40-C41-C42-C43
35	AJ	401	DGD	C4A-C5A-C6A-C7A
23	AH	607	CHL	C8-C10-C11-C12
26	9	617	NEX	C39-C29-C30-C31
26	AA	616	NEX	C39-C29-C30-C31
26	AC	616	NEX	C39-C29-C30-C31
26	AE	615	NEX	C39-C29-C30-C31
26	p	616	NEX	C39-C29-C30-C31
26	q	615	NEX	C39-C29-C30-C31
26	AR	615	NEX	C39-C29-C30-C31
29	f	101	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
35	J	411	DGD	O1G-C1G-C2G-C3G
35	AJ	412	DGD	O1G-C1G-C2G-C3G
33	O	624	LMG	C4-C5-C6-O5
33	AK	601	LMG	C4-C5-C6-O5
24	AE	611	CLA	CAA-CBA-CGA-O2A
28	AK	624	LHG	C11-C12-C13-C14
33	AL	501	LMG	C38-C39-C40-C41
33	J	409	LMG	C38-C39-C40-C41
23	AD	308	CHL	C11-C12-C13-C14
23	AD	308	CHL	C11-C12-C13-C15
24	O	614	CLA	C16-C17-C18-C20
24	AL	503	CLA	C16-C17-C18-C19
35	j	102	DGD	O6E-C1E-O5D-C6D
28	AH	616	LHG	C25-C26-C27-C28
23	9	605	CHL	CAA-CBA-CGA-O2A
23	AC	605	CHL	CAA-CBA-CGA-O2A
26	AA	616	NEX	C31-C32-C33-C40
33	P	518	LMG	C16-C17-C18-C19
23	AU	608	CHL	C3-C5-C6-C7
35	J	411	DGD	C4A-C5A-C6A-C7A
33	O	620	LMG	C15-C16-C17-C18
24	9	611	CLA	CAA-CBA-CGA-O2A
24	AF	610	CLA	CAA-CBA-CGA-O1A
24	AR	617	CLA	CAA-CBA-CGA-O1A
24	AR	617	CLA	CAA-CBA-CGA-O2A
28	O	621	LHG	C4-C5-O7-C7
28	O	621	LHG	C6-C5-O7-C7
23	AD	301	CHL	C5-C6-C7-C8
23	AH	601	CHL	C1A-C2A-CAA-CBA
23	AU	601	CHL	C1A-C2A-CAA-CBA
24	9	602	CLA	C1A-C2A-CAA-CBA
24	AB	611	CLA	C1A-C2A-CAA-CBA
24	J	407	CLA	C1A-C2A-CAA-CBA
24	q	601	CLA	C1A-C2A-CAA-CBA
24	AH	613	CLA	C1A-C2A-CAA-CBA
24	AL	512	CLA	C1A-C2A-CAA-CBA
24	AN	612	CLA	C1A-C2A-CAA-CBA
34	Q	402	SQD	C12-C13-C14-C15
24	O	610	CLA	C16-C17-C18-C19
33	AK	622	LMG	O9-C10-O7-C8
23	0	601	CHL	C11-C10-C8-C7
23	AA	606	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	V	607	CHL	C11-C10-C8-C7
23	p	609	CHL	C11-C12-C13-C15
24	O	611	CLA	C12-C13-C15-C16
24	O	612	CLA	C6-C7-C8-C10
24	AK	613	CLA	C12-C13-C15-C16
24	AK	614	CLA	C6-C7-C8-C10
24	AL	504	CLA	C12-C13-C15-C16
24	AS	303	CLA	C11-C10-C8-C7
33	AL	520	LMG	C16-C17-C18-C19
35	AJ	412	DGD	C4A-C5A-C6A-C7A
23	AD	301	CHL	C8-C10-C11-C12
28	q	616	LHG	O10-C23-O8-C6
29	AK	602	BCR	C9-C10-C11-C12
23	0	601	CHL	C3C-C2C-CMC-OMC
23	AC	605	CHL	C3C-C2C-CMC-OMC
23	AD	307	CHL	C3C-C2C-CMC-OMC
23	V	606	CHL	C3C-C2C-CMC-OMC
23	AN	601	CHL	C3C-C2C-CMC-OMC
34	AM	401	SQD	C24-C23-O48-C46
23	AC	601	CHL	CAA-CBA-CGA-O2A
35	AL	518	DGD	C5B-C6B-C7B-C8B
33	O	624	LMG	O6-C5-C6-O5
28	AU	617	LHG	C12-C13-C14-C15
23	AU	605	CHL	C2A-CAA-CBA-CGA
24	9	612	CLA	C2A-CAA-CBA-CGA
24	V	609	CLA	C2A-CAA-CBA-CGA
24	q	612	CLA	C2A-CAA-CBA-CGA
24	AL	504	CLA	C2A-CAA-CBA-CGA
35	J	411	DGD	O6D-C5D-C6D-O5D
33	AK	601	LMG	O6-C5-C6-O5
23	AC	605	CHL	CAA-CBA-CGA-O1A
28	AQ	618	LHG	C32-C33-C34-C35
28	AK	624	LHG	O6-C4-C5-C6
35	AJ	412	DGD	O6D-C5D-C6D-O5D
24	J	403	CLA	C13-C15-C16-C17
24	AU	602	CLA	C15-C16-C17-C18
23	9	605	CHL	CAA-CBA-CGA-O1A
24	v	313	CLA	C4-C3-C5-C6
24	P	503	CLA	C13-C15-C16-C17
24	AJ	404	CLA	C13-C15-C16-C17
24	AL	504	CLA	C13-C15-C16-C17
24	AS	313	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
37	AM	405	PL9	C13-C14-C16-C17
23	AC	605	CHL	C2B-C3B-CAB-CBB
23	AR	605	CHL	C2B-C3B-CAB-CBB
23	AU	608	CHL	C2B-C3B-CAB-CBB
24	AA	610	CLA	C2B-C3B-CAB-CBB
24	AA	611	CLA	C2B-C3B-CAB-CBB
24	AE	609	CLA	C2B-C3B-CAB-CBB
24	O	612	CLA	C2B-C3B-CAB-CBB
24	P	510	CLA	C2B-C3B-CAB-CBB
24	V	609	CLA	C2B-C3B-CAB-CBB
24	p	603	CLA	C2B-C3B-CAB-CBB
24	p	611	CLA	C2B-C3B-CAB-CBB
24	AL	511	CLA	C2B-C3B-CAB-CBB
24	AL	512	CLA	C2B-C3B-CAB-CBB
24	AN	603	CLA	C2B-C3B-CAB-CBB
24	AQ	611	CLA	C2B-C3B-CAB-CBB
24	AS	303	CLA	C2B-C3B-CAB-CBB
24	AS	305	CLA	C2B-C3B-CAB-CBB
24	AU	603	CLA	C2B-C3B-CAB-CBB
24	AU	610	CLA	C2B-C3B-CAB-CBB
33	O	624	LMG	C29-C30-C31-C32
23	v	307	CHL	CAA-CBA-CGA-O2A
24	AH	602	CLA	C15-C16-C17-C18
34	AM	401	SQD	O10-C23-O48-C46
28	p	617	LHG	C29-C30-C31-C32
23	AH	608	CHL	C3-C5-C6-C7
24	AL	512	CLA	CBD-CGD-O2D-CED
33	O	620	LMG	O9-C10-O7-C8
26	AA	616	NEX	C28-C29-C30-C31
26	AC	616	NEX	C28-C29-C30-C31
26	AE	615	NEX	C28-C29-C30-C31
26	p	616	NEX	C28-C29-C30-C31
26	q	615	NEX	C28-C29-C30-C31
26	AR	615	NEX	C28-C29-C30-C31
24	AN	602	CLA	C10-C11-C12-C13
29	O	625	BCR	C9-C10-C11-C12
23	AB	605	CHL	CAA-CBA-CGA-O1A
23	AU	607	CHL	C8-C10-C11-C12
24	q	602	CLA	C8-C10-C11-C12
24	AL	512	CLA	C10-C11-C12-C13
24	V	609	CLA	O1A-CGA-O2A-C1
24	AQ	602	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
23	AD	301	CHL	C2-C1-O2A-CGA
23	p	609	CHL	C2-C1-O2A-CGA
23	AN	607	CHL	C2-C1-O2A-CGA
23	AQ	609	CHL	C2-C1-O2A-CGA
24	AK	617	CLA	C2-C1-O2A-CGA
24	AL	513	CLA	C2-C1-O2A-CGA
24	O	601	CLA	O1D-CGD-O2D-CED
23	p	605	CHL	C2-C1-O2A-CGA
33	AL	520	LMG	C36-C37-C38-C39
23	p	607	CHL	CAA-CBA-CGA-O2A
23	AQ	608	CHL	C11-C12-C13-C14
24	V	610	CLA	C6-C7-C8-C9
32	J	406	PHO	C11-C10-C8-C9
32	AJ	408	PHO	C11-C10-C8-C9
28	0	616	LHG	C11-C12-C13-C14
28	w	201	LHG	C15-C16-C17-C18
23	AB	605	CHL	CAA-CBA-CGA-O2A
24	AF	614	CLA	CAA-CBA-CGA-O2A
38	f	102	HEM	CAD-CBD-CGD-O2D
23	AQ	607	CHL	CAA-CBA-CGA-O2A
23	AQ	605	CHL	C2-C1-O2A-CGA
34	J	410	SQD	C15-C16-C17-C18
23	AB	606	CHL	CAA-CBA-CGA-O1A
24	O	604	CLA	C4C-C3C-CAC-CBC
23	AE	605	CHL	O1A-CGA-O2A-C1
23	AS	307	CHL	O1A-CGA-O2A-C1
33	AL	501	LMG	O10-C28-O8-C9
25	9	615	LUT	C1-C6-C7-C8
25	q	614	LUT	C1-C6-C7-C8
25	AN	614	LUT	C1-C6-C7-C8
25	AR	614	LUT	C1-C6-C7-C8
25	AS	316	LUT	C5-C6-C7-C8
29	AF	612	BCR	C23-C24-C25-C30
29	P	513	BCR	C23-C24-C25-C30
29	F	101	BCR	C23-C24-C25-C30
29	j	101	BCR	C1-C6-C7-C8
29	AL	515	BCR	C23-C24-C25-C30
29	f	101	BCR	C23-C24-C25-C30
29	AO	101	BCR	C1-C6-C7-C8
33	AK	622	LMG	C15-C16-C17-C18
23	AA	608	CHL	O1D-CGD-O2D-CED
23	AA	606	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	p	617	LHG	C32-C33-C34-C35
34	AM	401	SQD	C12-C13-C14-C15
33	P	518	LMG	C37-C38-C39-C40
34	AJ	411	SQD	C15-C16-C17-C18
24	AU	612	CLA	O1A-CGA-O2A-C1
28	p	617	LHG	O10-C23-O8-C6
29	O	625	BCR	C15-C16-C17-C18
24	AD	309	CLA	C4-C3-C5-C6
24	O	608	CLA	C4-C3-C5-C6
24	AN	602	CLA	C4-C3-C5-C6
32	J	406	PHO	C4-C3-C5-C6
37	AM	405	PL9	C35-C34-C36-C37
24	AE	602	CLA	C1A-C2A-CAA-CBA
25	AS	315	LUT	C7-C8-C9-C10
29	AL	516	BCR	C7-C8-C9-C10
23	AN	607	CHL	C3-C5-C6-C7
33	Q	407	LMG	C8-C7-O1-C1
33	AM	407	LMG	C8-C7-O1-C1
24	AN	613	CLA	O2A-C1-C2-C3
28	AQ	618	LHG	C29-C30-C31-C32
23	AA	617	CHL	CAA-CBA-CGA-O2A
24	0	611	CLA	CAA-CBA-CGA-O2A
24	AE	603	CLA	C6-C7-C8-C9
24	O	601	CLA	C16-C17-C18-C19
28	W	201	LHG	C28-C29-C30-C31
24	AR	602	CLA	C8-C10-C11-C12
28	O	623	LHG	O6-C4-C5-O7
24	9	602	CLA	C14-C13-C15-C16
24	AK	606	CLA	C4C-C3C-CAC-CBC
23	AA	605	CHL	CAA-CBA-CGA-O2A
23	AE	617	CHL	CAA-CBA-CGA-O2A
24	P	503	CLA	C2A-CAA-CBA-CGA
24	AK	604	CLA	C2A-CAA-CBA-CGA
23	AE	605	CHL	CAA-CBA-CGA-O2A
35	AO	102	DGD	O2G-C1B-C2B-C3B
24	AU	612	CLA	CBA-CGA-O2A-C1
24	AS	303	CLA	C3-C5-C6-C7
23	v	302	CHL	CAA-CBA-CGA-O2A
24	AB	611	CLA	CAA-CBA-CGA-O1A
24	AD	310	CLA	C4B-C3B-CAB-CBB
24	AE	602	CLA	C4B-C3B-CAB-CBB
24	O	612	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	V	603	CLA	C4B-C3B-CAB-CBB
24	V	609	CLA	C4B-C3B-CAB-CBB
24	AS	312	CLA	C4B-C3B-CAB-CBB
23	0	601	CHL	C8-C10-C11-C12
24	AH	612	CLA	C8-C10-C11-C12
28	0	616	LHG	O8-C23-C24-C25
23	9	607	CHL	O1A-CGA-O2A-C1
37	Q	405	PL9	C35-C34-C36-C37
23	AA	608	CHL	C11-C10-C8-C7
23	AE	607	CHL	C11-C10-C8-C7
23	p	601	CHL	C11-C12-C13-C15
24	AK	611	CLA	C11-C12-C13-C15
32	J	406	PHO	C6-C7-C8-C10
23	AE	616	CHL	CAA-CBA-CGA-O2A
23	AE	605	CHL	CBA-CGA-O2A-C1
28	w	201	LHG	C28-C29-C30-C31
24	AR	604	CLA	O2A-C1-C2-C3
35	J	411	DGD	C2D-C1D-O3G-C3G
35	AJ	412	DGD	C2D-C1D-O3G-C3G
24	AK	603	CLA	C16-C17-C18-C19
35	J	413	DGD	O6D-C5D-C6D-O5D
28	AD	316	LHG	C2-C3-O3-P
24	V	609	CLA	CBA-CGA-O2A-C1
28	v	301	LHG	C24-C23-O8-C6
34	AP	101	SQD	C13-C14-C15-C16
24	O	604	CLA	C3-C5-C6-C7
24	AB	603	CLA	CAA-CBA-CGA-O2A
24	AC	610	CLA	CAA-CBA-CGA-O1A
23	AH	606	CHL	O2A-C1-C2-C3
23	AU	606	CHL	O2A-C1-C2-C3
24	O	602	CLA	CAA-CBA-CGA-O2A
23	AN	608	CHL	C10-C11-C12-C13
23	AE	617	CHL	CAA-CBA-CGA-O1A
24	AF	603	CLA	CAA-CBA-CGA-O2A
23	AD	302	CHL	CBA-CGA-O2A-C1
28	AD	316	LHG	C24-C23-O8-C6
33	AK	601	LMG	C29-C28-O8-C9
26	v	317	NEX	C39-C29-C30-C31
26	AQ	617	NEX	C39-C29-C30-C31
26	AU	616	NEX	C39-C29-C30-C31
24	P	501	CLA	CAA-CBA-CGA-O2A
24	AL	502	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	AQ	612	CLA	CAA-CBA-CGA-O2A
23	q	605	CHL	C4-C3-C5-C6
24	AN	611	CLA	C4-C3-C5-C6
24	AN	603	CLA	C10-C11-C12-C13
23	AF	608	CHL	C2C-C3C-CAC-CBC
24	AA	612	CLA	CAA-CBA-CGA-O1A
33	J	409	LMG	O10-C28-O8-C9
24	p	610	CLA	C2-C3-C5-C6
24	v	313	CLA	C2-C3-C5-C6
24	AK	610	CLA	C2-C3-C5-C6
24	V	603	CLA	C10-C11-C12-C13
24	AK	611	CLA	CBA-CGA-O2A-C1
23	V	607	CHL	CAA-CBA-CGA-O2A
24	P	507	CLA	C6-C7-C8-C9
24	Q	403	CLA	C11-C10-C8-C9
24	AH	603	CLA	C14-C13-C15-C16
24	AK	603	CLA	C11-C12-C13-C14
24	AK	608	CLA	C14-C13-C15-C16
24	AL	508	CLA	C6-C7-C8-C9
24	AM	403	CLA	C11-C10-C8-C9
24	AN	603	CLA	C6-C7-C8-C9
24	AU	603	CLA	C14-C13-C15-C16
24	AK	606	CLA	C3-C5-C6-C7
24	AF	610	CLA	CAA-CBA-CGA-O2A
24	q	608	CLA	CAA-CBA-CGA-O2A
28	AL	519	LHG	C24-C25-C26-C27
33	AL	520	LMG	C37-C38-C39-C40
24	v	314	CLA	C3A-C2A-CAA-CBA
24	AR	601	CLA	C3A-C2A-CAA-CBA
24	AS	314	CLA	C3A-C2A-CAA-CBA
32	J	406	PHO	C3A-C2A-CAA-CBA
24	AQ	602	CLA	C10-C11-C12-C13
35	j	102	DGD	O1A-C1A-O1G-C1G
35	AJ	401	DGD	O6D-C5D-C6D-O5D
24	9	610	CLA	CAA-CBA-CGA-O2A
24	AK	618	CLA	CAA-CBA-CGA-O2A
24	AL	513	CLA	CAA-CBA-CGA-O2A
34	M	101	SQD	O47-C7-C8-C9
34	m	101	SQD	O47-C7-C8-C9
38	f	102	HEM	CAD-CBD-CGD-O1D
23	AA	606	CHL	CAD-CBD-CGD-O2D
23	AB	607	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	AC	606	CHL	CAD-CBD-CGD-O2D
23	AD	301	CHL	CAD-CBD-CGD-O2D
23	AE	605	CHL	CAD-CBD-CGD-O2D
23	AF	607	CHL	CAD-CBD-CGD-O2D
23	V	607	CHL	CAD-CBD-CGD-O2D
23	v	308	CHL	CAD-CBD-CGD-O2D
23	AN	607	CHL	CAD-CBD-CGD-O2D
23	AQ	606	CHL	CAD-CBD-CGD-O2D
23	AQ	609	CHL	CAD-CBD-CGD-O2D
23	AR	606	CHL	CAD-CBD-CGD-O2D
24	9	602	CLA	CAD-CBD-CGD-O2D
24	0	602	CLA	CAD-CBD-CGD-O2D
24	0	611	CLA	CAD-CBD-CGD-O2D
24	AA	602	CLA	CAD-CBD-CGD-O2D
24	AA	611	CLA	CAD-CBD-CGD-O2D
24	AA	612	CLA	CAD-CBD-CGD-O2D
24	AD	303	CLA	CAD-CBD-CGD-O2D
24	AD	311	CLA	CAD-CBD-CGD-O2D
24	AD	312	CLA	CAD-CBD-CGD-O2D
24	AD	313	CLA	CAD-CBD-CGD-O2D
24	AE	610	CLA	CAD-CBD-CGD-O2D
24	AE	611	CLA	CAD-CBD-CGD-O2D
24	AF	614	CLA	CAD-CBD-CGD-O2D
24	J	404	CLA	CAD-CBD-CGD-O2D
24	O	602	CLA	CAD-CBD-CGD-O2D
24	O	604	CLA	CAD-CBD-CGD-O2D
24	O	612	CLA	CAD-CBD-CGD-O2D
24	P	503	CLA	CAD-CBD-CGD-O2D
24	P	511	CLA	CAD-CBD-CGD-O2D
24	Q	404	CLA	CAD-CBD-CGD-O2D
24	V	603	CLA	CAD-CBD-CGD-O2D
24	K	101	CLA	CAD-CBD-CGD-O2D
24	p	604	CLA	CAD-CBD-CGD-O2D
24	q	604	CLA	CAD-CBD-CGD-O2D
24	AH	602	CLA	CAD-CBD-CGD-O2D
24	AH	611	CLA	CAD-CBD-CGD-O2D
24	AH	612	CLA	CAD-CBD-CGD-O2D
24	AJ	405	CLA	CAD-CBD-CGD-O2D
24	AK	604	CLA	CAD-CBD-CGD-O2D
24	AK	606	CLA	CAD-CBD-CGD-O2D
24	AK	607	CLA	CAD-CBD-CGD-O2D
24	AK	614	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	AL	503	CLA	CAD-CBD-CGD-O2D
24	AL	505	CLA	CAD-CBD-CGD-O2D
24	AL	512	CLA	CAD-CBD-CGD-O2D
24	AL	513	CLA	CAD-CBD-CGD-O2D
24	AM	404	CLA	CAD-CBD-CGD-O2D
24	AN	613	CLA	CAD-CBD-CGD-O2D
24	AQ	604	CLA	CAD-CBD-CGD-O2D
24	AU	602	CLA	CAD-CBD-CGD-O2D
24	AU	611	CLA	CAD-CBD-CGD-O2D
24	AU	612	CLA	CAD-CBD-CGD-O2D
24	P	502	CLA	C16-C17-C18-C19
24	AQ	603	CLA	C16-C17-C18-C19
33	AM	407	LMG	C11-C12-C13-C14
29	AF	612	BCR	C13-C14-C15-C16
24	AJ	404	CLA	C15-C16-C17-C18
23	AC	608	CHL	C2-C1-O2A-CGA
23	AE	607	CHL	C2-C1-O2A-CGA
24	AD	309	CLA	C2-C1-O2A-CGA
23	AS	302	CHL	CAA-CBA-CGA-O2A
24	9	613	CLA	CAA-CBA-CGA-O2A
24	O	616	CLA	CAA-CBA-CGA-O2A
24	P	511	CLA	CAA-CBA-CGA-O2A
28	0	616	LHG	C27-C28-C29-C30
25	AC	614	LUT	C6-C7-C8-C9
28	AS	301	LHG	C24-C23-O8-C6
24	V	610	CLA	C4-C3-C5-C6
23	v	302	CHL	CAA-CBA-CGA-O1A
23	AS	302	CHL	CAA-CBA-CGA-O1A
24	0	611	CLA	CAA-CBA-CGA-O1A
24	O	611	CLA	CAA-CBA-CGA-O2A
24	P	504	CLA	CAA-CBA-CGA-O2A
24	V	612	CLA	CAA-CBA-CGA-O2A
24	p	610	CLA	CAA-CBA-CGA-O2A
28	W	201	LHG	C15-C16-C17-C18
25	AH	614	LUT	C7-C8-C9-C10
26	AA	616	NEX	C31-C32-C33-C34
26	AC	616	NEX	C31-C32-C33-C34
29	P	514	BCR	C7-C8-C9-C10
33	P	518	LMG	C7-C8-C9-O8
33	AL	520	LMG	C7-C8-C9-O8
35	AO	102	DGD	C1G-C2G-C3G-O3G
24	AD	311	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	AN	607	CHL	C4C-C3C-CAC-CBC
24	AJ	405	CLA	C2C-C3C-CAC-CBC
28	AD	316	LHG	O6-C4-C5-O7
28	AS	301	LHG	O8-C23-C24-C25
28	AH	616	LHG	C30-C31-C32-C33
23	AA	605	CHL	CAA-CBA-CGA-O1A
24	AB	603	CLA	CAA-CBA-CGA-O1A
24	AC	611	CLA	CAA-CBA-CGA-O2A
24	AF	614	CLA	CAA-CBA-CGA-O1A
23	q	607	CHL	O2A-C1-C2-C3
23	AR	607	CHL	O2A-C1-C2-C3
24	9	613	CLA	O2A-C1-C2-C3
24	J	403	CLA	O2A-C1-C2-C3
24	p	610	CLA	O2A-C1-C2-C3
24	AJ	404	CLA	O2A-C1-C2-C3
24	AQ	610	CLA	O2A-C1-C2-C3
33	Q	407	LMG	C11-C12-C13-C14
24	O	609	CLA	CBA-CGA-O2A-C1
24	AD	309	CLA	C2A-CAA-CBA-CGA
24	AE	603	CLA	C2A-CAA-CBA-CGA
24	J	403	CLA	C15-C16-C17-C18
24	O	613	CLA	CAA-CBA-CGA-O2A
24	AK	615	CLA	CAA-CBA-CGA-O2A
23	AA	617	CHL	CAA-CBA-CGA-O1A
24	9	612	CLA	CAA-CBA-CGA-O1A
24	AF	603	CLA	CAA-CBA-CGA-O1A
24	q	608	CLA	CAA-CBA-CGA-O1A
24	O	607	CLA	C16-C17-C18-C20
28	Q	406	LHG	O2-C2-C3-O3
23	AA	601	CHL	CHA-CBD-CGD-O1D
23	AE	607	CHL	CHA-CBD-CGD-O2D
24	0	602	CLA	CHA-CBD-CGD-O1D
24	AA	604	CLA	CHA-CBD-CGD-O2D
24	AB	611	CLA	CHA-CBD-CGD-O1D
24	AB	611	CLA	CHA-CBD-CGD-O2D
24	AD	305	CLA	CHA-CBD-CGD-O1D
24	AD	305	CLA	CHA-CBD-CGD-O2D
24	AD	313	CLA	CHA-CBD-CGD-O2D
24	AE	604	CLA	CHA-CBD-CGD-O2D
24	O	601	CLA	CHA-CBD-CGD-O1D
24	O	601	CLA	CHA-CBD-CGD-O2D
24	O	604	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	O	605	CLA	CHA-CBD-CGD-O2D
24	P	502	CLA	CHA-CBD-CGD-O1D
24	P	508	CLA	CHA-CBD-CGD-O1D
24	P	508	CLA	CHA-CBD-CGD-O2D
24	V	612	CLA	CHA-CBD-CGD-O2D
24	p	604	CLA	CHA-CBD-CGD-O2D
24	q	603	CLA	CHA-CBD-CGD-O2D
24	q	604	CLA	CHA-CBD-CGD-O2D
24	AH	604	CLA	CHA-CBD-CGD-O1D
24	AH	604	CLA	CHA-CBD-CGD-O2D
24	AJ	405	CLA	CHA-CBD-CGD-O2D
24	AK	603	CLA	CHA-CBD-CGD-O1D
24	AK	603	CLA	CHA-CBD-CGD-O2D
24	AK	606	CLA	CHA-CBD-CGD-O2D
24	AK	607	CLA	CHA-CBD-CGD-O1D
24	AK	614	CLA	CHA-CBD-CGD-O1D
24	AL	504	CLA	CHA-CBD-CGD-O2D
24	AL	505	CLA	CHA-CBD-CGD-O1D
24	AL	505	CLA	CHA-CBD-CGD-O2D
24	AL	509	CLA	CHA-CBD-CGD-O1D
24	AL	509	CLA	CHA-CBD-CGD-O2D
24	AL	513	CLA	CHA-CBD-CGD-O2D
24	AN	613	CLA	CHA-CBD-CGD-O2D
24	AQ	603	CLA	CHA-CBD-CGD-O2D
24	AQ	604	CLA	CHA-CBD-CGD-O1D
24	AQ	604	CLA	CHA-CBD-CGD-O2D
24	AR	601	CLA	CHA-CBD-CGD-O1D
24	AR	601	CLA	CHA-CBD-CGD-O2D
24	AR	603	CLA	CHA-CBD-CGD-O1D
24	AR	612	CLA	CHA-CBD-CGD-O1D
24	AR	612	CLA	CHA-CBD-CGD-O2D
24	AU	602	CLA	CHA-CBD-CGD-O2D
24	AU	603	CLA	CHA-CBD-CGD-O2D
24	AU	604	CLA	CHA-CBD-CGD-O1D
24	AU	604	CLA	CHA-CBD-CGD-O2D
24	9	612	CLA	CAA-CBA-CGA-O2A
23	AA	608	CHL	CAA-CBA-CGA-O2A
24	AL	503	CLA	CAA-CBA-CGA-O2A
24	AL	505	CLA	CAA-CBA-CGA-O2A
24	AN	613	CLA	CAA-CBA-CGA-O2A
23	p	609	CHL	C3-C5-C6-C7
23	AQ	609	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	9	617	NEX	C28-C29-C30-C31
26	v	317	NEX	C28-C29-C30-C31
26	AQ	617	NEX	C28-C29-C30-C31
26	AU	616	NEX	C28-C29-C30-C31
23	AE	616	CHL	CAA-CBA-CGA-O1A
28	O	621	LHG	C13-C14-C15-C16
24	p	603	CLA	C16-C17-C18-C19
24	AL	508	CLA	C8-C10-C11-C12
24	AK	613	CLA	CAA-CBA-CGA-O2A
24	AU	610	CLA	CAA-CBA-CGA-O2A
28	v	301	LHG	O8-C23-C24-C25
34	o	101	SQD	O48-C23-C24-C25
35	J	411	DGD	O2G-C1B-C2B-C3B
35	AJ	412	DGD	O2G-C1B-C2B-C3B
28	AD	316	LHG	C26-C27-C28-C29
28	AN	616	LHG	O7-C5-C6-O8
33	P	518	LMG	O7-C8-C9-O8
33	AL	520	LMG	O7-C8-C9-O8
35	J	411	DGD	O1G-C1G-C2G-O2G
35	AJ	412	DGD	O1G-C1G-C2G-O2G
23	9	607	CHL	CBA-CGA-O2A-C1
24	AM	404	CLA	C8-C10-C11-C12
23	AB	607	CHL	CAA-CBA-CGA-O1A
23	AE	606	CHL	CAA-CBA-CGA-O2A
23	AD	308	CHL	C4C-C3C-CAC-CBC
24	J	404	CLA	C4C-C3C-CAC-CBC
35	P	516	DGD	O2G-C1B-C2B-C3B
35	AL	517	DGD	O2G-C1B-C2B-C3B
23	AR	607	CHL	C2A-CAA-CBA-CGA
23	AA	607	CHL	CAA-CBA-CGA-O2A
23	AD	307	CHL	CAA-CBA-CGA-O2A
23	AQ	609	CHL	C10-C11-C12-C13
24	AC	609	CLA	CAA-CBA-CGA-O2A
24	AH	610	CLA	CAA-CBA-CGA-O2A
34	AP	101	SQD	O48-C23-C24-C25
35	AL	518	DGD	O2G-C1B-C2B-C3B
38	F	102	HEM	CAA-CBA-CGA-O2A
23	AU	605	CHL	O1A-CGA-O2A-C1
24	AK	611	CLA	O1A-CGA-O2A-C1
23	9	607	CHL	C6-C7-C8-C10
23	AD	302	CHL	C12-C13-C15-C16
23	AN	607	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	AQ	609	CHL	C11-C12-C13-C15
24	AK	606	CLA	C6-C7-C8-C10
24	AL	505	CLA	C11-C10-C8-C7
32	AJ	408	PHO	C6-C7-C8-C10
28	AH	616	LHG	C5-C4-O6-P
23	V	605	CHL	CAA-CBA-CGA-O2A
23	AS	307	CHL	CAA-CBA-CGA-O2A
24	0	613	CLA	CAA-CBA-CGA-O2A
24	P	502	CLA	CAA-CBA-CGA-O2A
24	V	609	CLA	CAA-CBA-CGA-O2A
24	AR	612	CLA	CAA-CBA-CGA-O2A
24	AU	611	CLA	CAA-CBA-CGA-O2A
24	AB	611	CLA	CAA-CBA-CGA-O2A
28	p	617	LHG	C12-C13-C14-C15
23	AQ	609	CHL	C11-C12-C13-C14
24	P	504	CLA	C11-C10-C8-C9
24	AL	514	CLA	C6-C7-C8-C9
24	AS	303	CLA	C6-C7-C8-C9
28	p	617	LHG	O10-C23-C24-C25
23	9	605	CHL	C2B-C3B-CAB-CBB
23	p	605	CHL	C2B-C3B-CAB-CBB
24	9	613	CLA	C2B-C3B-CAB-CBB
28	AM	406	LHG	O2-C2-C3-O3
24	AD	313	CLA	CAA-CBA-CGA-O2A
24	p	612	CLA	CAA-CBA-CGA-O2A
24	AH	611	CLA	CAA-CBA-CGA-O2A
24	AK	616	CLA	CAA-CBA-CGA-O2A
34	J	410	SQD	C4-C5-C6-S
34	AJ	411	SQD	C4-C5-C6-S
24	P	505	CLA	C16-C17-C18-C19
23	AH	605	CHL	O1A-CGA-O2A-C1
23	0	605	CHL	CAA-CBA-CGA-O2A
23	AB	606	CHL	CAA-CBA-CGA-O2A
24	AD	311	CLA	CAA-CBA-CGA-O1A
24	AN	613	CLA	C2A-CAA-CBA-CGA
24	AS	312	CLA	C2A-CAA-CBA-CGA
24	O	614	CLA	CAA-CBA-CGA-O2A
23	AF	607	CHL	CAA-CBA-CGA-O1A
24	AA	612	CLA	CAA-CBA-CGA-O2A
24	AC	610	CLA	CAA-CBA-CGA-O2A
24	AC	611	CLA	CAA-CBA-CGA-O1A
24	9	613	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	AK	618	CLA	C16-C17-C18-C20
24	AL	506	CLA	C16-C17-C18-C19
28	P	517	LHG	C30-C31-C32-C33
24	AJ	404	CLA	C4-C3-C5-C6
24	AL	502	CLA	C4-C3-C5-C6
28	AL	519	LHG	C30-C31-C32-C33
35	j	102	DGD	C4A-C5A-C6A-C7A
24	P	501	CLA	CAA-CBA-CGA-O1A
24	p	610	CLA	CAA-CBA-CGA-O1A
25	AU	614	LUT	C7-C8-C9-C10
23	AH	605	CHL	CBA-CGA-O2A-C1
23	p	609	CHL	C10-C11-C12-C13
23	AQ	605	CHL	O1A-CGA-O2A-C1
23	9	606	CHL	C1A-C2A-CAA-CBA
23	AA	606	CHL	C1A-C2A-CAA-CBA
23	AE	605	CHL	C1A-C2A-CAA-CBA
24	AK	604	CLA	C1A-C2A-CAA-CBA
28	V	615	LHG	C11-C12-C13-C14
32	J	406	PHO	C16-C17-C18-C20
24	AD	313	CLA	CAA-CBA-CGA-O1A
24	AK	618	CLA	CAA-CBA-CGA-O1A
24	AL	513	CLA	CAA-CBA-CGA-O1A
24	O	609	CLA	O1A-CGA-O2A-C1
24	V	603	CLA	C2-C1-O2A-CGA
24	AJ	404	CLA	C2-C1-O2A-CGA
24	AN	603	CLA	C2-C1-O2A-CGA
23	AU	605	CHL	CBA-CGA-O2A-C1
33	O	624	LMG	C29-C28-O8-C9
23	AA	608	CHL	CAA-CBA-CGA-O1A
24	O	613	CLA	CAA-CBA-CGA-O1A
24	O	616	CLA	CAA-CBA-CGA-O1A
24	P	504	CLA	CAA-CBA-CGA-O1A
24	P	511	CLA	CAA-CBA-CGA-O1A
24	AL	502	CLA	CAA-CBA-CGA-O1A
23	AN	601	CHL	CAA-CBA-CGA-O2A
23	AC	608	CHL	C2A-CAA-CBA-CGA
24	0	612	CLA	C2A-CAA-CBA-CGA
24	AA	602	CLA	C2A-CAA-CBA-CGA
24	AA	611	CLA	C2A-CAA-CBA-CGA
24	v	312	CLA	C2A-CAA-CBA-CGA
24	AR	609	CLA	C2A-CAA-CBA-CGA
24	V	612	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	AQ	612	CLA	CAA-CBA-CGA-O1A
23	V	601	CHL	CAA-CBA-CGA-O2A
24	AH	612	CLA	CAA-CBA-CGA-O2A
28	p	617	LHG	O8-C23-C24-C25
28	AU	617	LHG	C5-C4-O6-P
23	AH	605	CHL	C2-C1-O2A-CGA
23	V	607	CHL	CAA-CBA-CGA-O1A
24	AC	609	CLA	CAA-CBA-CGA-O1A
28	v	301	LHG	O10-C23-C24-C25
24	V	612	CLA	O2A-C1-C2-C3
23	AU	605	CHL	C2-C1-O2A-CGA
23	9	605	CHL	C4B-C3B-CAB-CBB
23	0	607	CHL	C4B-C3B-CAB-CBB
23	AC	605	CHL	C4B-C3B-CAB-CBB
23	AD	306	CHL	C4B-C3B-CAB-CBB
23	AF	601	CHL	C4B-C3B-CAB-CBB
23	p	605	CHL	C4B-C3B-CAB-CBB
24	AF	603	CLA	C4B-C3B-CAB-CBB
24	O	601	CLA	C4B-C3B-CAB-CBB
24	O	603	CLA	C4B-C3B-CAB-CBB
24	q	611	CLA	C4B-C3B-CAB-CBB
24	AH	610	CLA	C4B-C3B-CAB-CBB
24	AR	611	CLA	C4B-C3B-CAB-CBB
24	AS	310	CLA	C4B-C3B-CAB-CBB
28	O	623	LHG	C4-O6-P-O5
28	P	517	LHG	C4-O6-P-O5
28	AL	519	LHG	C4-O6-P-O5
23	AH	608	CHL	C16-C17-C18-C19
24	AN	611	CLA	C11-C12-C13-C14
24	AH	611	CLA	CAA-CBA-CGA-O1A
24	AN	613	CLA	CAA-CBA-CGA-O1A
24	AR	612	CLA	CAA-CBA-CGA-O1A
23	AH	601	CHL	CAA-CBA-CGA-O2A
28	w	201	LHG	O10-C23-O8-C6
29	F	101	BCR	C35-C13-C14-C15
35	AO	102	DGD	C8A-C9A-CAA-CBA
25	p	614	LUT	C1-C6-C7-C8
25	AQ	615	LUT	C1-C6-C7-C8
29	F	101	BCR	C23-C24-C25-C26
29	f	101	BCR	C23-C24-C25-C26
24	P	507	CLA	C8-C10-C11-C12
26	q	615	NEX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
26	AR	615	NEX	C26-C27-C28-C29
27	AF	613	XAT	C6-C7-C8-C9
27	q	617	XAT	C6-C7-C8-C9
27	AR	616	XAT	C6-C7-C8-C9
24	9	610	CLA	CAA-CBA-CGA-O1A
24	AH	610	CLA	CAA-CBA-CGA-O1A
24	AK	615	CLA	CAA-CBA-CGA-O1A
24	AL	503	CLA	CAA-CBA-CGA-O1A
28	W	201	LHG	O9-C7-C8-C9
33	Q	407	LMG	C20-C21-C22-C23
23	AD	302	CHL	O1A-CGA-O2A-C1
23	0	606	CHL	CAA-CBA-CGA-O2A
24	AC	604	CLA	CAA-CBA-CGA-O2A
24	p	602	CLA	C10-C11-C12-C13
24	AA	610	CLA	CAA-CBA-CGA-O2A
24	AK	609	CLA	C16-C17-C18-C20
24	AK	616	CLA	C16-C17-C18-C19
27	q	617	XAT	C30-C31-C32-C33
29	AI	101	BCR	C18-C19-C20-C21
24	0	613	CLA	CAA-CBA-CGA-O1A
24	AK	613	CLA	CAA-CBA-CGA-O1A
24	AL	505	CLA	CAA-CBA-CGA-O1A
24	AU	611	CLA	CAA-CBA-CGA-O1A
28	AS	301	LHG	O10-C23-C24-C25
23	V	608	CHL	C10-C11-C12-C13
23	AQ	601	CHL	CAA-CBA-CGA-O2A
28	q	616	LHG	O7-C7-C8-C9
33	AK	601	LMG	C34-C35-C36-C37
33	AM	407	LMG	C20-C21-C22-C23
35	j	102	DGD	C8A-C9A-CAA-CBA
24	O	614	CLA	C16-C17-C18-C19
32	AJ	408	PHO	C16-C17-C18-C20
34	M	101	SQD	C31-C32-C33-C34
23	0	607	CHL	CAD-CBD-CGD-O1D
23	q	607	CHL	CAD-CBD-CGD-O1D
24	AA	604	CLA	CAD-CBD-CGD-O1D
24	O	605	CLA	CAD-CBD-CGD-O1D
24	AR	601	CLA	CAD-CBD-CGD-O1D
24	AS	305	CLA	CAD-CBD-CGD-O1D
34	J	410	SQD	O5-C5-C6-S
34	AJ	411	SQD	O5-C5-C6-S
24	9	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	V	605	CHL	CAA-CBA-CGA-O1A
24	O	611	CLA	CAA-CBA-CGA-O1A
24	p	612	CLA	CAA-CBA-CGA-O1A
24	AU	610	CLA	CAA-CBA-CGA-O1A
34	o	101	SQD	O10-C23-C24-C25
24	AK	612	CLA	CAA-CBA-CGA-O2A
24	AN	609	CLA	CAA-CBA-CGA-O2A
28	AD	316	LHG	O8-C23-C24-C25
23	AQ	608	CHL	C8-C10-C11-C12
23	AE	607	CHL	C11-C10-C8-C9
23	p	601	CHL	C11-C12-C13-C14
23	p	609	CHL	C11-C12-C13-C14
23	AR	605	CHL	C6-C7-C8-C9
24	P	512	CLA	C6-C7-C8-C9
24	V	603	CLA	C6-C7-C8-C9
24	v	303	CLA	C6-C7-C8-C9
24	AL	505	CLA	C11-C10-C8-C9
23	AA	607	CHL	CAA-CBA-CGA-O1A
23	AB	607	CHL	CAA-CBA-CGA-O2A
23	AE	606	CHL	CAA-CBA-CGA-O1A
24	AC	613	CLA	CAA-CBA-CGA-O2A
38	F	102	HEM	CAA-CBA-CGA-O1A
23	p	605	CHL	O1A-CGA-O2A-C1
33	O	624	LMG	C34-C35-C36-C37
24	V	610	CLA	C11-C12-C13-C14
23	AN	605	CHL	CAA-CBA-CGA-O2A
34	M	101	SQD	C30-C31-C32-C33
23	AD	307	CHL	CAA-CBA-CGA-O1A
35	AO	102	DGD	C4A-C5A-C6A-C7A
24	AE	610	CLA	C2A-CAA-CBA-CGA
24	p	603	CLA	C2A-CAA-CBA-CGA
23	q	605	CHL	CAA-CBA-CGA-O2A
24	AC	602	CLA	CAA-CBA-CGA-O2A
24	O	605	CLA	CAA-CBA-CGA-O2A
24	O	607	CLA	CAA-CBA-CGA-O2A
24	q	612	CLA	CAA-CBA-CGA-O2A
24	AL	504	CLA	CAA-CBA-CGA-O2A
24	AS	313	CLA	CAA-CBA-CGA-O2A
23	AC	608	CHL	C2C-C3C-CAC-CBC
28	0	616	LHG	C26-C27-C28-C29
28	AU	617	LHG	C18-C19-C20-C21
34	m	101	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
23	V	601	CHL	CAA-CBA-CGA-O1A
23	AS	307	CHL	CAA-CBA-CGA-O1A
24	P	502	CLA	CAA-CBA-CGA-O1A
23	AA	608	CHL	C4-C3-C5-C6
23	AE	607	CHL	C4-C3-C5-C6
23	AR	605	CHL	C4-C3-C5-C6
24	AH	602	CLA	C4-C3-C5-C6
24	AQ	610	CLA	C4-C3-C5-C6
24	AJ	405	CLA	C4C-C3C-CAC-CBC
23	V	607	CHL	C11-C12-C13-C15
23	AN	607	CHL	C11-C12-C13-C15
24	O	604	CLA	C6-C7-C8-C10
24	O	610	CLA	C11-C10-C8-C7
24	P	504	CLA	C11-C10-C8-C7
24	V	602	CLA	C2-C3-C5-C6
24	p	603	CLA	C12-C13-C15-C16
24	q	612	CLA	C3A-C2A-CAA-CBA
24	v	303	CLA	C11-C10-C8-C7
24	AH	610	CLA	C11-C10-C8-C7
24	AL	514	CLA	C6-C7-C8-C10
24	AN	609	CLA	C6-C7-C8-C10
24	AQ	603	CLA	C12-C13-C15-C16
24	AR	603	CLA	C6-C7-C8-C10
24	AS	303	CLA	C6-C7-C8-C10
24	AU	610	CLA	C11-C10-C8-C7
32	AJ	408	PHO	C3A-C2A-CAA-CBA
32	AJ	408	PHO	C2-C3-C5-C6
28	q	616	LHG	O9-C7-C8-C9
34	AP	101	SQD	O10-C23-C24-C25
23	0	605	CHL	CAA-CBA-CGA-O1A
24	AA	604	CLA	CAA-CBA-CGA-O2A
28	AH	616	LHG	C26-C27-C28-C29
23	AR	605	CHL	CAA-CBA-CGA-O2A
23	AU	601	CHL	CAA-CBA-CGA-O2A
24	v	313	CLA	CAA-CBA-CGA-O2A
24	AK	609	CLA	CAA-CBA-CGA-O2A
24	AR	610	CLA	CAA-CBA-CGA-O2A
24	AU	612	CLA	CAA-CBA-CGA-O2A
25	9	616	LUT	C7-C8-C9-C10
25	AA	614	LUT	C7-C8-C9-C10
26	AU	616	NEX	C27-C28-C29-C30
29	AF	612	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
29	O	625	BCR	C17-C18-C19-C20
24	O	614	CLA	CAA-CBA-CGA-O1A
24	V	609	CLA	CAA-CBA-CGA-O1A
24	AH	612	CLA	CAA-CBA-CGA-O1A
24	AK	616	CLA	CAA-CBA-CGA-O1A
24	AS	313	CLA	CAA-CBA-CGA-O1A
28	W	201	LHG	O7-C7-C8-C9
24	AH	609	CLA	C8-C10-C11-C12
24	AL	506	CLA	C13-C15-C16-C17
23	q	605	CHL	CAA-CBA-CGA-O1A
23	AN	601	CHL	CAA-CBA-CGA-O1A
24	AL	504	CLA	CAA-CBA-CGA-O1A
24	AU	612	CLA	CAA-CBA-CGA-O1A
24	AC	613	CLA	CAA-CBA-CGA-O1A
28	AD	316	LHG	O10-C23-O8-C6
24	P	503	CLA	CAA-CBA-CGA-O2A
24	p	618	CLA	CAA-CBA-CGA-O2A
24	AK	607	CLA	CAA-CBA-CGA-O2A
28	w	201	LHG	O9-C7-C8-C9
35	AL	518	DGD	O1B-C1B-C2B-C3B
24	O	611	CLA	C2A-CAA-CBA-CGA
24	Q	404	CLA	C8-C10-C11-C12
28	AN	616	LHG	C16-C17-C18-C19
23	AN	605	CHL	CAA-CBA-CGA-O1A
24	P	503	CLA	CAA-CBA-CGA-O1A
24	AN	609	CLA	CAA-CBA-CGA-O1A
23	p	601	CHL	CAA-CBA-CGA-O2A
24	q	610	CLA	CAA-CBA-CGA-O2A
24	AS	311	CLA	CAA-CBA-CGA-O2A
28	AU	617	LHG	O8-C23-C24-C25
34	o	101	SQD	O47-C7-C8-C9
24	AE	609	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

404 monomers are involved in 1453 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	v	312	CLA	1	0
24	AQ	602	CLA	3	0
35	AL	517	DGD	1	0
24	O	601	CLA	10	0
23	9	601	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AC	607	CHL	4	0
26	AR	615	NEX	6	0
29	AK	602	BCR	2	0
23	p	606	CHL	7	0
24	O	603	CLA	4	0
24	AC	604	CLA	9	0
25	0	614	LUT	2	0
25	AC	614	LUT	7	0
23	AF	606	CHL	1	0
23	AD	302	CHL	15	0
24	AL	503	CLA	1	0
23	AN	617	CHL	5	0
23	AC	608	CHL	5	0
24	AK	618	CLA	3	0
23	AR	605	CHL	9	0
24	q	608	CLA	2	0
38	F	102	HEM	4	0
24	AU	613	CLA	3	0
24	Q	401	CLA	1	0
26	p	616	NEX	2	0
23	0	617	CHL	3	0
23	AD	306	CHL	3	0
23	AD	317	CHL	4	0
24	AN	612	CLA	4	0
24	AE	603	CLA	4	0
24	O	611	CLA	6	0
25	9	616	LUT	6	0
25	AN	614	LUT	10	0
25	AU	614	LUT	4	0
23	AF	605	CHL	3	0
23	0	608	CHL	7	0
34	J	410	SQD	7	0
27	9	618	XAT	2	0
24	V	611	CLA	2	0
25	0	615	LUT	2	0
25	AC	615	LUT	7	0
24	AF	614	CLA	1	0
23	0	607	CHL	3	0
26	9	617	NEX	4	0
23	AE	601	CHL	4	0
23	p	605	CHL	1	0
24	9	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	p	601	CHL	9	0
24	O	606	CLA	4	0
24	AD	310	CLA	1	0
24	O	609	CLA	7	0
25	AS	316	LUT	5	0
24	AM	403	CLA	4	0
24	AD	303	CLA	4	0
23	AQ	608	CHL	19	0
28	O	621	LHG	3	0
29	AO	101	BCR	3	0
29	AV	101	BCR	3	0
24	AS	303	CLA	2	0
24	AH	603	CLA	1	0
24	AJ	409	CLA	1	0
32	J	405	PHO	4	0
23	AH	608	CHL	17	0
28	AK	623	LHG	1	0
23	V	606	CHL	12	0
24	AA	609	CLA	1	0
24	K	101	CLA	2	0
23	AQ	607	CHL	12	0
24	AE	602	CLA	2	0
24	AN	611	CLA	3	0
33	P	518	LMG	2	0
24	AK	617	CLA	3	0
24	p	604	CLA	2	0
28	W	201	LHG	2	0
24	0	610	CLA	2	0
28	p	617	LHG	1	0
24	Q	404	CLA	4	0
29	AI	101	BCR	2	0
25	AR	614	LUT	12	0
24	V	604	CLA	1	0
25	V	614	LUT	6	0
24	V	610	CLA	4	0
24	AU	611	CLA	4	0
23	AU	605	CHL	3	0
35	AJ	412	DGD	1	0
24	AK	608	CLA	4	0
24	AK	604	CLA	2	0
29	O	619	BCR	5	0
25	AF	611	LUT	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AA	603	CLA	2	0
24	q	609	CLA	10	0
24	0	604	CLA	3	0
23	p	609	CHL	7	0
24	AA	613	CLA	1	0
24	P	506	CLA	2	0
24	AL	509	CLA	9	0
23	q	605	CHL	8	0
23	AN	607	CHL	24	0
24	O	613	CLA	1	0
23	AQ	605	CHL	1	0
24	AM	404	CLA	1	0
24	AN	603	CLA	4	0
29	O	617	BCR	5	0
23	AF	607	CHL	7	0
32	J	406	PHO	3	0
23	9	607	CHL	12	0
25	9	615	LUT	7	0
24	AR	612	CLA	7	0
23	p	608	CHL	17	0
29	k	101	BCR	4	0
29	P	515	BCR	5	0
33	AK	601	LMG	1	0
23	V	601	CHL	10	0
23	AU	606	CHL	4	0
26	q	615	NEX	3	0
29	AJ	410	BCR	4	0
25	v	316	LUT	6	0
24	9	604	CLA	6	0
23	AS	306	CHL	2	0
23	AB	605	CHL	3	0
24	O	608	CLA	5	0
23	AR	606	CHL	5	0
23	AD	307	CHL	3	0
23	AU	601	CHL	15	0
24	AR	609	CLA	5	0
29	AK	621	BCR	2	0
24	AB	602	CLA	2	0
25	AE	613	LUT	8	0
24	J	403	CLA	7	0
28	P	517	LHG	2	0
25	AN	615	LUT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AH	609	CLA	10	0
24	0	602	CLA	2	0
24	AE	611	CLA	2	0
24	P	507	CLA	3	0
24	AL	508	CLA	4	0
24	AS	311	CLA	6	0
29	AL	515	BCR	2	0
35	AJ	401	DGD	2	0
23	AB	607	CHL	5	0
24	AR	610	CLA	2	0
24	P	510	CLA	2	0
24	AK	607	CLA	8	0
23	AE	617	CHL	6	0
24	AS	312	CLA	1	0
24	O	610	CLA	9	0
34	AM	401	SQD	2	0
23	v	306	CHL	3	0
24	0	609	CLA	3	0
24	AC	602	CLA	5	0
27	AB	613	XAT	7	0
24	P	505	CLA	2	0
24	AK	603	CLA	9	0
28	AM	406	LHG	2	0
29	O	618	BCR	4	0
24	AF	603	CLA	2	0
24	AL	502	CLA	2	0
23	AA	617	CHL	4	0
23	AF	608	CHL	3	0
24	P	508	CLA	8	0
24	AH	602	CLA	5	0
24	9	610	CLA	7	0
24	AQ	613	CLA	5	0
24	AK	614	CLA	4	0
23	AE	606	CHL	7	0
24	AS	309	CLA	1	0
24	AL	507	CLA	3	0
24	AD	304	CLA	5	0
24	O	614	CLA	9	0
24	AQ	612	CLA	4	0
34	AJ	411	SQD	6	0
29	O	625	BCR	1	0
33	AK	622	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	AO	102	DGD	3	0
24	0	613	CLA	2	0
24	AC	613	CLA	3	0
24	AK	605	CLA	6	0
25	p	614	LUT	3	0
23	AB	606	CHL	3	0
25	V	613	LUT	7	0
23	V	605	CHL	7	0
28	O	622	LHG	1	0
33	AL	501	LMG	1	0
25	AS	315	LUT	3	0
28	AQ	618	LHG	1	0
24	p	603	CLA	3	0
24	AN	609	CLA	5	0
23	9	608	CHL	4	0
24	AA	602	CLA	5	0
24	O	604	CLA	6	0
24	9	602	CLA	5	0
24	0	603	CLA	2	0
24	AR	602	CLA	1	0
24	AH	610	CLA	5	0
24	O	612	CLA	6	0
25	AD	314	LUT	2	0
23	AA	606	CHL	9	0
24	AU	603	CLA	1	0
24	v	311	CLA	5	0
38	f	102	HEM	3	0
24	AH	613	CLA	1	0
24	AB	610	CLA	2	0
23	AQ	609	CHL	8	0
33	O	620	LMG	1	0
23	AA	605	CHL	4	0
24	AB	611	CLA	2	0
24	AH	611	CLA	5	0
29	AL	516	BCR	3	0
25	p	615	LUT	4	0
24	AJ	404	CLA	9	0
29	AK	619	BCR	5	0
29	P	514	BCR	3	0
24	AL	505	CLA	2	0
26	AA	616	NEX	1	0
24	q	603	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	P	513	BCR	2	0
24	AA	610	CLA	1	0
23	p	607	CHL	14	0
24	q	602	CLA	3	0
29	f	101	BCR	3	0
23	AD	301	CHL	8	0
24	AK	606	CLA	4	0
35	J	413	DGD	2	0
29	AF	612	BCR	2	0
24	P	501	CLA	3	0
24	AH	612	CLA	2	0
28	q	616	LHG	2	0
28	AS	301	LHG	1	0
25	v	315	LUT	4	0
34	M	101	SQD	3	0
23	AE	607	CHL	8	0
24	AS	310	CLA	3	0
28	AL	519	LHG	2	0
24	AC	612	CLA	3	0
28	w	201	LHG	2	0
24	AB	609	CLA	2	0
24	O	615	CLA	5	0
23	AH	607	CHL	9	0
25	AQ	615	LUT	3	0
23	AD	308	CHL	9	0
23	0	606	CHL	2	0
24	v	309	CLA	1	0
23	AH	606	CHL	4	0
23	AN	608	CHL	8	0
24	AD	309	CLA	5	0
24	AR	604	CLA	4	0
23	q	613	CHL	1	0
24	AC	611	CLA	1	0
24	p	610	CLA	10	0
24	AN	602	CLA	5	0
34	m	101	SQD	3	0
24	AS	304	CLA	1	0
29	AK	620	BCR	2	0
24	AU	604	CLA	3	0
23	q	606	CHL	6	0
23	AS	307	CHL	5	0
24	AB	604	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	AQ	617	NEX	2	0
24	P	502	CLA	1	0
24	p	613	CLA	2	0
24	AL	511	CLA	2	0
24	AK	611	CLA	10	0
24	O	607	CLA	3	0
23	AR	607	CHL	7	0
27	AF	613	XAT	7	0
24	AL	512	CLA	3	0
24	v	310	CLA	4	0
24	AL	514	CLA	4	0
23	AE	605	CHL	6	0
24	AA	612	CLA	2	0
23	V	608	CHL	4	0
33	AL	520	LMG	1	0
24	AS	313	CLA	4	0
23	AC	606	CHL	5	0
25	AH	615	LUT	6	0
24	AC	609	CLA	8	0
24	q	610	CLA	2	0
24	AN	613	CLA	2	0
23	AE	616	CHL	5	0
24	J	407	CLA	3	0
35	P	516	DGD	1	0
23	AH	605	CHL	2	0
24	O	602	CLA	1	0
24	J	404	CLA	3	0
24	AE	609	CLA	1	0
24	AK	616	CLA	8	0
23	V	607	CHL	20	0
23	AC	601	CHL	3	0
28	0	616	LHG	3	0
24	AB	603	CLA	3	0
28	AK	624	LHG	2	0
27	q	617	XAT	1	0
23	AB	608	CHL	4	0
26	AC	616	NEX	4	0
24	AS	305	CLA	1	0
24	p	618	CLA	2	0
24	AQ	603	CLA	3	0
28	v	301	LHG	1	0
33	O	624	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	F	101	BCR	2	0
23	AS	302	CHL	3	0
24	AF	609	CLA	3	0
24	AQ	610	CLA	10	0
24	AR	601	CLA	1	0
24	v	313	CLA	6	0
24	O	605	CLA	6	0
24	AR	608	CLA	4	0
23	9	605	CHL	2	0
24	AE	604	CLA	2	0
24	V	602	CLA	6	0
23	AS	308	CHL	7	0
23	0	605	CHL	2	0
24	AH	604	CLA	2	0
24	AK	610	CLA	6	0
24	p	602	CLA	3	0
23	AH	601	CHL	15	0
35	J	411	DGD	1	0
23	9	606	CHL	4	0
29	j	101	BCR	5	0
25	AD	315	LUT	4	0
29	AB	612	BCR	4	0
24	AF	610	CLA	3	0
24	Q	403	CLA	4	0
24	AC	610	CLA	2	0
24	AA	611	CLA	1	0
26	v	317	NEX	1	0
24	v	314	CLA	1	0
24	AU	602	CLA	3	0
24	q	612	CLA	5	0
23	AN	605	CHL	5	0
35	AL	518	DGD	1	0
25	AE	614	LUT	8	0
25	AA	614	LUT	5	0
25	AU	615	LUT	8	0
24	P	504	CLA	3	0
28	AN	616	LHG	2	0
23	0	601	CHL	16	0
23	AR	613	CHL	1	0
34	Q	402	SQD	2	0
23	AQ	606	CHL	5	0
28	V	615	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	V	616	CHL	4	0
24	AF	602	CLA	7	0
23	v	307	CHL	7	0
24	q	601	CLA	2	0
24	V	609	CLA	7	0
24	AQ	604	CLA	1	0
23	AQ	601	CHL	9	0
28	Q	406	LHG	2	0
24	AK	609	CLA	5	0
23	AA	601	CHL	3	0
25	q	614	LUT	10	0
24	P	512	CLA	4	0
24	AK	612	CLA	3	0
24	AU	609	CLA	8	0
24	0	611	CLA	1	0
24	AE	608	CLA	2	0
23	v	302	CHL	3	0
24	V	603	CLA	4	0
24	AF	604	CLA	2	0
23	AN	606	CHL	12	0
34	o	101	SQD	5	0
28	O	623	LHG	3	0
23	v	308	CHL	3	0
26	AE	615	NEX	1	0
24	AD	313	CLA	2	0
23	AN	601	CHL	8	0
24	AR	617	CLA	7	0
24	v	303	CLA	3	0
24	9	613	CLA	4	0
35	j	102	DGD	2	0
24	AL	513	CLA	2	0
24	q	618	CLA	6	0
24	AJ	405	CLA	4	0
23	9	609	CHL	8	0
24	q	604	CLA	3	0
23	AU	607	CHL	7	0
25	AH	614	LUT	5	0
29	J	408	BCR	4	0
25	AA	615	LUT	3	0
24	AL	506	CLA	3	0
26	AS	317	NEX	1	0
24	AQ	611	CLA	2	0

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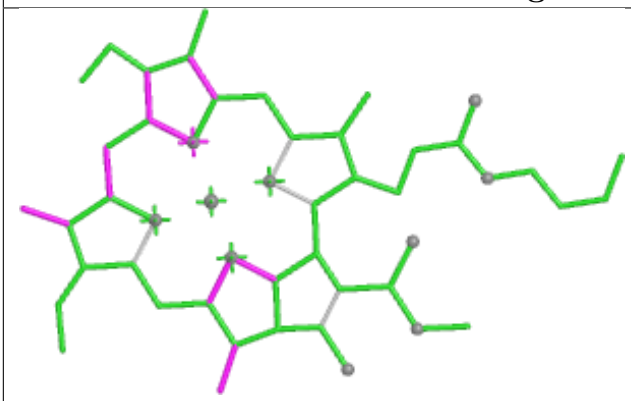
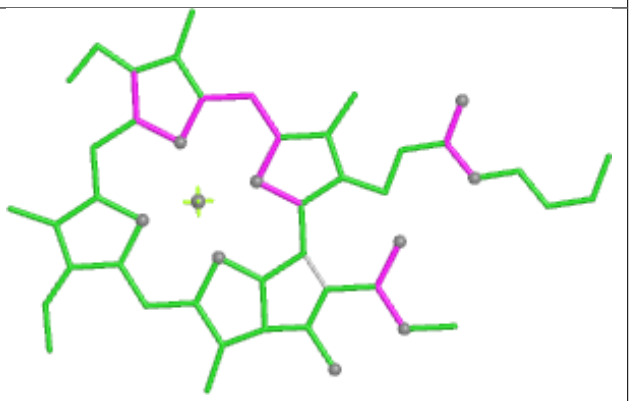
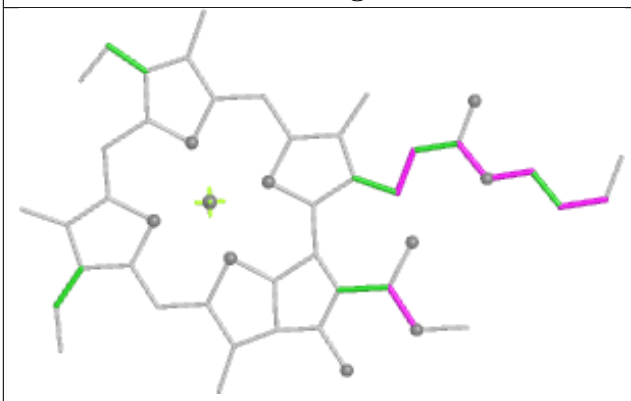
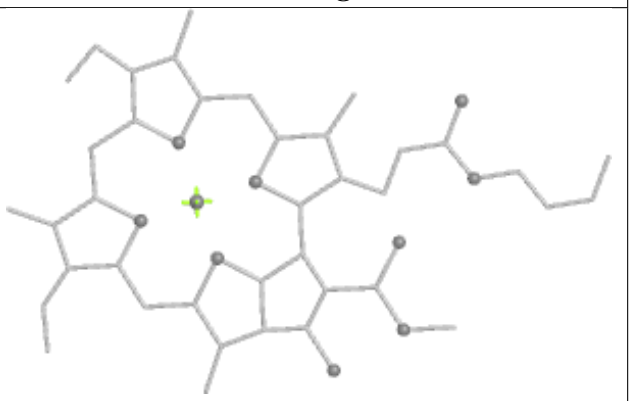
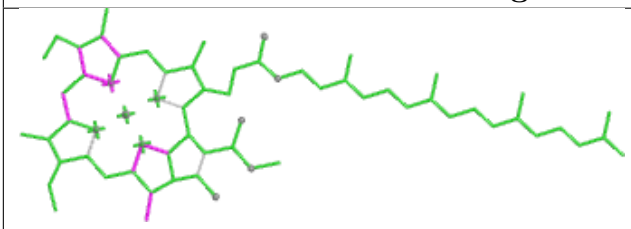
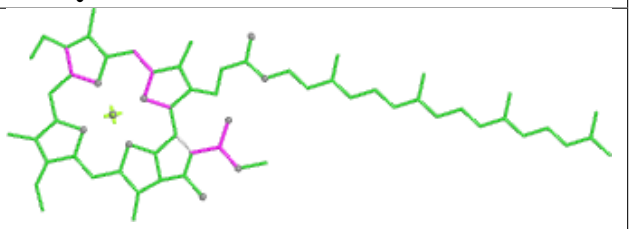
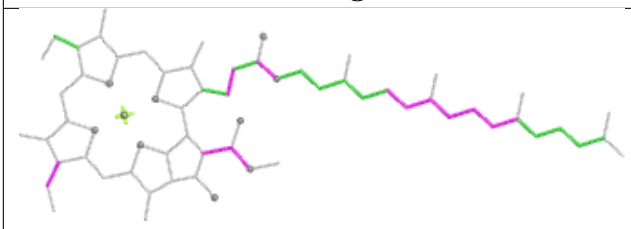
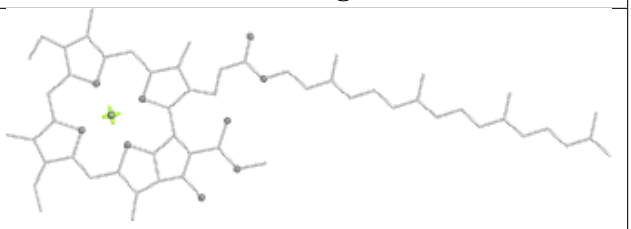
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	AJ	407	PHO	5	0
24	AD	305	CLA	3	0
24	0	612	CLA	1	0
23	AA	607	CHL	4	0
24	AU	612	CLA	3	0
24	AK	615	CLA	2	0
34	AP	101	SQD	5	0
23	AC	605	CHL	3	0
24	AD	311	CLA	2	0
26	AU	616	NEX	1	0
24	O	616	CLA	2	0
24	P	511	CLA	2	0
23	AU	608	CHL	18	0
24	AA	604	CLA	4	0
24	AK	613	CLA	8	0
32	AJ	408	PHO	3	0
24	AU	610	CLA	5	0
23	q	607	CHL	7	0
25	AQ	616	LUT	3	0
23	AA	608	CHL	5	0
24	P	503	CLA	1	0

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

Ligand CLA v 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AQ 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

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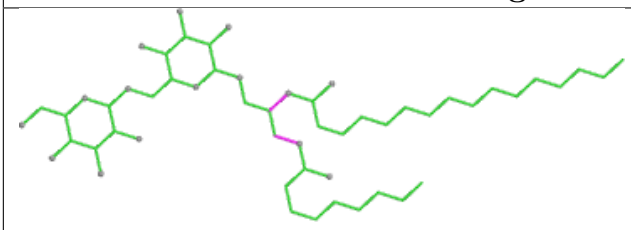
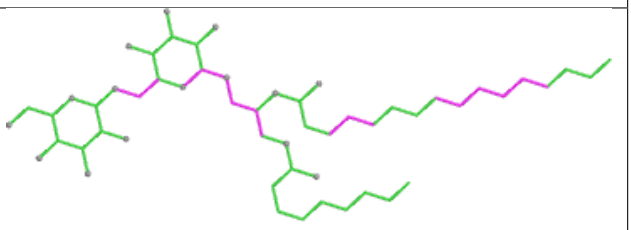
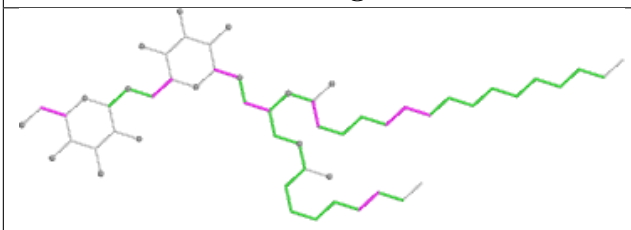
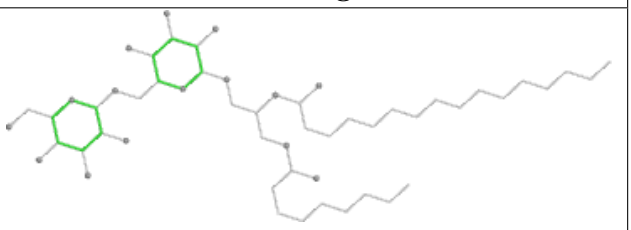
 Bond lengths	 Bond angles
 Torsions	 Rings

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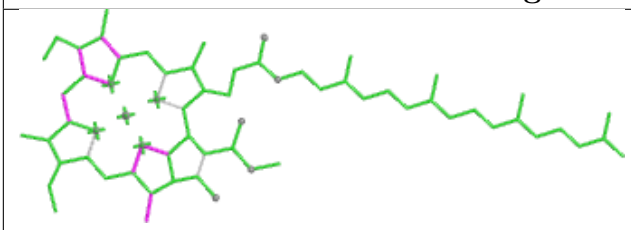
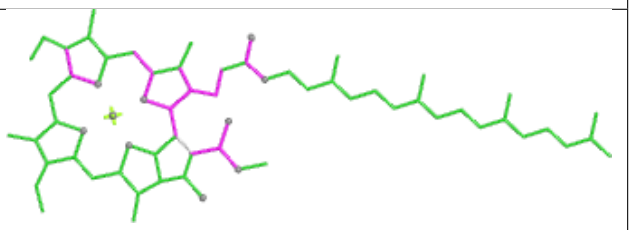
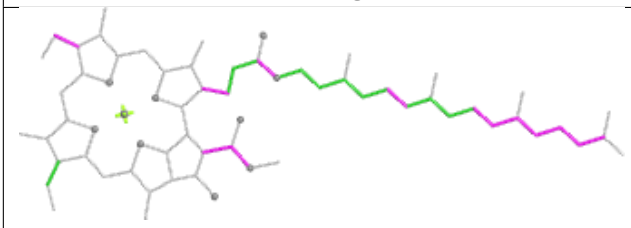
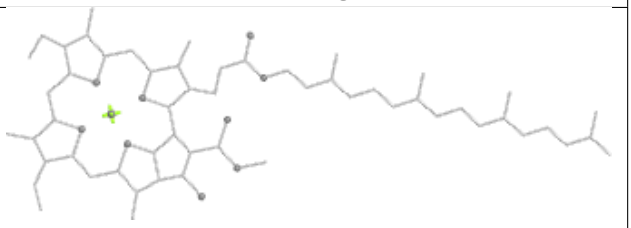
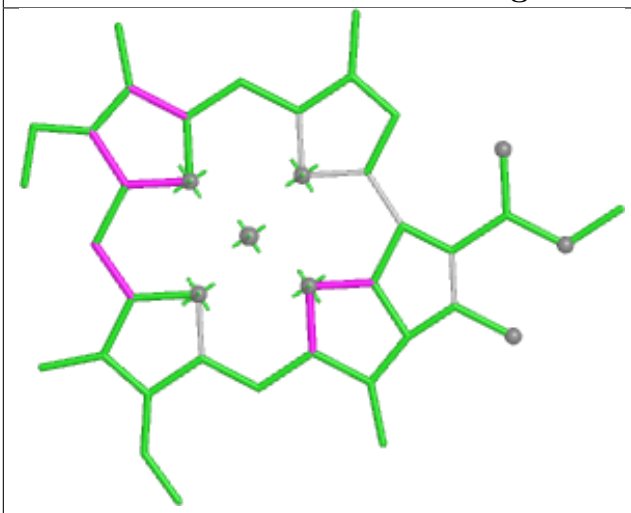
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AQ 614



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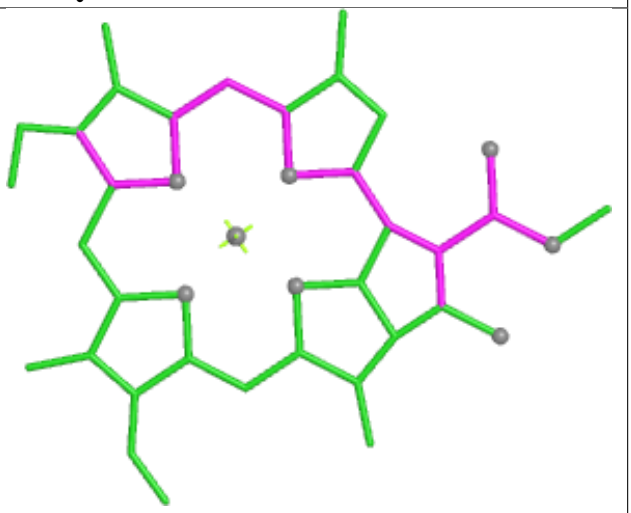

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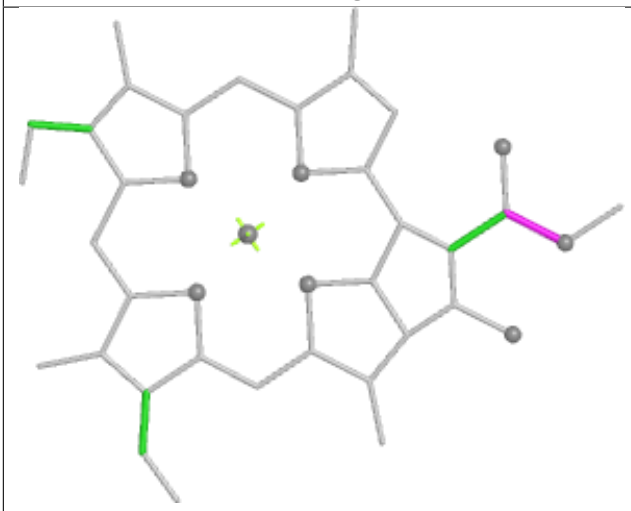

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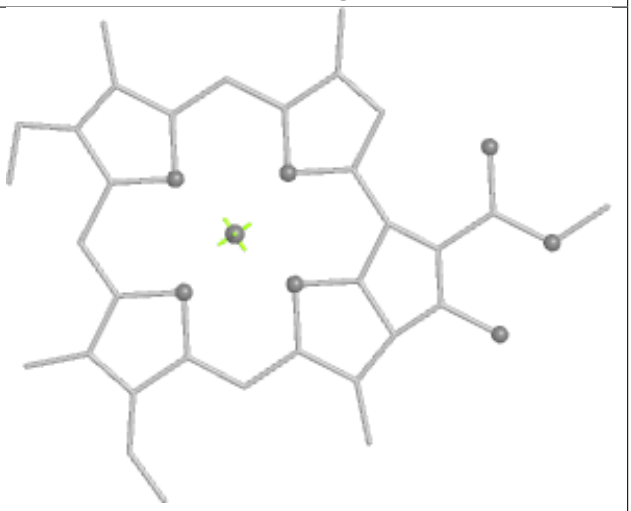
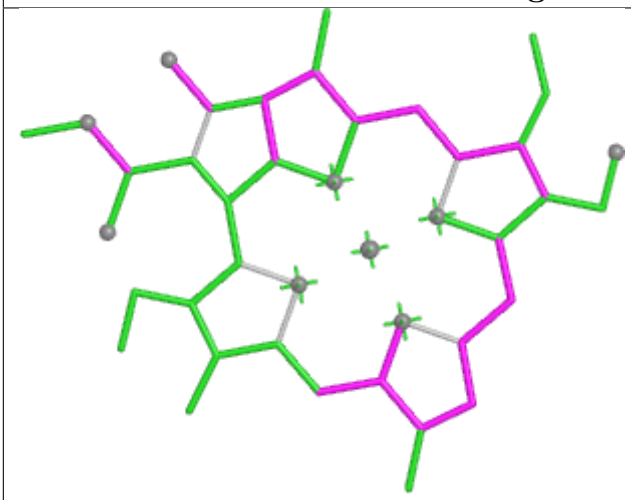
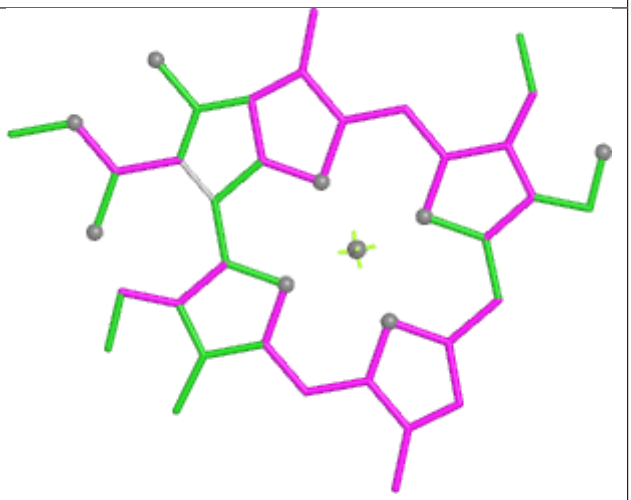
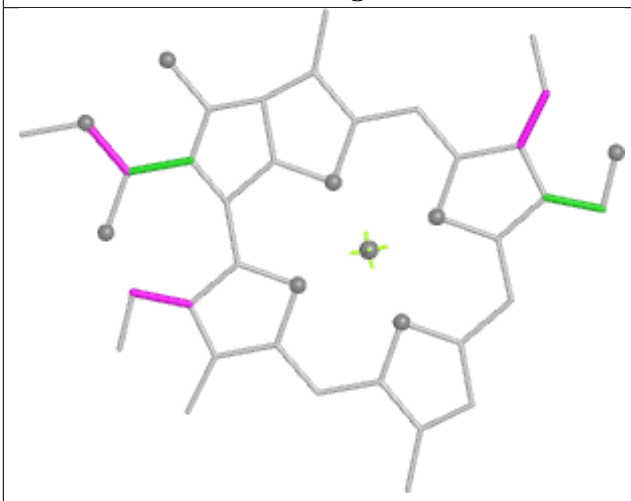
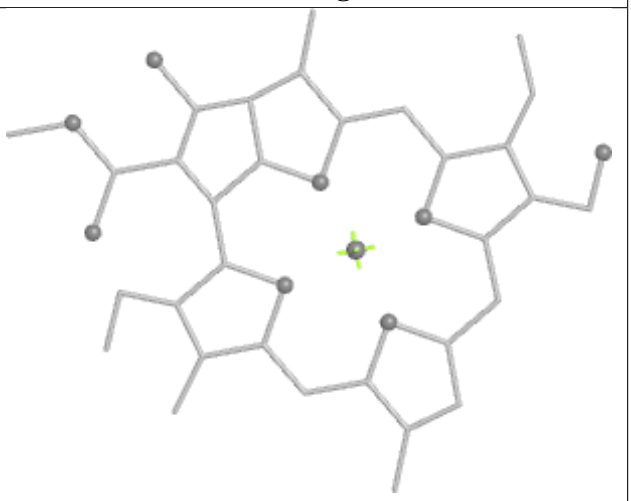


Rings

Ligand CHL 9 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

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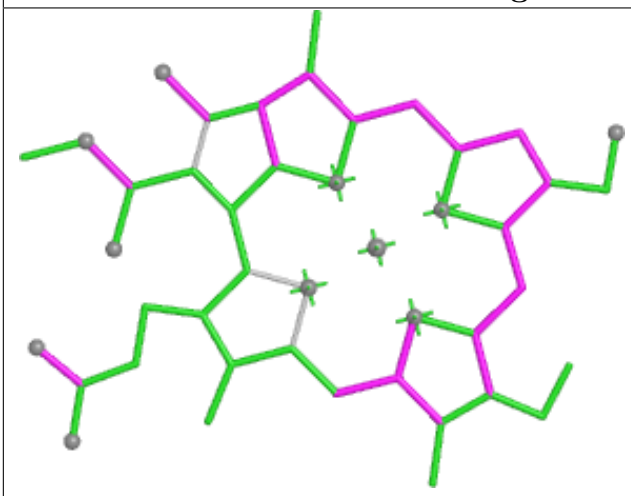

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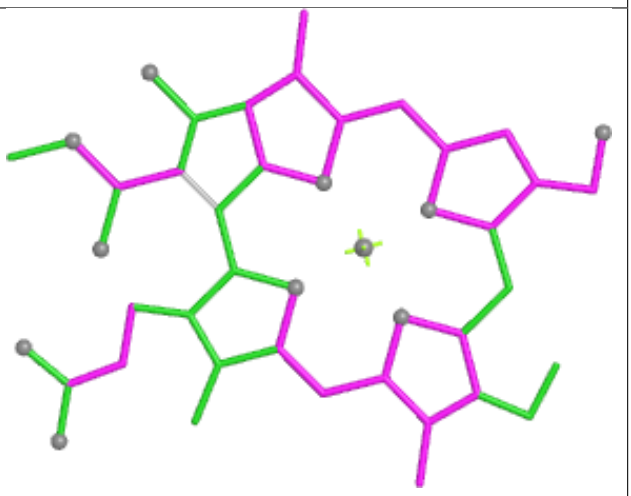

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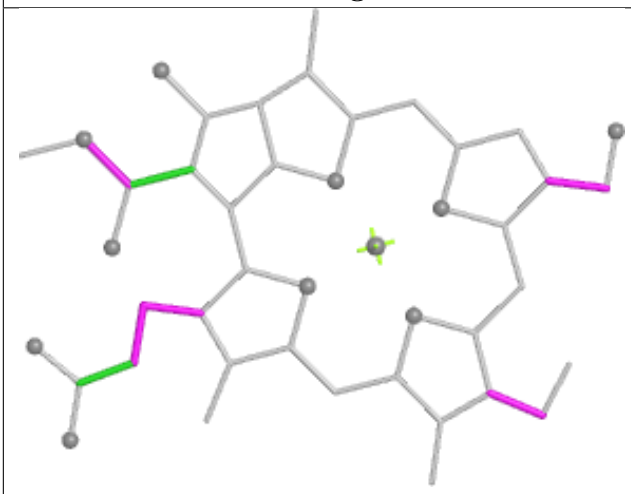

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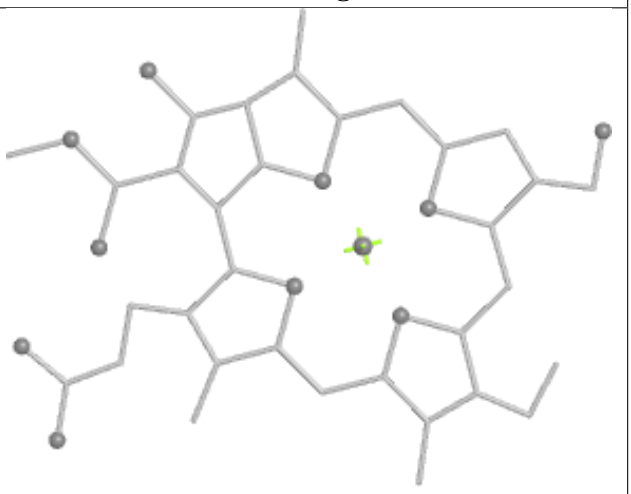
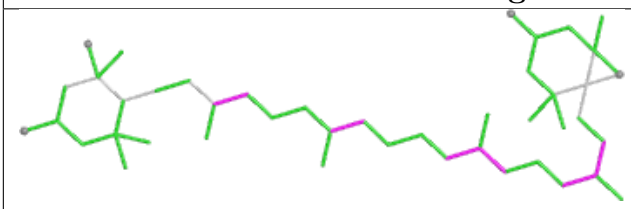


Rings

Ligand NEX AR 615



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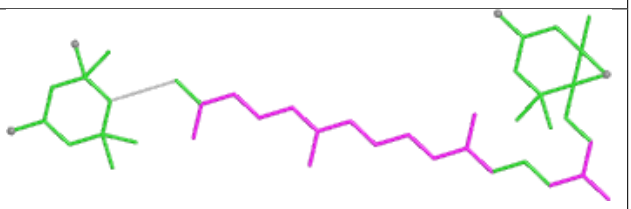

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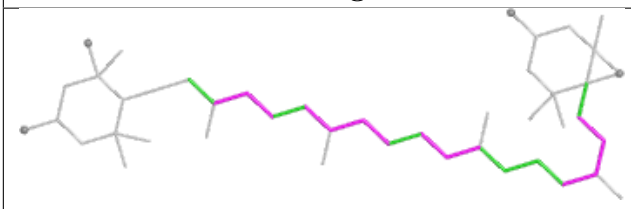

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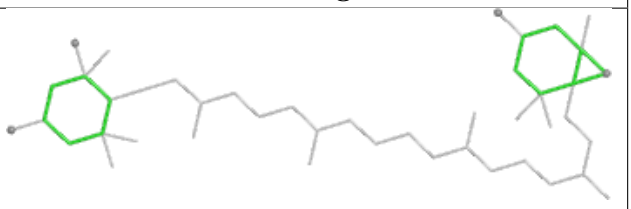

Rings

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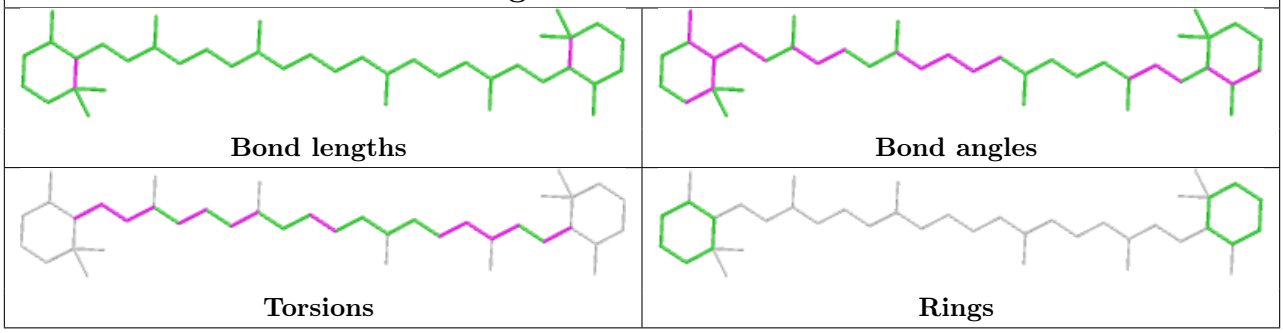
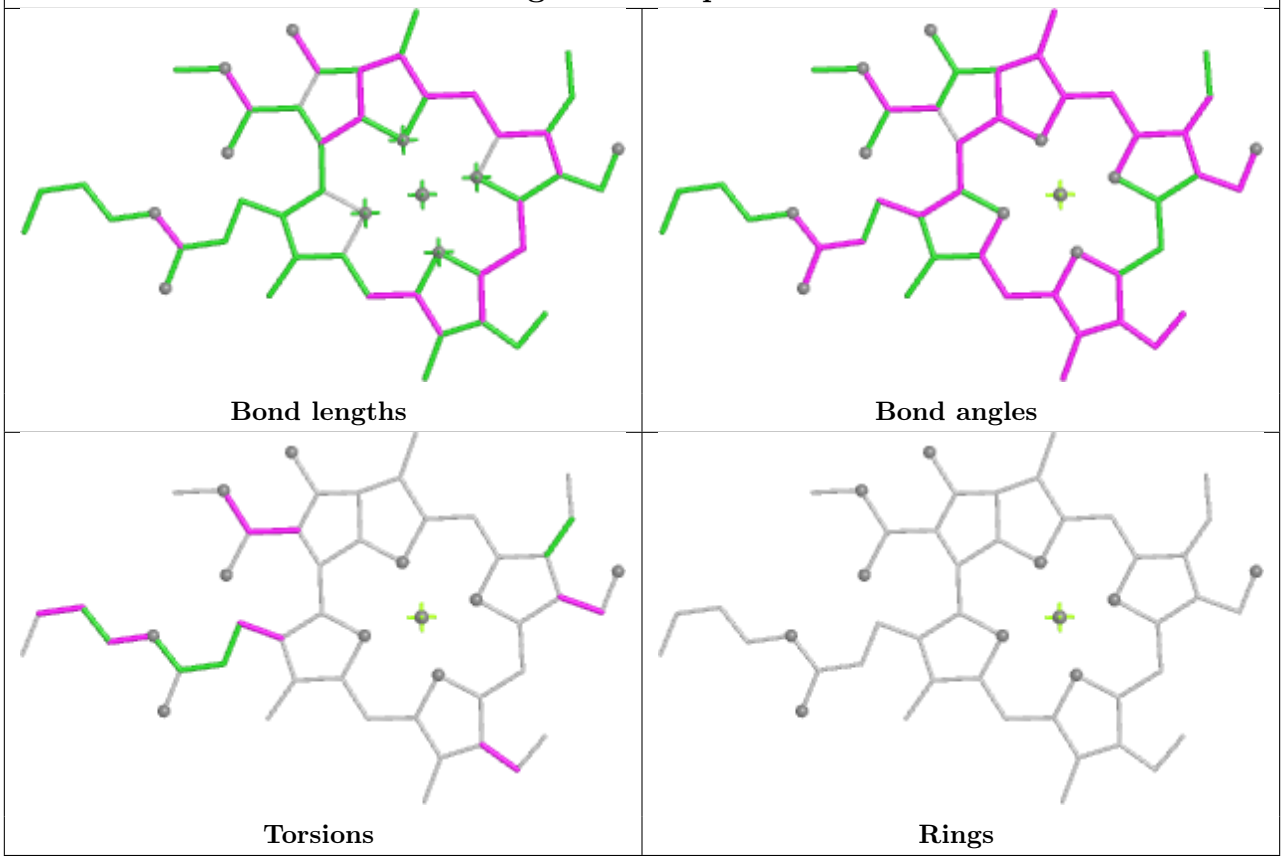


Ligand CHL p 606



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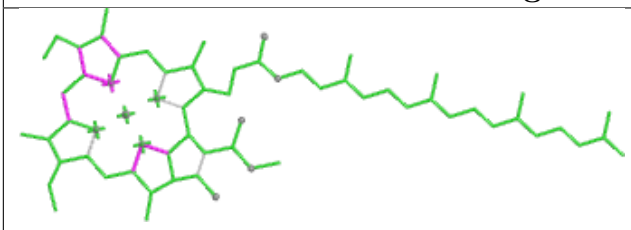
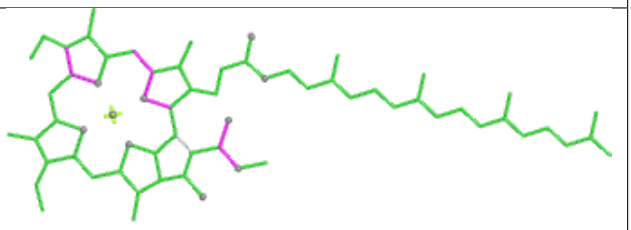
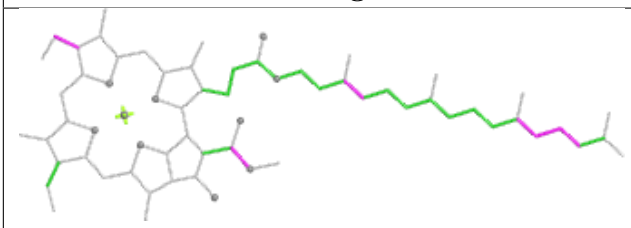
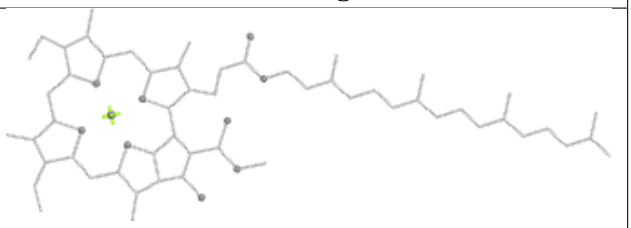
 Bond lengths	 Bond angles
 Torsions	 Rings

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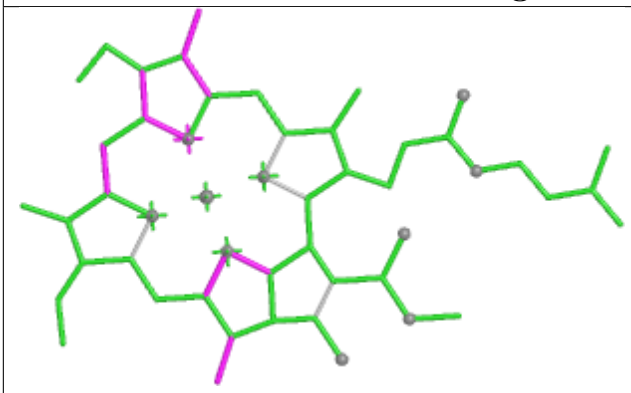
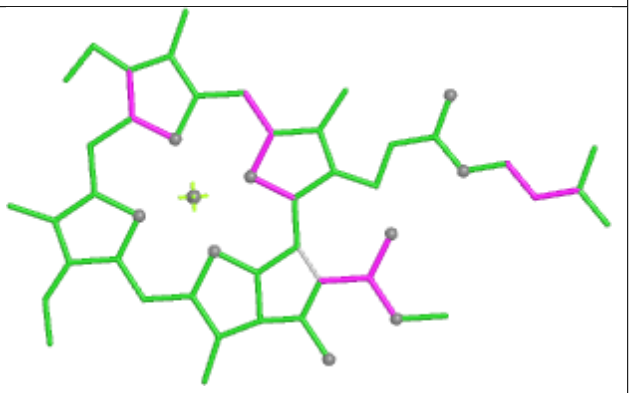
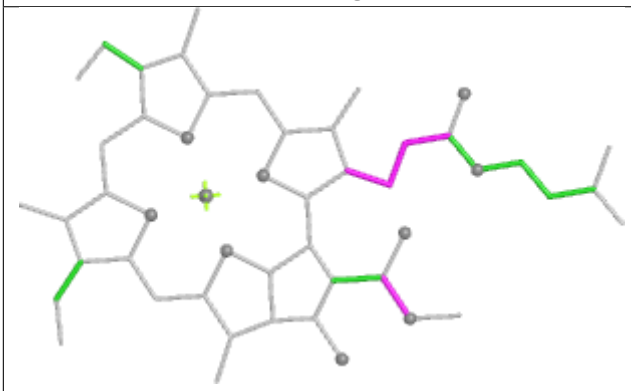
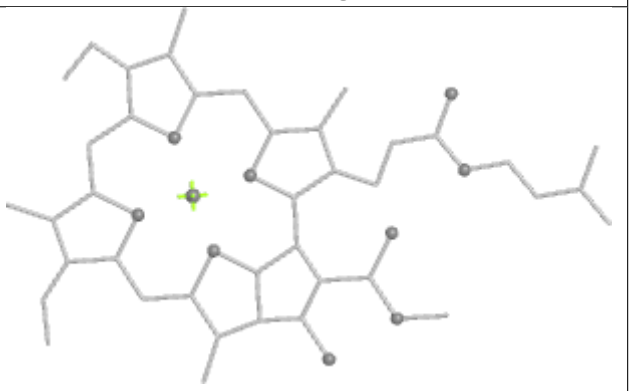
 Bond lengths	 Bond angles
 Torsions	 Rings

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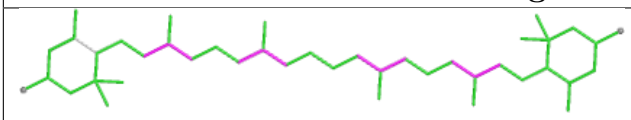
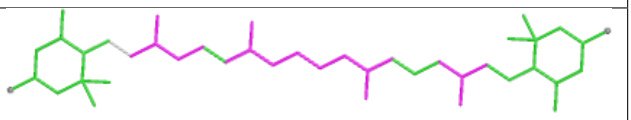
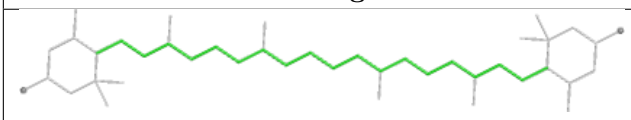
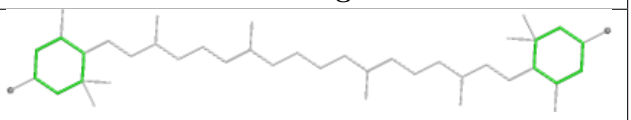
 Bond lengths	 Bond angles
 Torsions	 Rings

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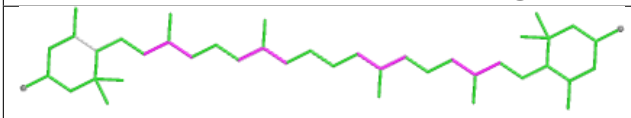
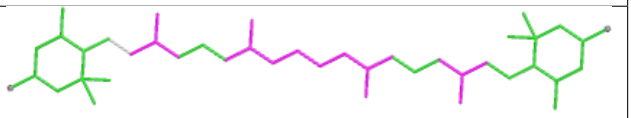
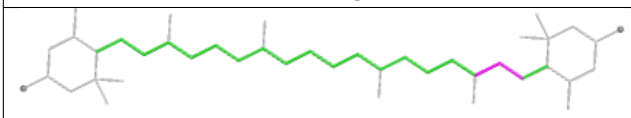
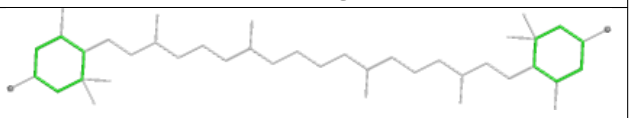
 Bond lengths	 Bond angles
 Torsions	 Rings

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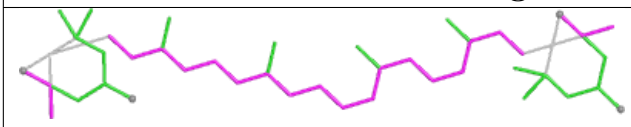
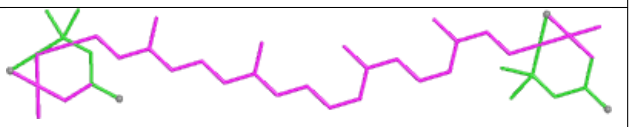
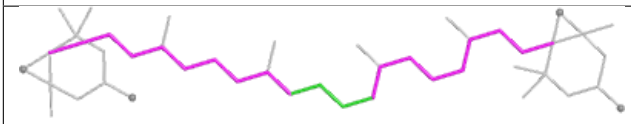
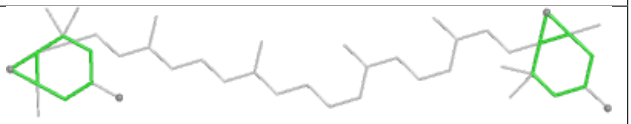
 Bond lengths	 Bond angles
 Torsions	 Rings

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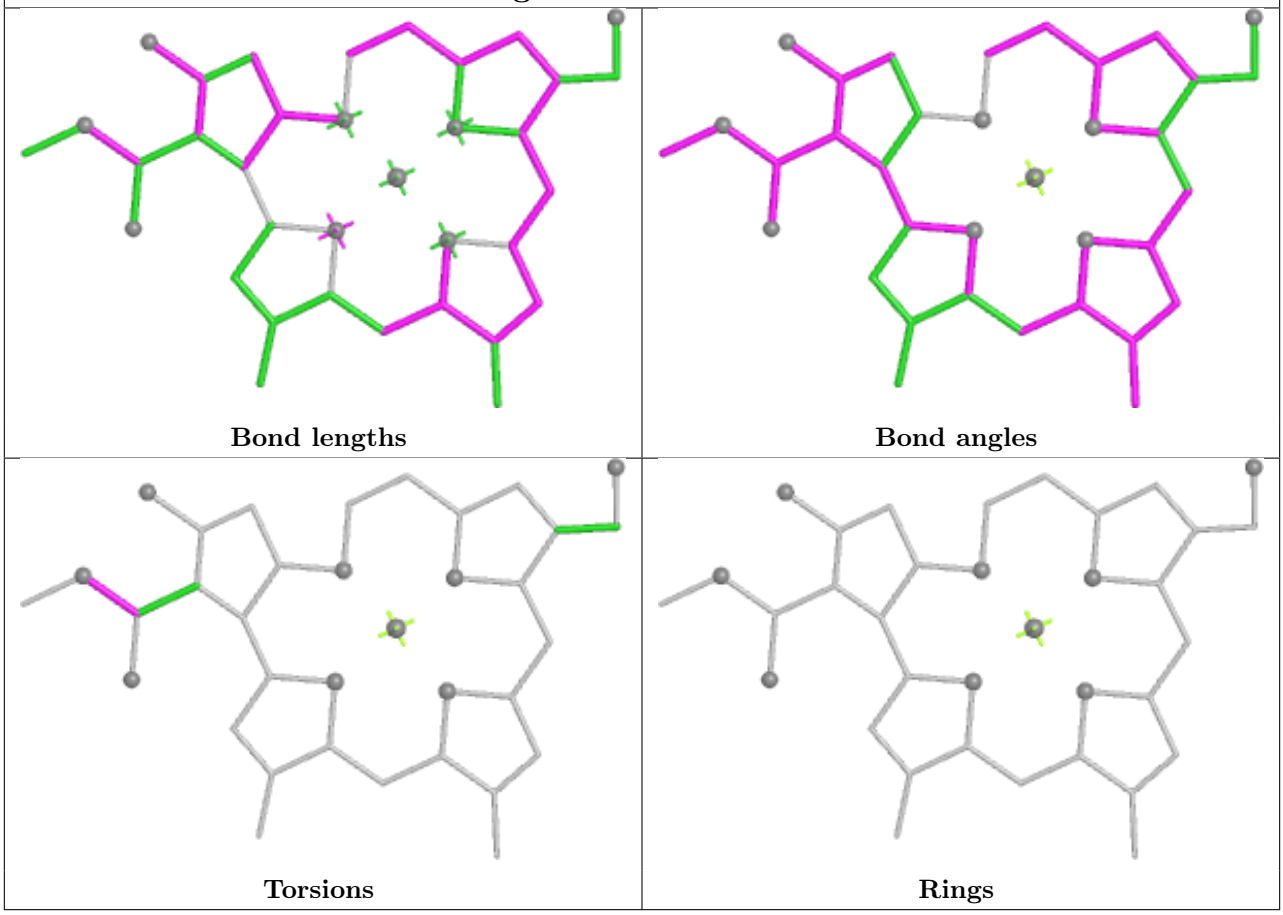
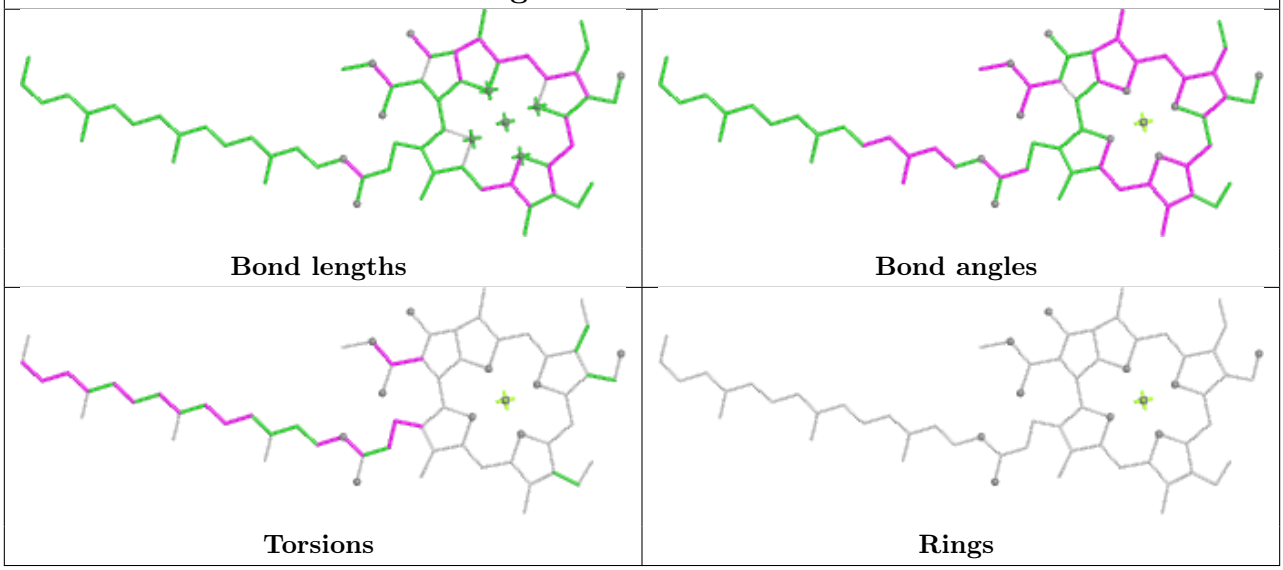
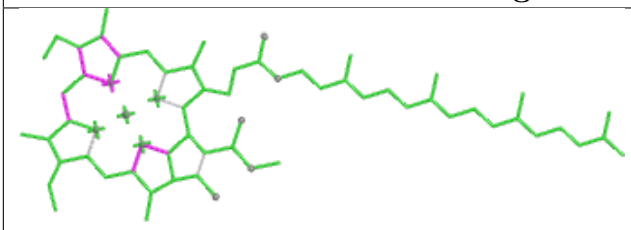


Ligand CHL AD 302



Ligand CLA AL 503



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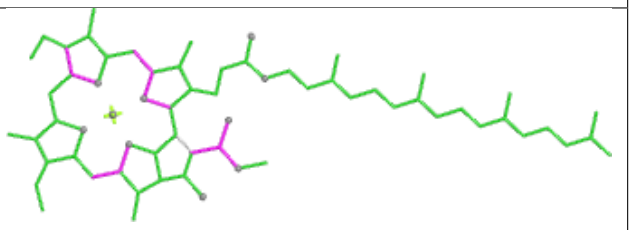

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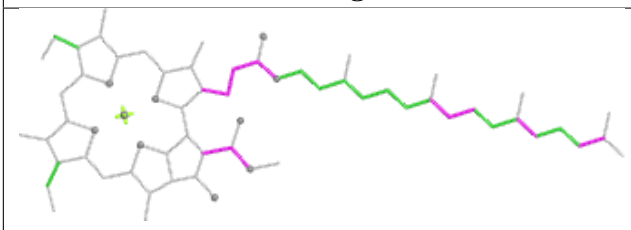

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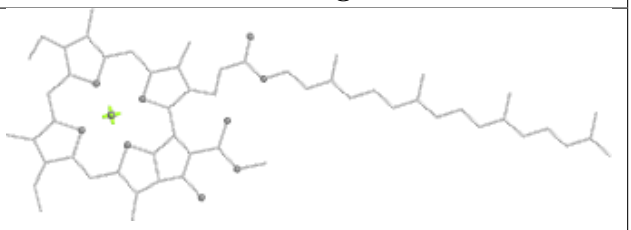
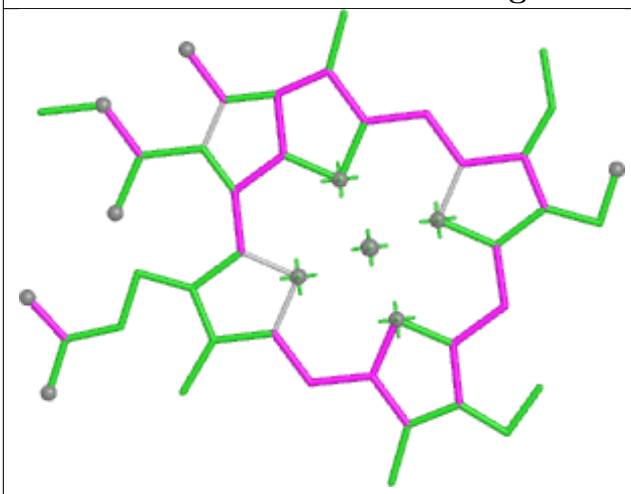


Rings

Ligand CHL AN 617



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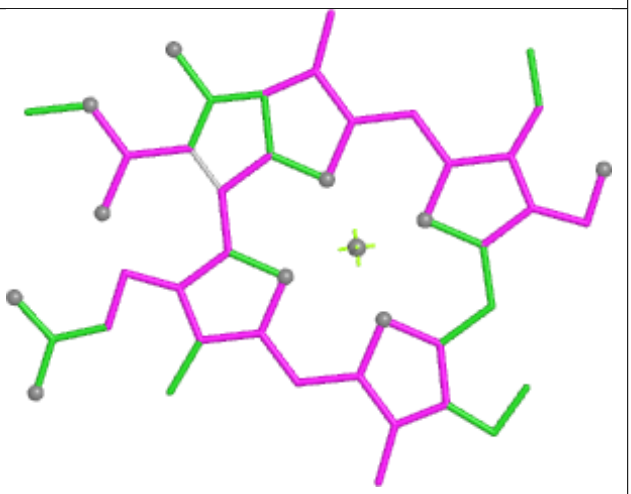

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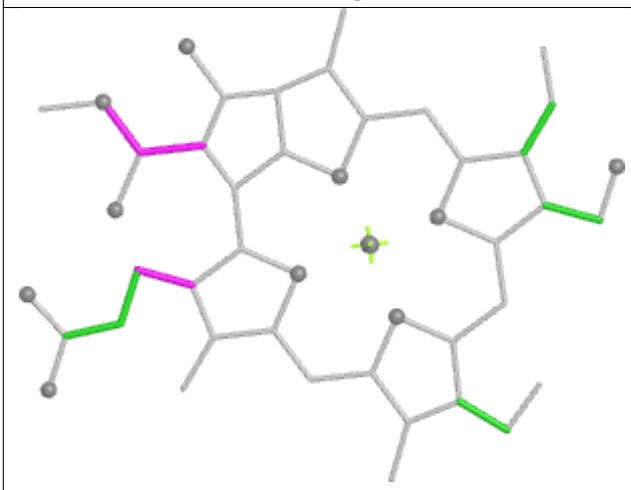

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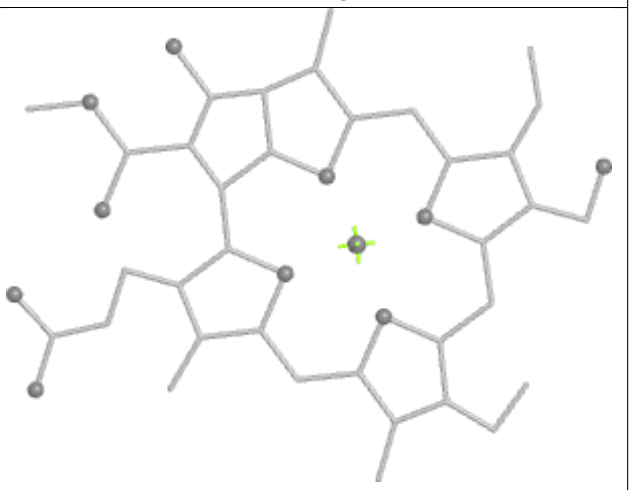

Rings

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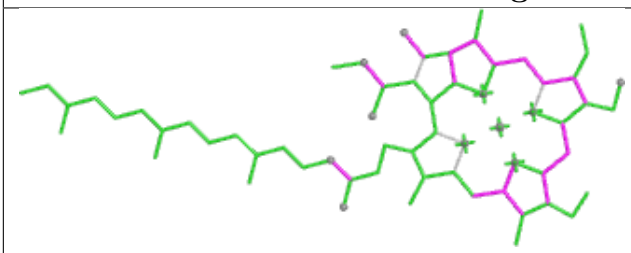
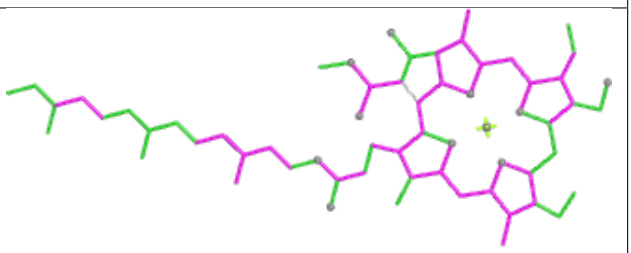
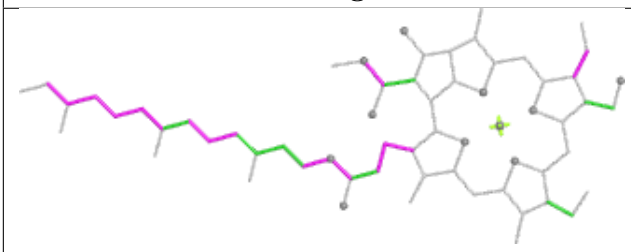
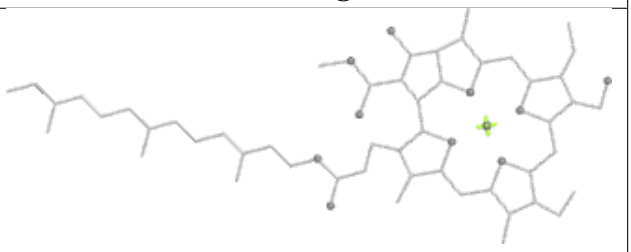
 Bond lengths	 Bond angles
 Torsions	 Rings

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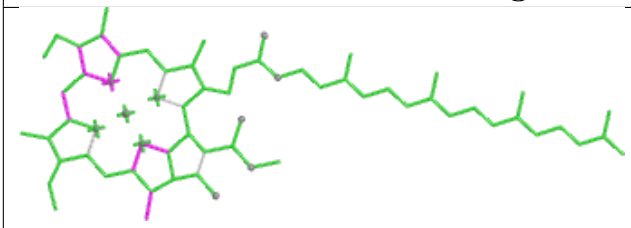
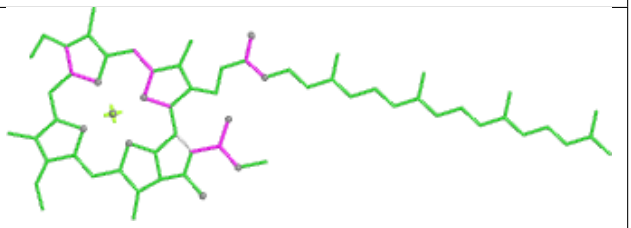
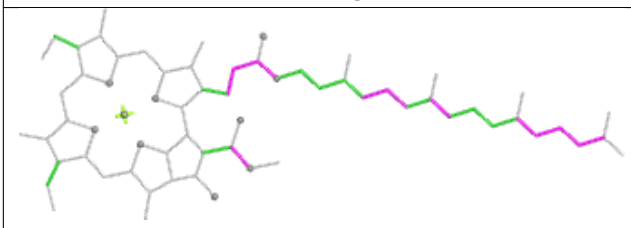
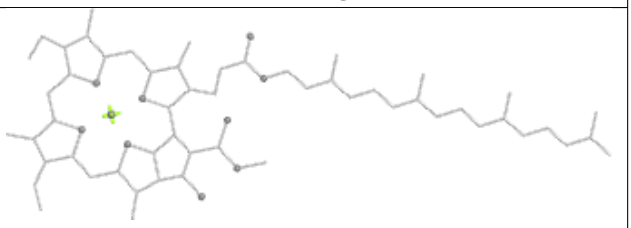
 Bond lengths	 Bond angles
 Torsions	 Rings

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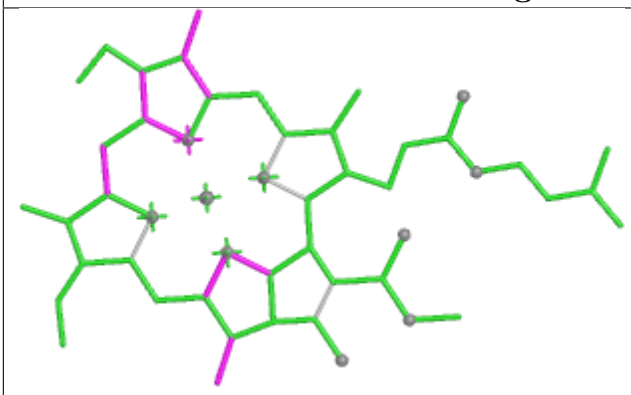

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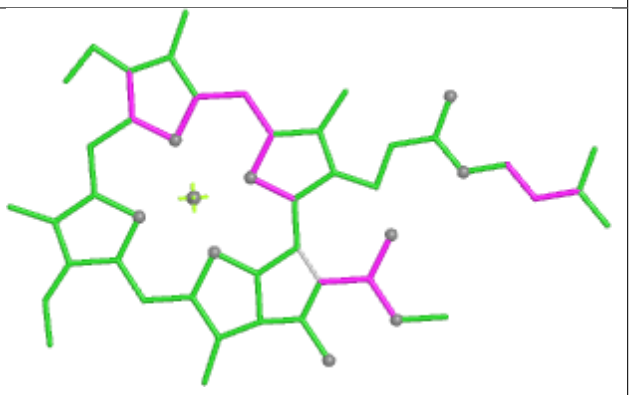

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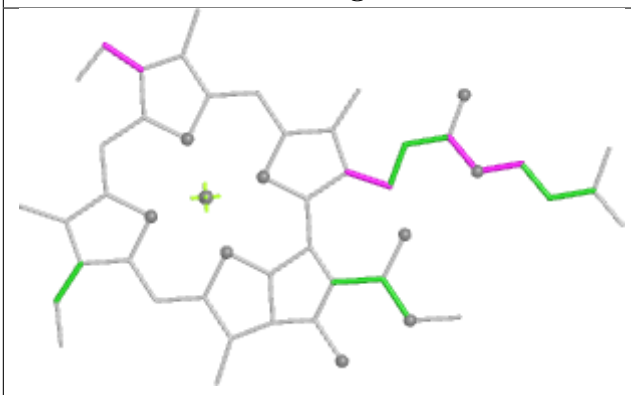

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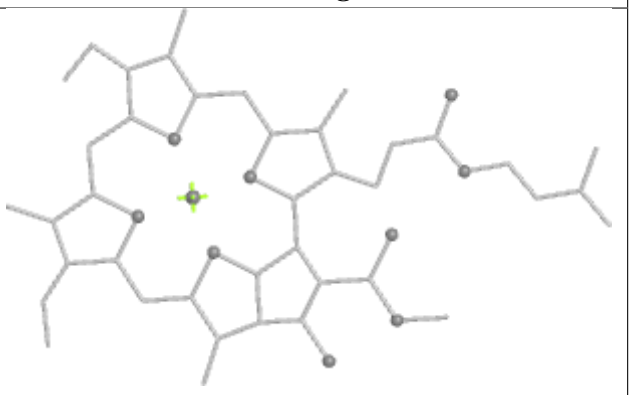
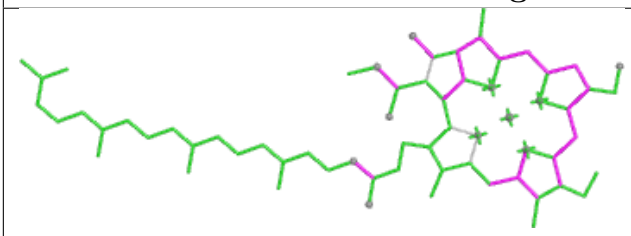


Rings

Ligand CHL AR 605



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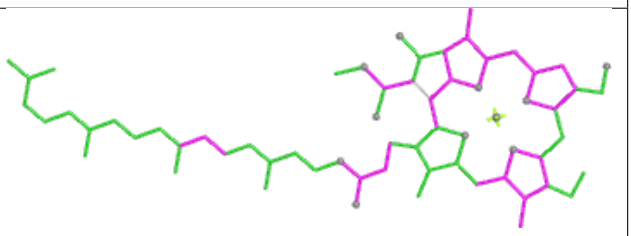

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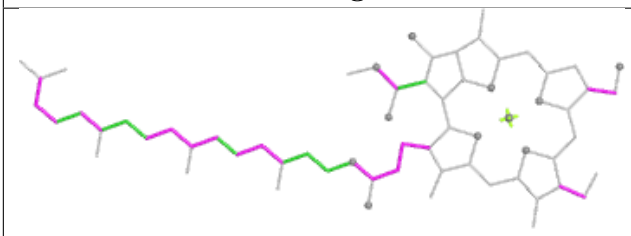

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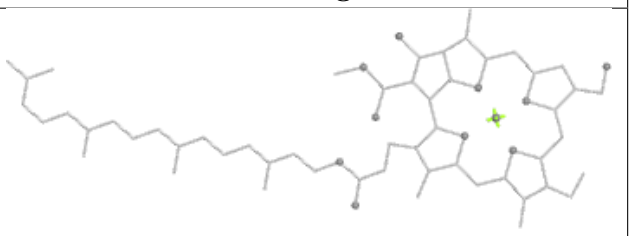
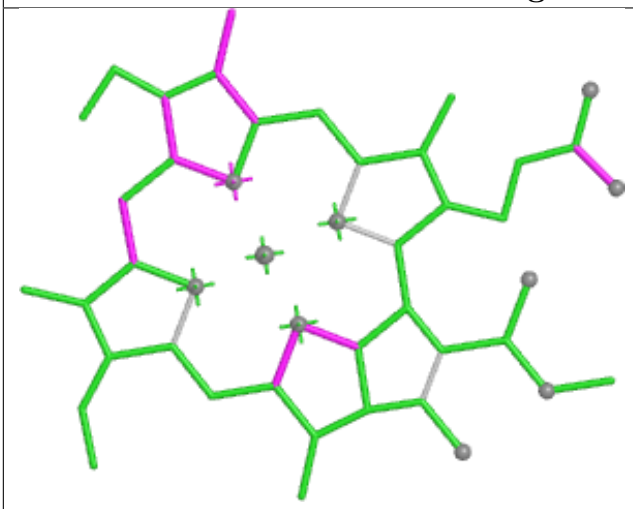


Rings

Ligand CLA q 608



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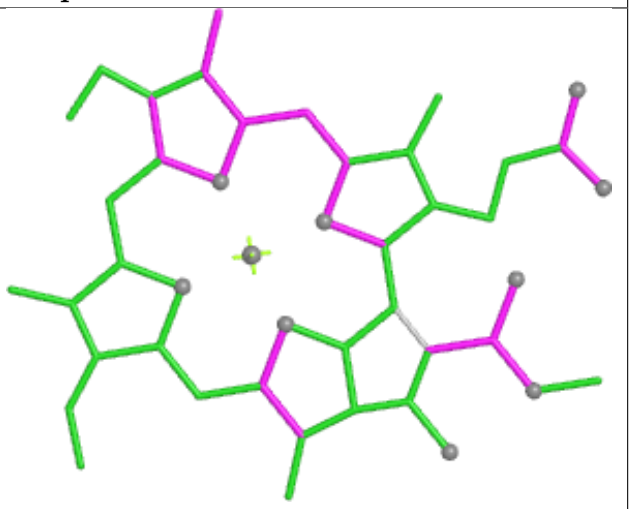

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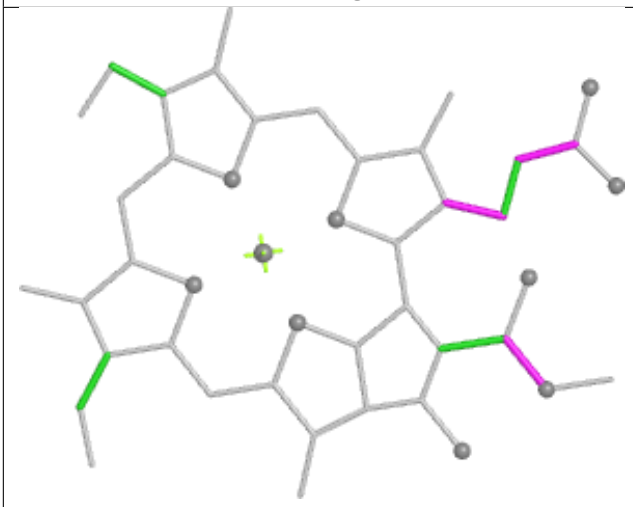
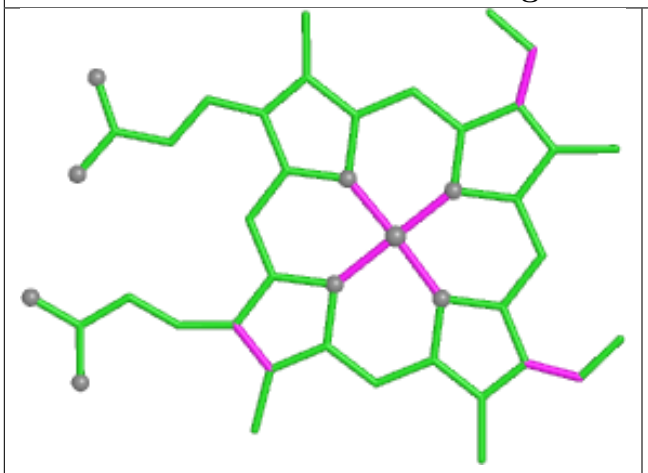


Torsions

Rings

Ligand HEM F 102



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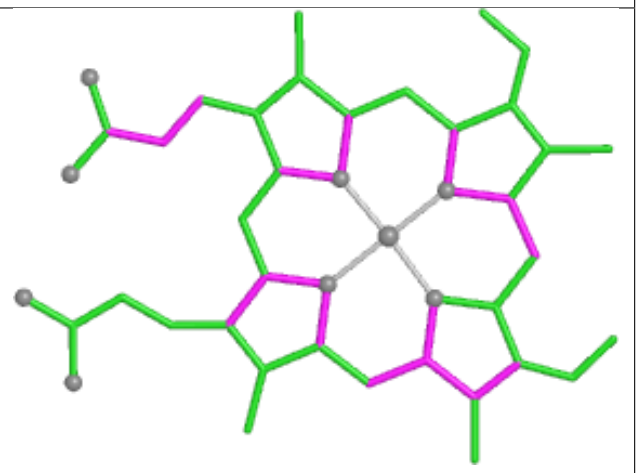

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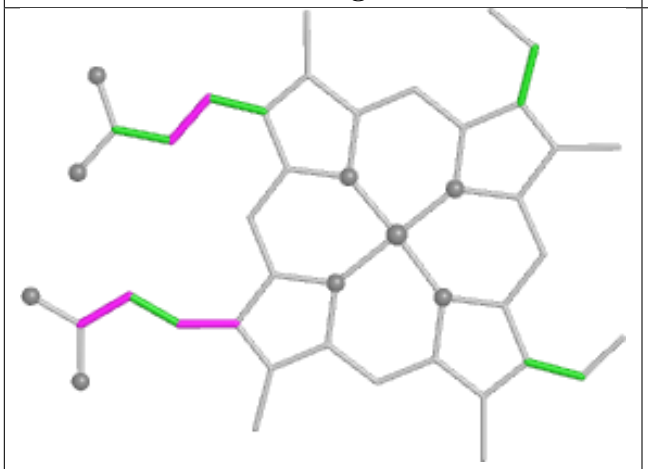

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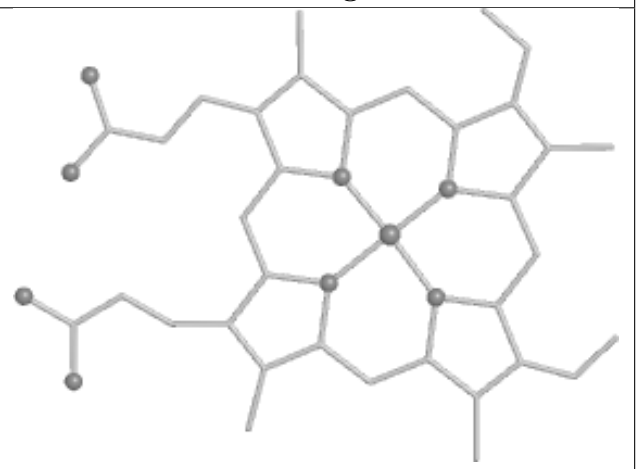

Rings

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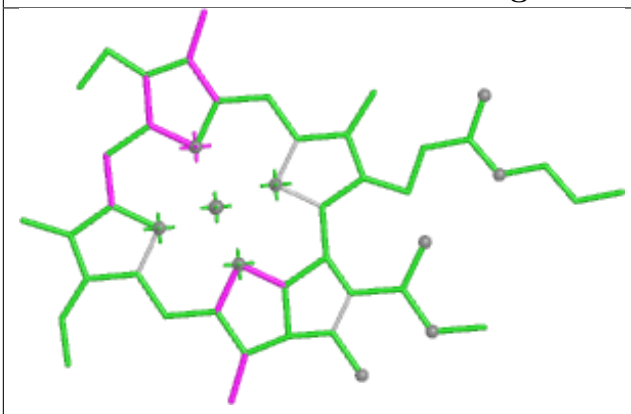
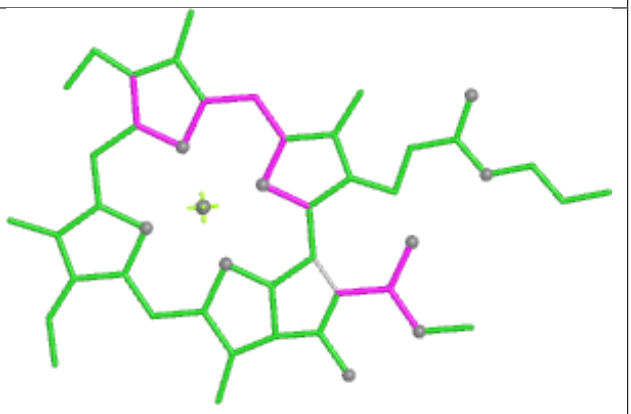
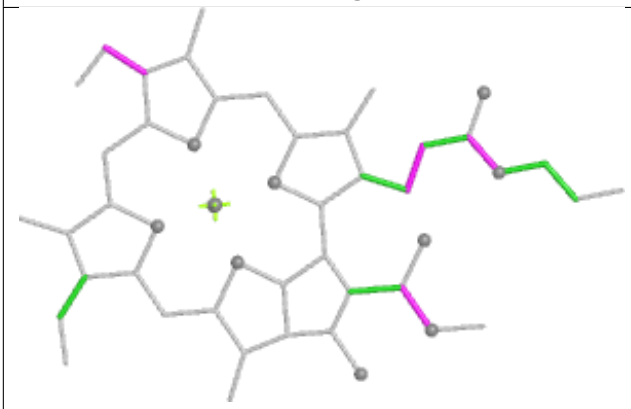
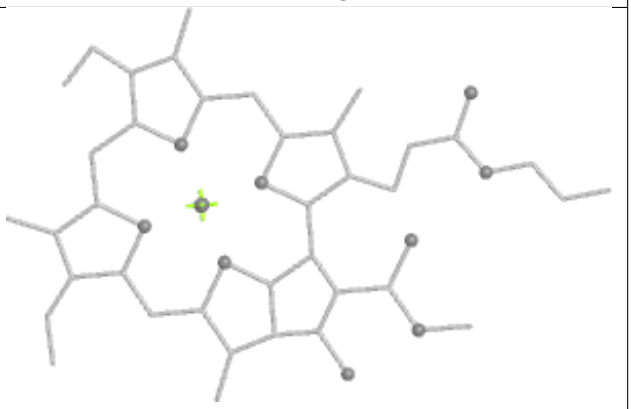
 Bond lengths	 Bond angles
 Torsions	 Rings

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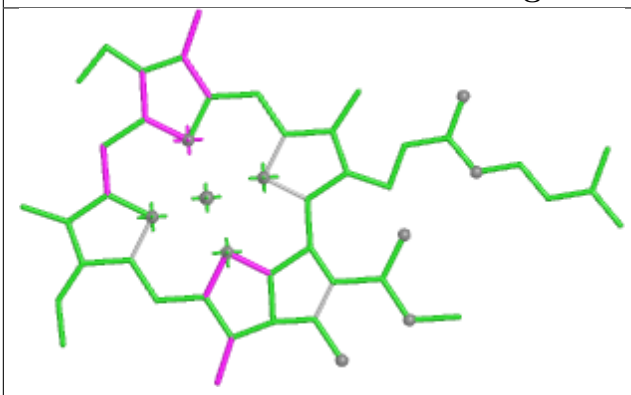
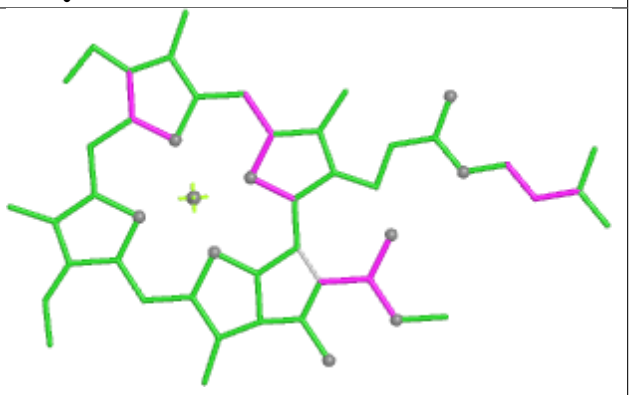
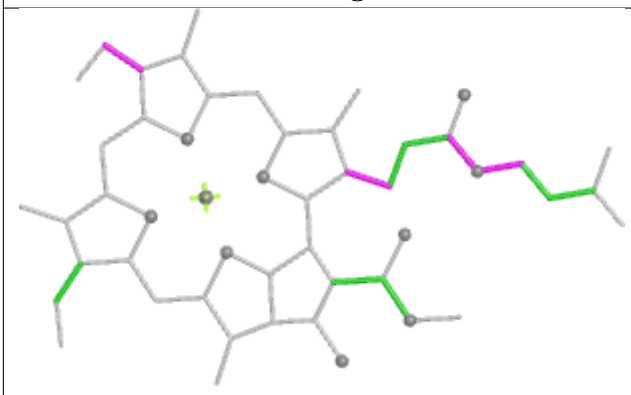
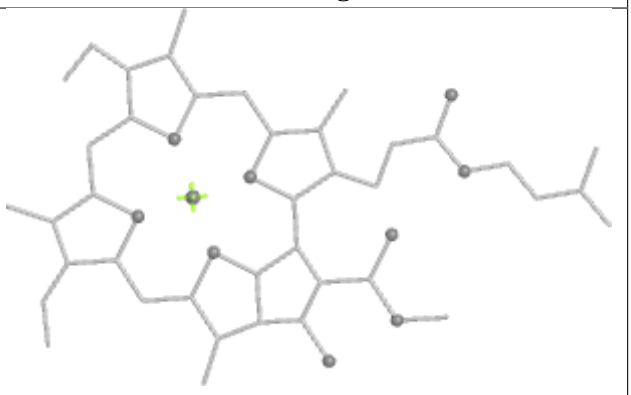
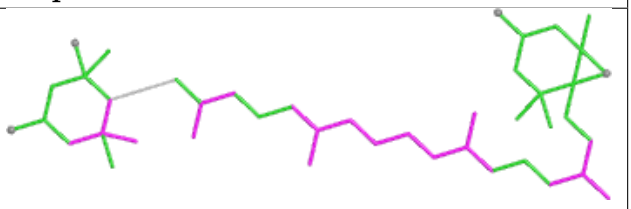
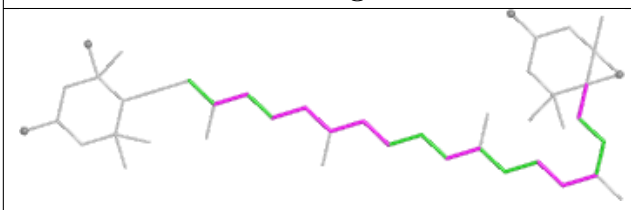
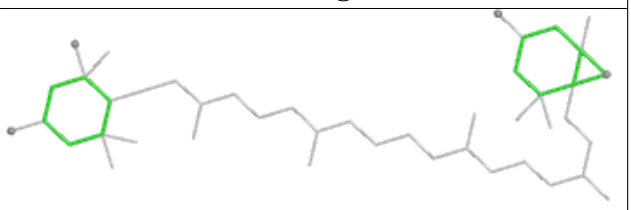
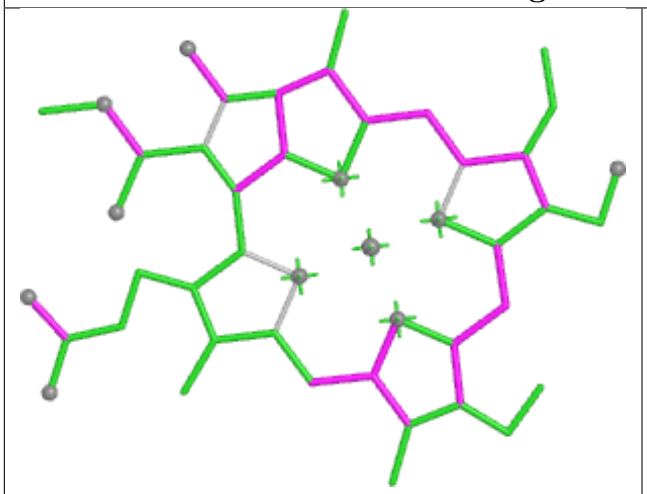
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NEX p 616	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 0 617



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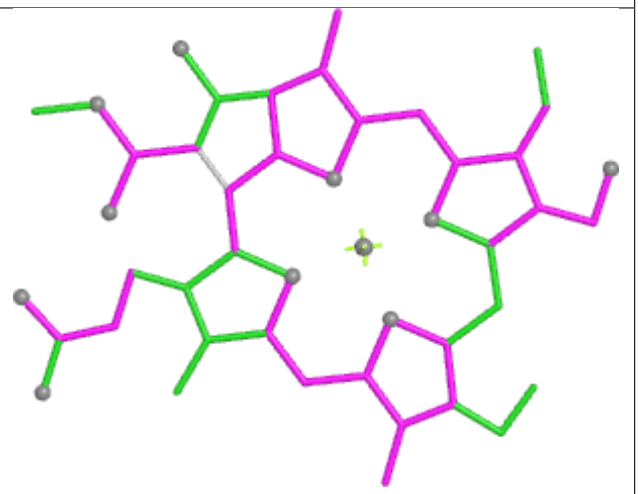

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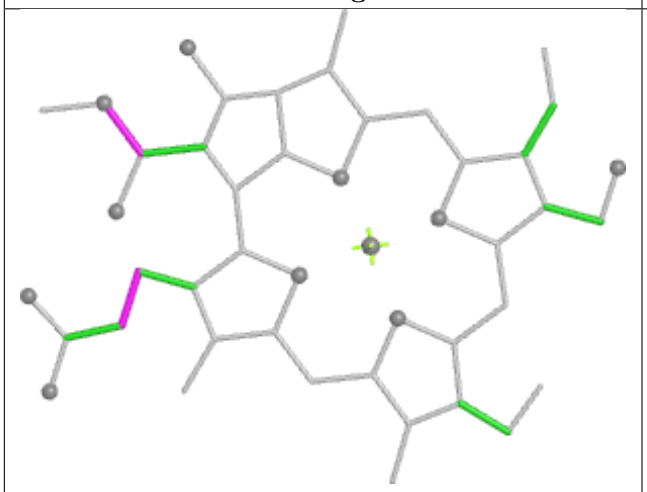

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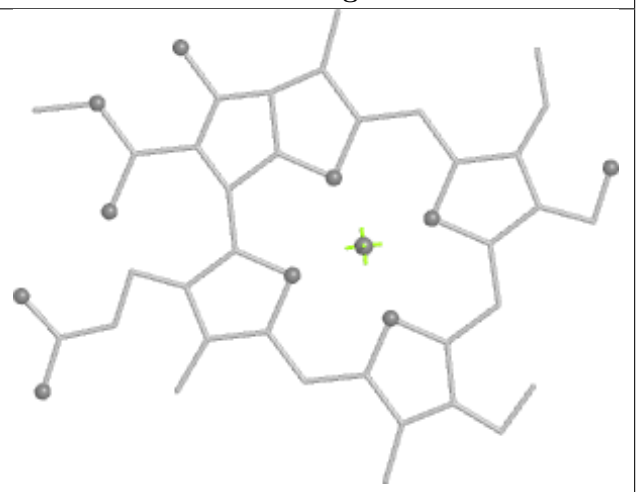
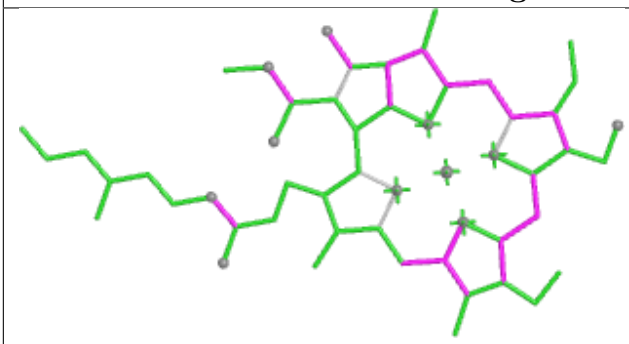
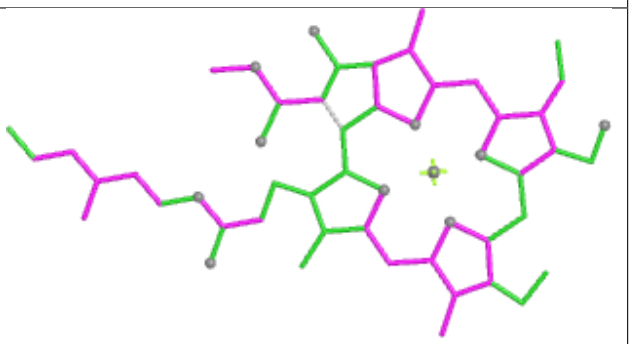
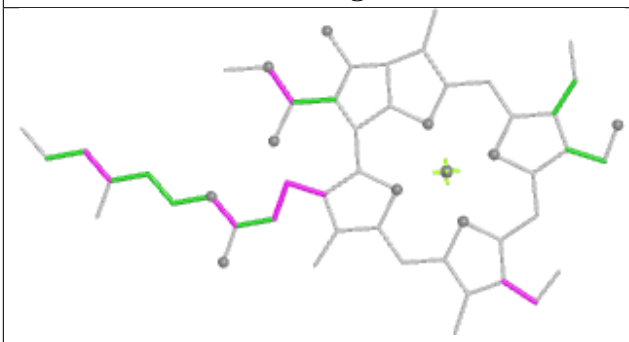
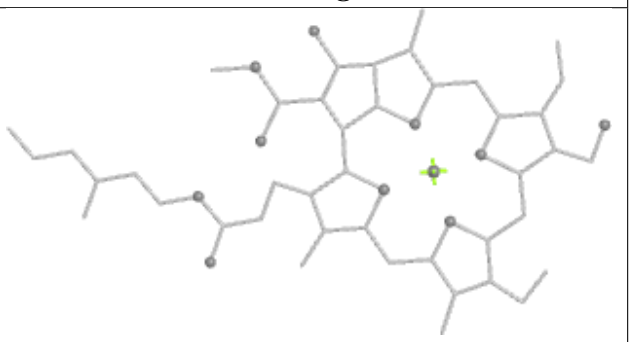
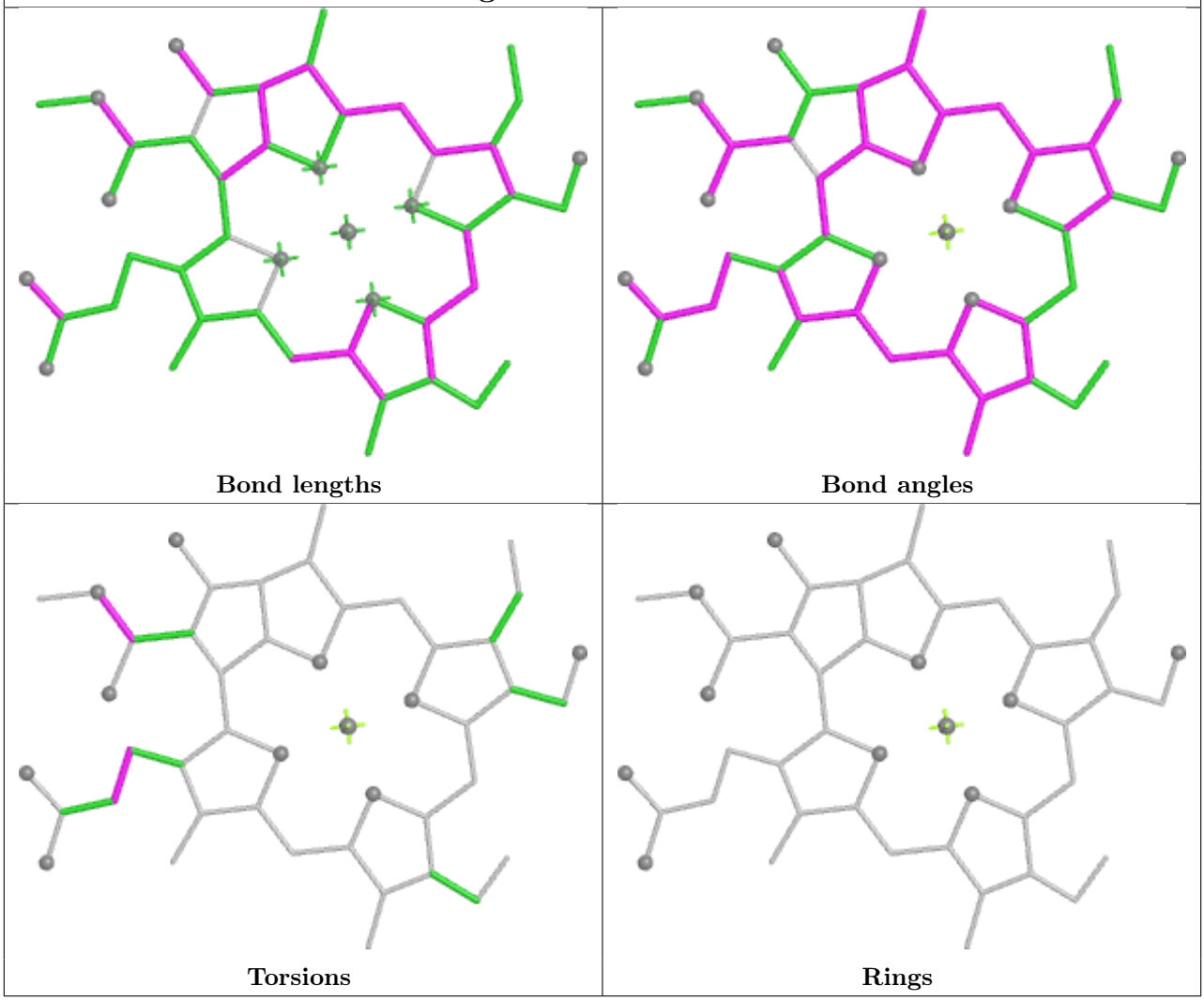


Rings

Ligand CHL AD 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL AD 317



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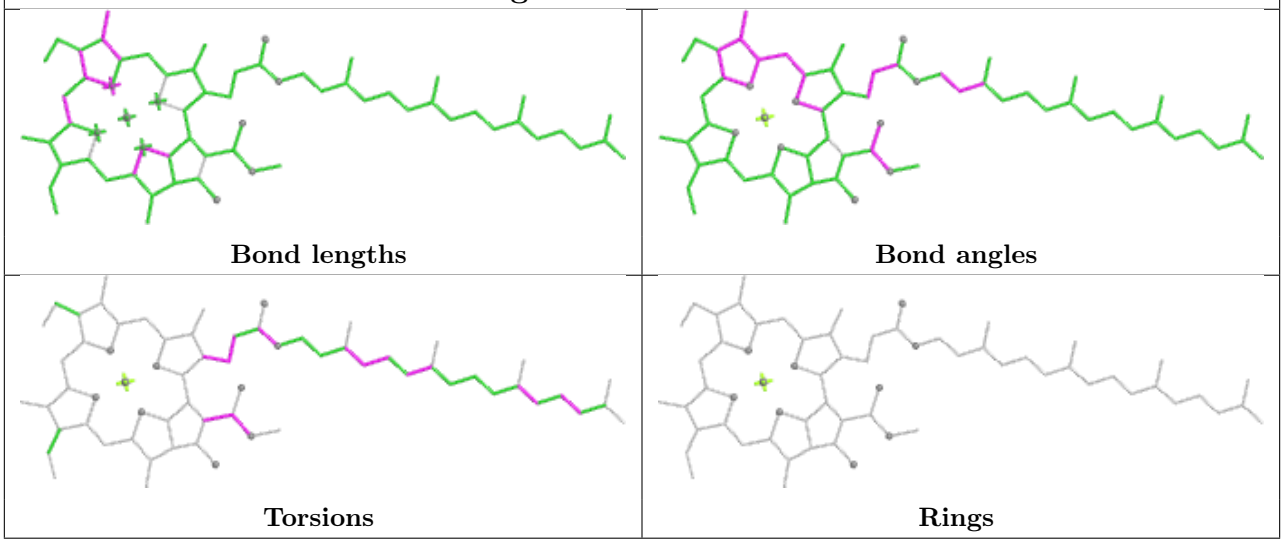

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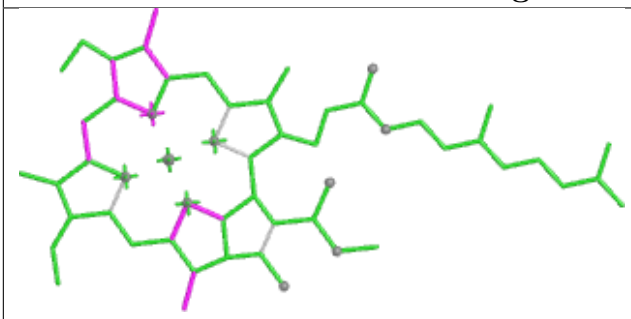
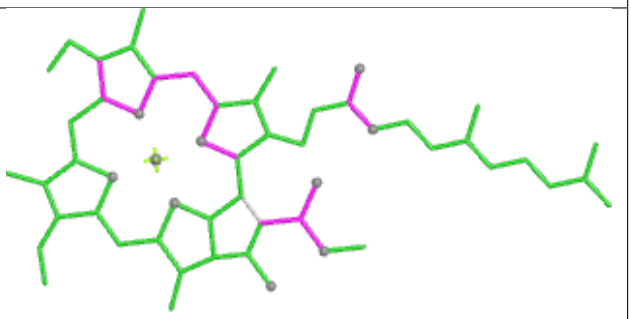


Bond lengths



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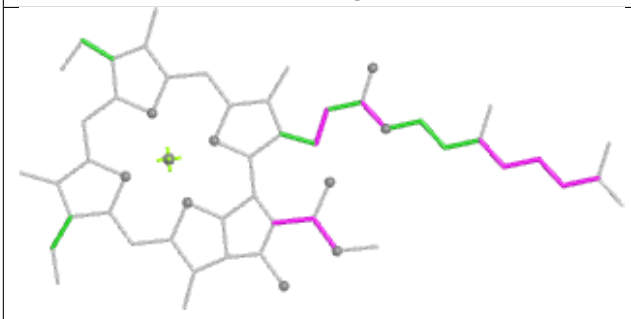

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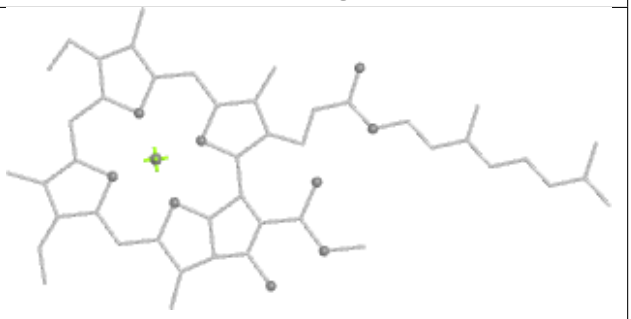
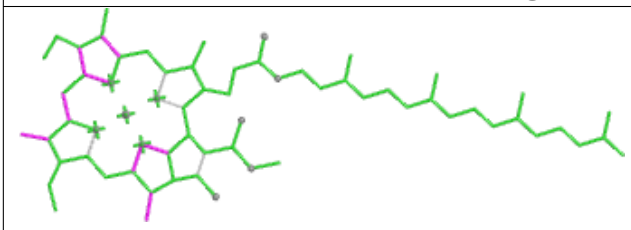


Rings

Ligand CLA O 611



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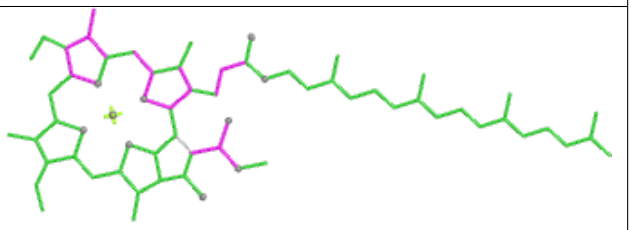

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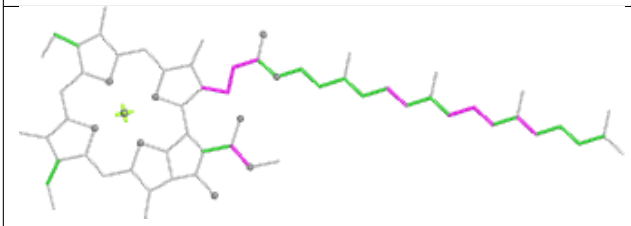

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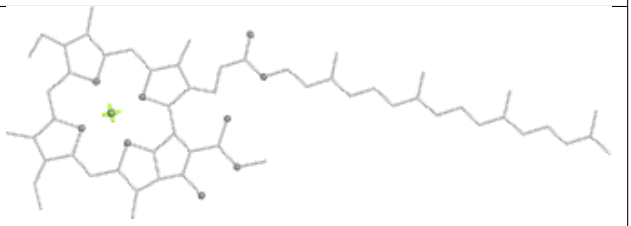

Rings

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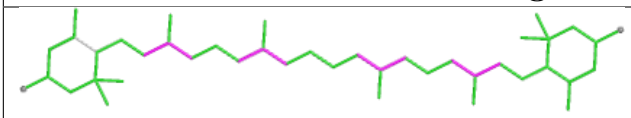

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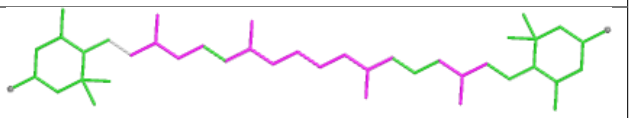

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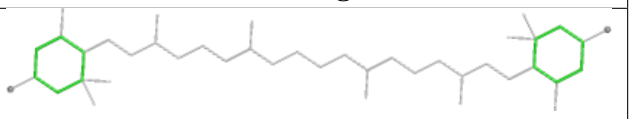

Rings

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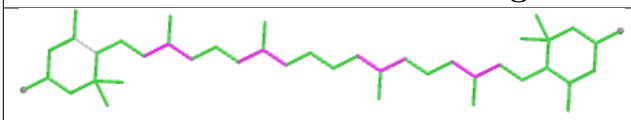
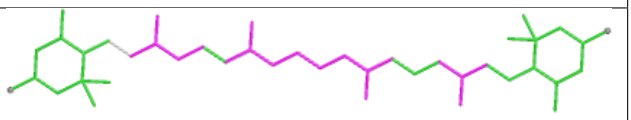
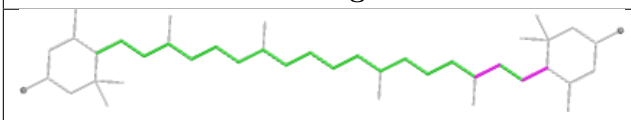
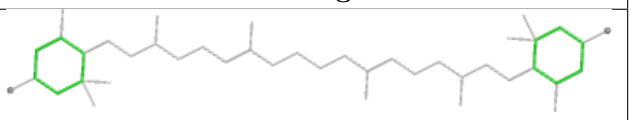
 Bond lengths	 Bond angles
 Torsions	 Rings

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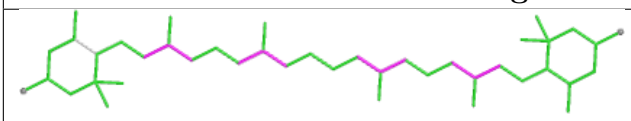
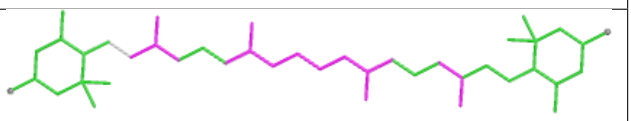
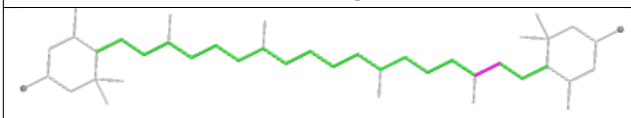
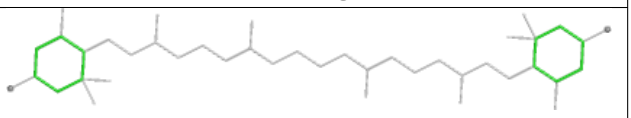
 Bond lengths	 Bond angles
 Torsions	 Rings

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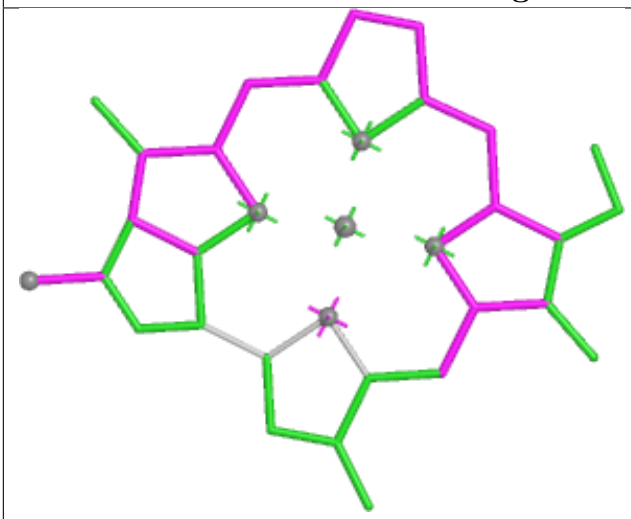
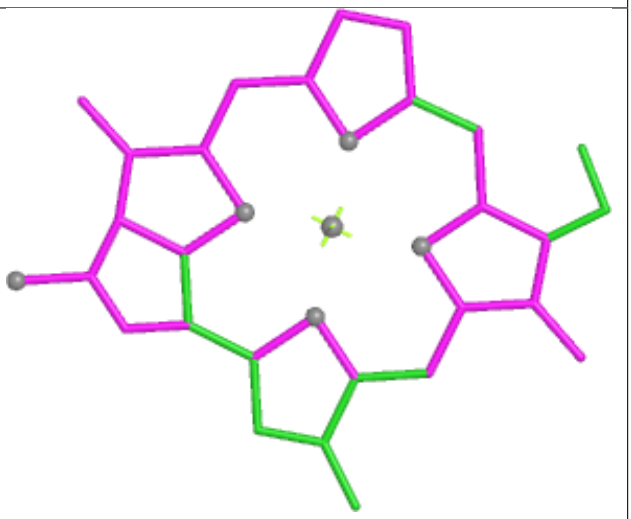
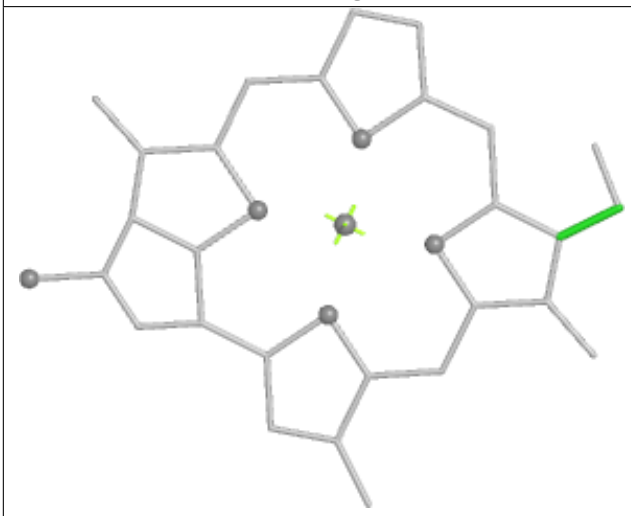
 Bond lengths	 Bond angles
 Torsions	Rings

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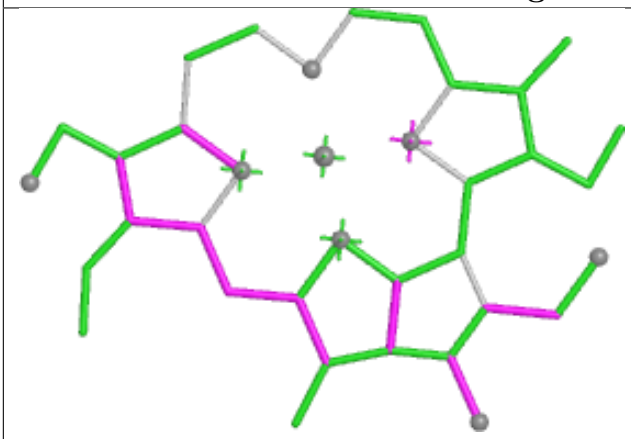
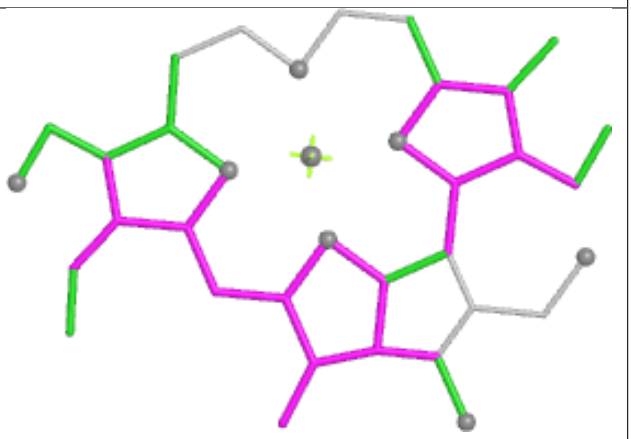
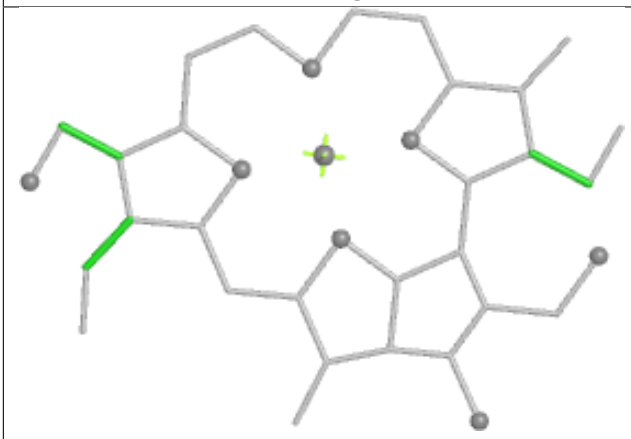
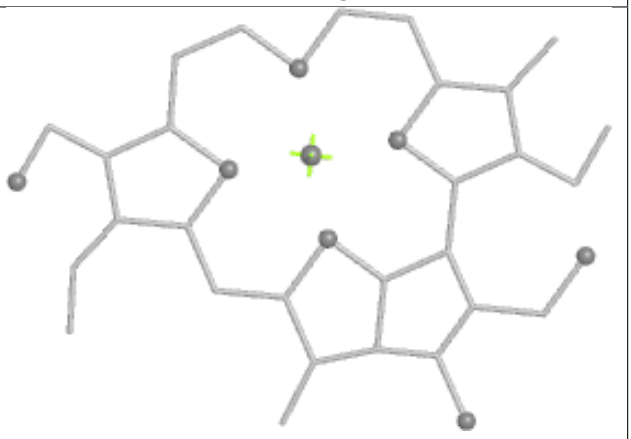
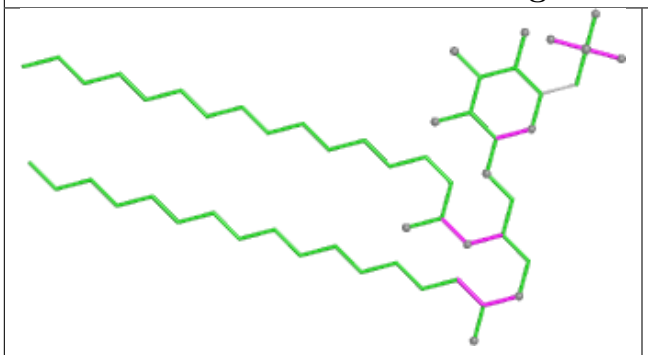
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD J 410



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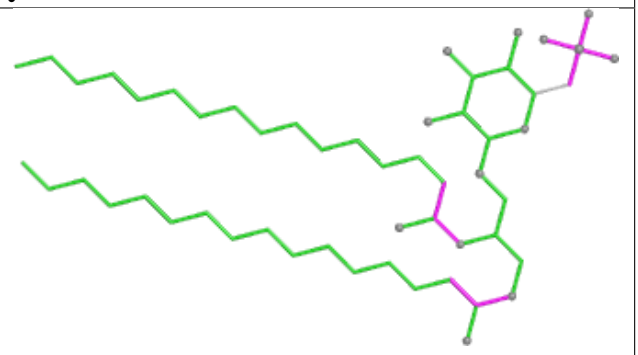

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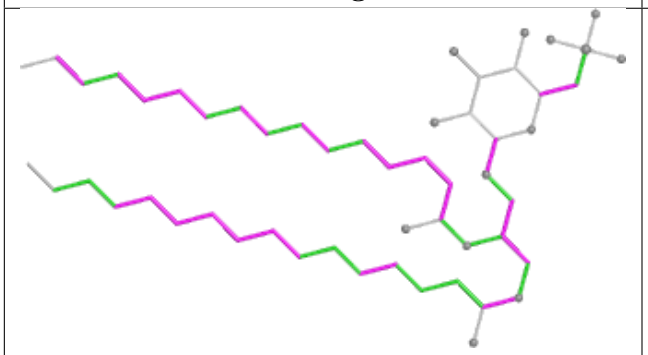

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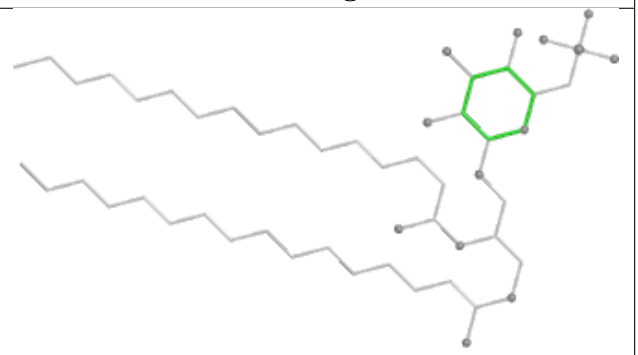
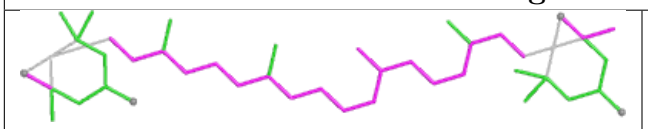


Rings

Ligand XAT 9 618



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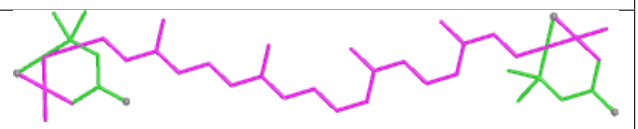

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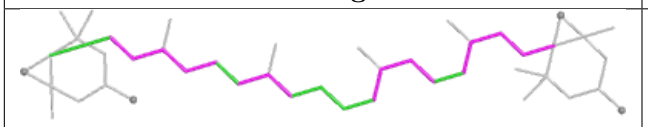

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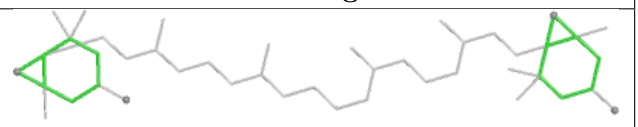

Rings

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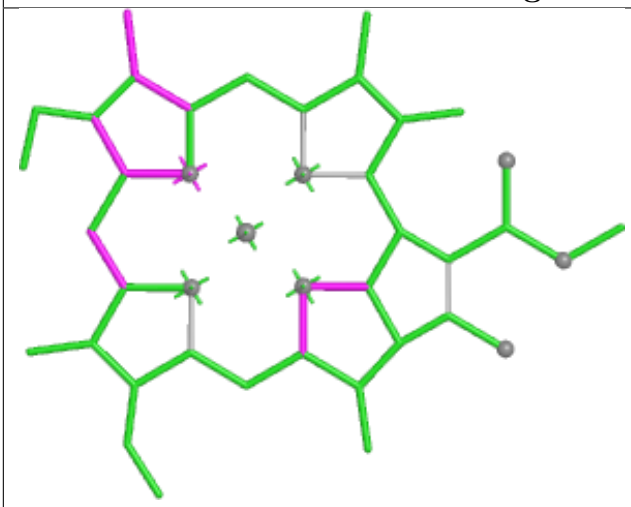

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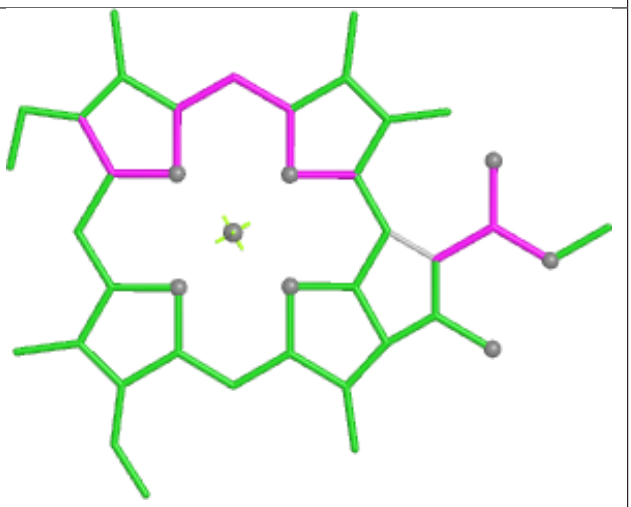

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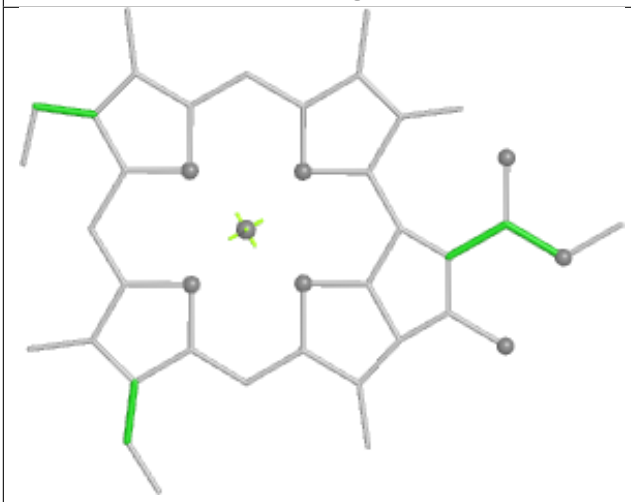

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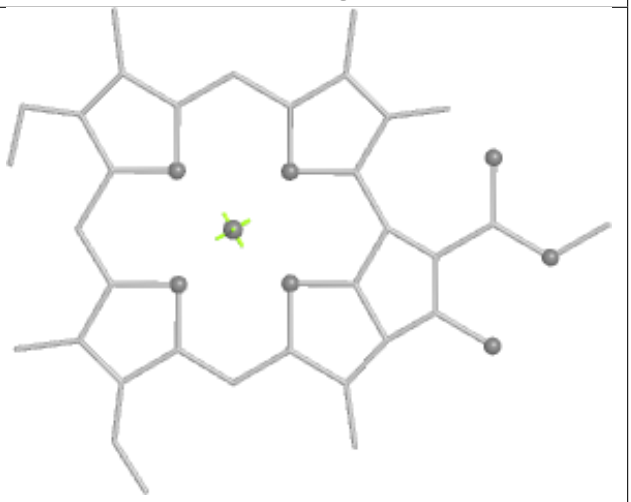

Rings

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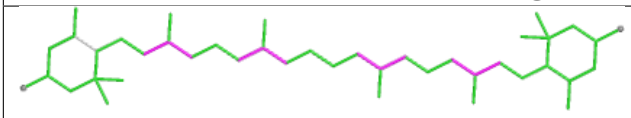

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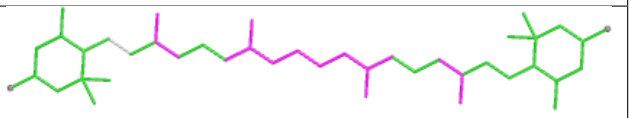
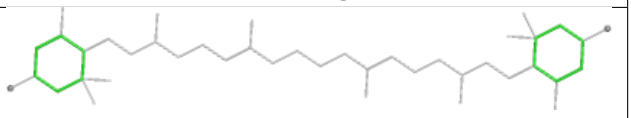


Bond angles

Torsions



Rings

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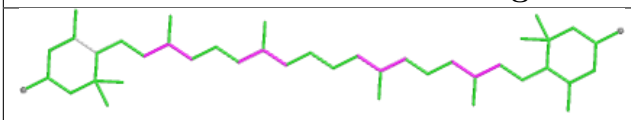
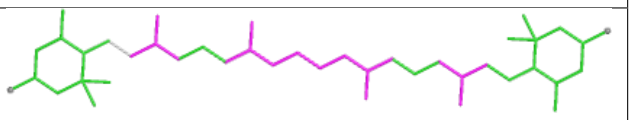
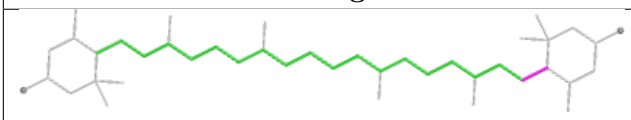
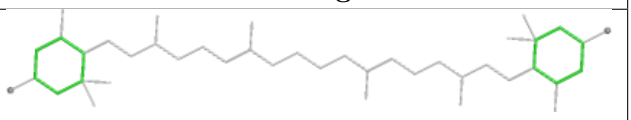
 Bond lengths	 Bond angles
 Torsions	 Rings

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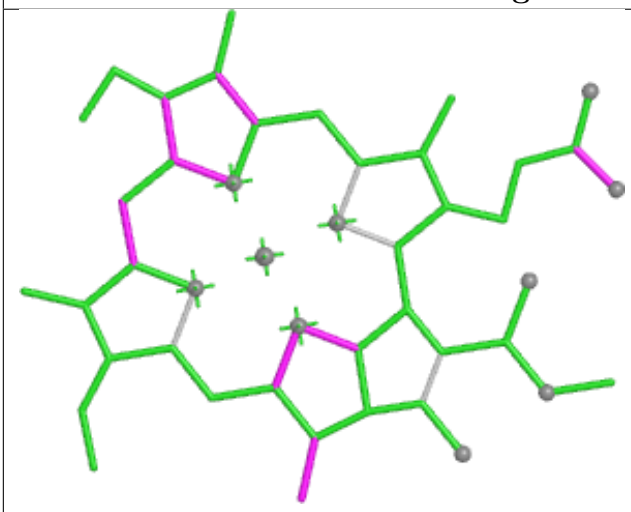
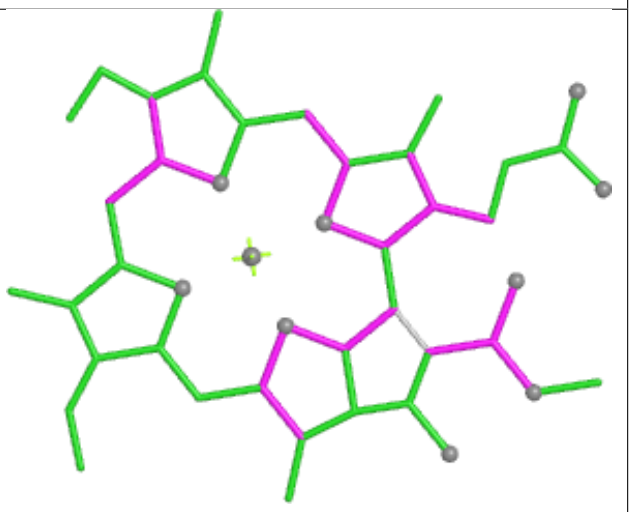
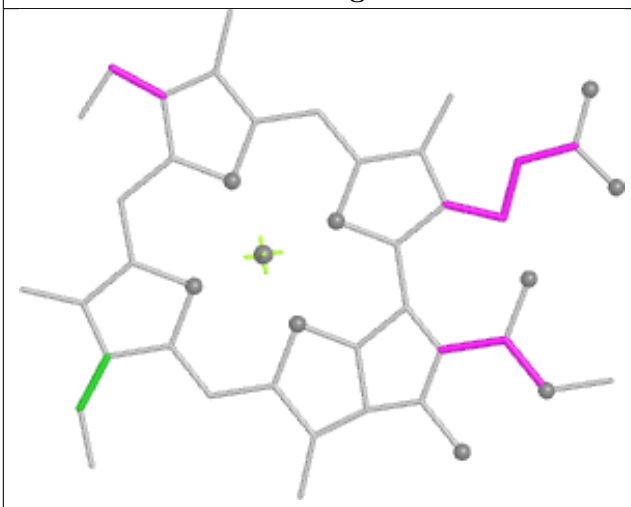
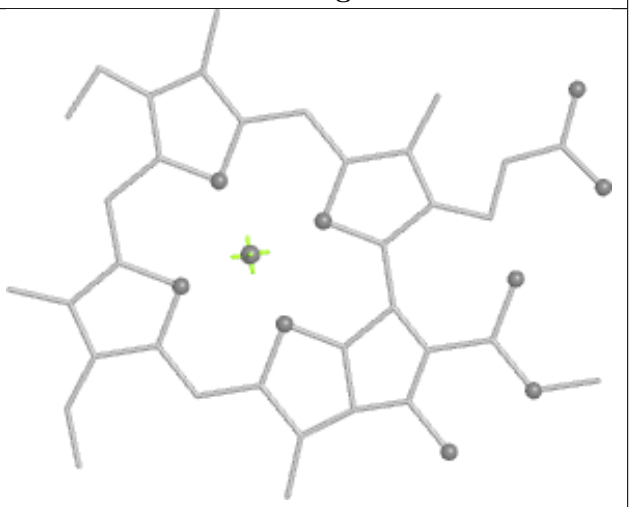
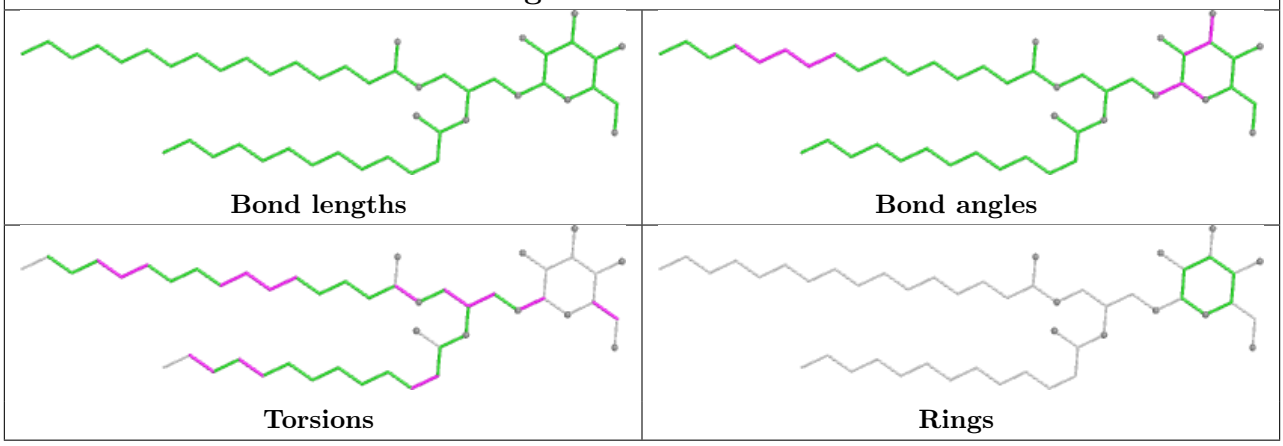
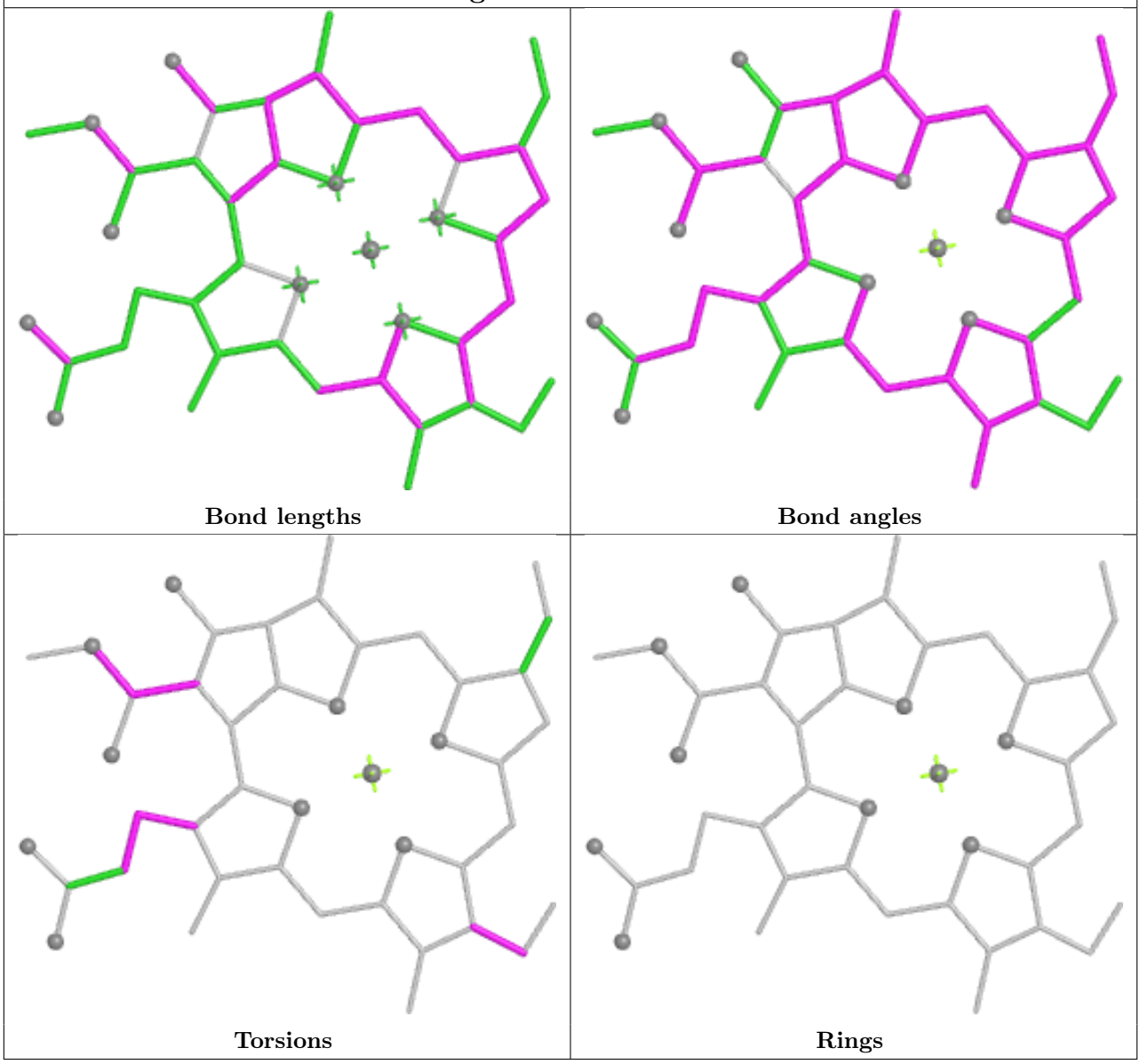
 Bond lengths	 Bond angles
 Torsions	 Rings

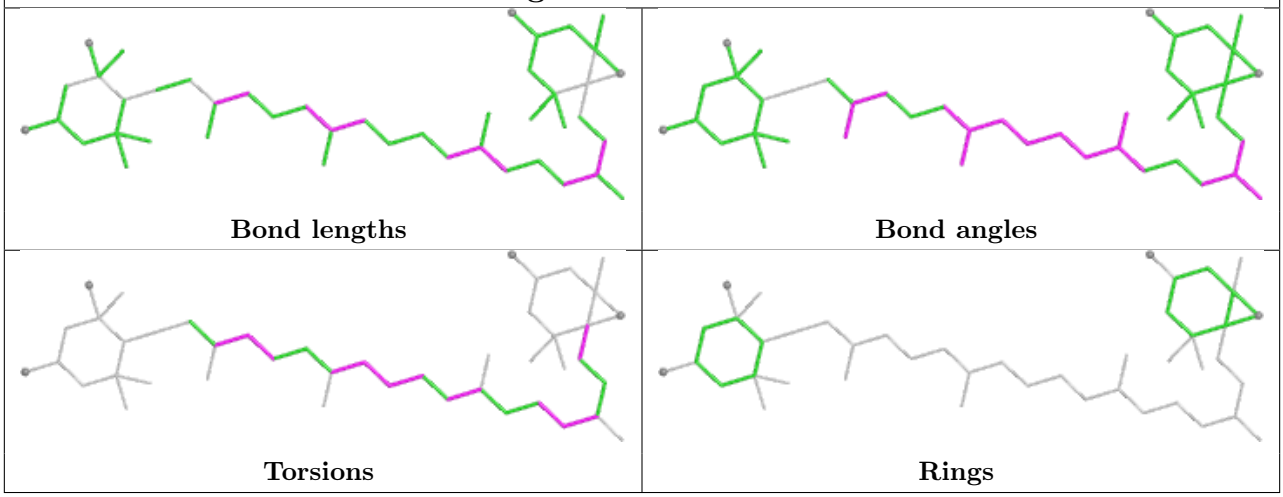
Ligand LMG J 409



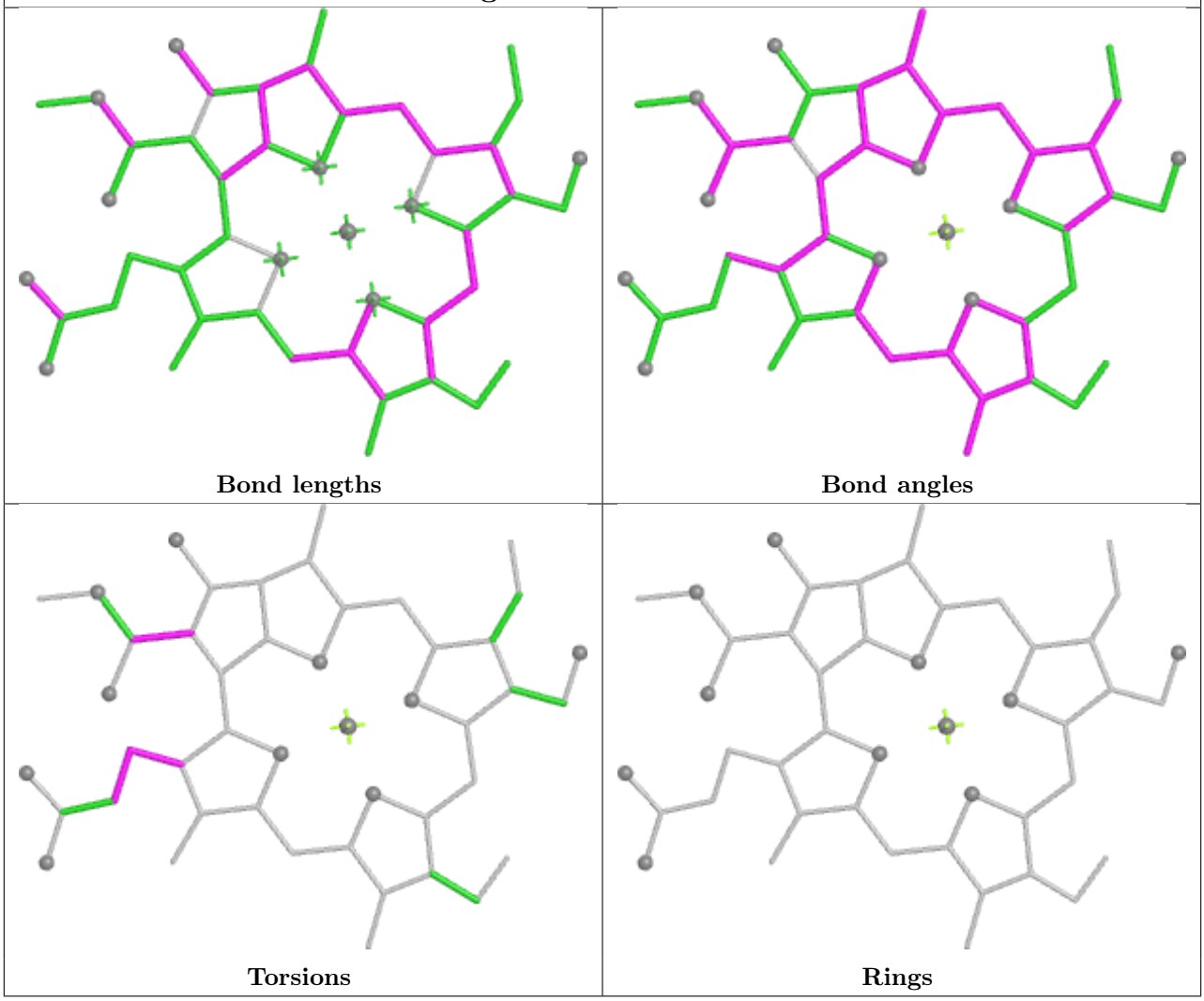
Ligand CHL 0 607

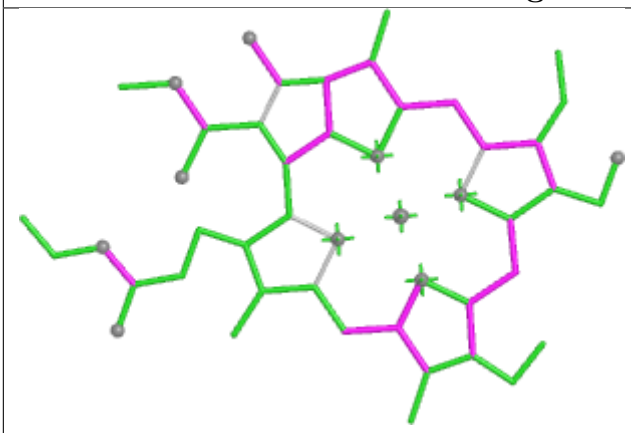
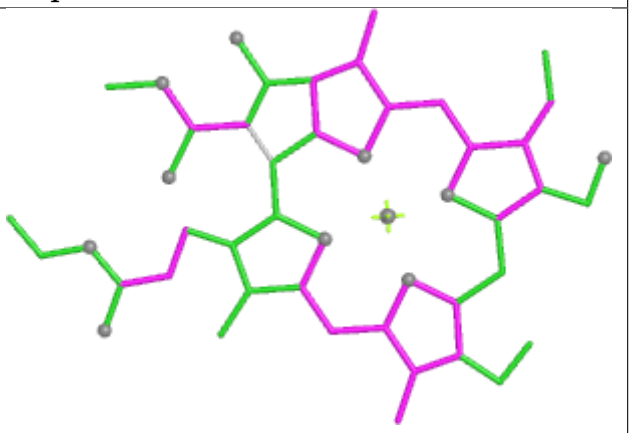
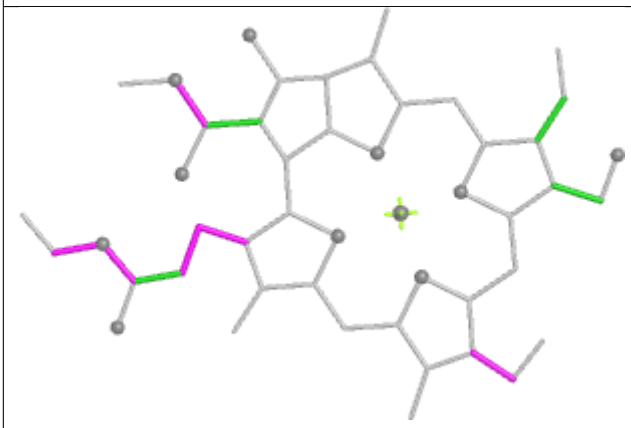
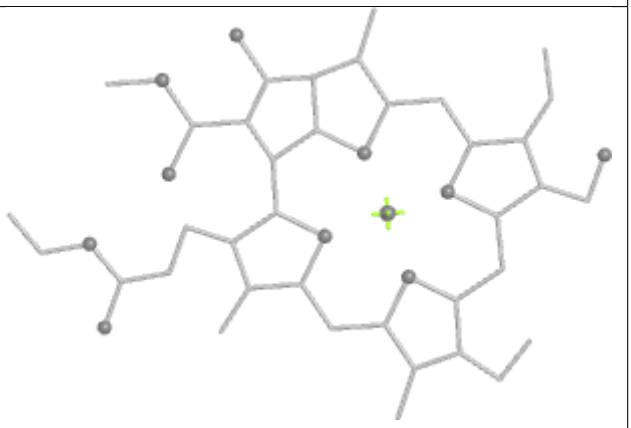


Ligand NEX 9 617

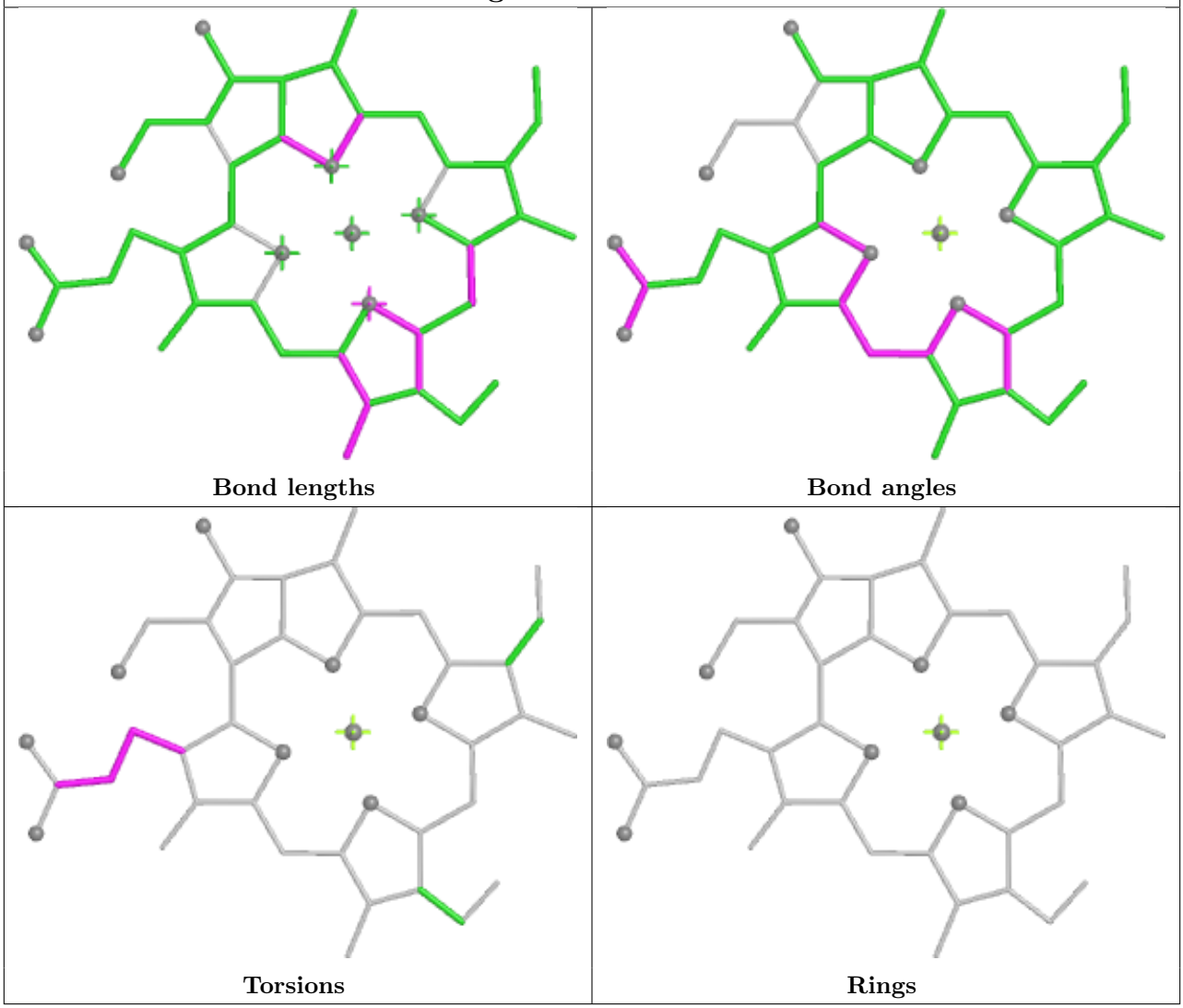


Ligand CHL AE 601

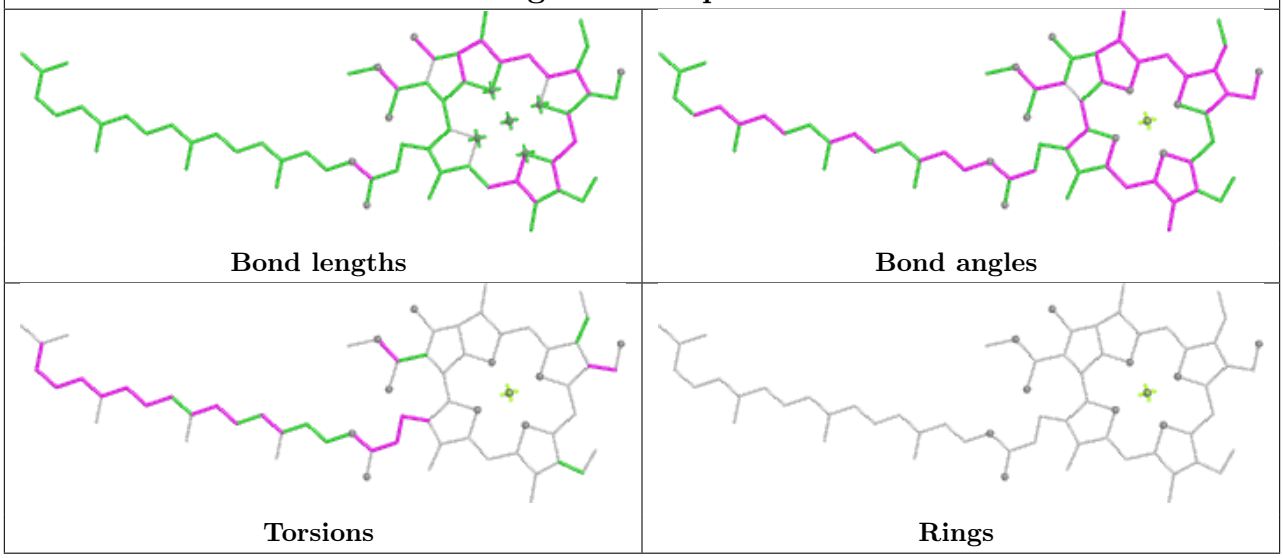


Ligand CHL p 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 611



Ligand CHL p 601



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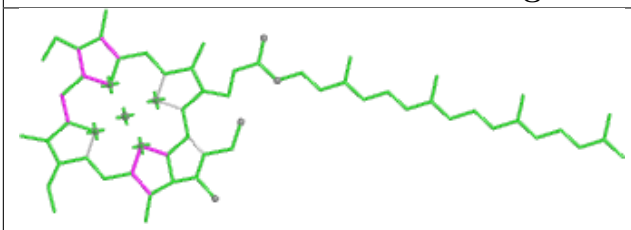
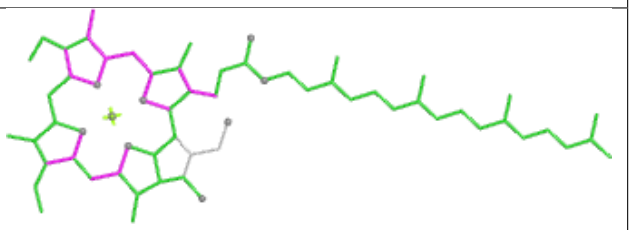
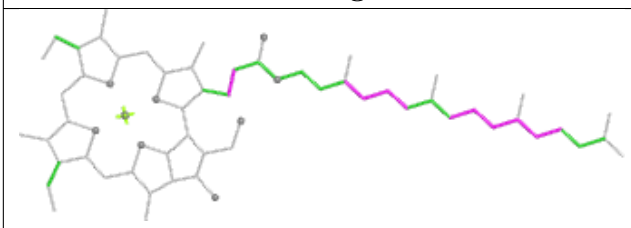
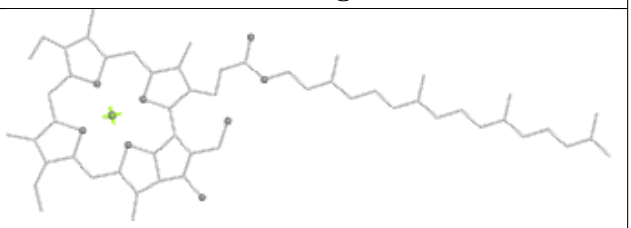
 Bond lengths	 Bond angles
 Torsions	 Rings

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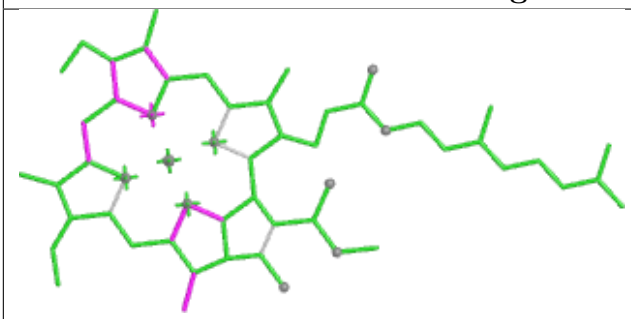
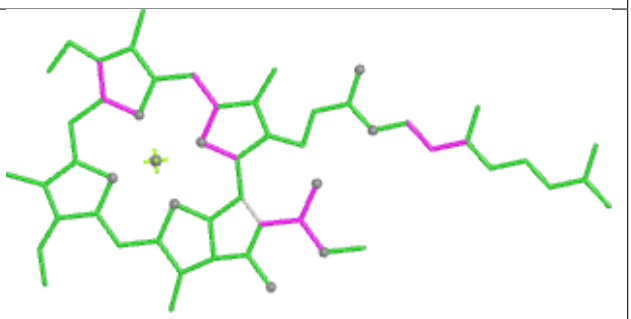
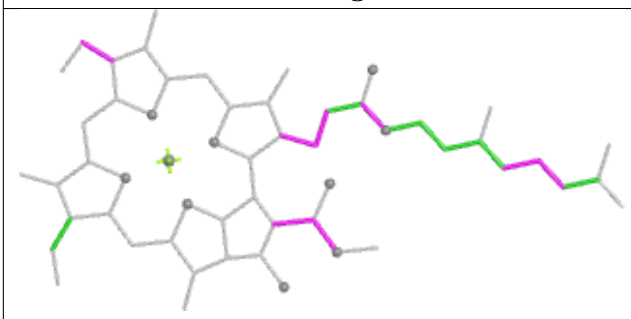
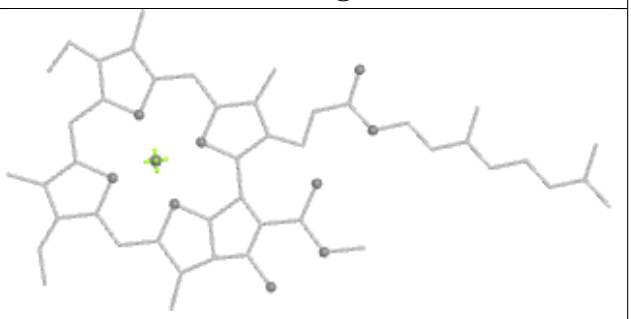
 Bond lengths	 Bond angles
 Torsions	 Rings

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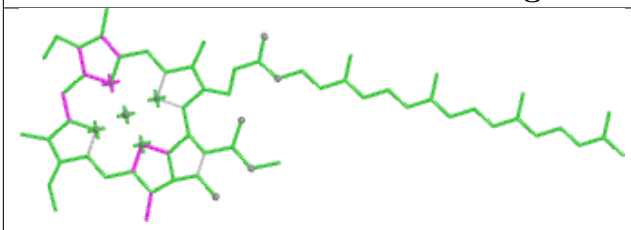
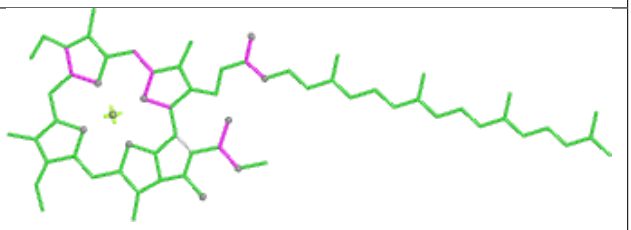
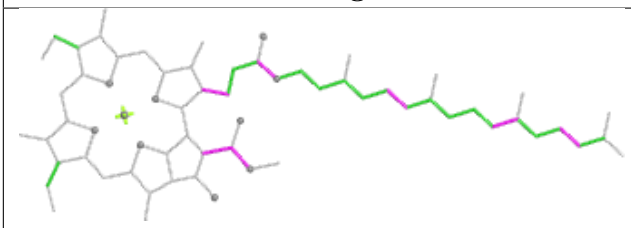
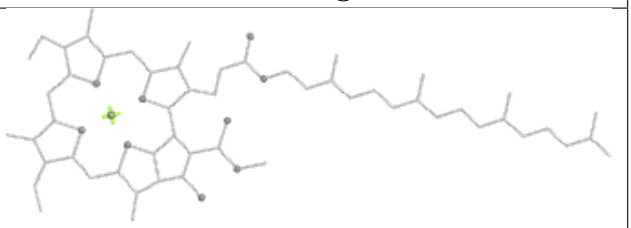
 Bond lengths	 Bond angles
 Torsions	 Rings

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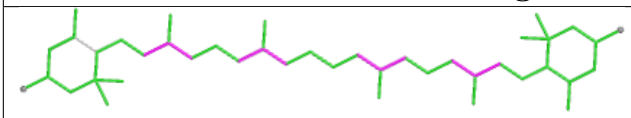
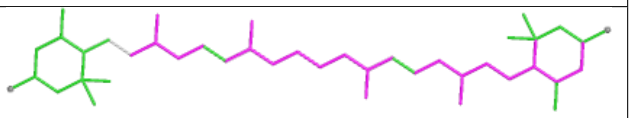
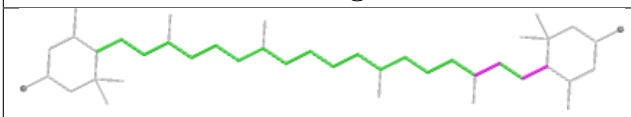
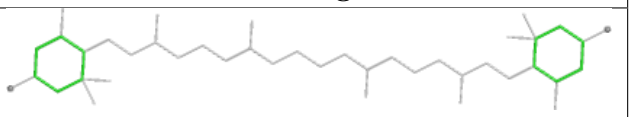
 Bond lengths	 Bond angles
 Torsions	 Rings

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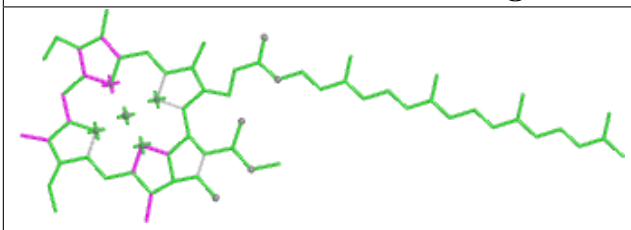
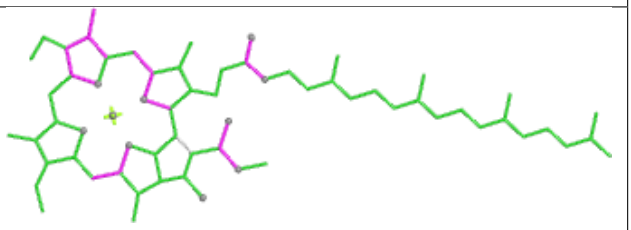
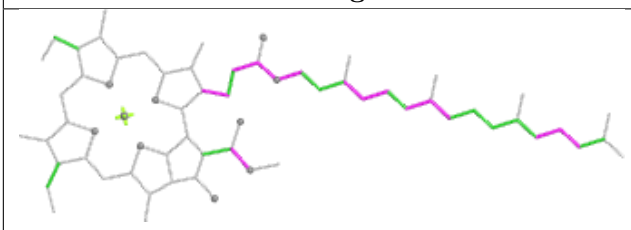
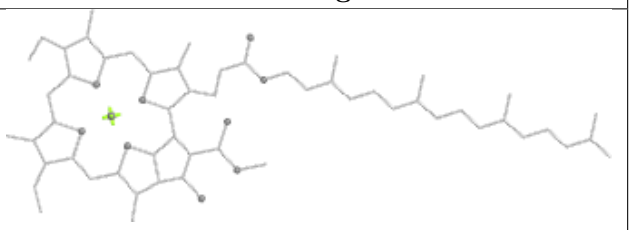
 Bond lengths	 Bond angles
 Torsions	 Rings

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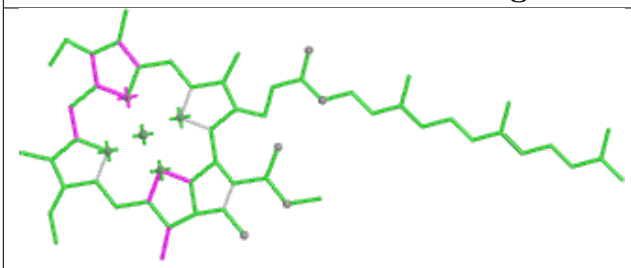
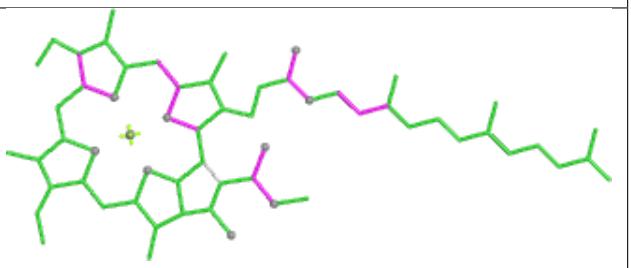
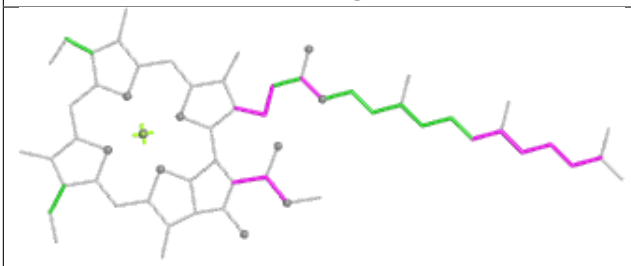
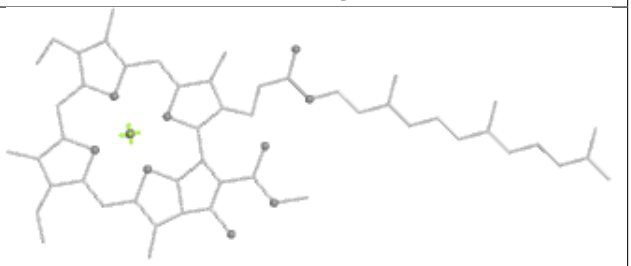
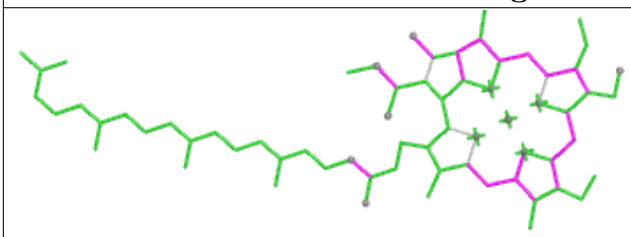
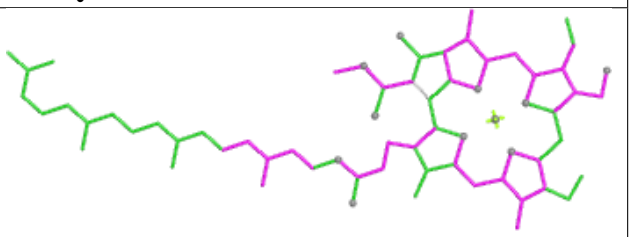
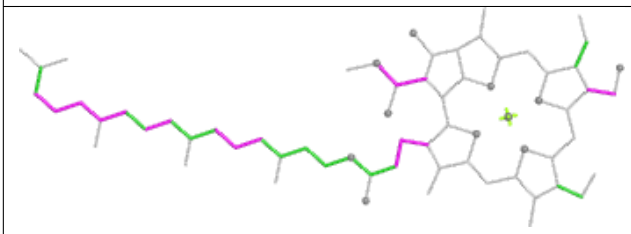
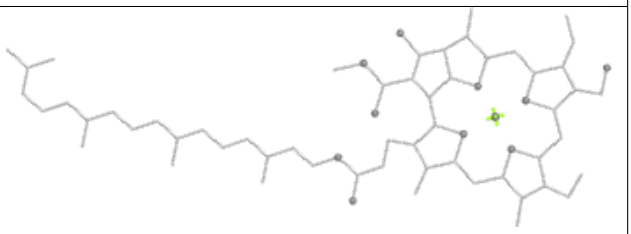
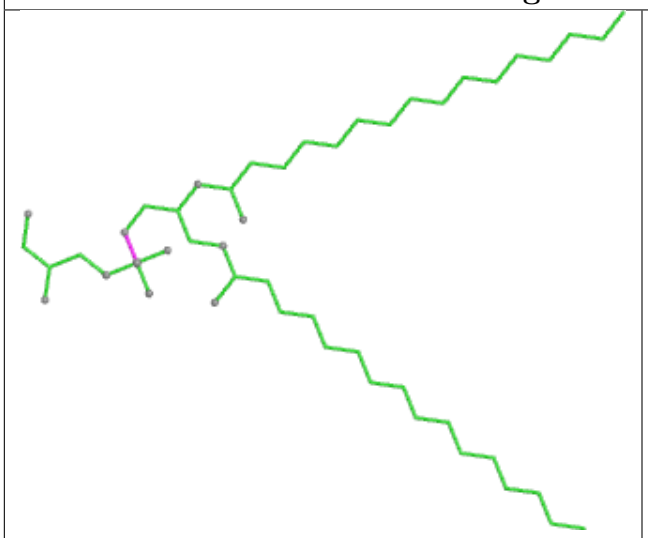
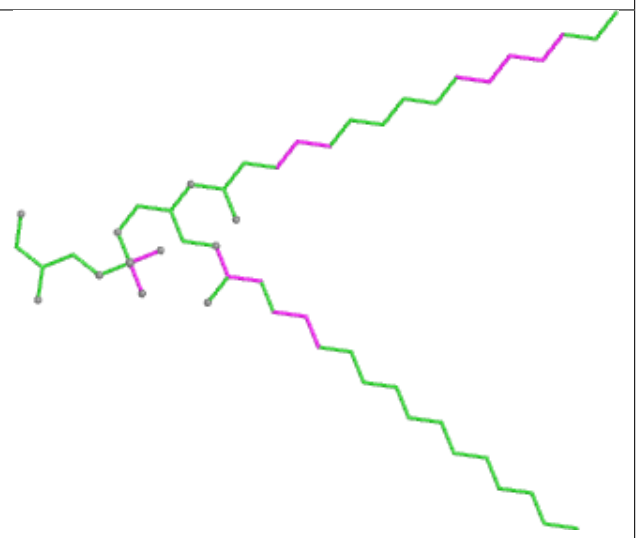
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL AQ 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

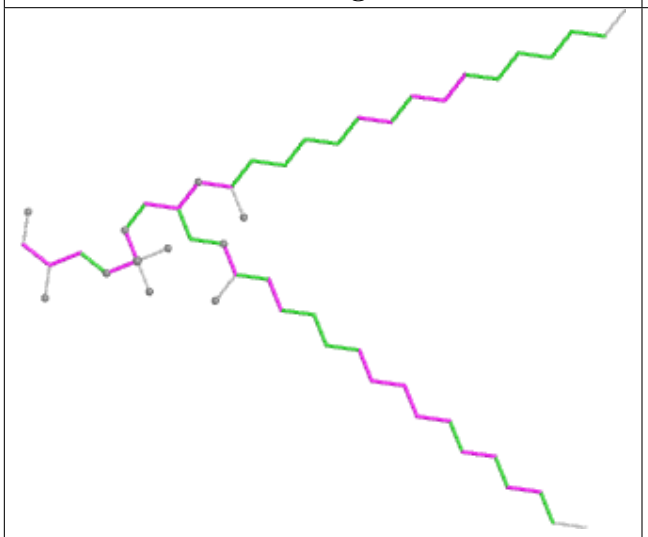
Ligand LHG O 621



Bond lengths



Bond angles



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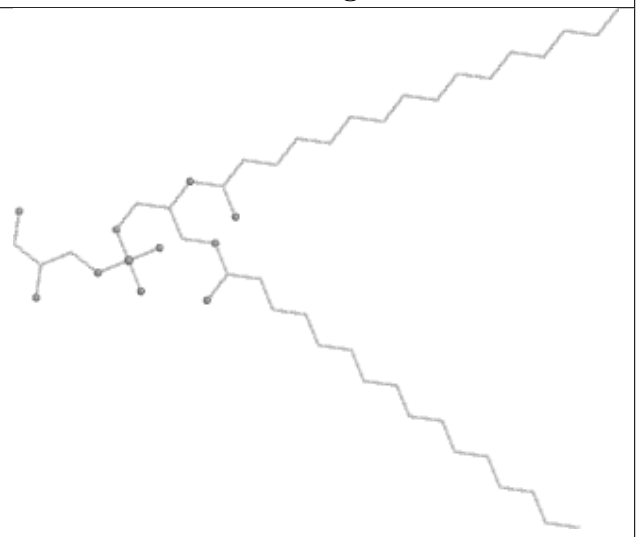
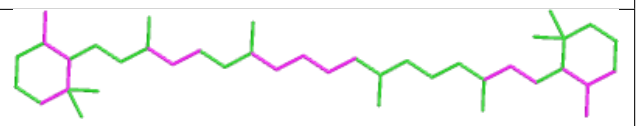


Rings

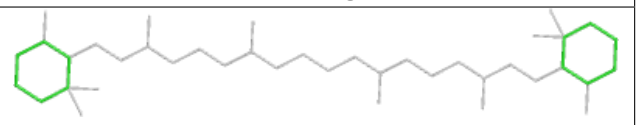
Ligand BCR AO 101

Bond lengths



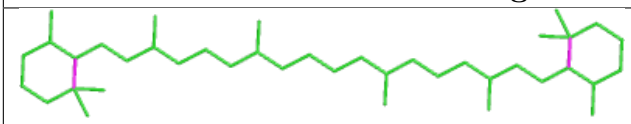
Bond angles

Torsions



Rings

Ligand BCR AV 101



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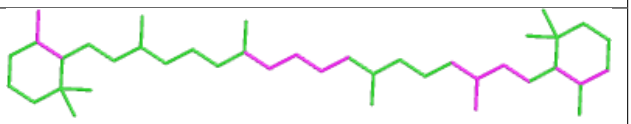

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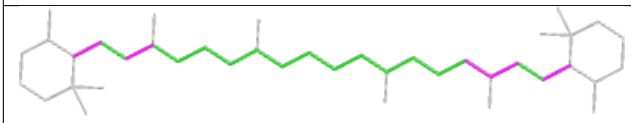

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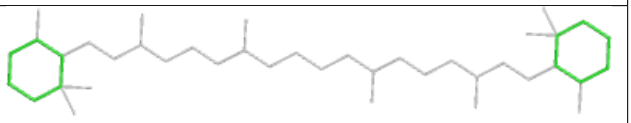
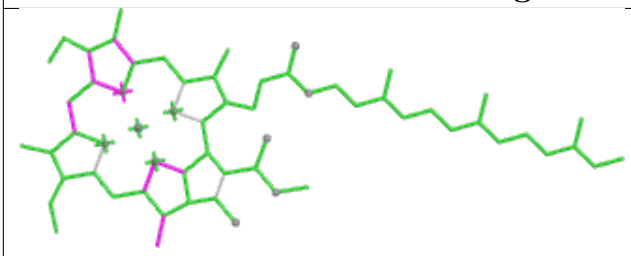
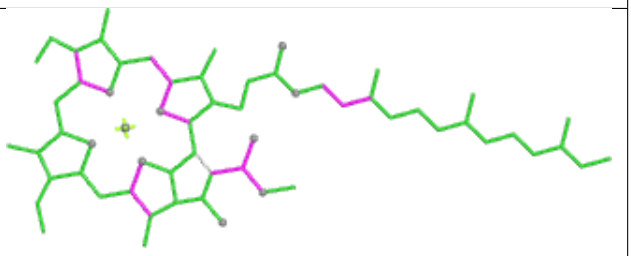


Rings

Ligand CLA AS 303



Bond lengths



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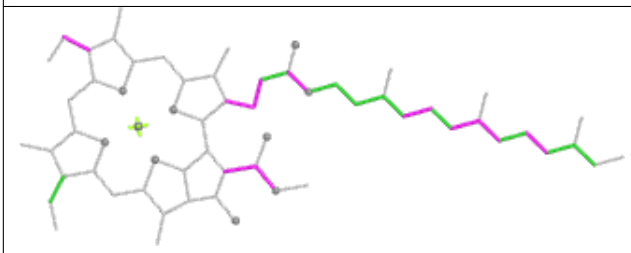

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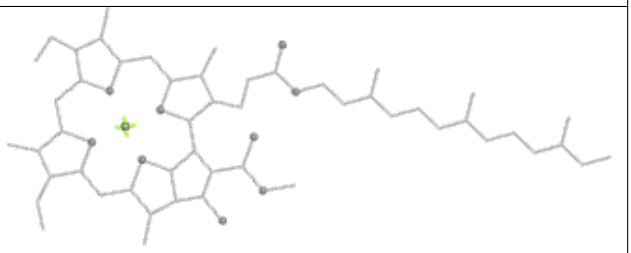
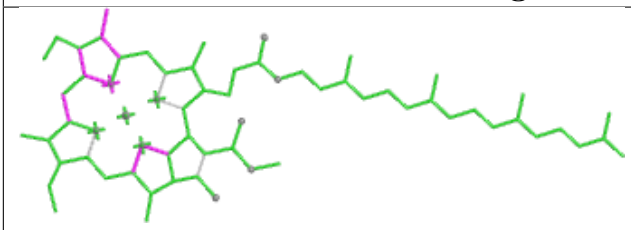
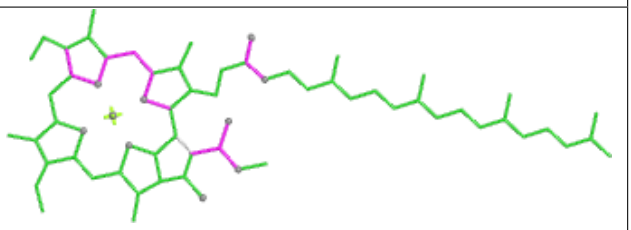


Rings

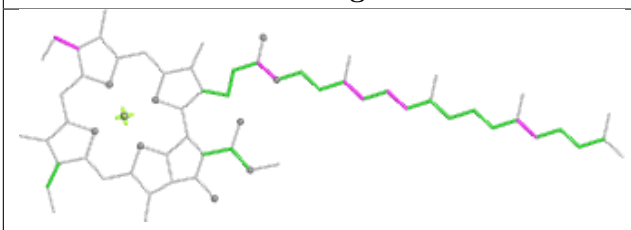
Ligand CLA AH 603



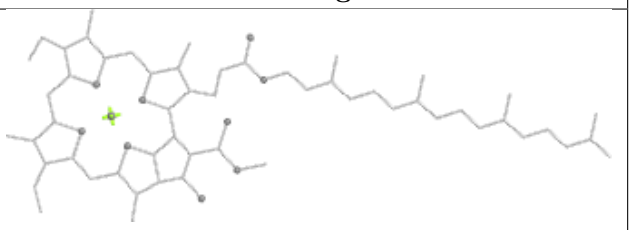
Bond lengths



Bond angles

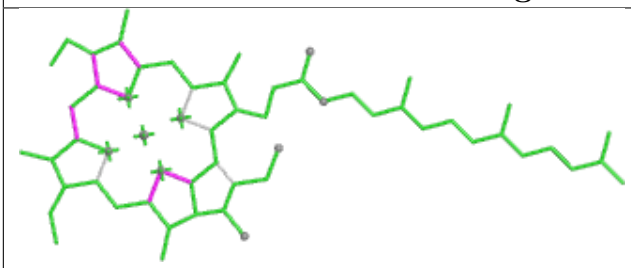


Torsions

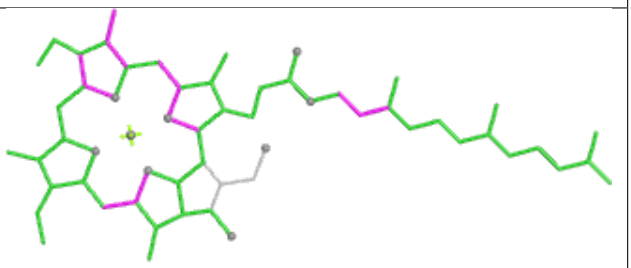


Rings

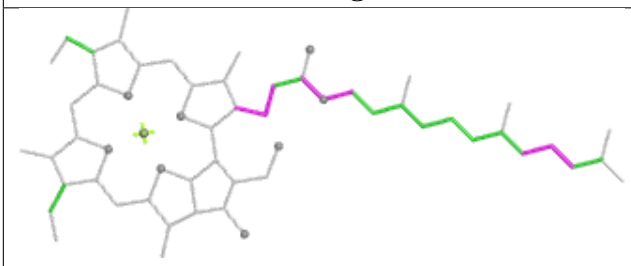
Ligand CLA AJ 409



Bond lengths



Bond angles



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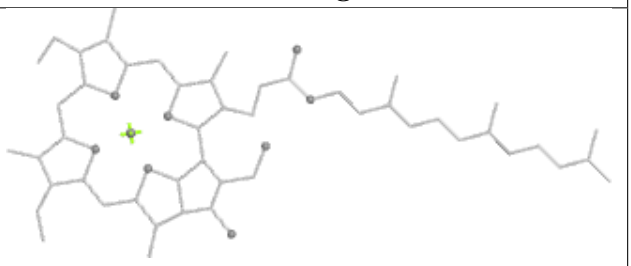
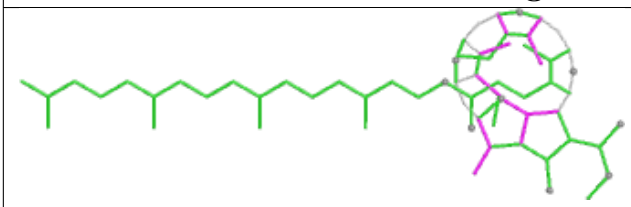
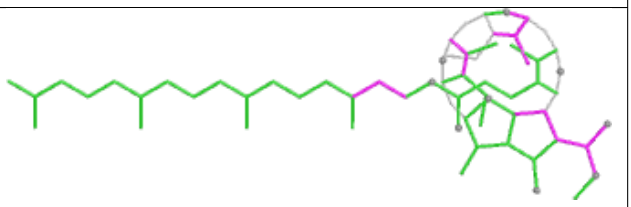


Rings

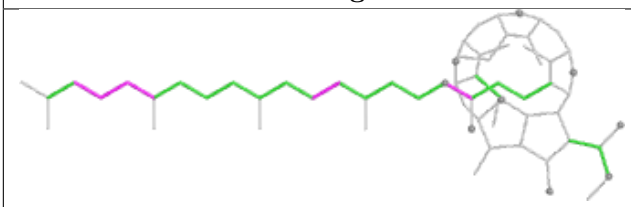
Ligand PHO J 405



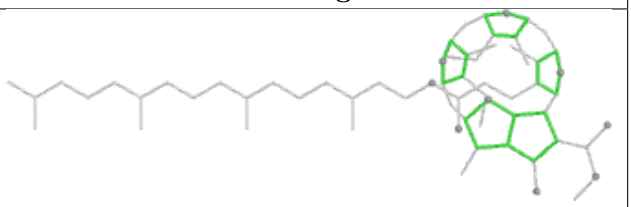
Bond lengths



Bond angles

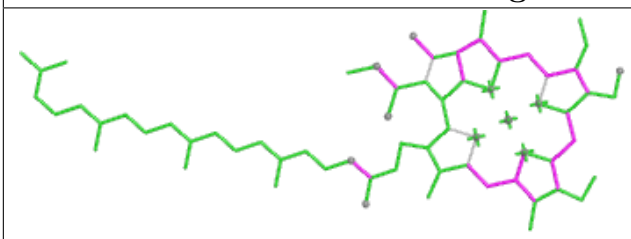


Torsions



Rings

Ligand CHL AH 608



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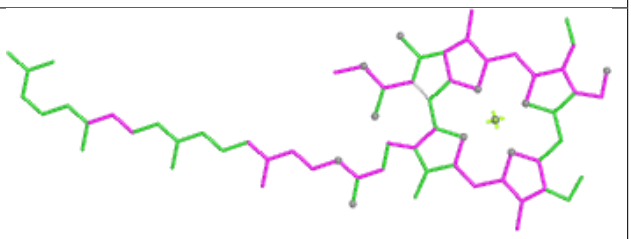

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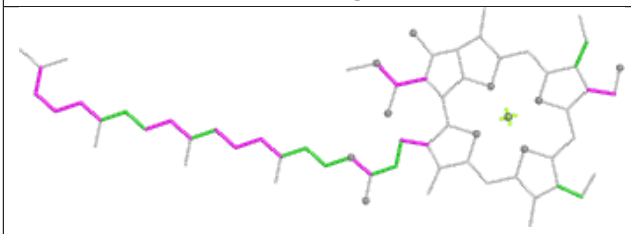

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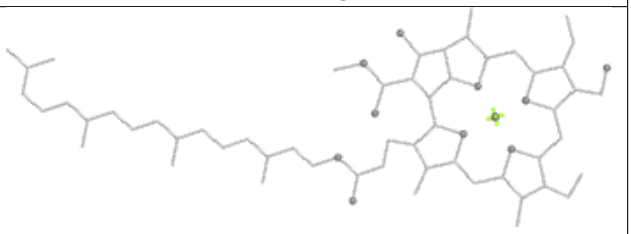
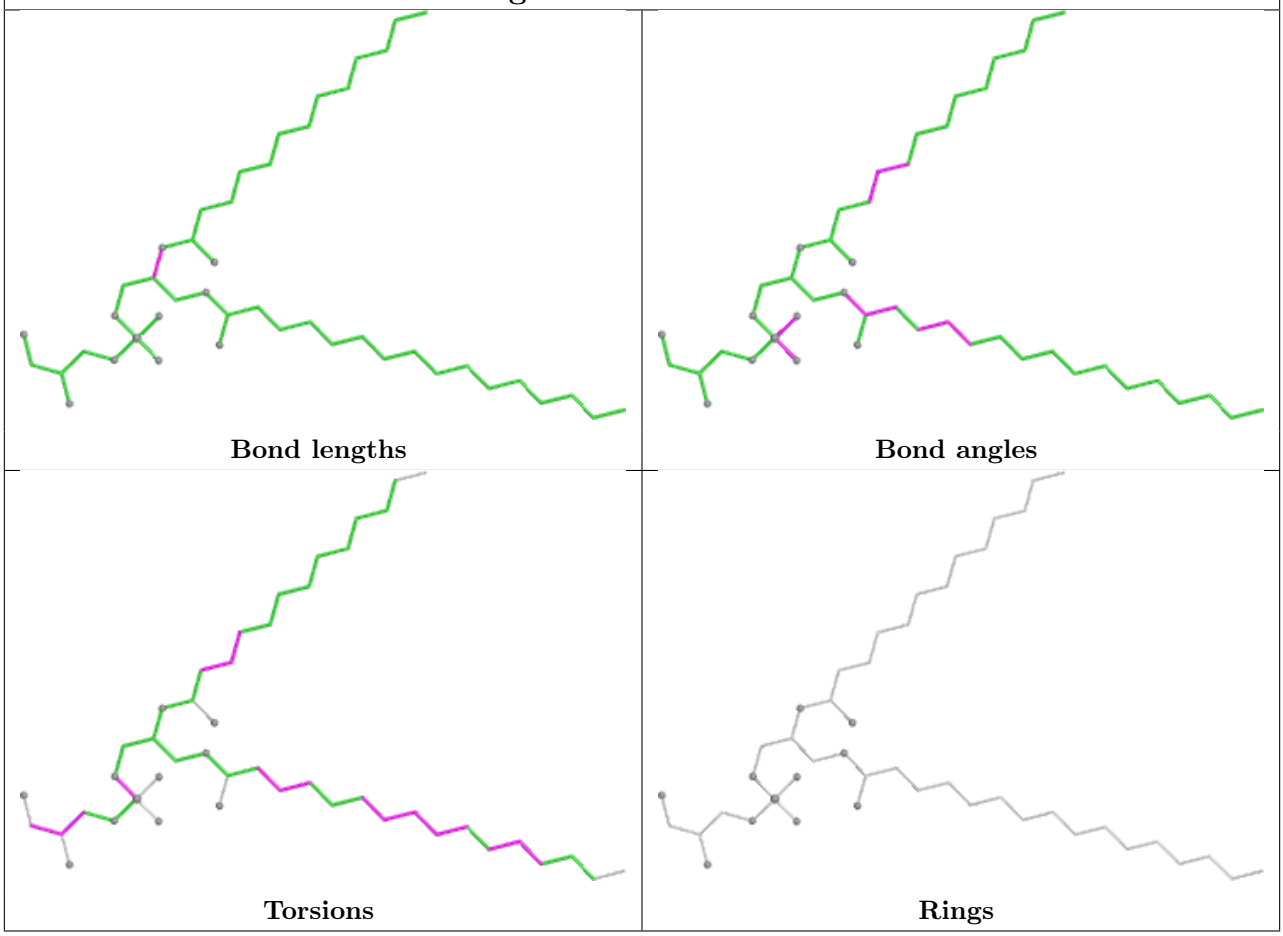
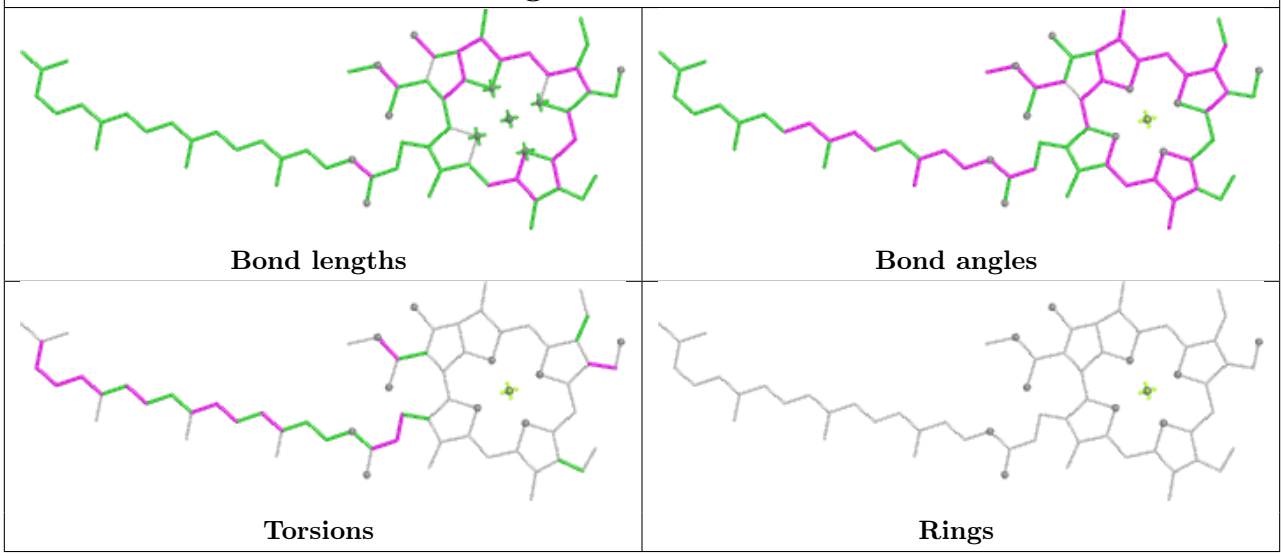


Rings

Ligand LHG AK 623



Ligand CHL V 606



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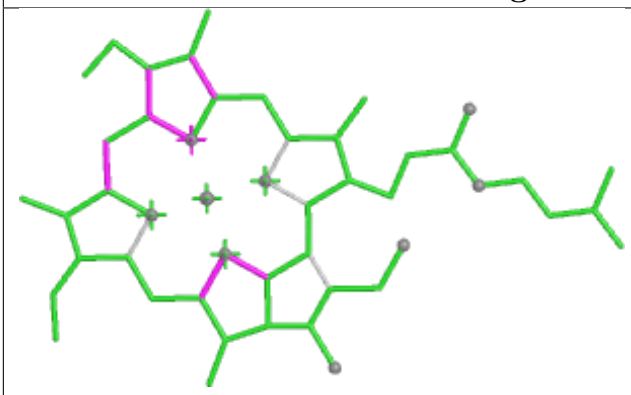
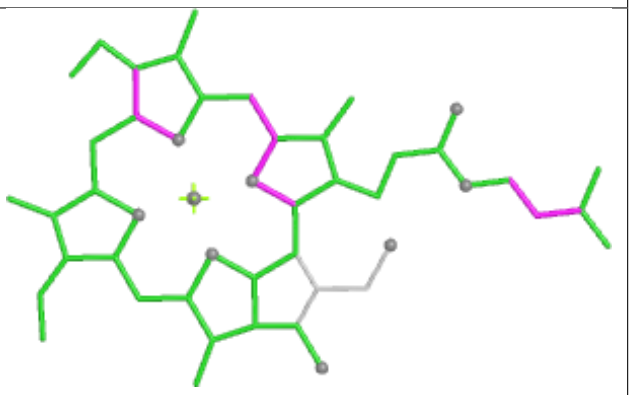
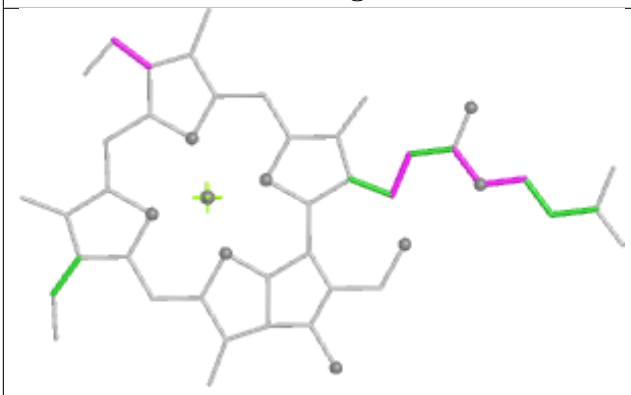
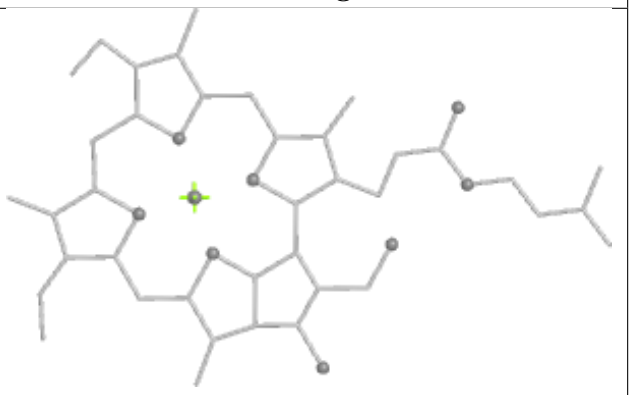
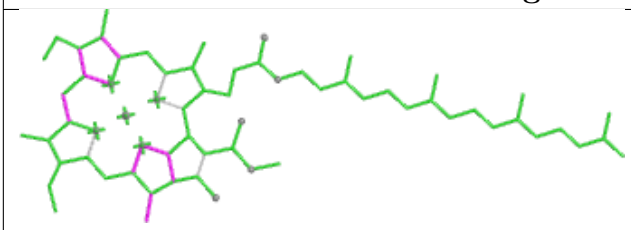
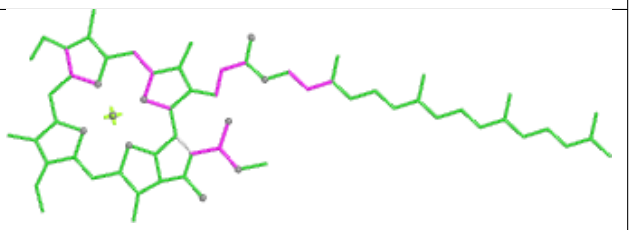
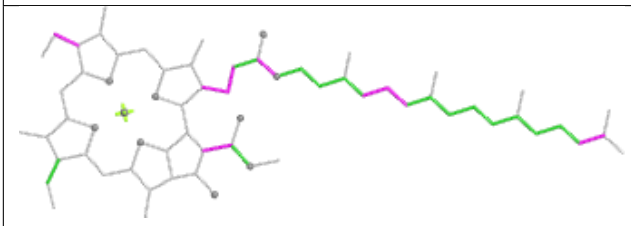
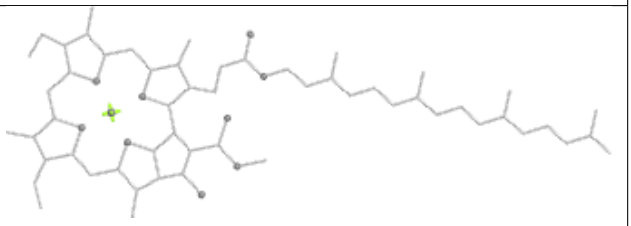
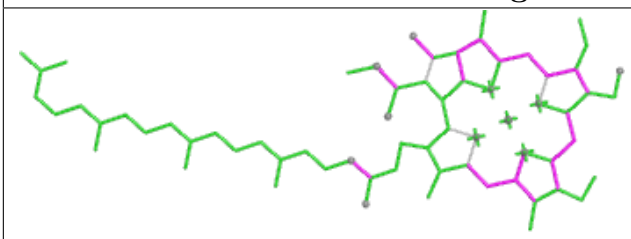
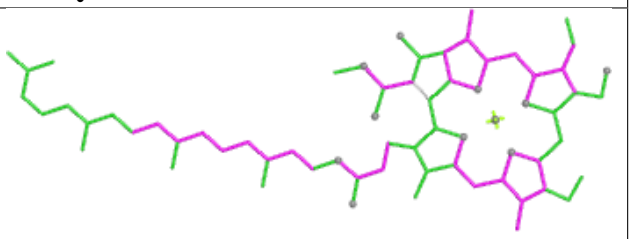
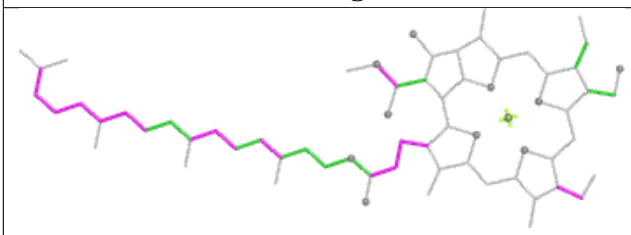
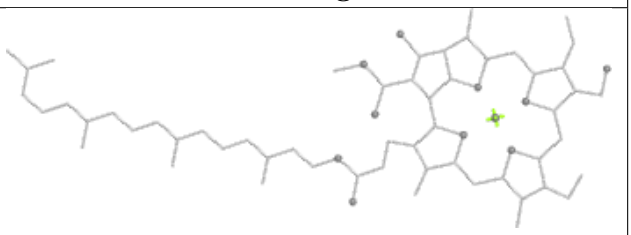
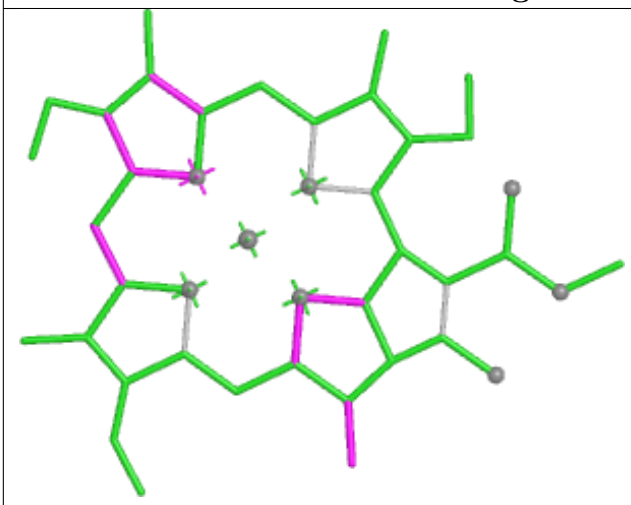
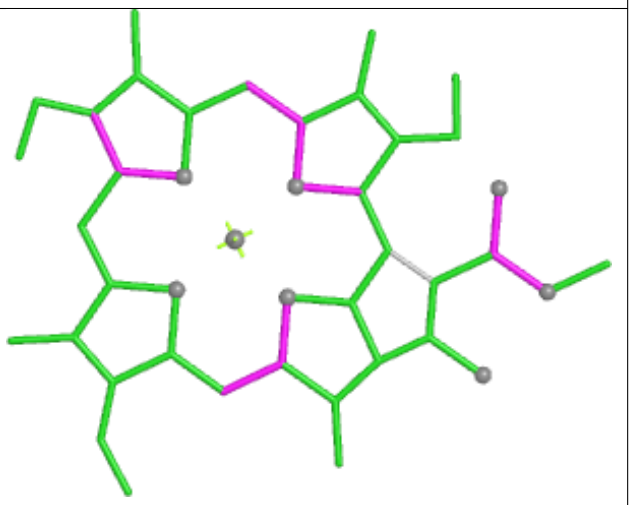
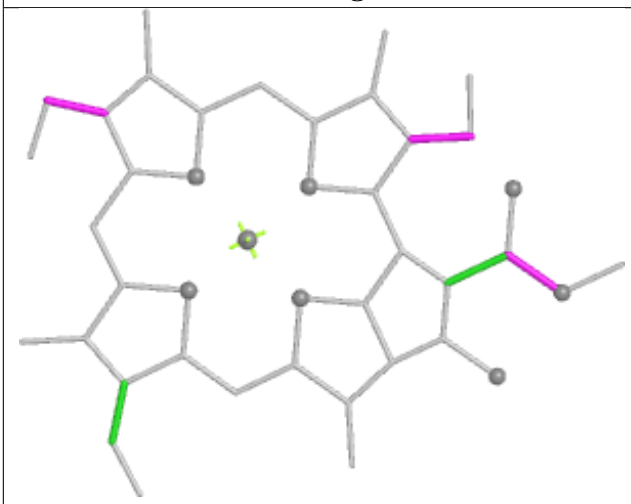
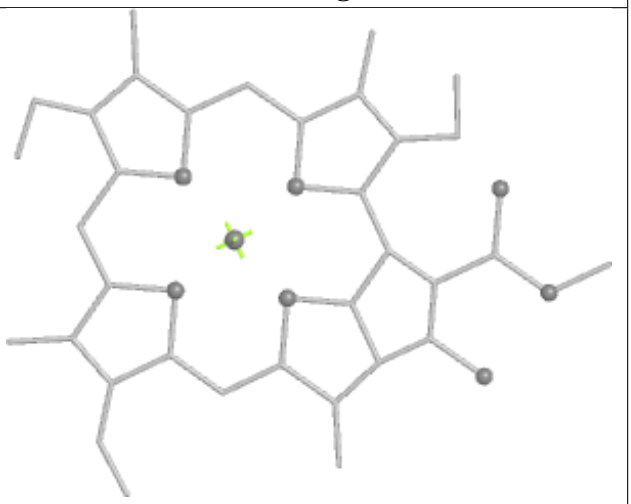
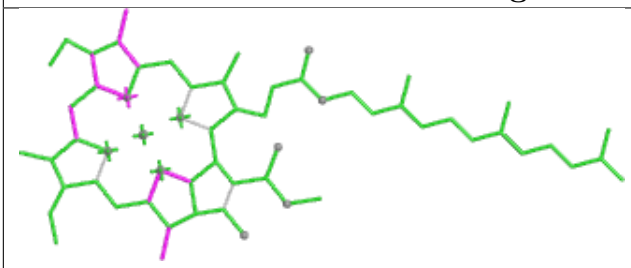
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

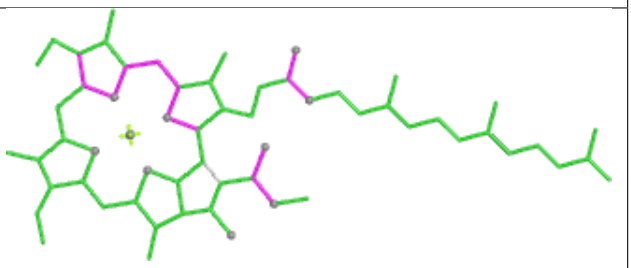
Ligand CHL AQ 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AE 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

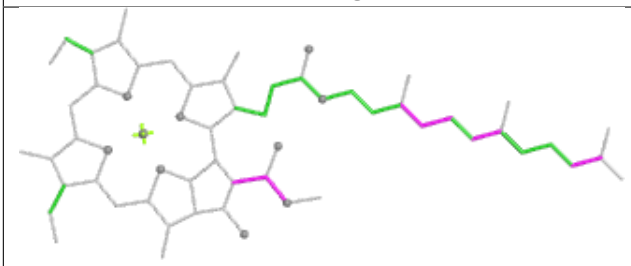
Ligand CLA AN 611



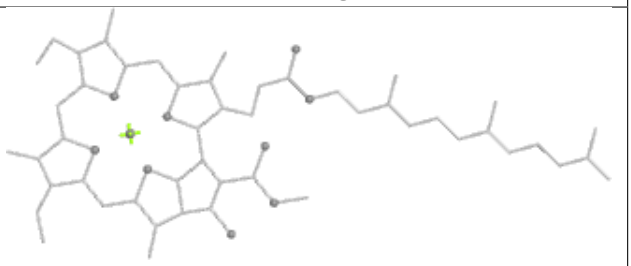
Bond lengths



Bond angles

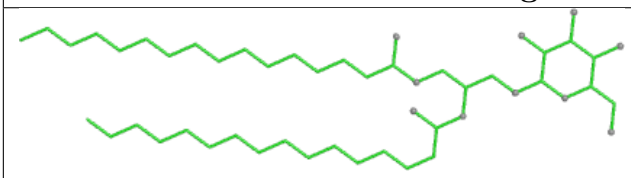


Torsions



Rings

Ligand LMG P 518



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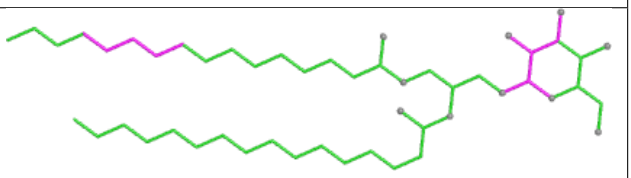
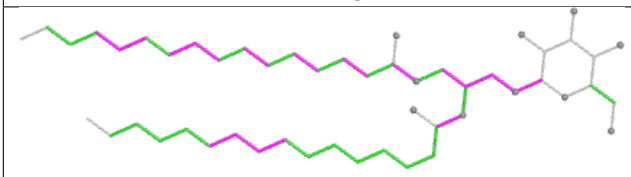


Bond angles



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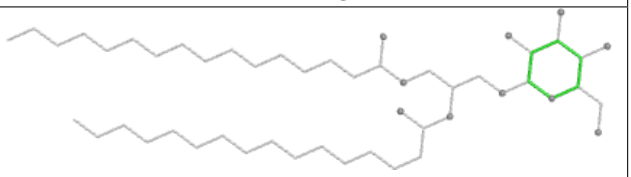
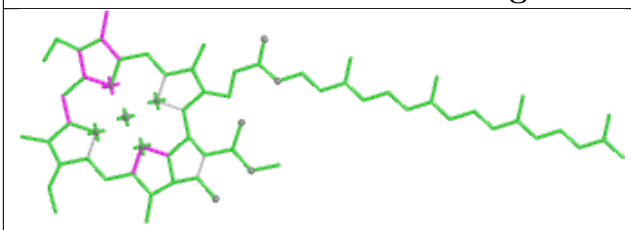
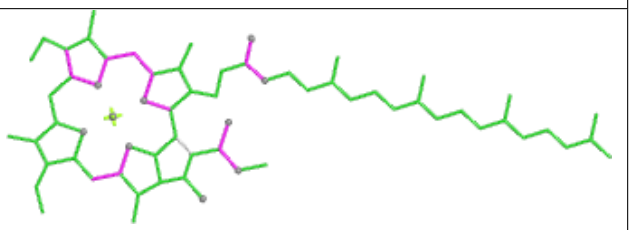


Rings

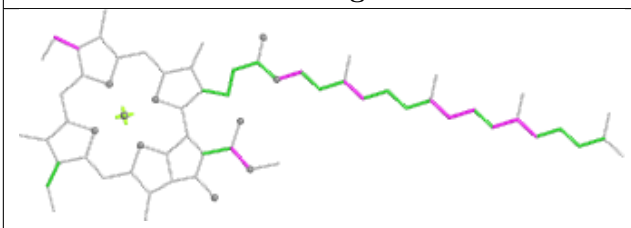
Ligand CLA AK 617



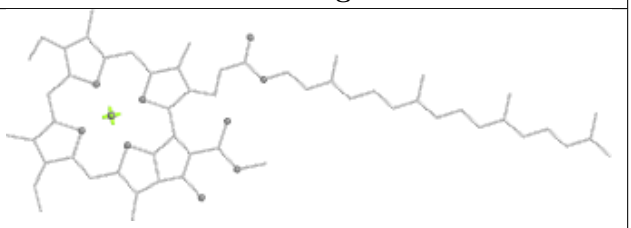
Bond lengths



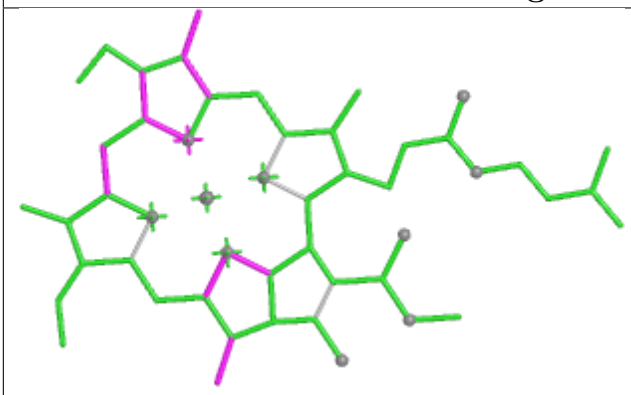
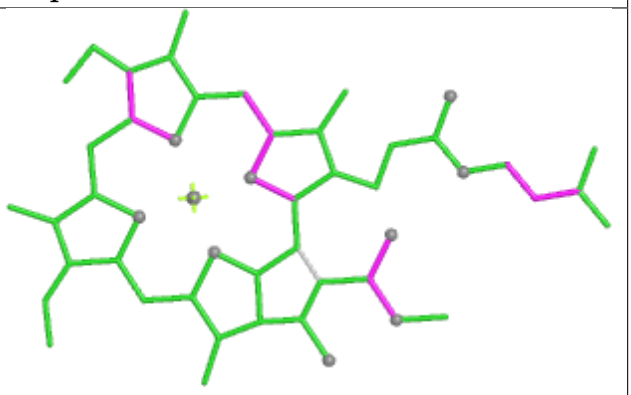
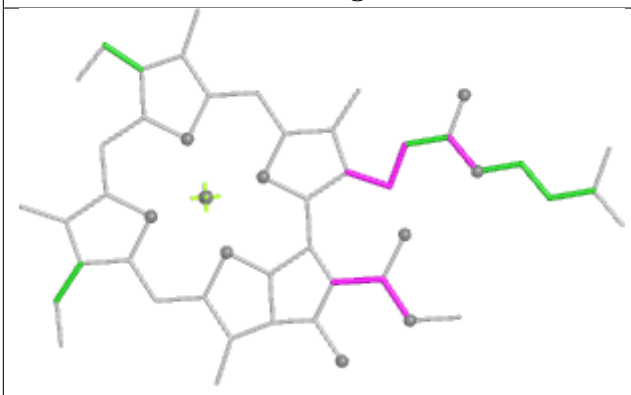
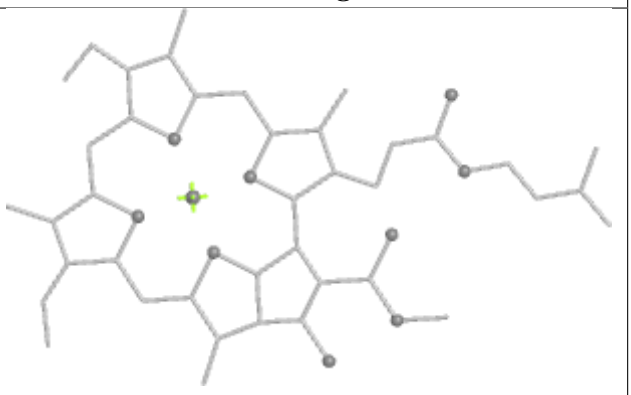
Bond angles

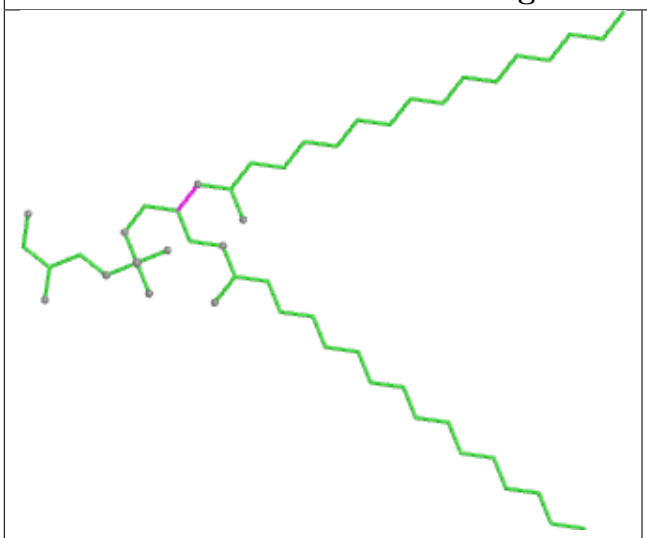
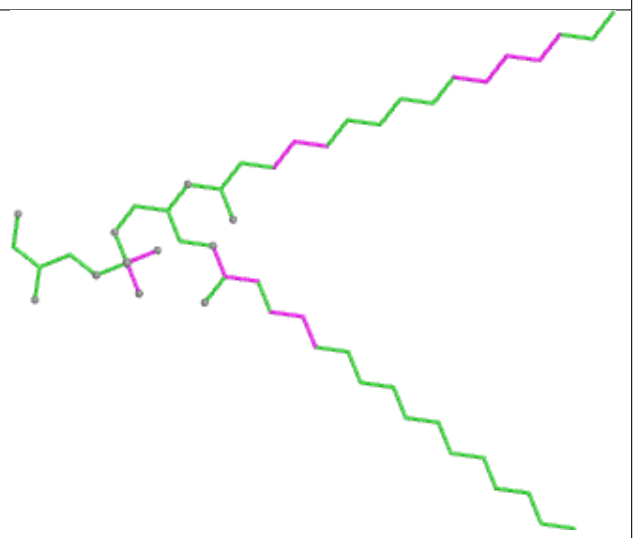
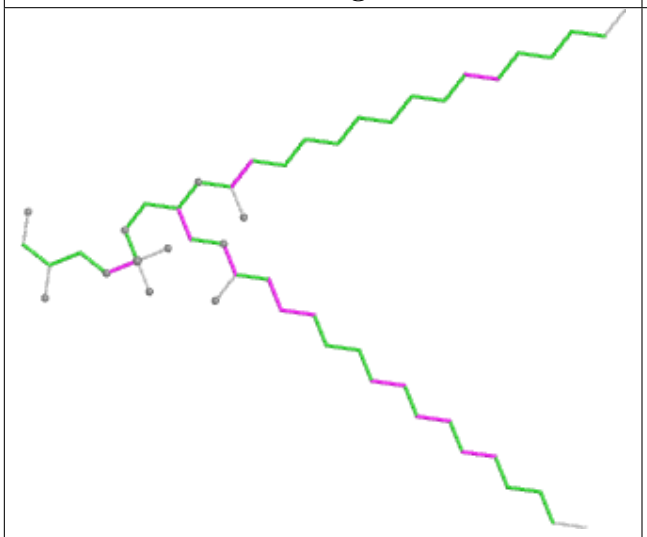
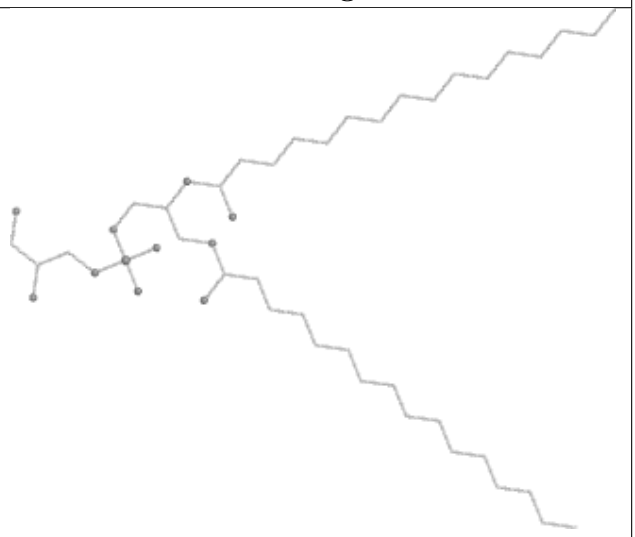


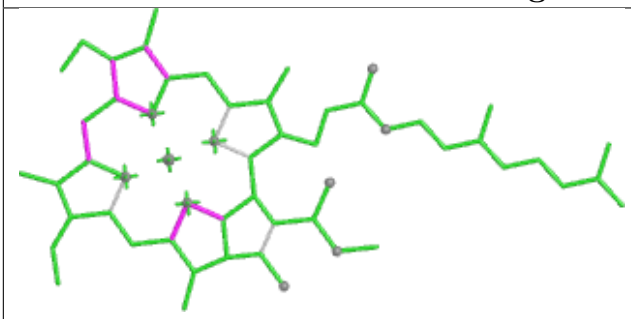
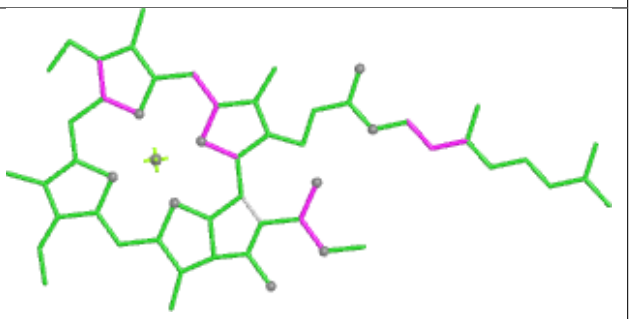
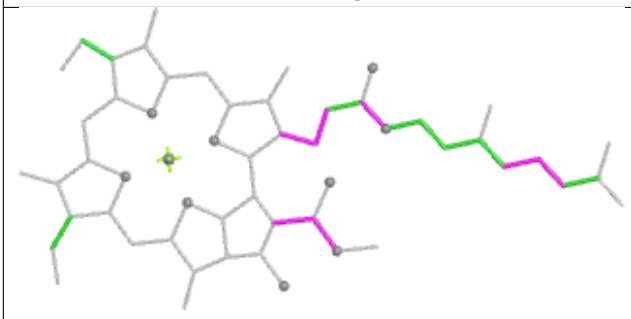
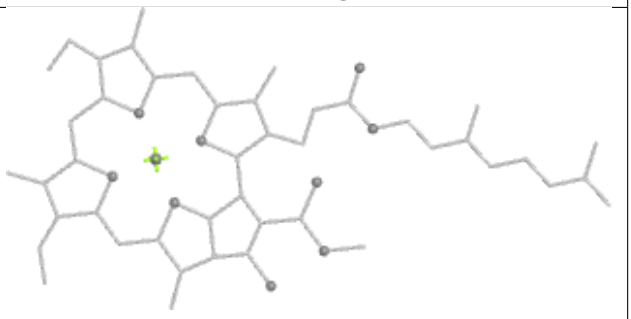
Torsions



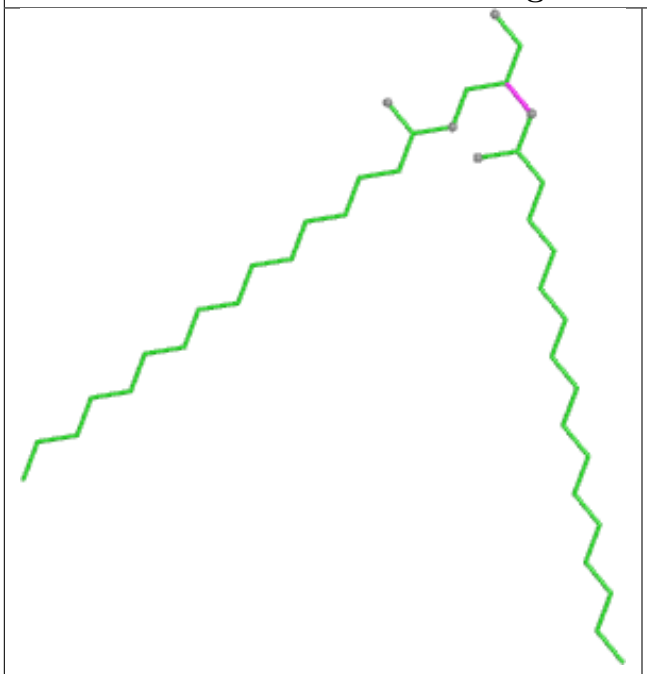
Rings

Ligand CLA p 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

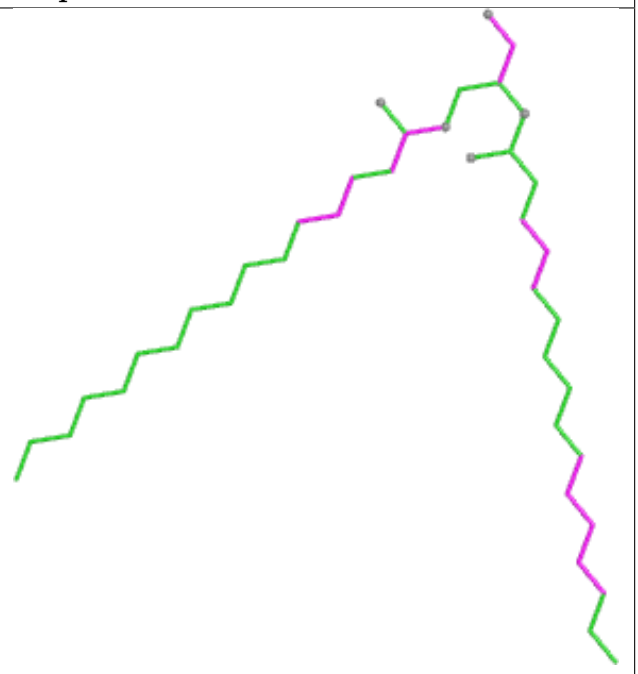
Ligand LHG W 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 0 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

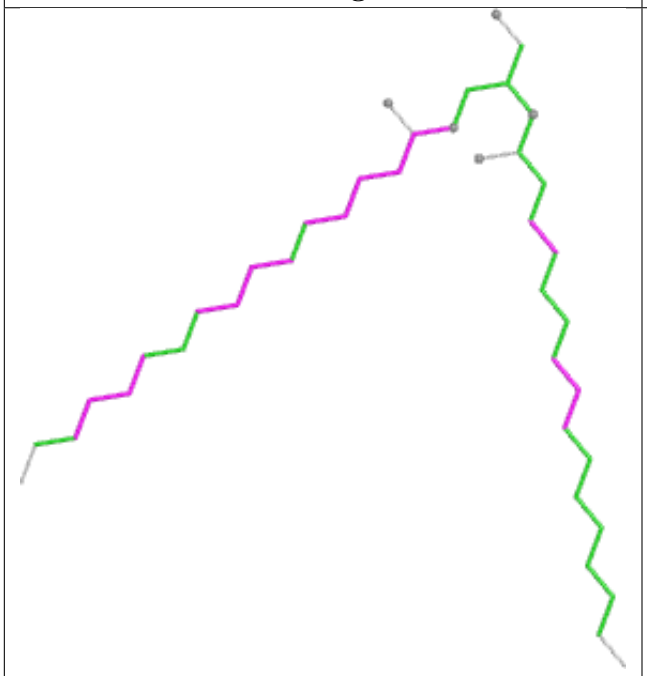
Ligand LHG p 617



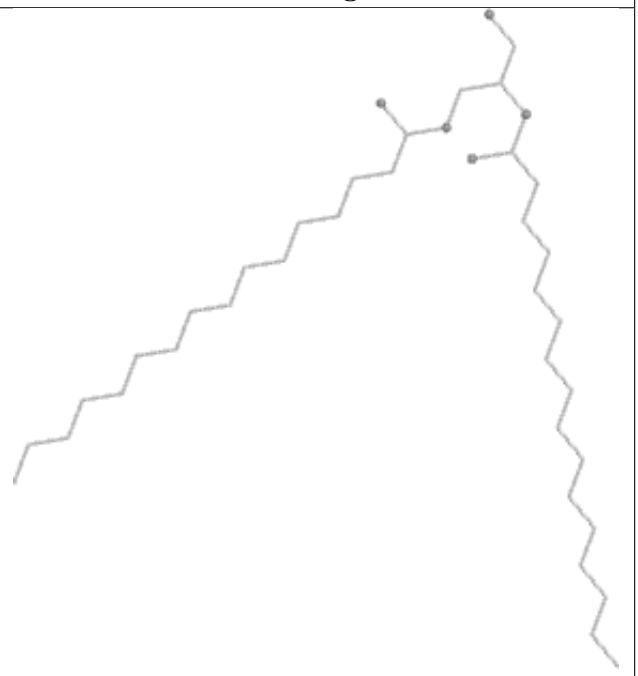
Bond lengths



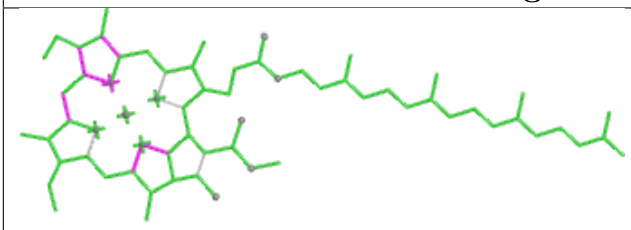
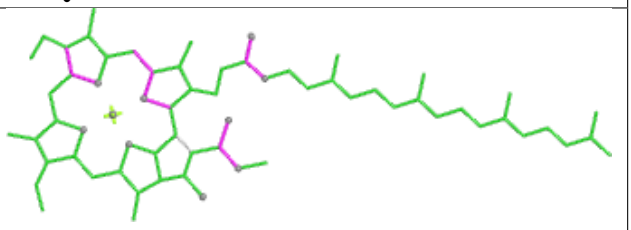
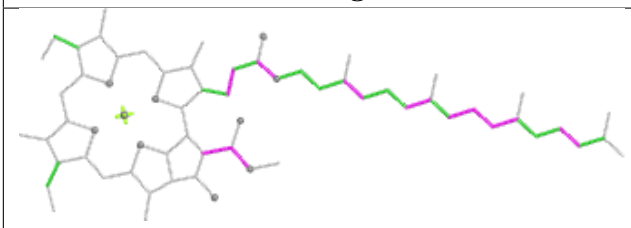
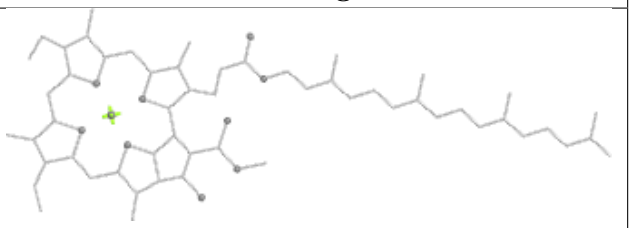
Bond angles

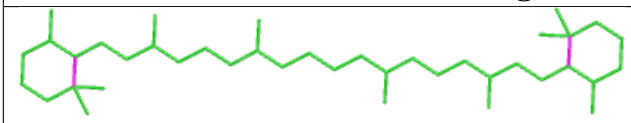
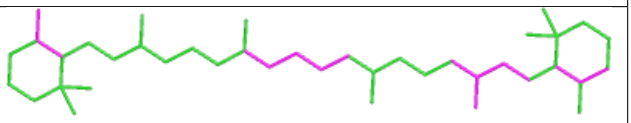
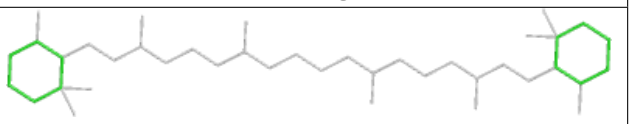


Torsions



Rings

Ligand CLA Q 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR AI 101	
 Bond lengths	 Bond angles
Torsions	 Rings

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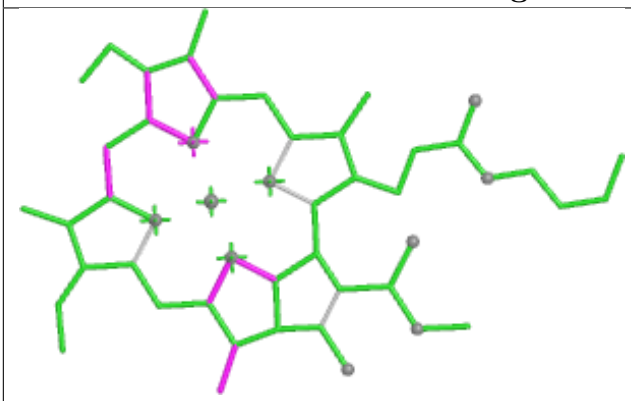

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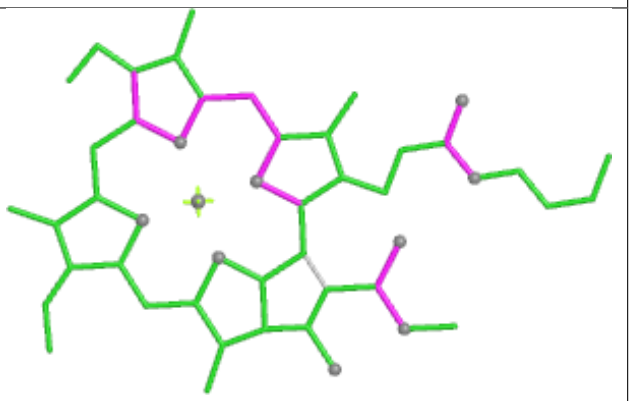

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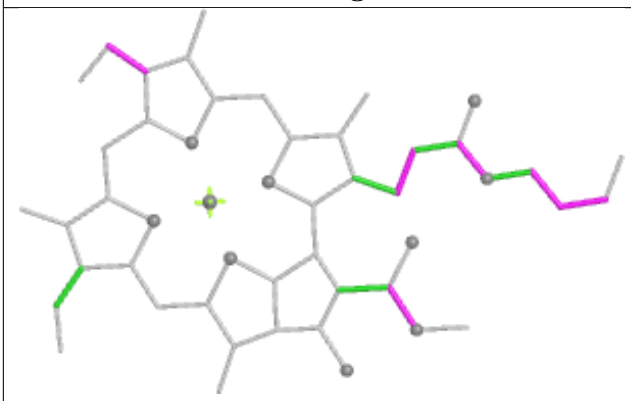

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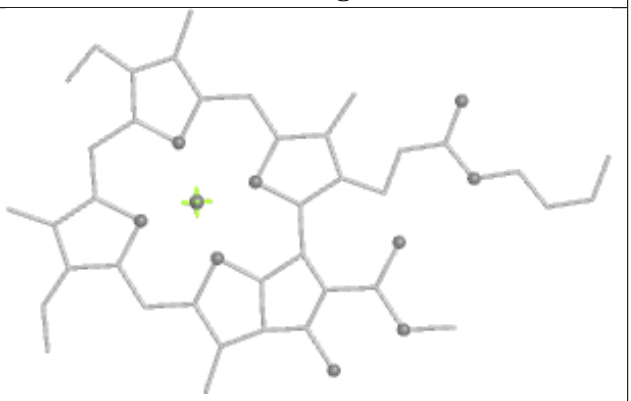

Rings

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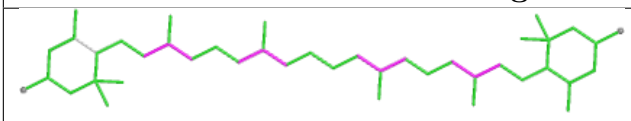

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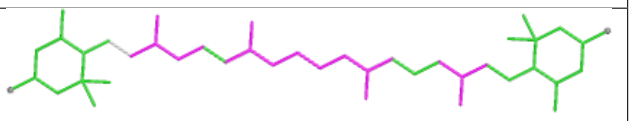

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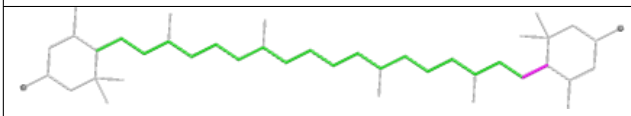

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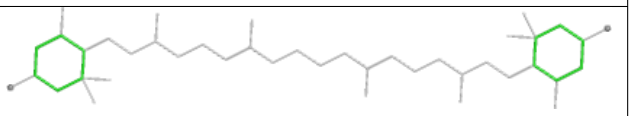
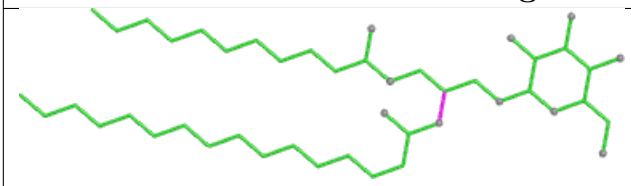


Rings

Ligand LMG Q 407



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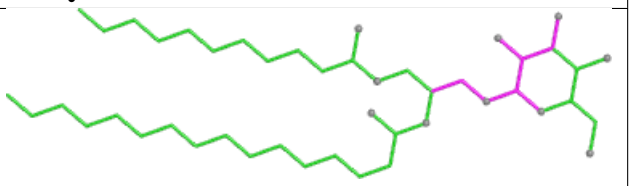

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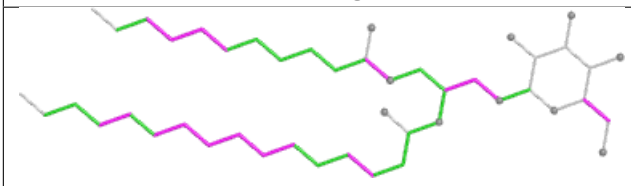

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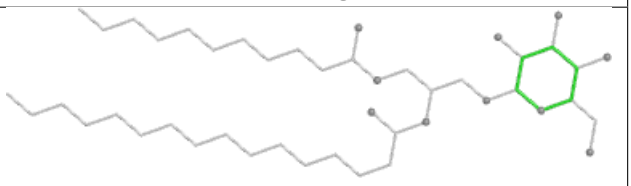
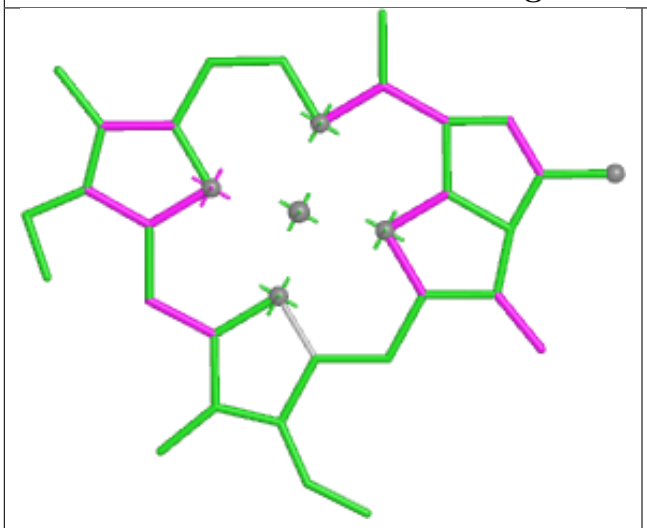


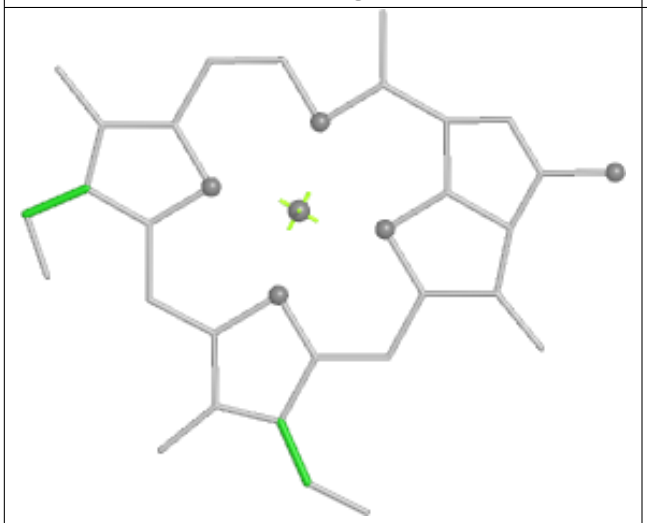
Rings

Ligand CLA V 604



Bond lengths

Bond angles



Torsions

Rings

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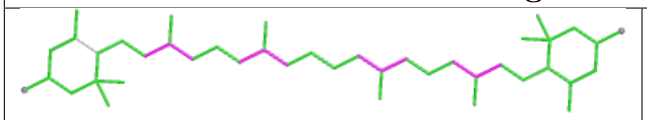

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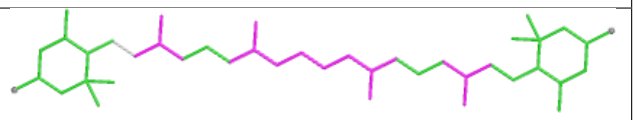

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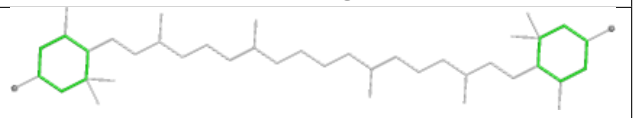

Rings

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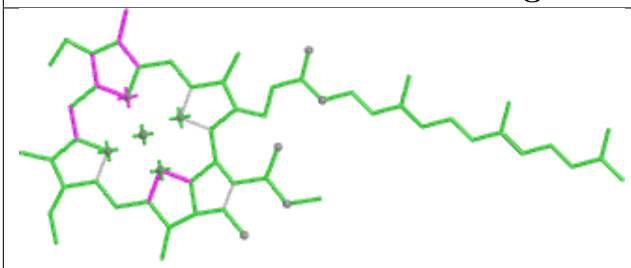
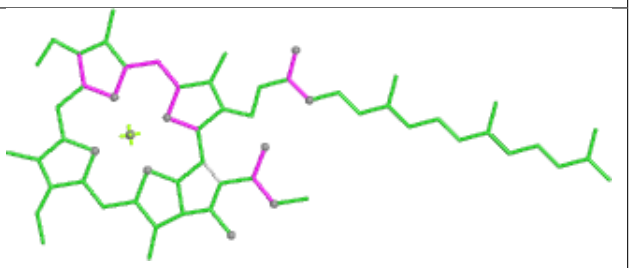
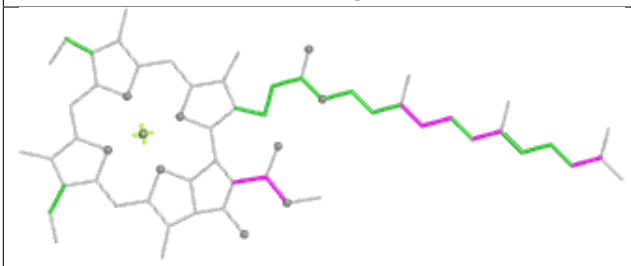
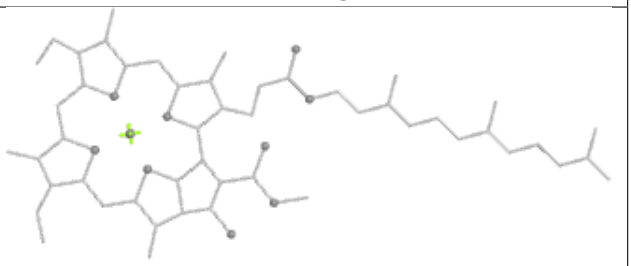
 Bond lengths	 Bond angles
 Torsions	 Rings

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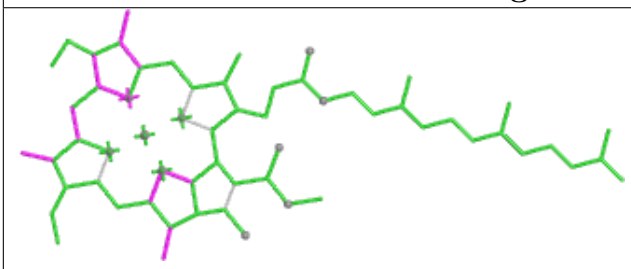
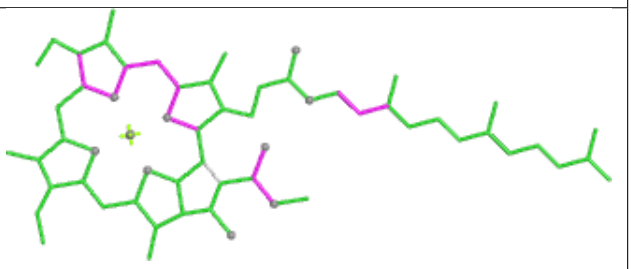
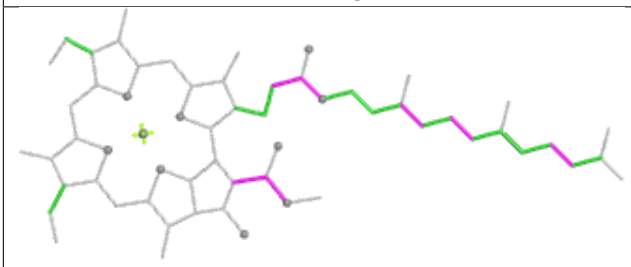
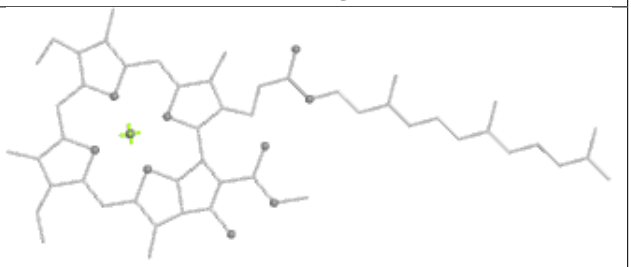
 Bond lengths	 Bond angles
 Torsions	 Rings

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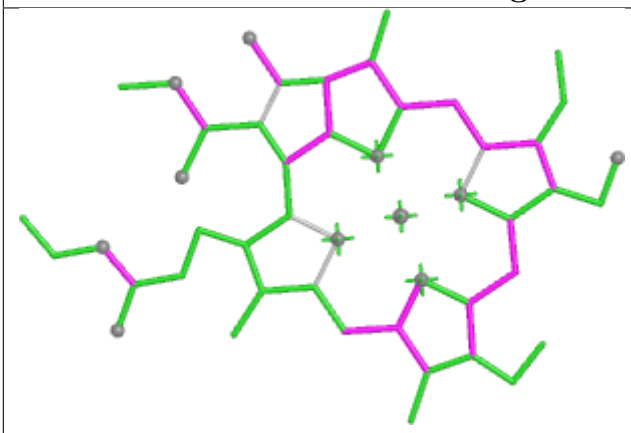

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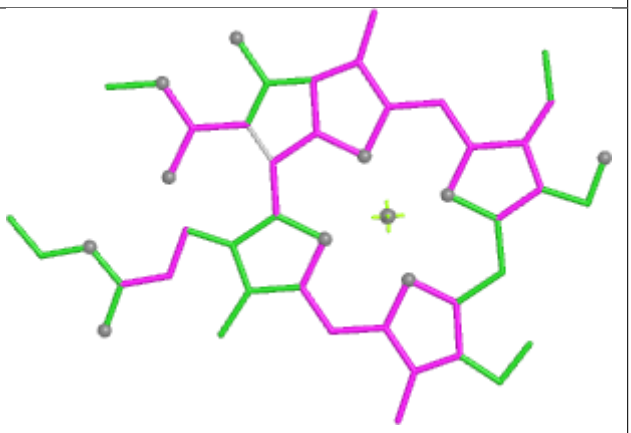

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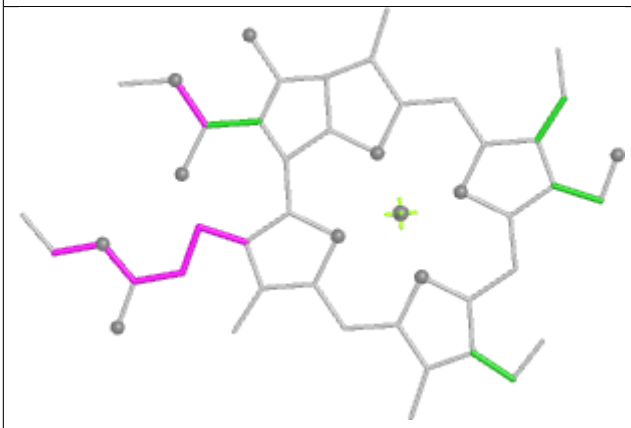

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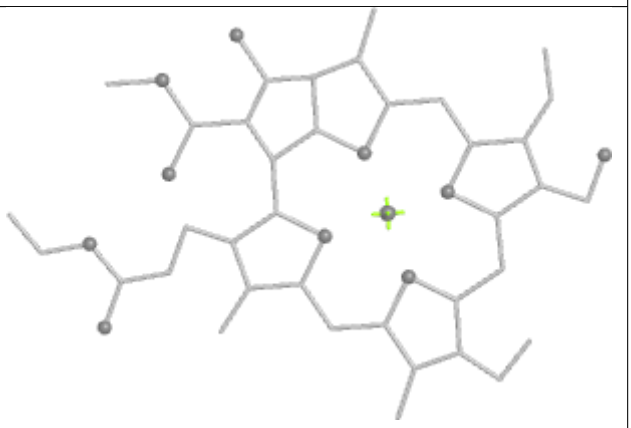
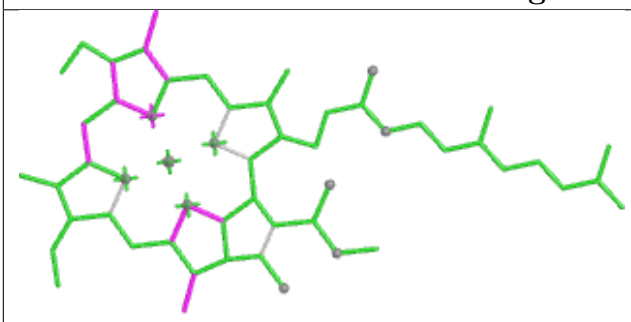


Rings

Ligand CLA 9 603



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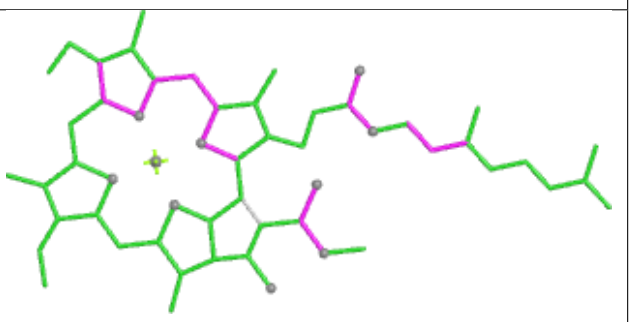

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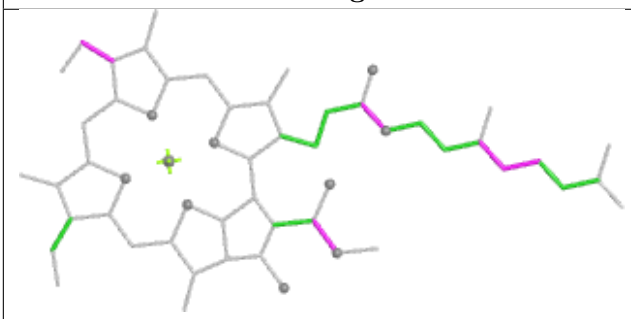

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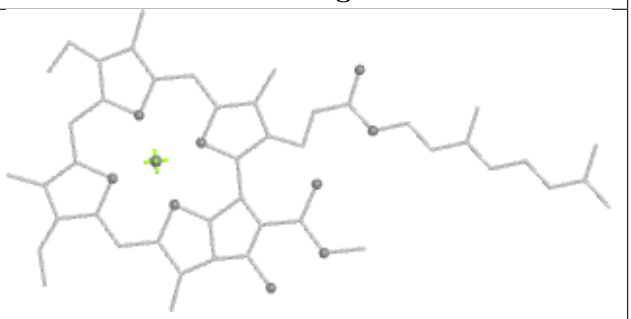

Rings

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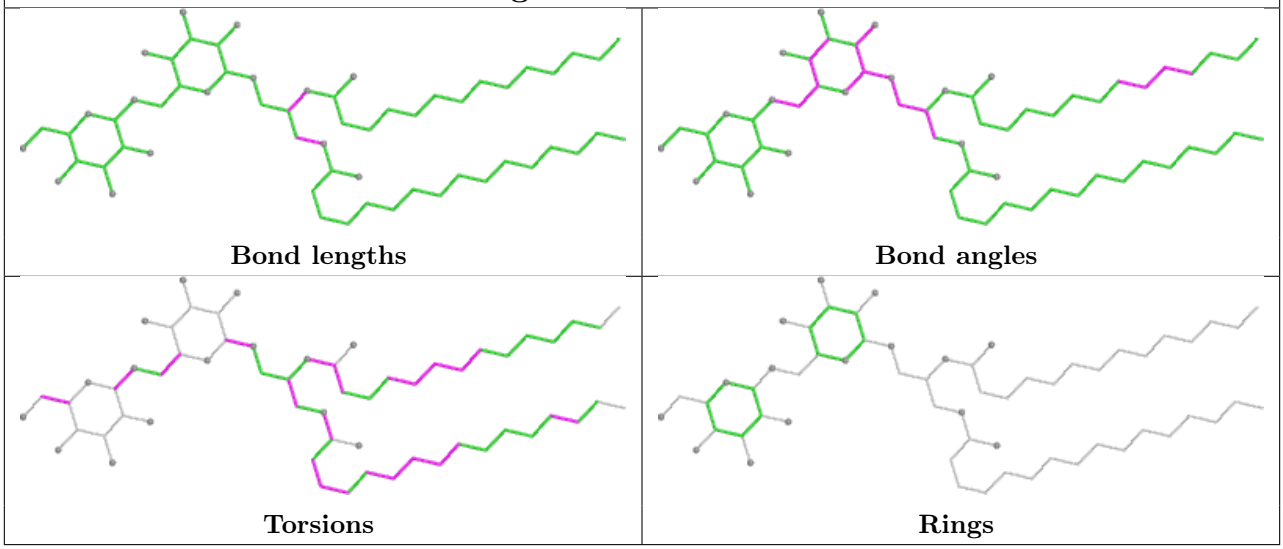

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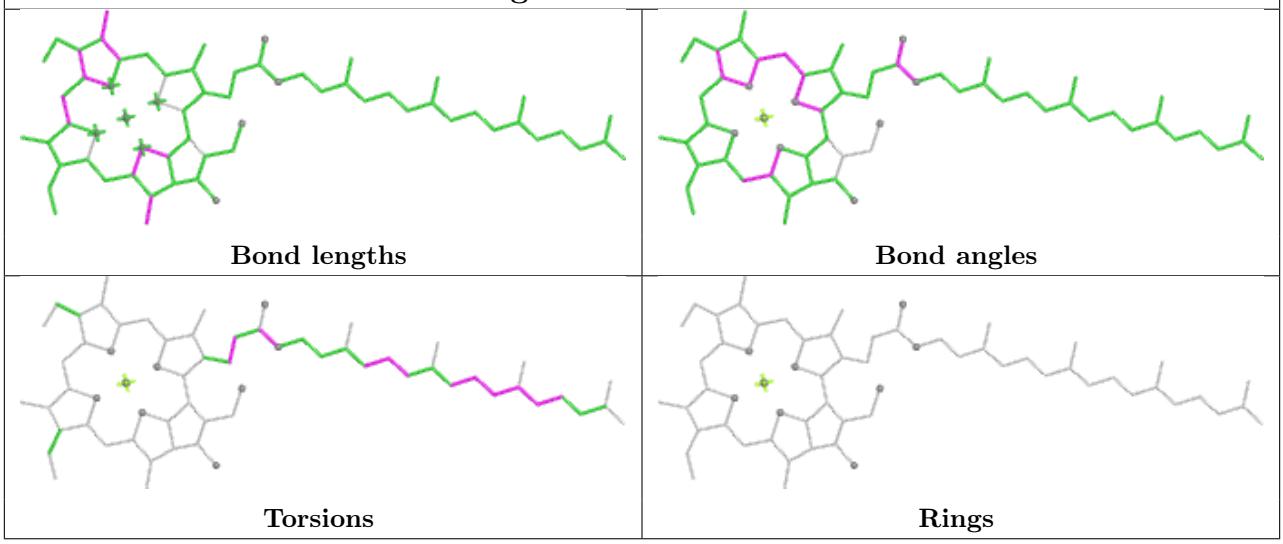

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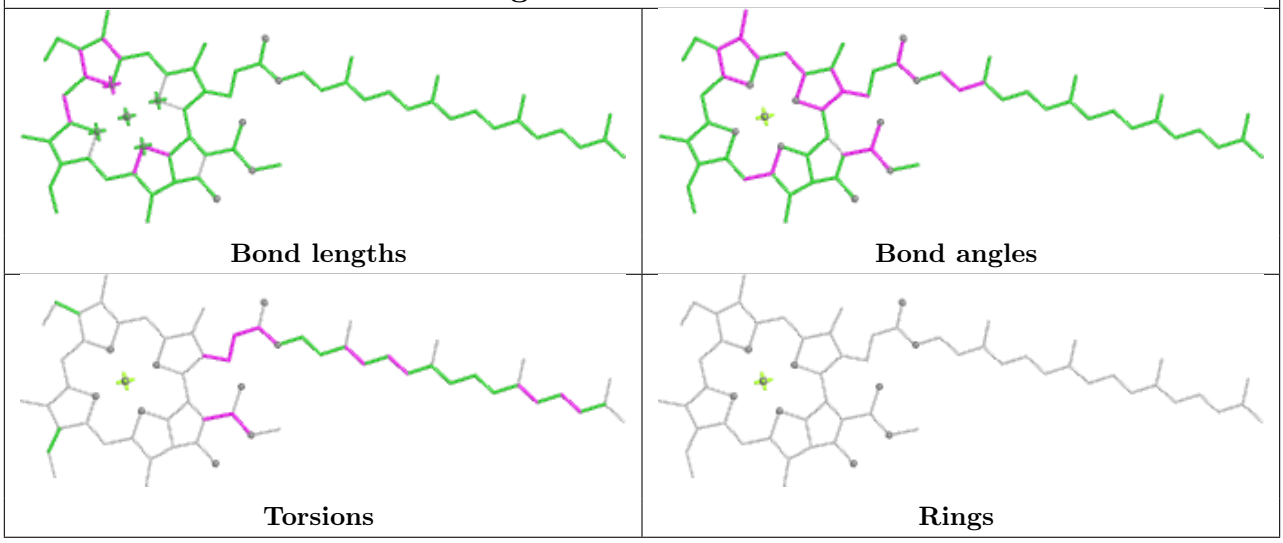

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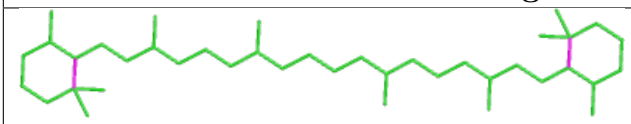

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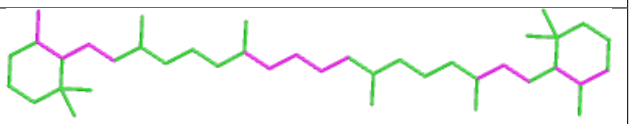
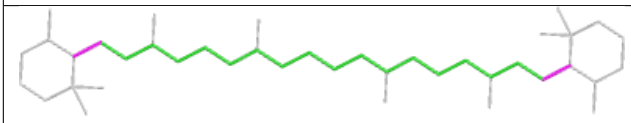


Bond angles



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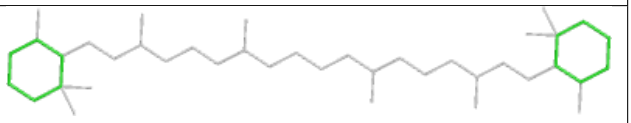
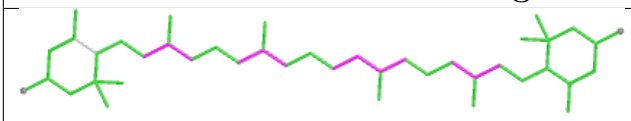


Rings

Ligand LUT AF 611



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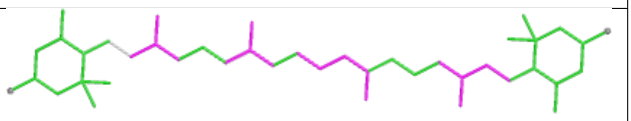

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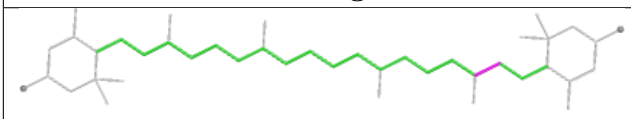

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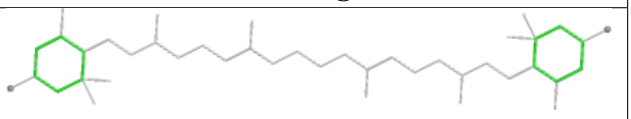

Rings

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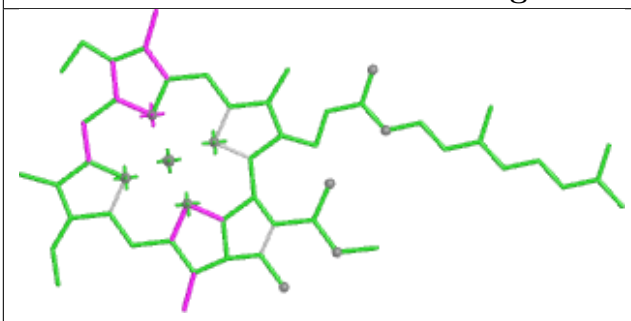

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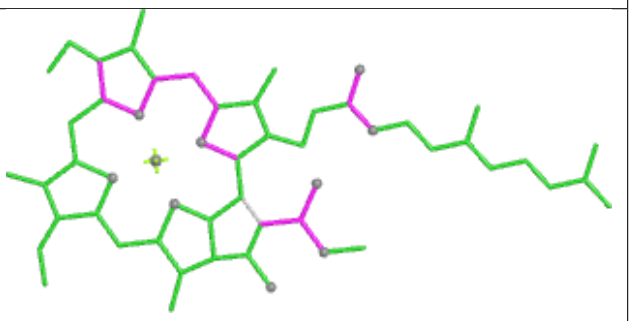

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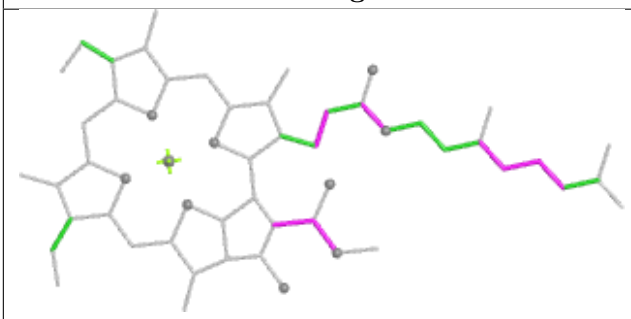

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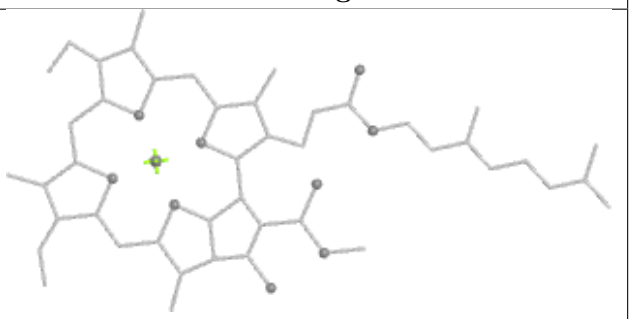

Rings

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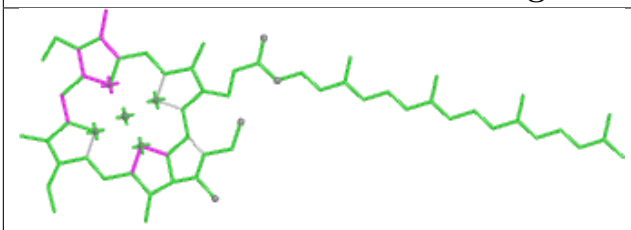
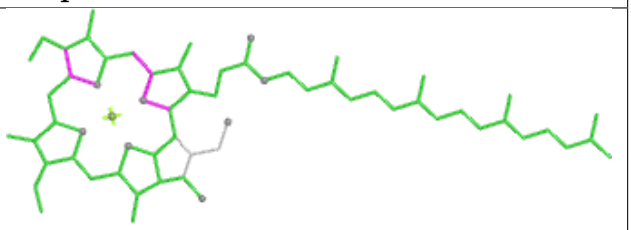
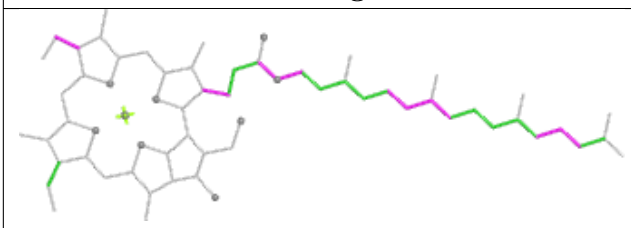
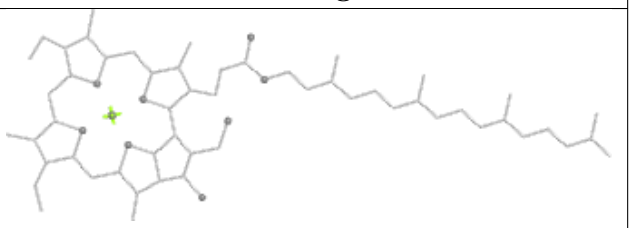
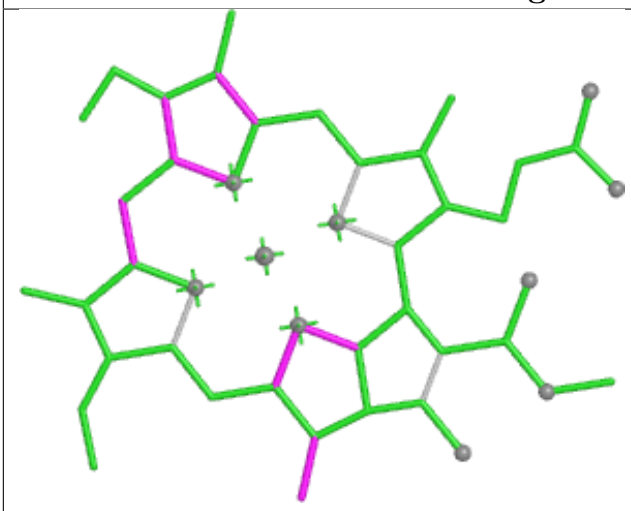
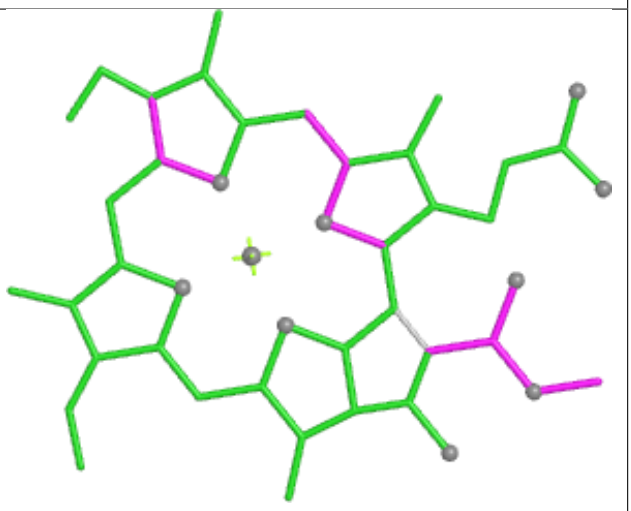
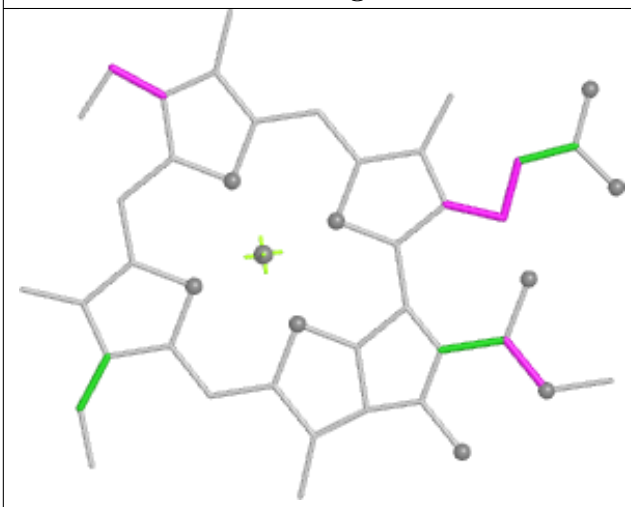
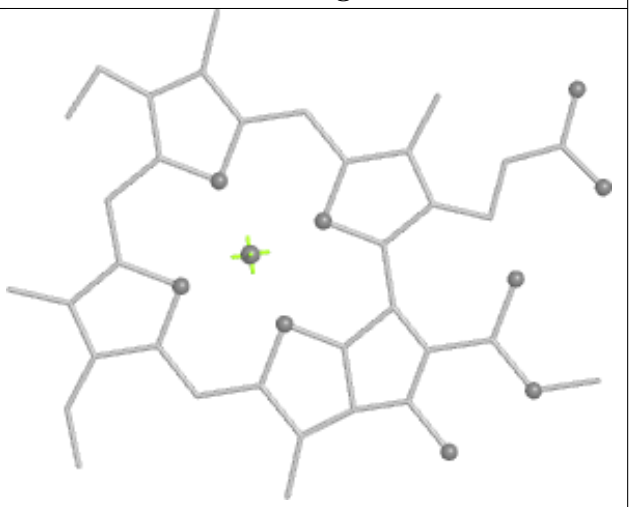
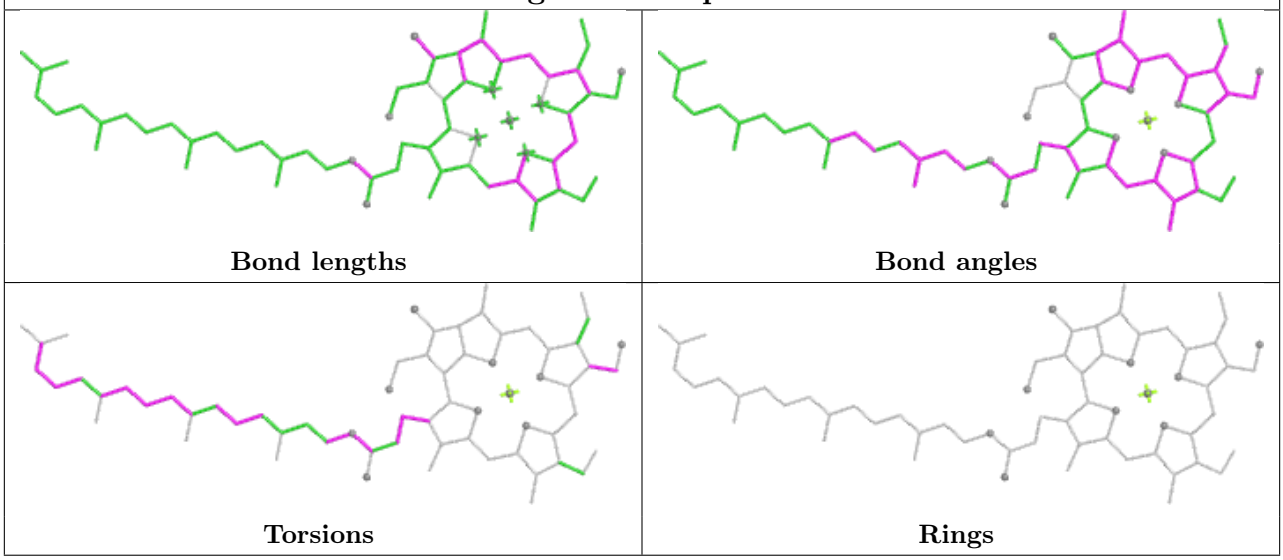
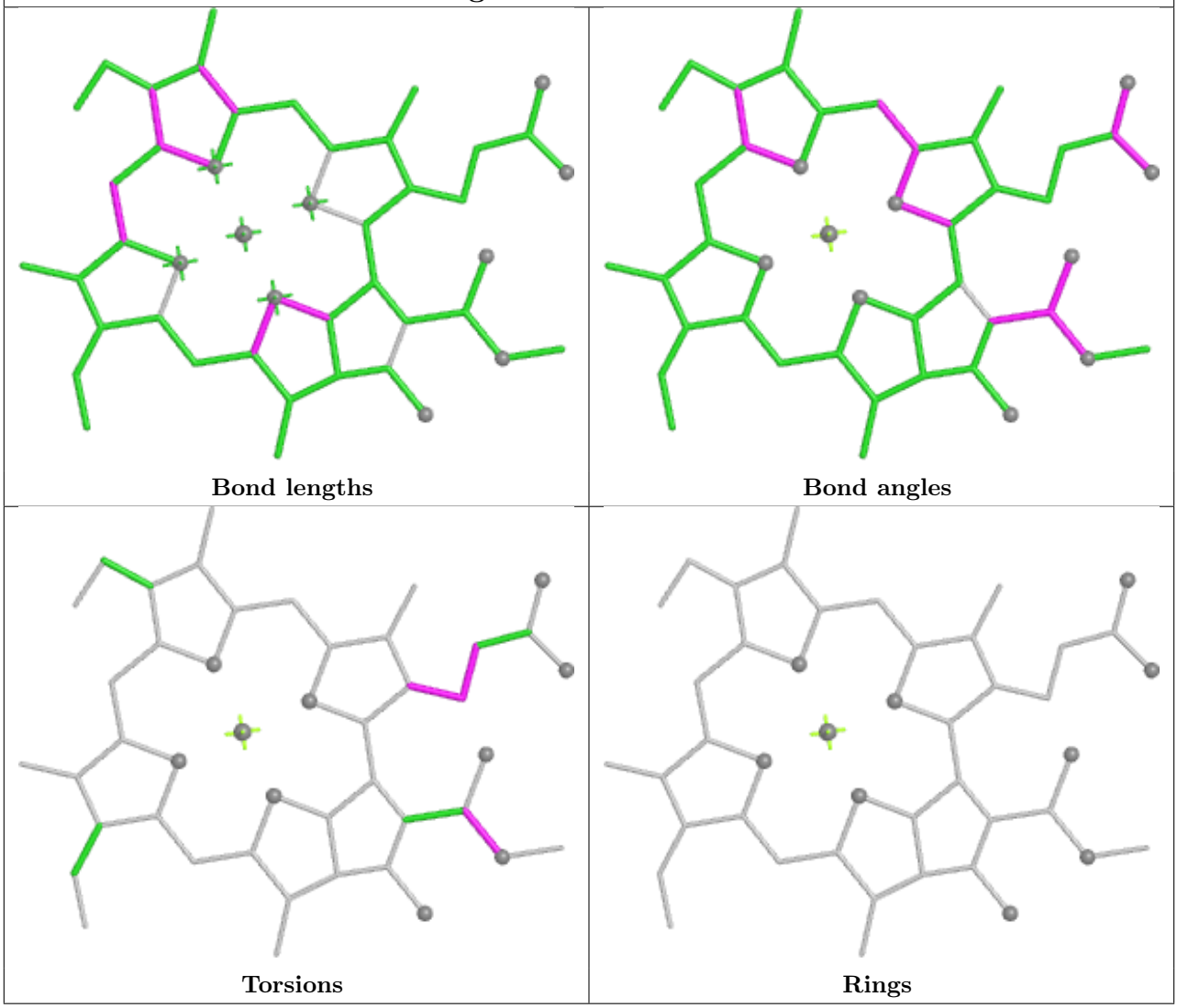
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 0 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL p 609



Ligand CLA AA 613



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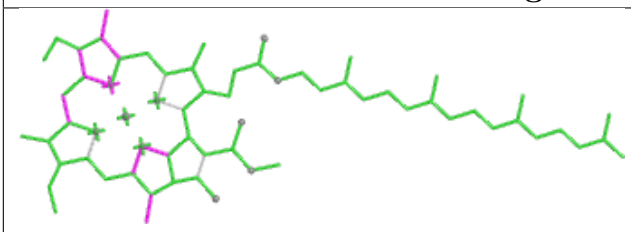

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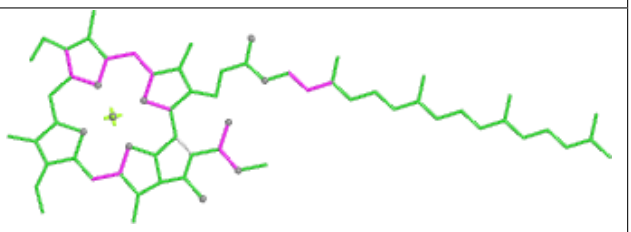

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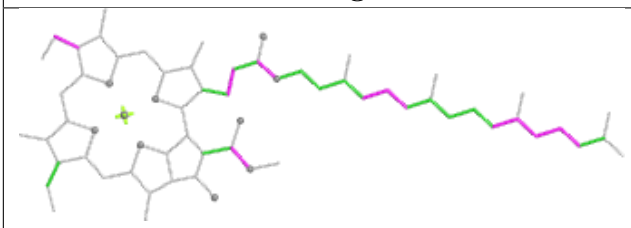

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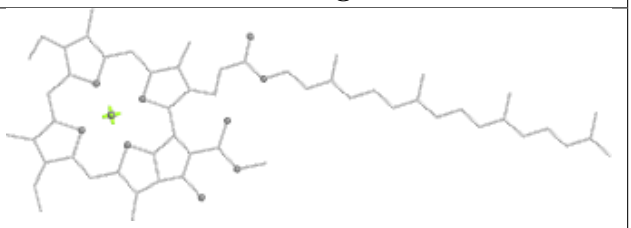
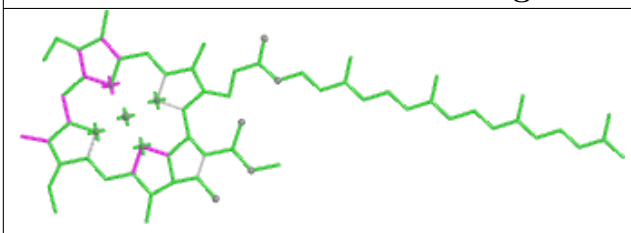


Rings

Ligand CLA AL 509



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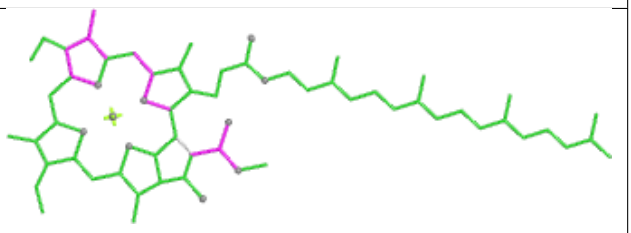

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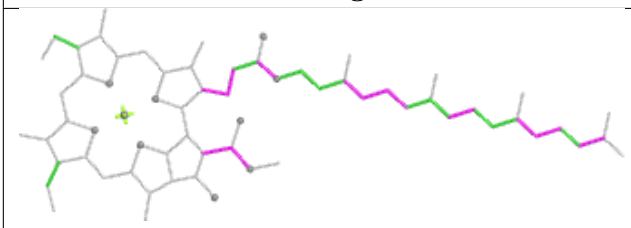

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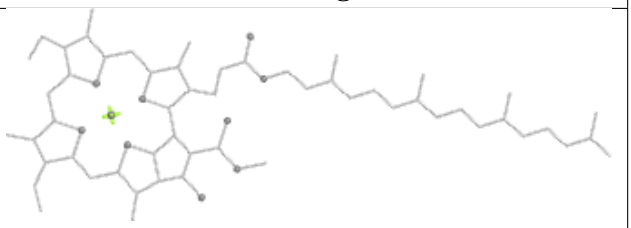
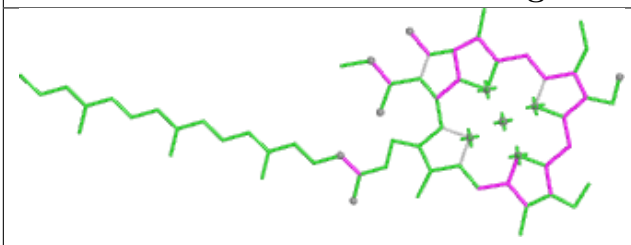


Rings

Ligand CHL q 605



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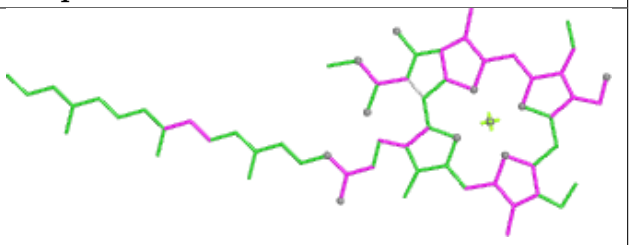

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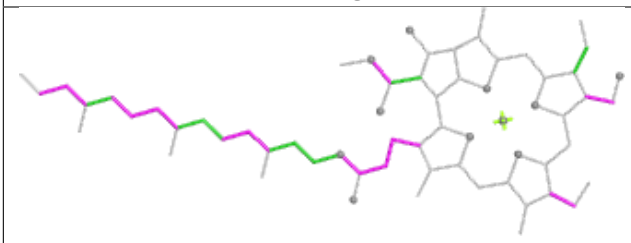

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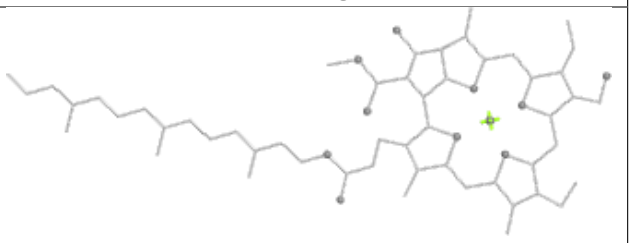
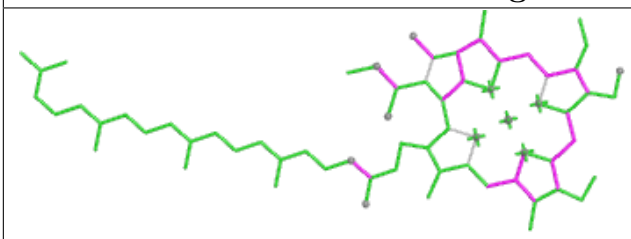
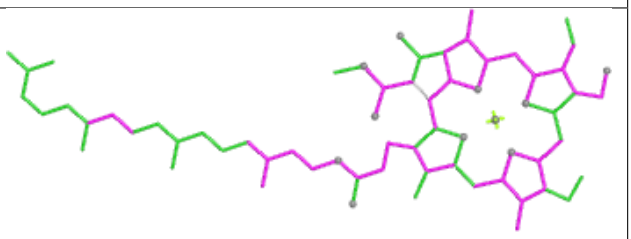
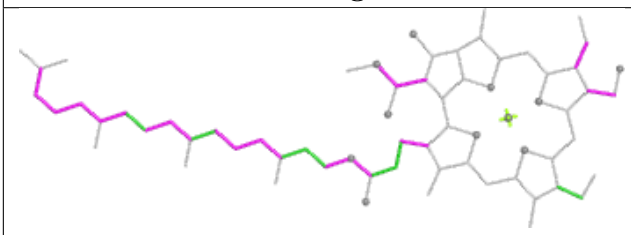
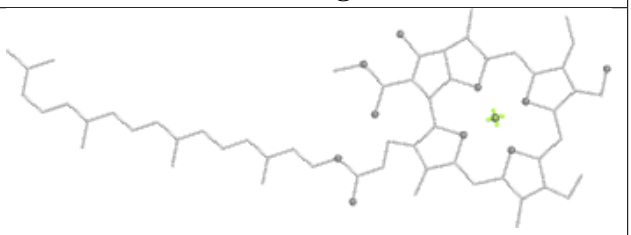
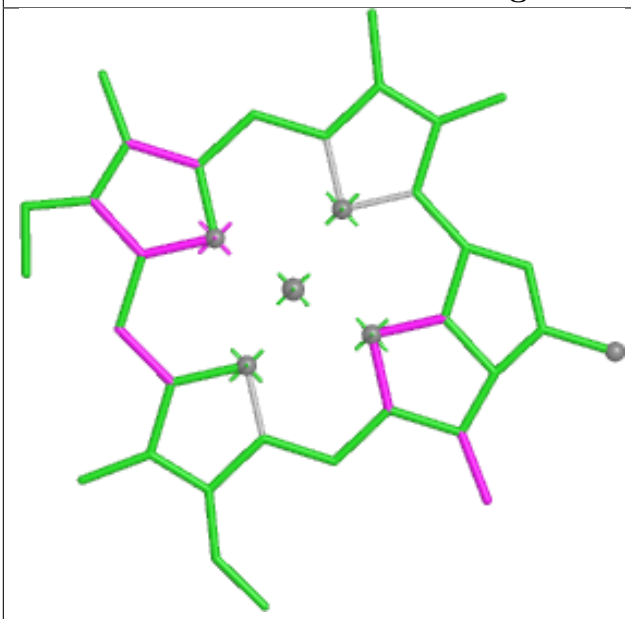


Rings

Ligand CHL AN 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AN 604



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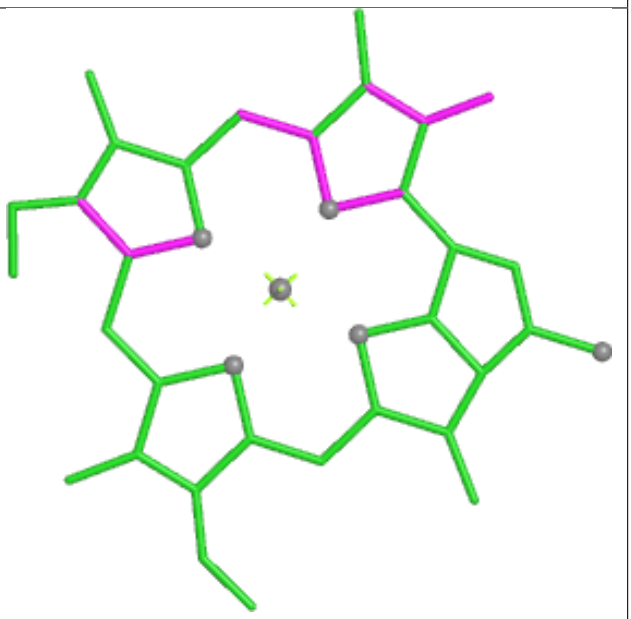
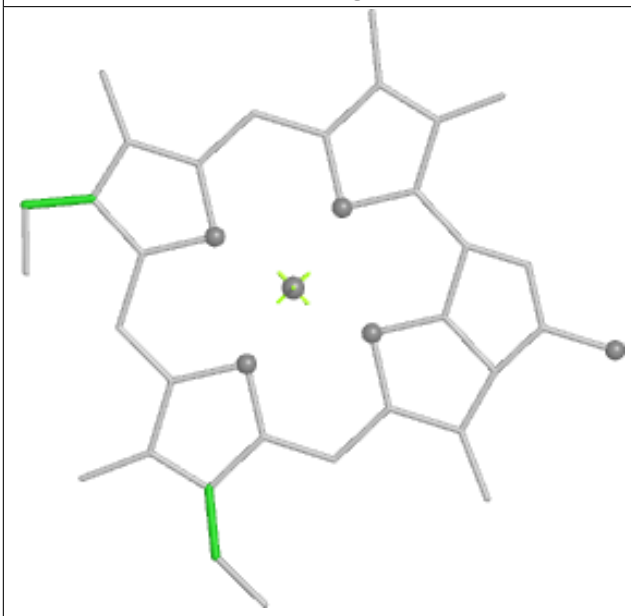


Bond angles



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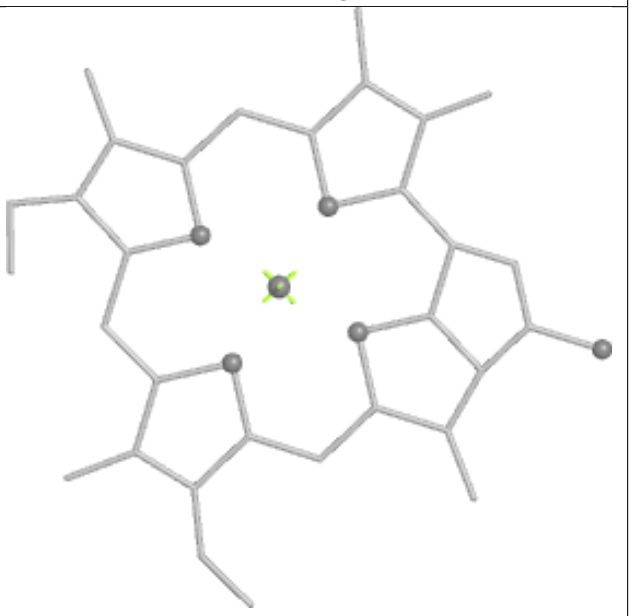
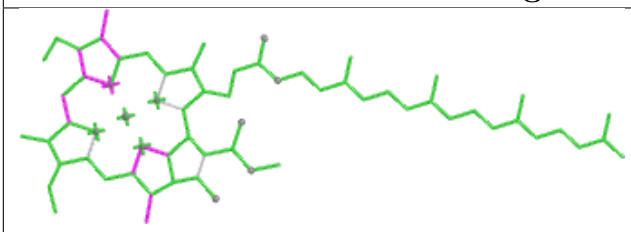


Rings

Ligand CLA O 613



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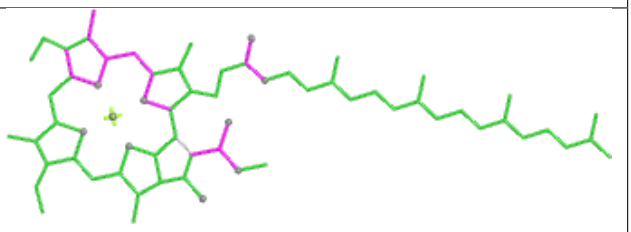
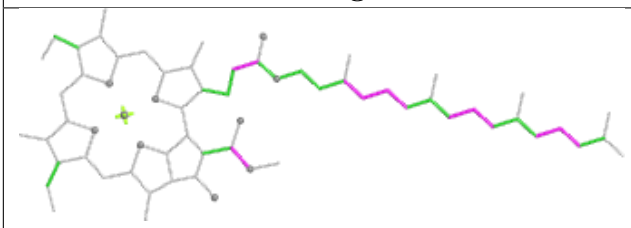


Bond angles



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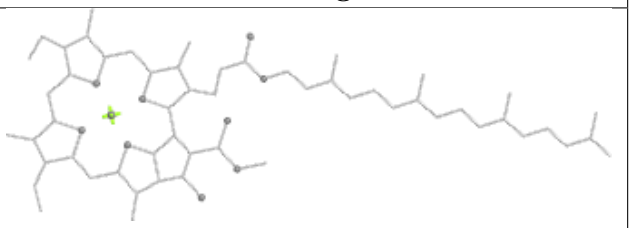
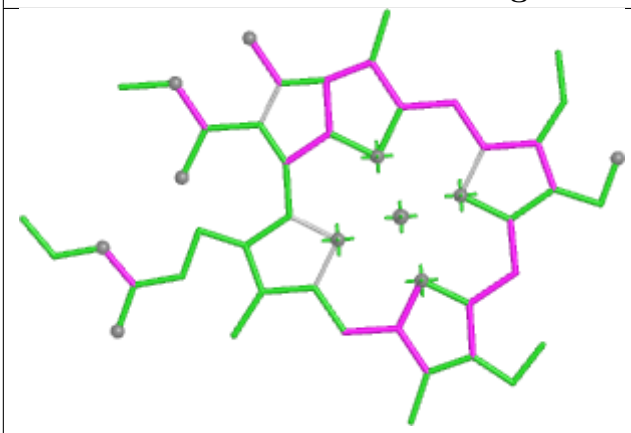


Rings

Ligand CHL AQ 605



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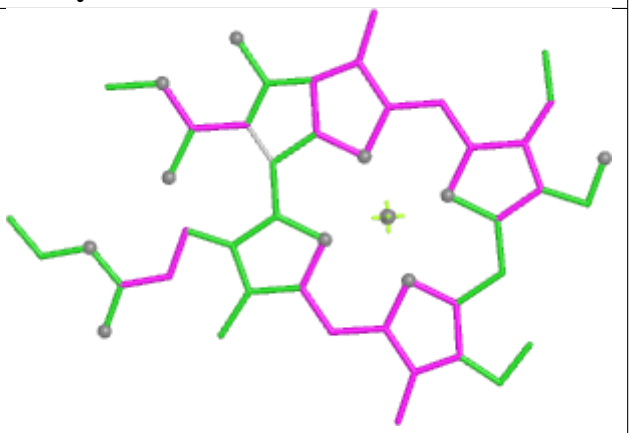

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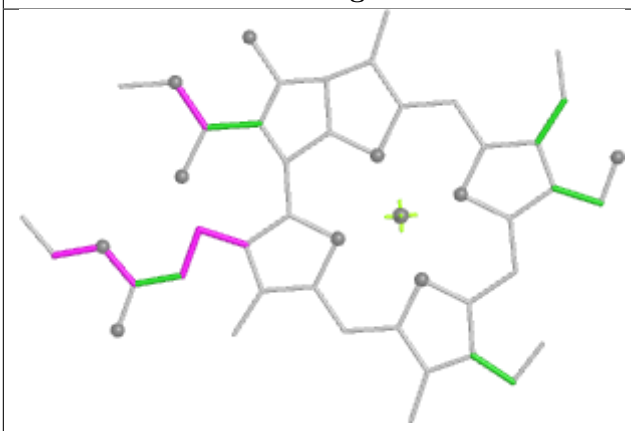

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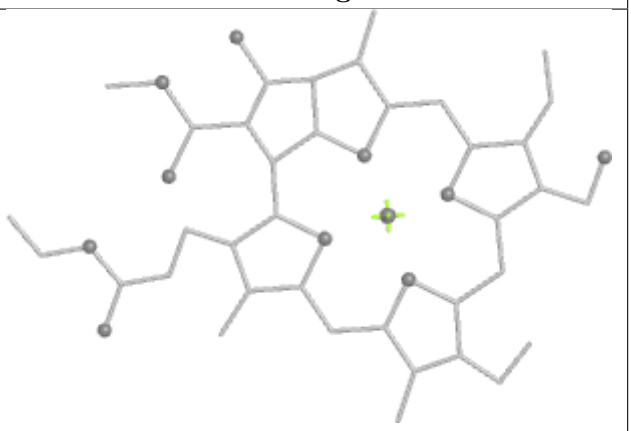
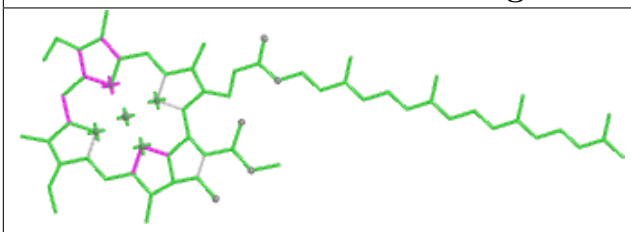


Rings

Ligand CLA AM 404



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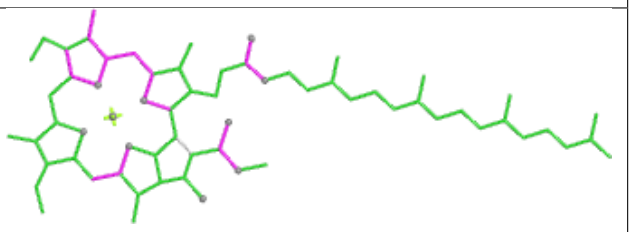

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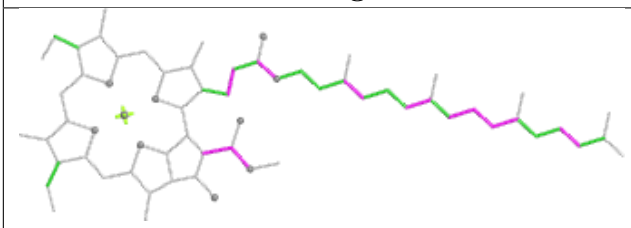

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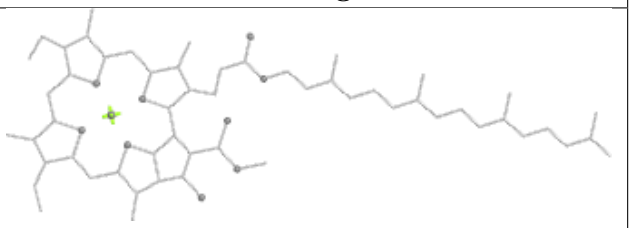
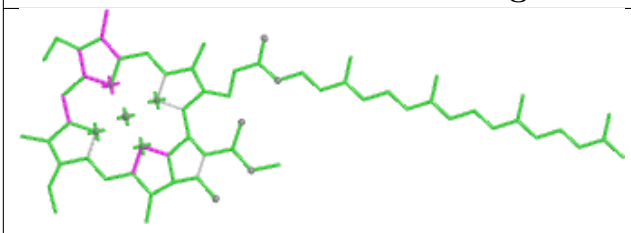


Rings

Ligand CLA AN 603



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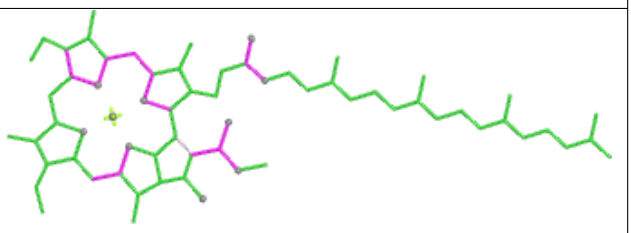
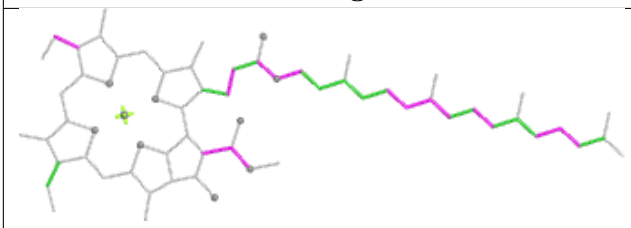


Bond angles



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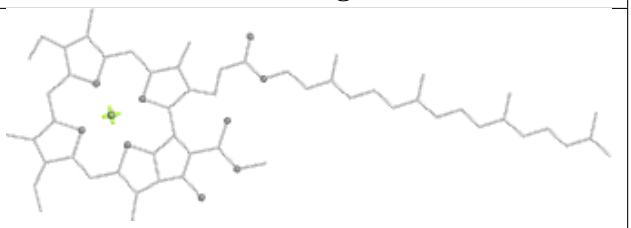
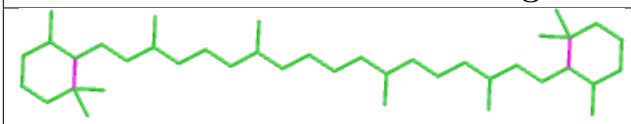


Rings

Ligand BCR O 617



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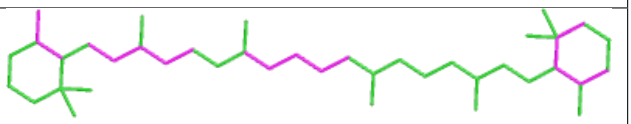
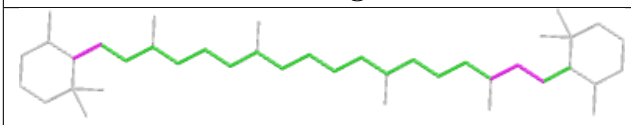


Bond angles



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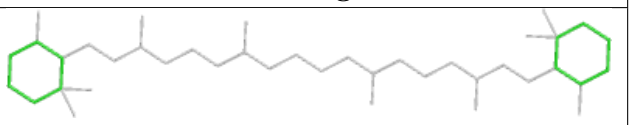
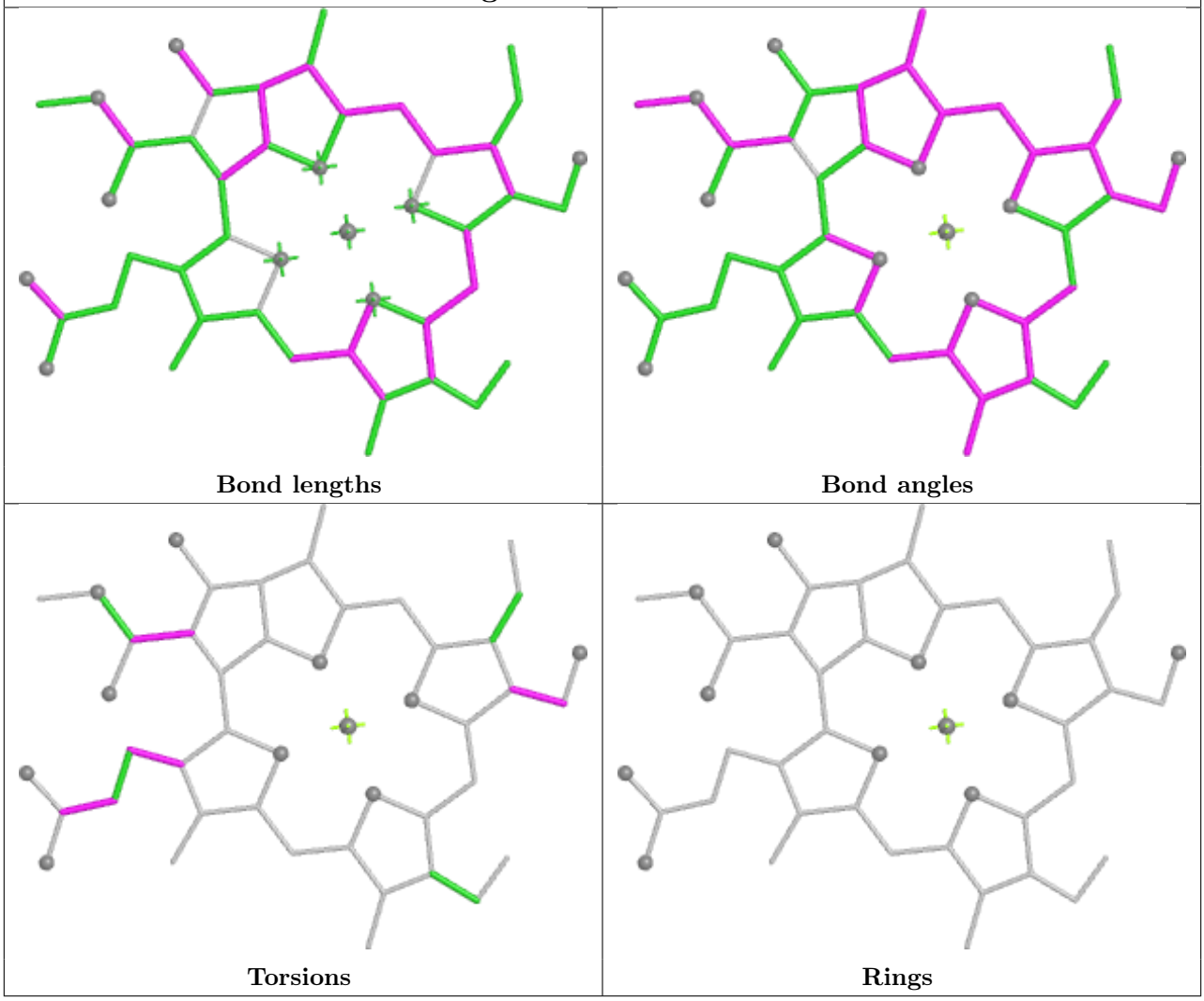
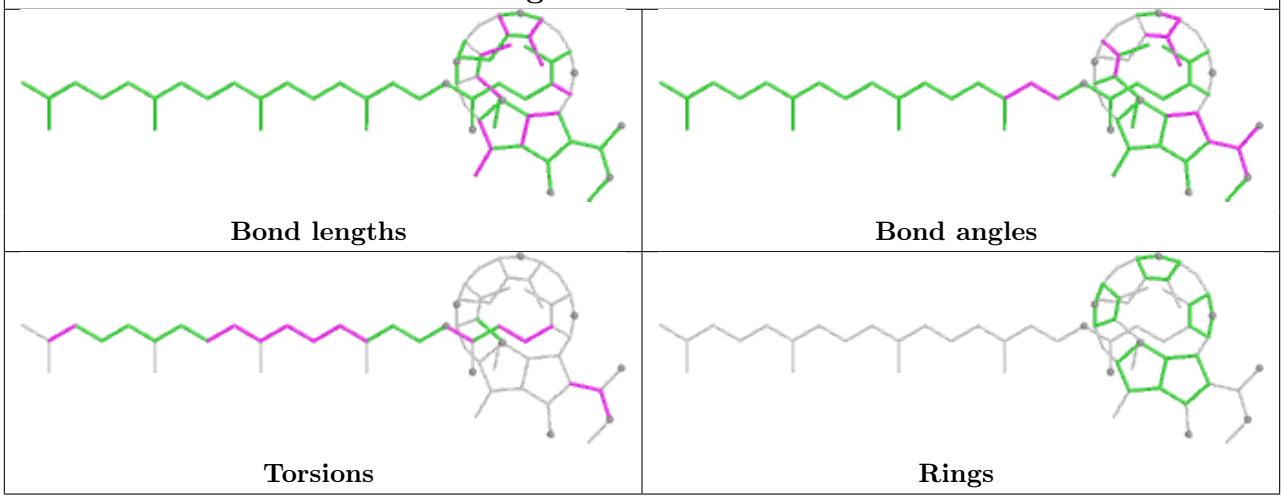


Rings

Ligand CHL AF 607



Ligand PHO J 406



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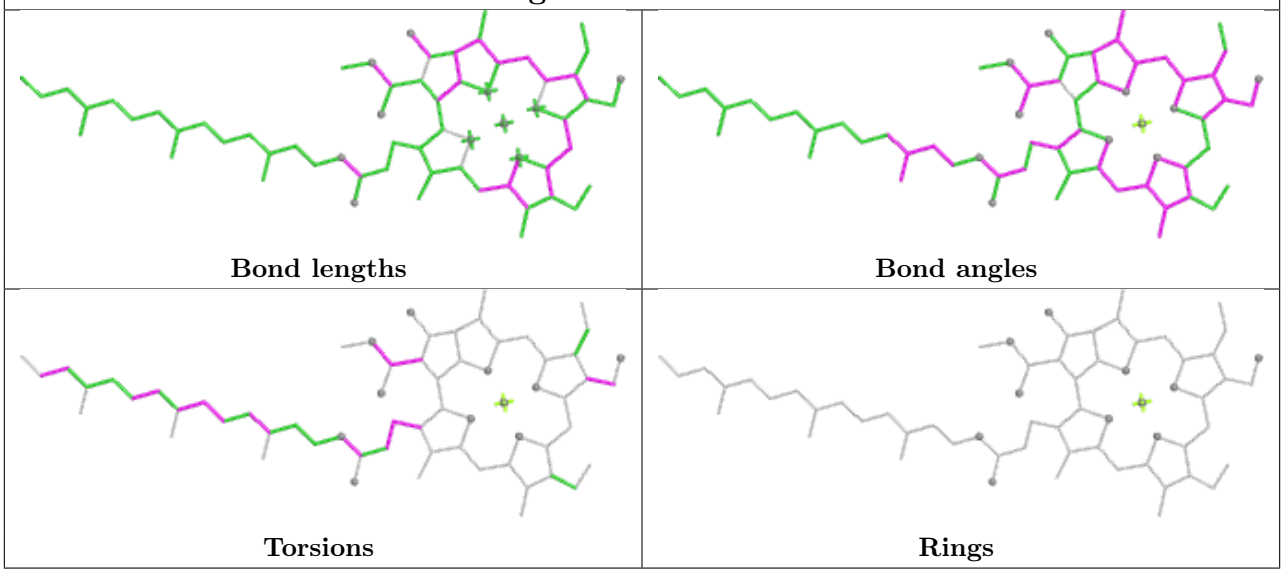

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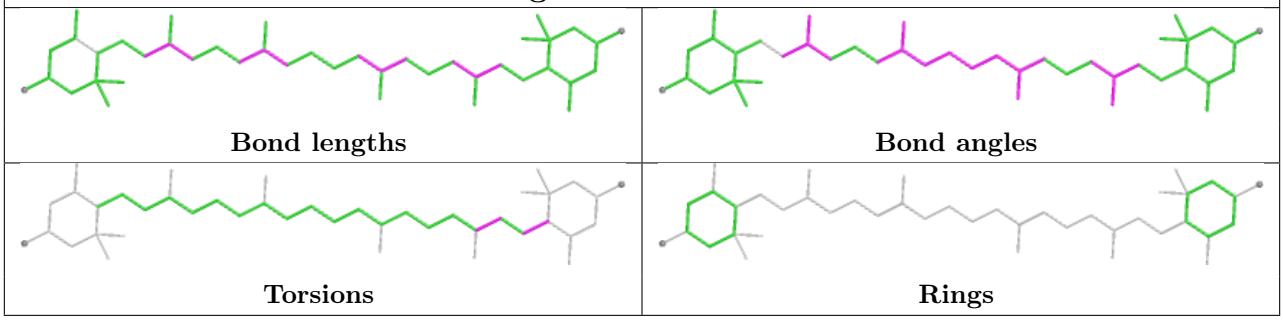
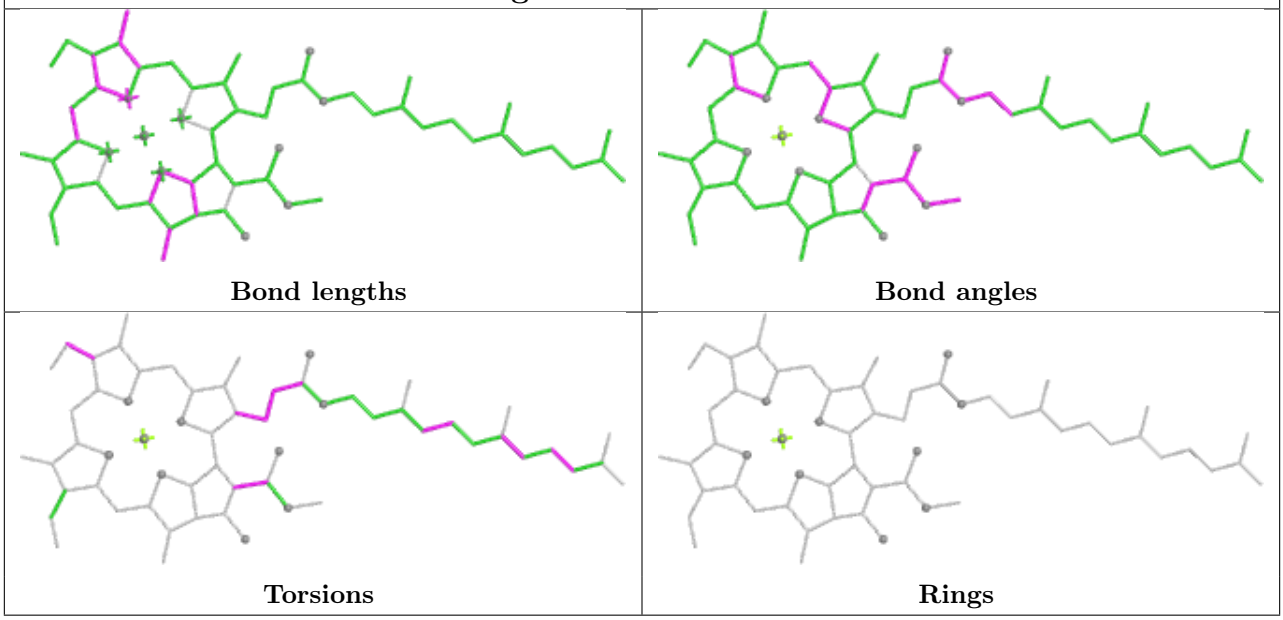
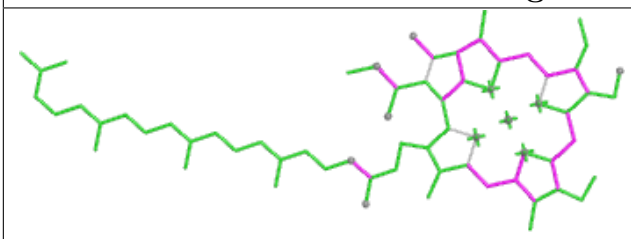
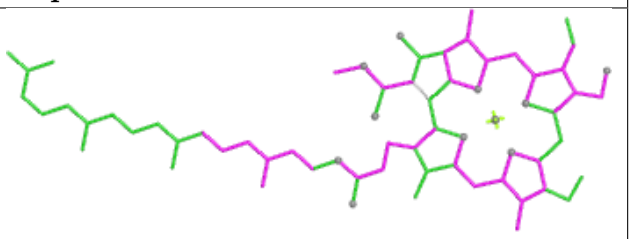
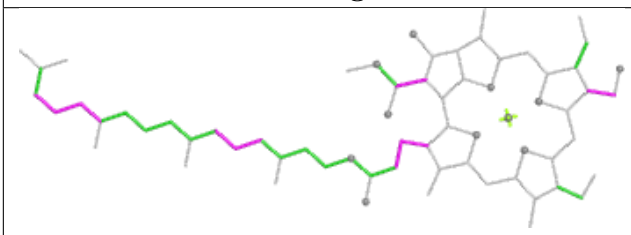
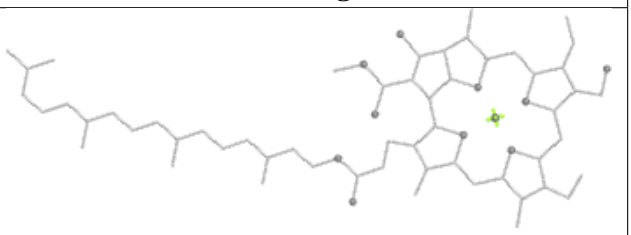
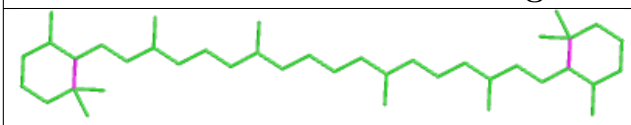
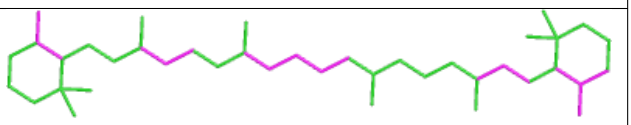
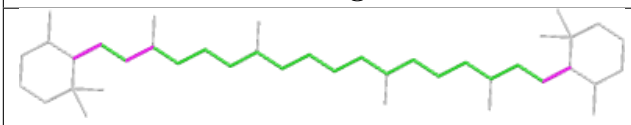
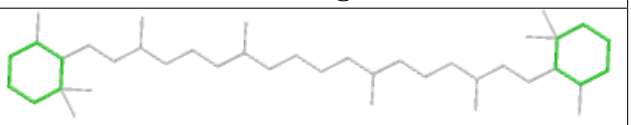


Ligand CLA AR 612



Ligand CHL p 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR k 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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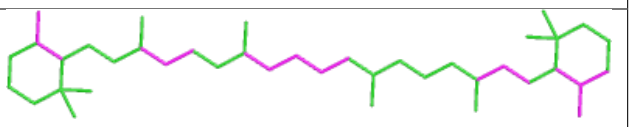
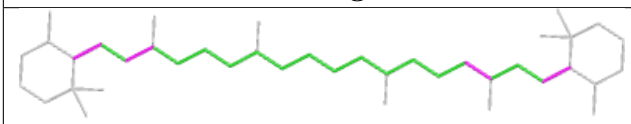
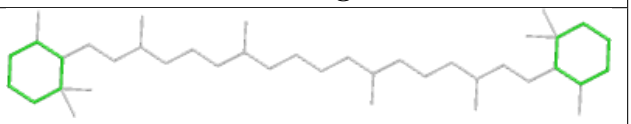
Bond lengths	 Bond angles
 Torsions	 Rings

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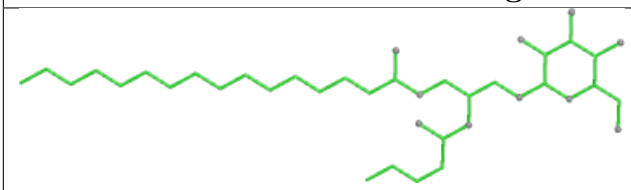
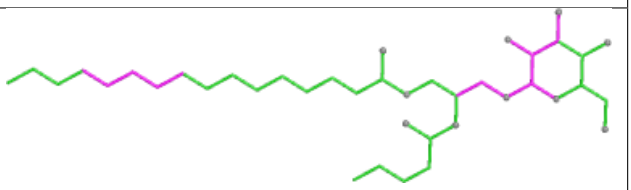
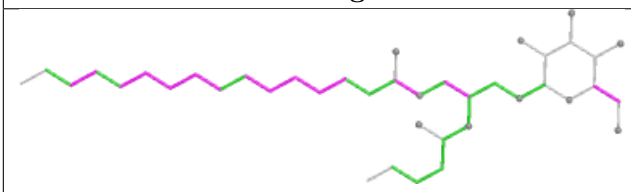
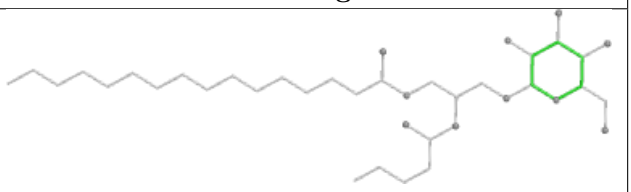
 Bond lengths	 Bond angles
 Torsions	 Rings

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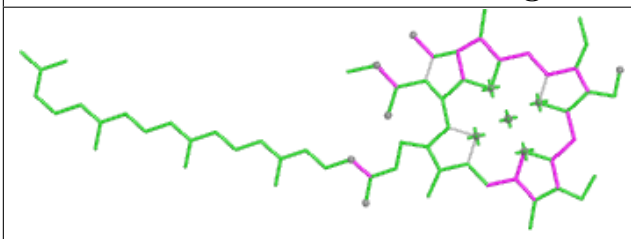
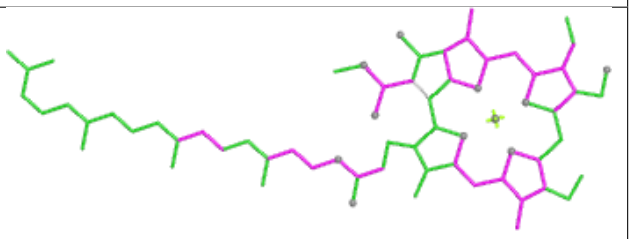
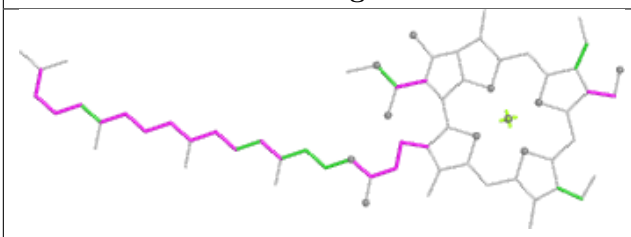
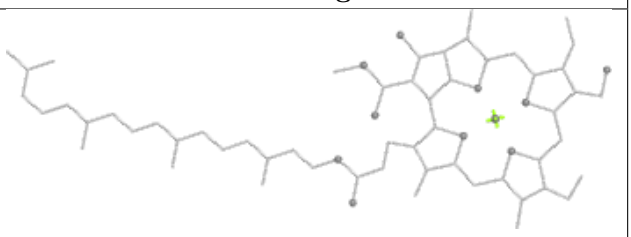
 Bond lengths	 Bond angles
 Torsions	 Rings

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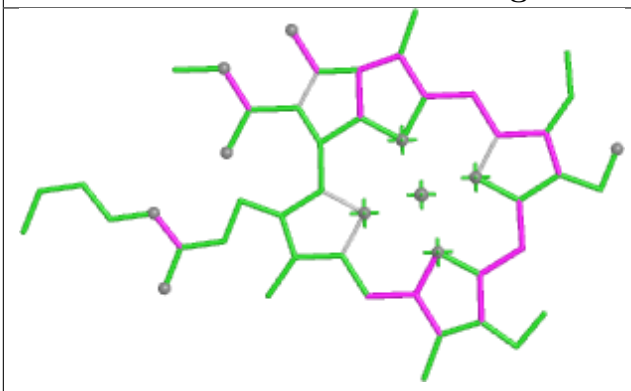
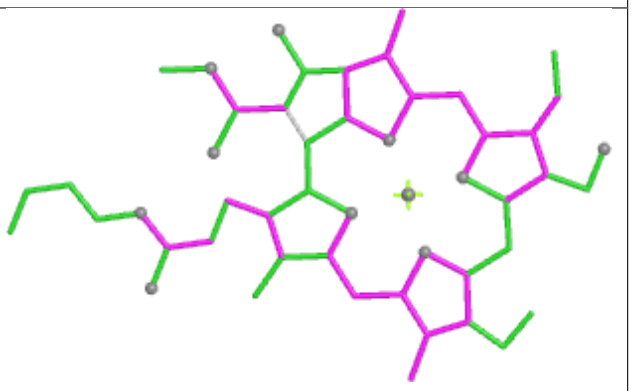
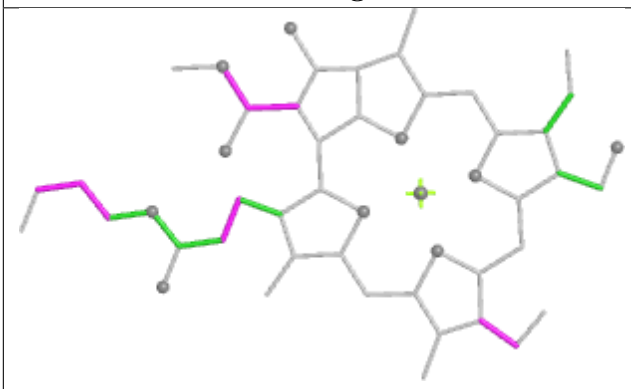
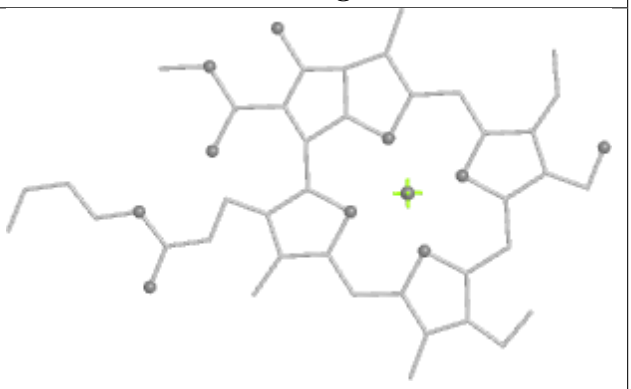
 Bond lengths	 Bond angles
 Torsions	 Rings

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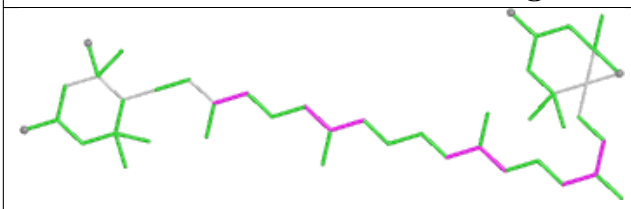
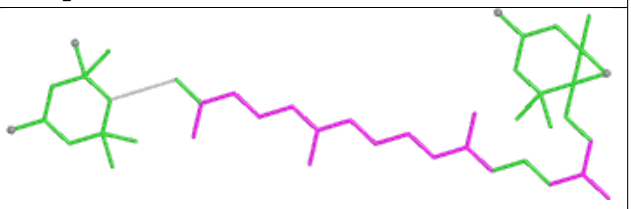
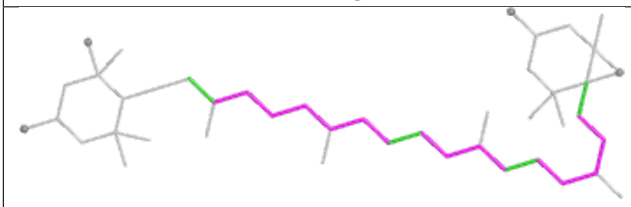
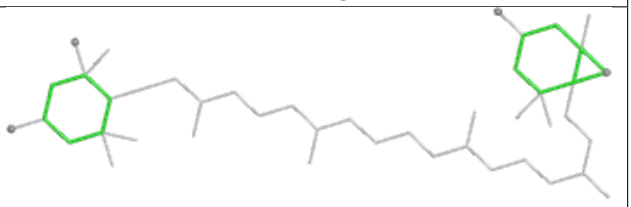
 Bond lengths	 Bond angles
 Torsions	 Rings

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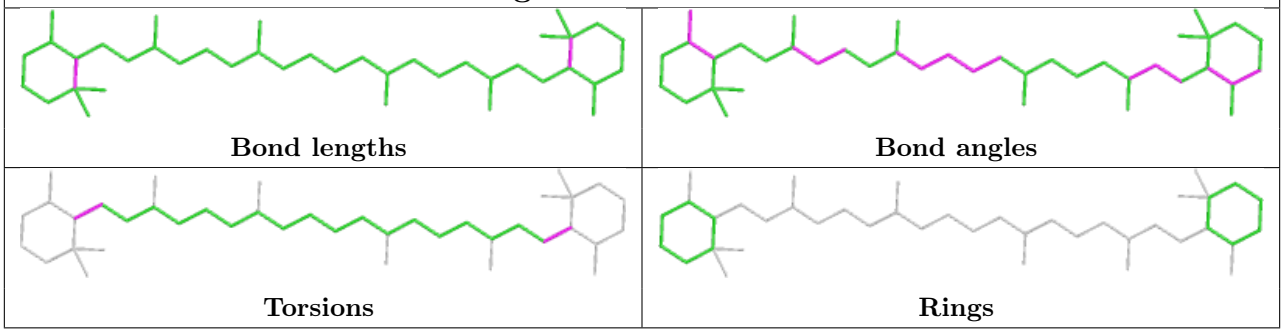
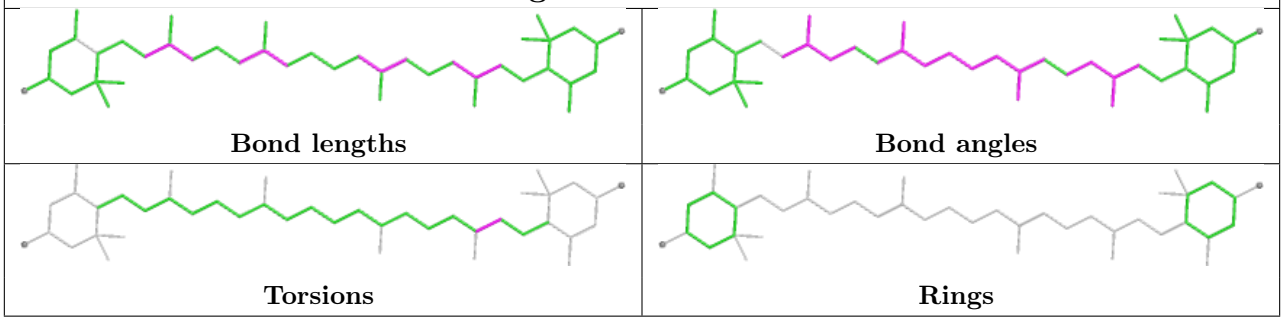
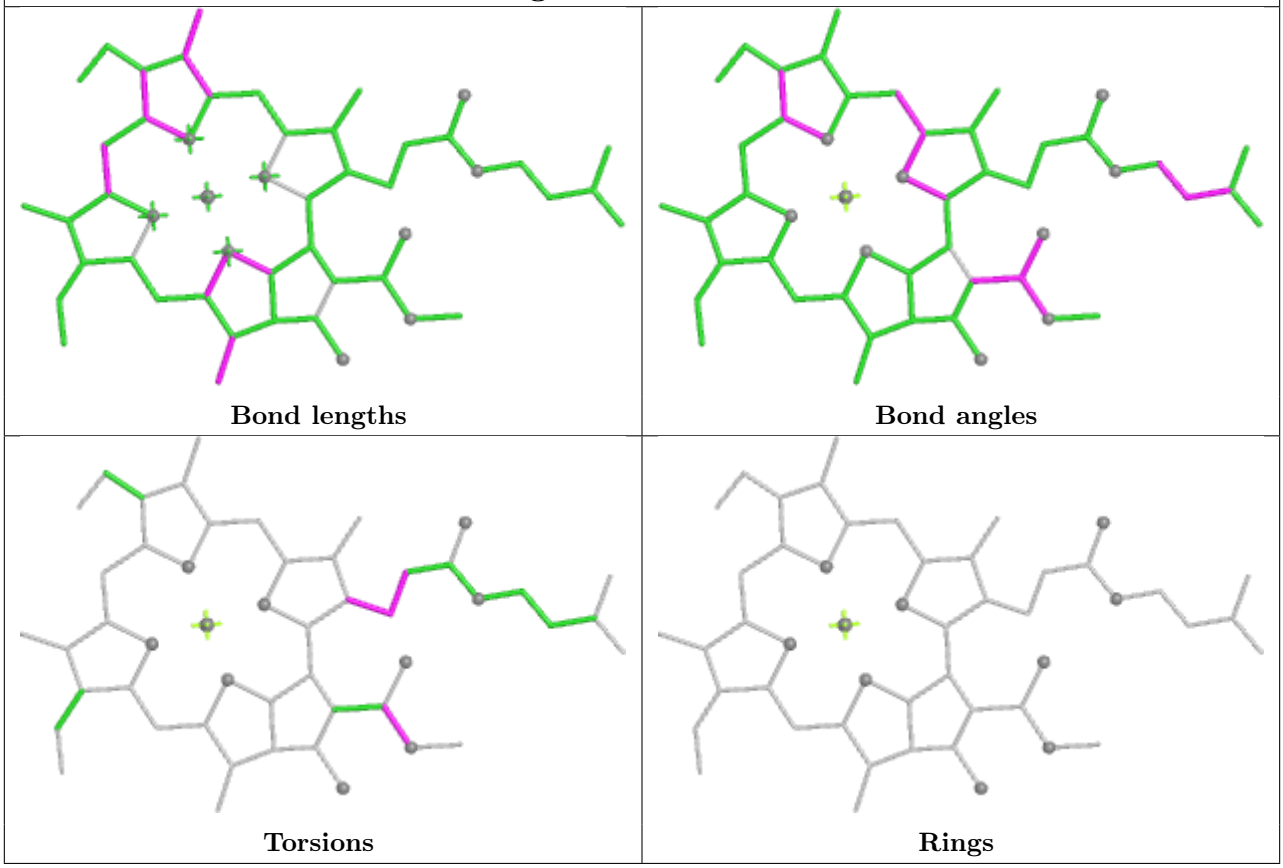


Ligand LUT v 316



Ligand CLA 9 604



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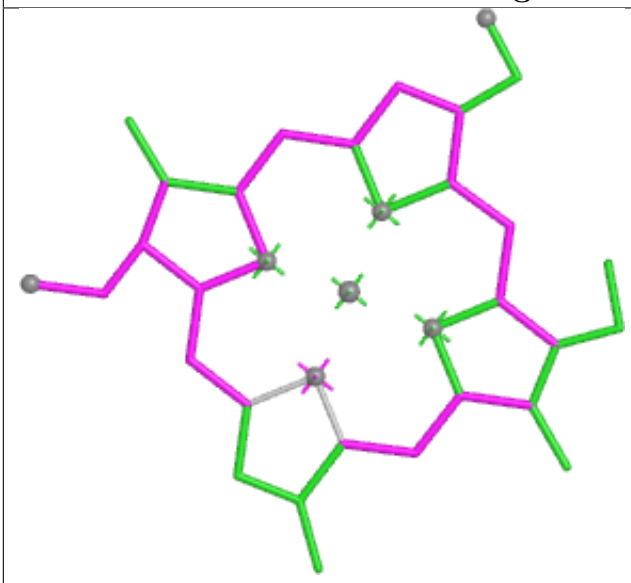
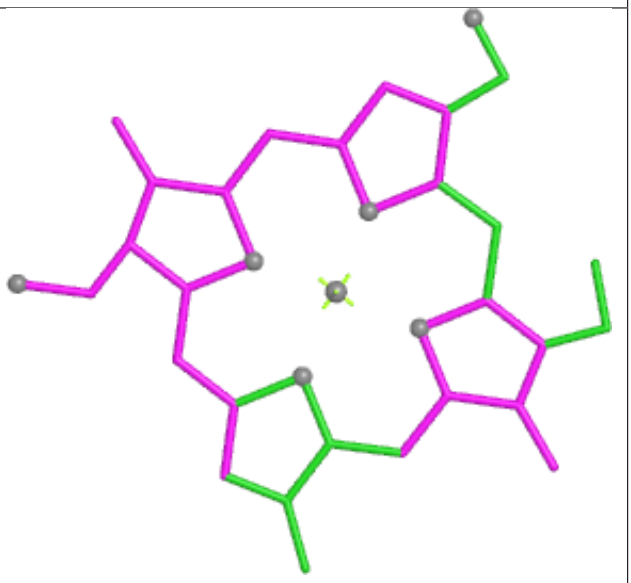
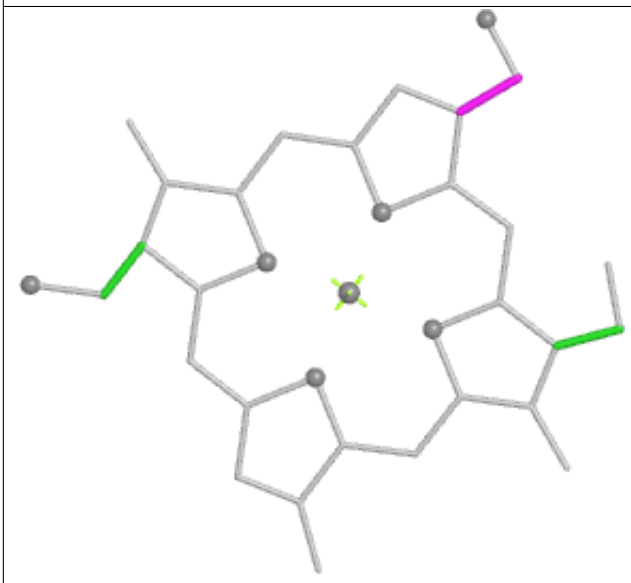
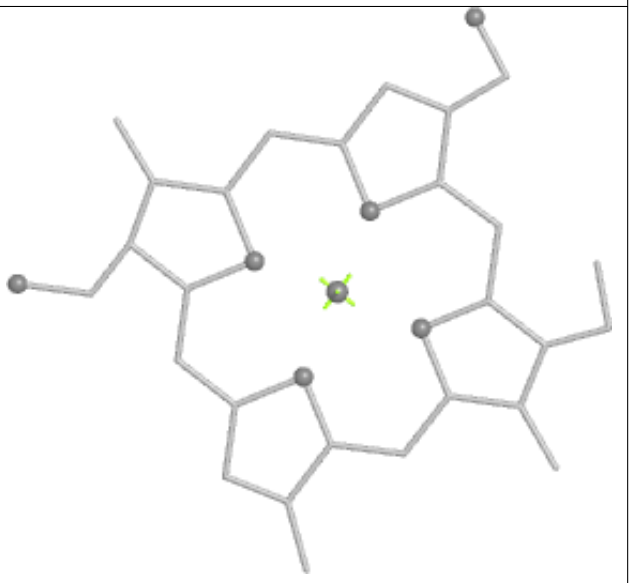
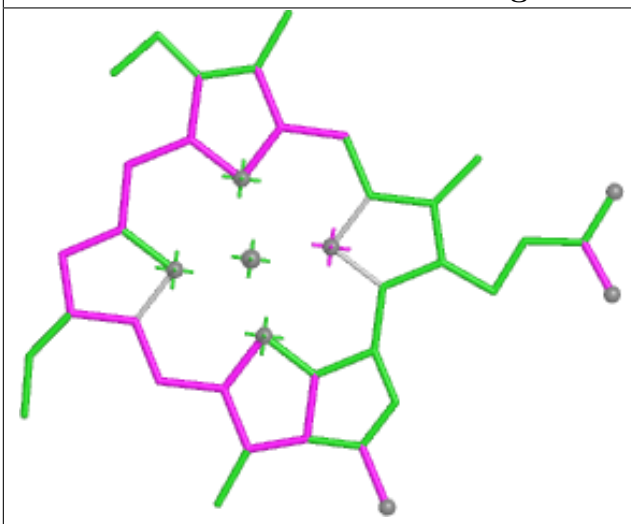
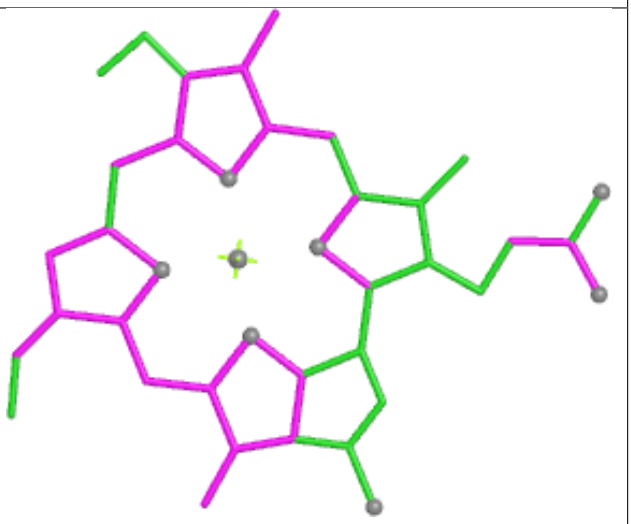
 Bond lengths	 Bond angles
 Torsions	 Rings

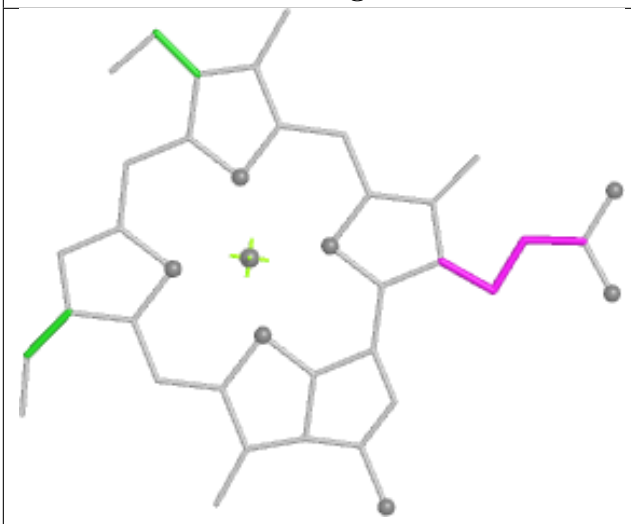
Ligand CHL AB 605



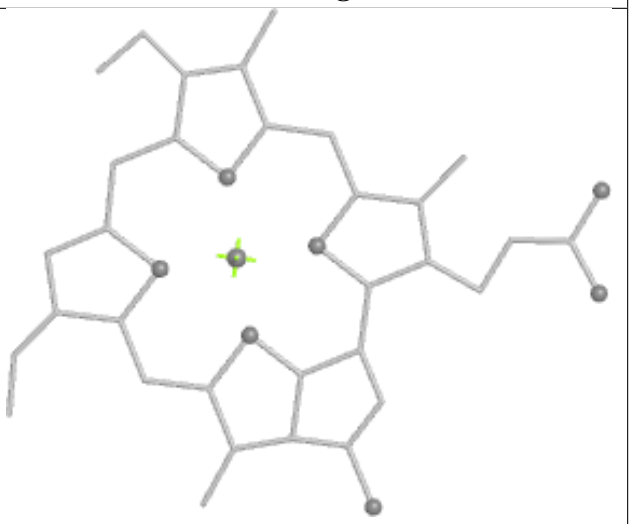
Bond lengths



Bond angles

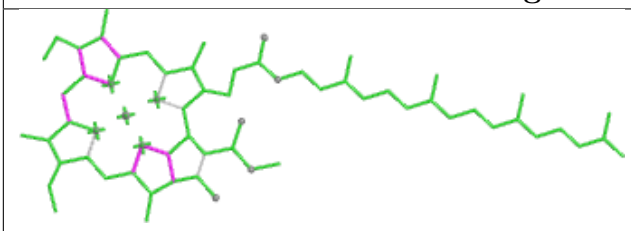


Torsions



Rings

Ligand CLA O 608



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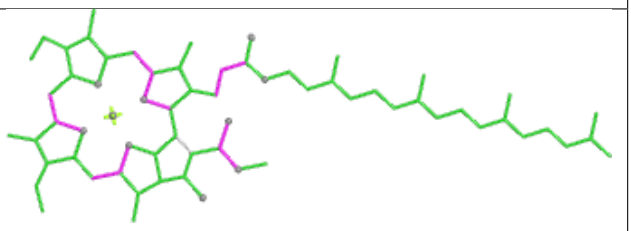
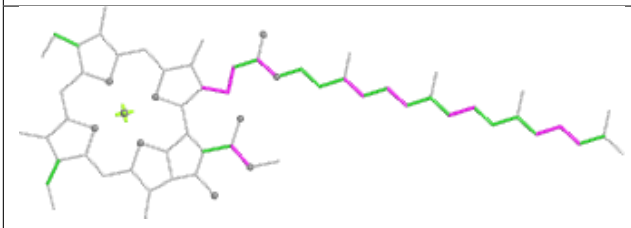


Bond angles



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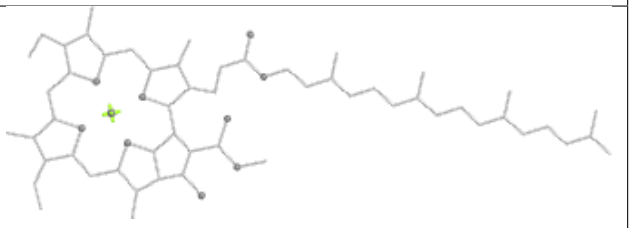

Rings

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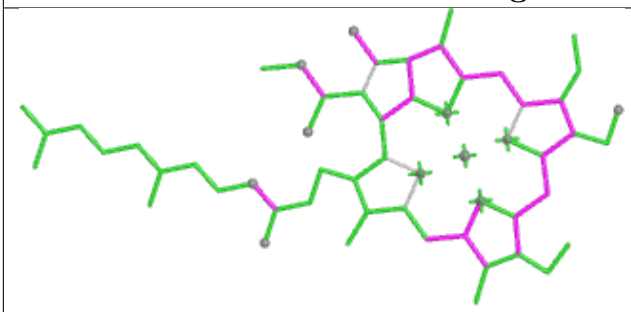
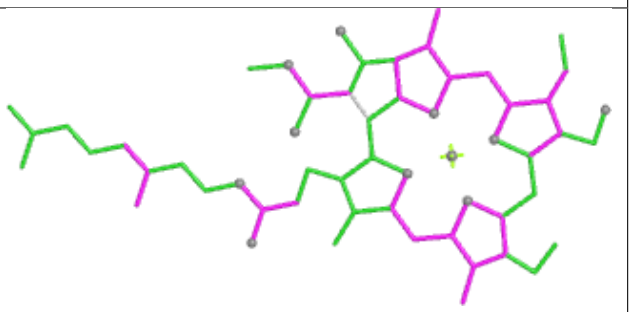
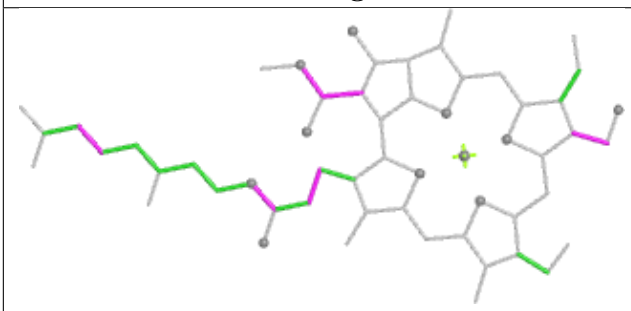
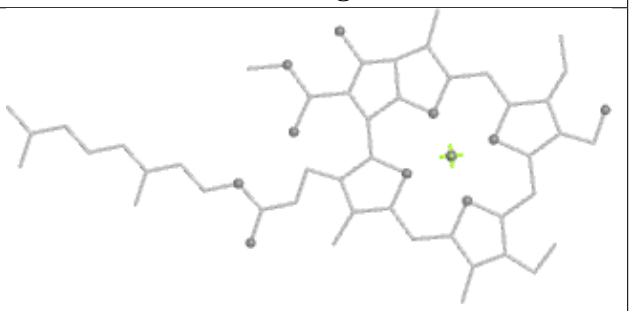
 Bond lengths	 Bond angles
 Torsions	 Rings

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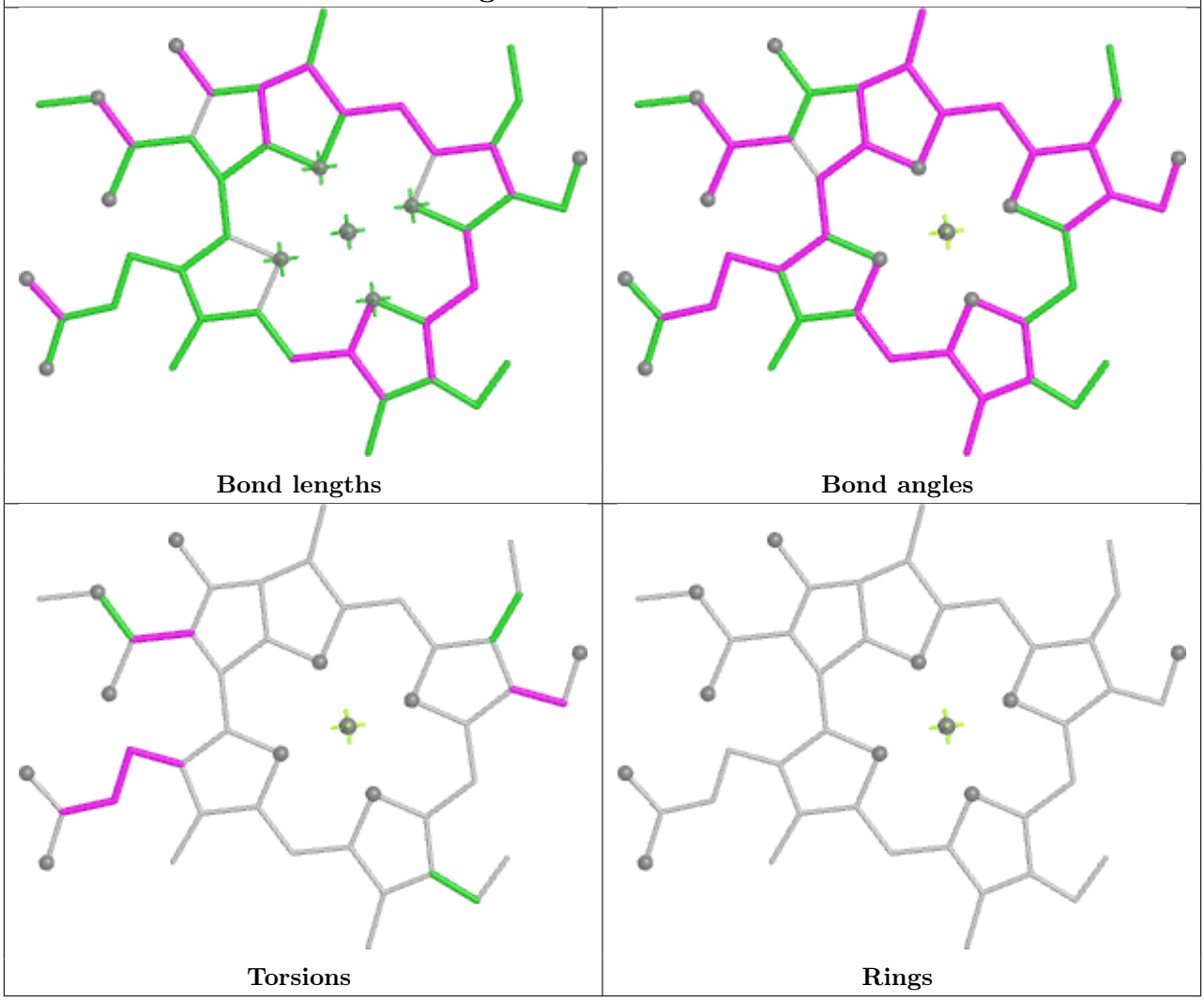

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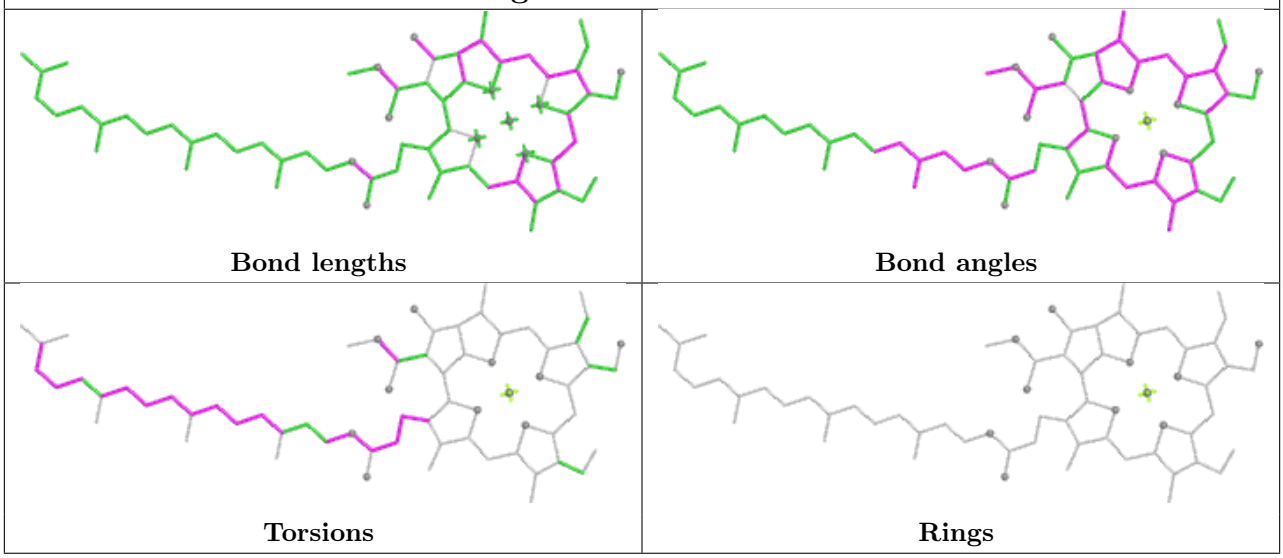

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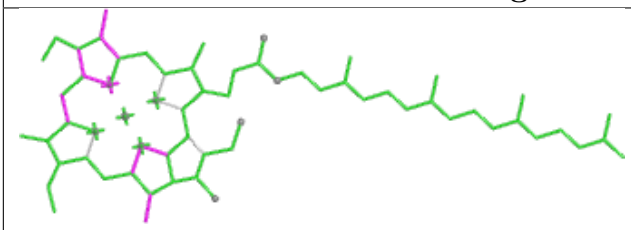
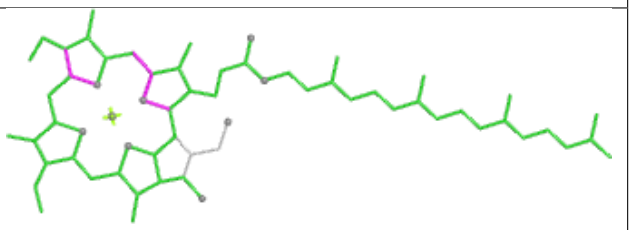
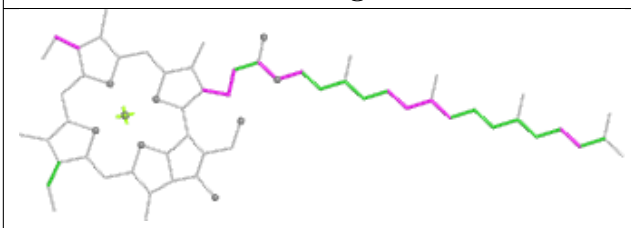
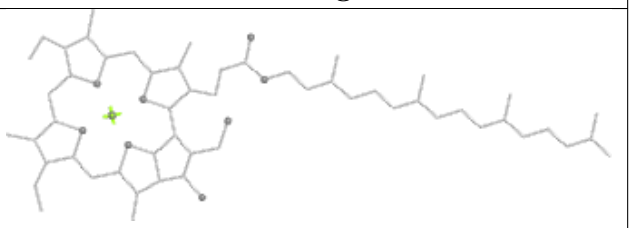
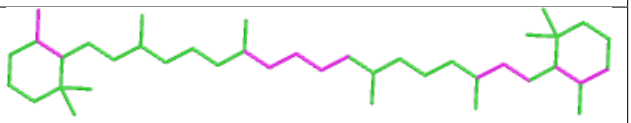
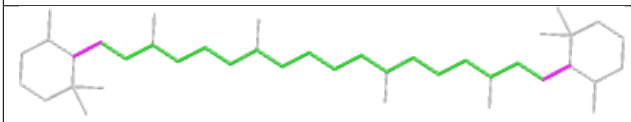
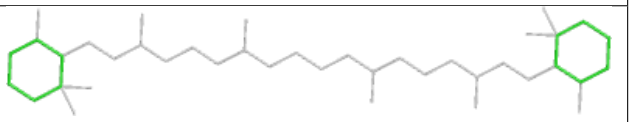
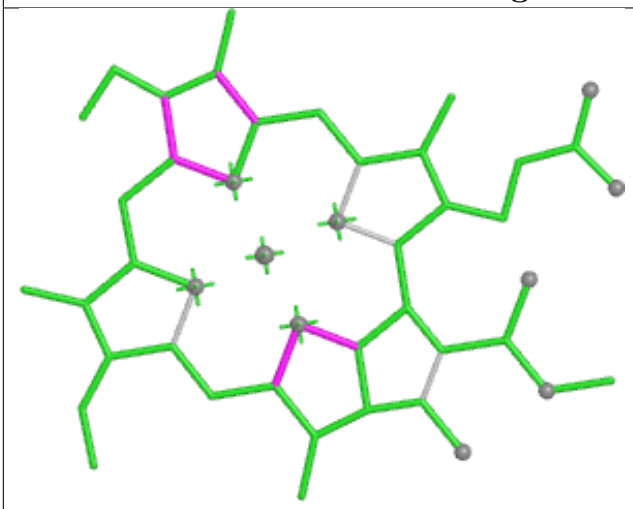
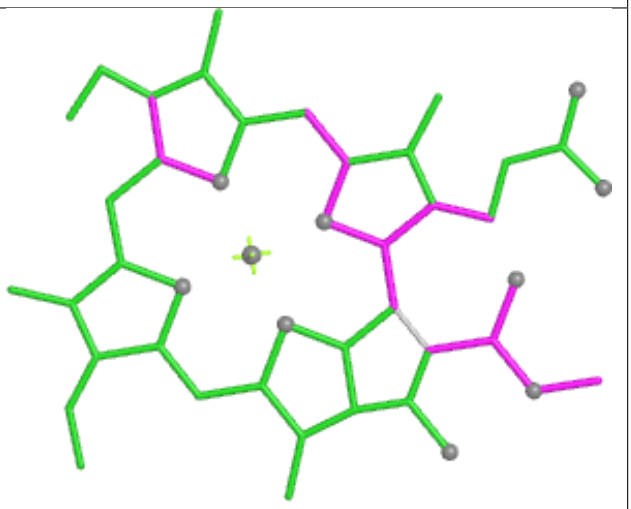
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR AK 621	
Bond lengths	 Bond angles
 Torsions	 Rings

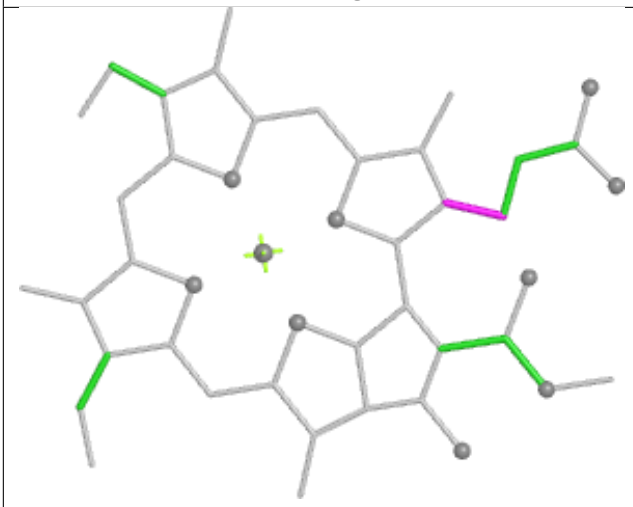
Ligand CLA AB 602



Bond lengths



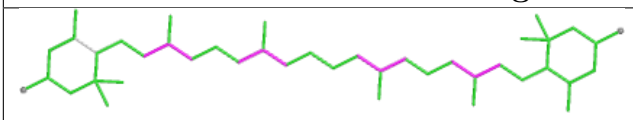
Bond angles



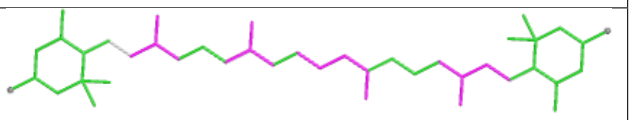
Torsions

Rings

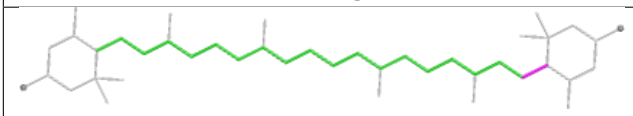
Ligand LUT AE 613



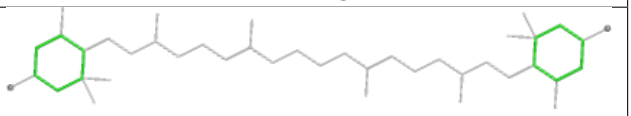
Bond lengths



Bond angles

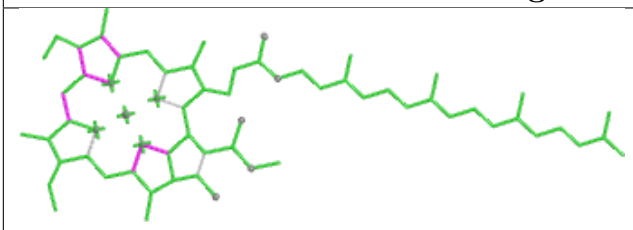


Torsions



Rings

Ligand CLA J 403



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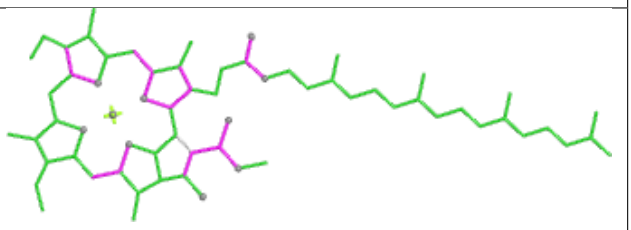

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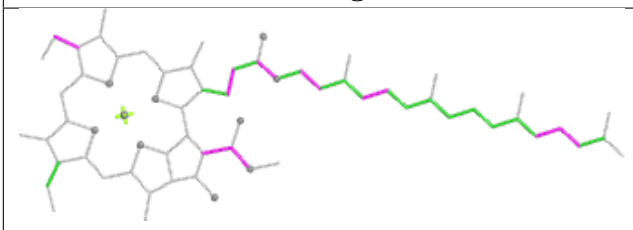

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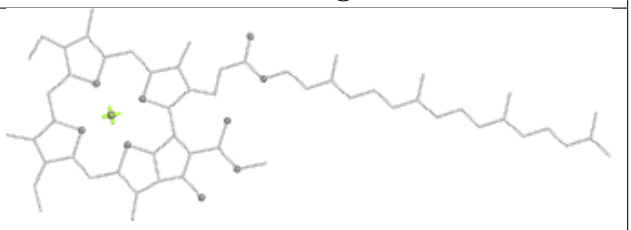
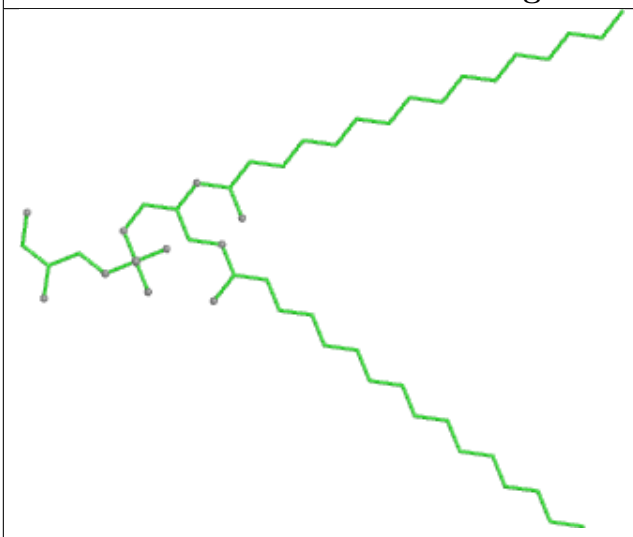


Rings

Ligand LHG P 517



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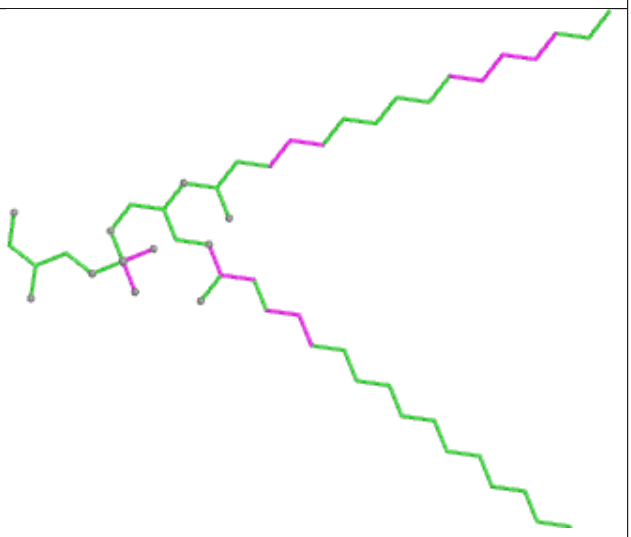
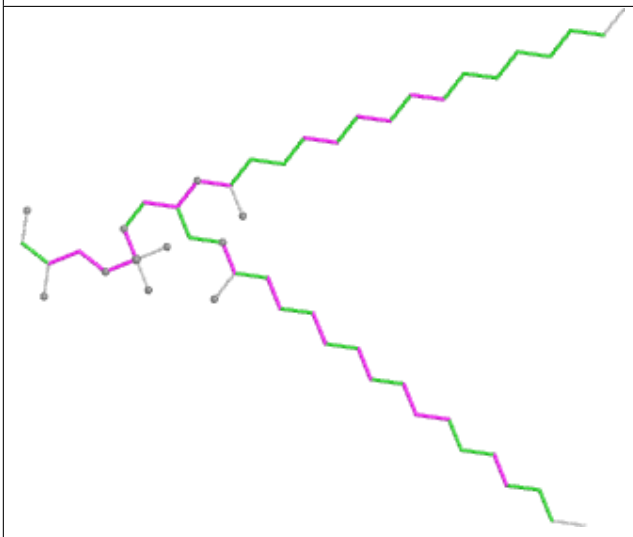


Bond angles



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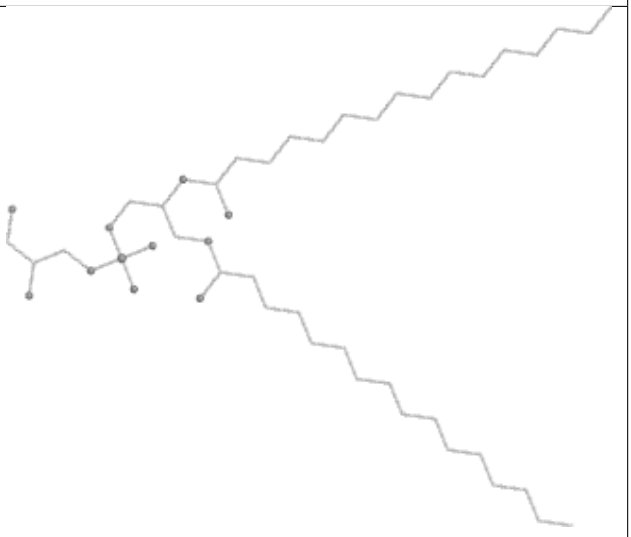
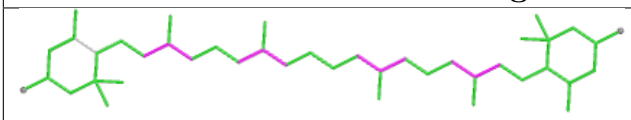


Rings

Ligand LUT AN 615



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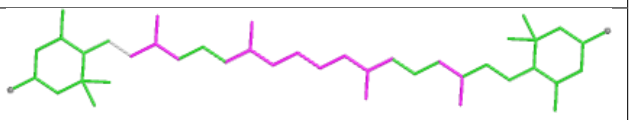
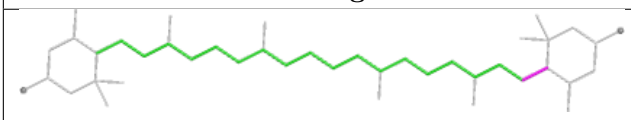


Bond angles



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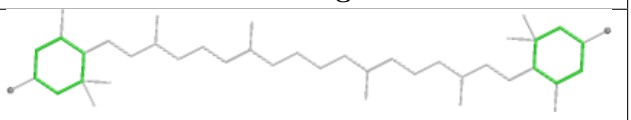
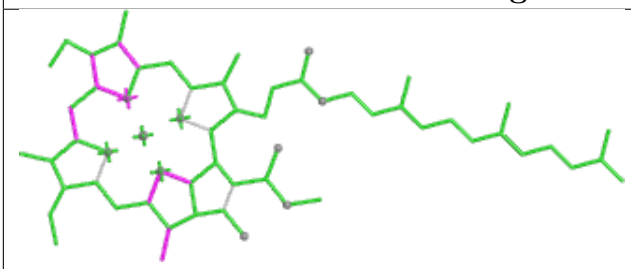


Rings

Ligand CLA AH 609



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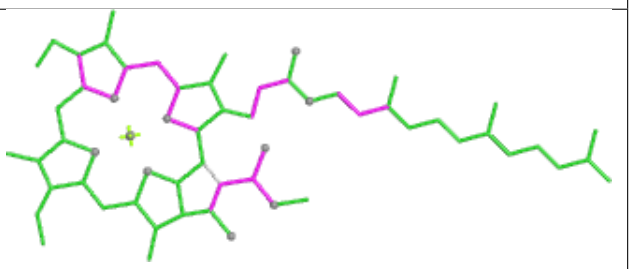
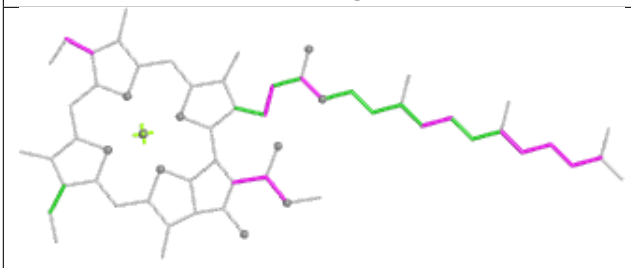


Bond angles



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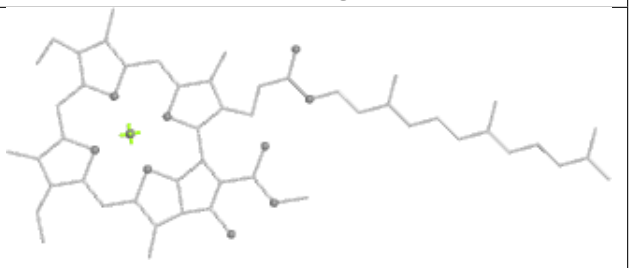
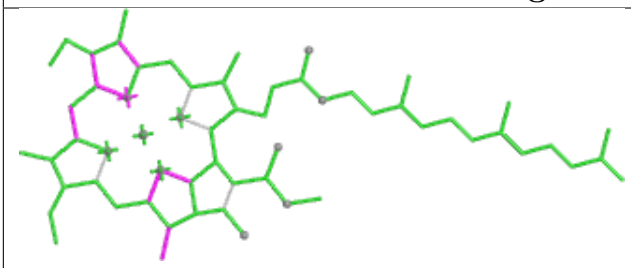


Rings

Ligand CLA 0 602



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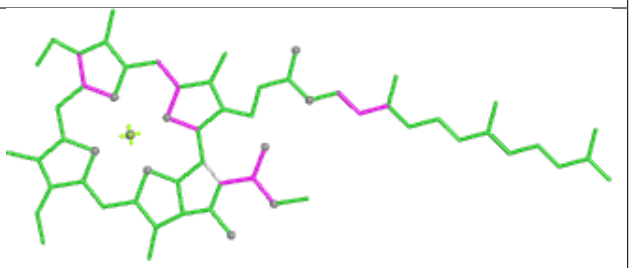

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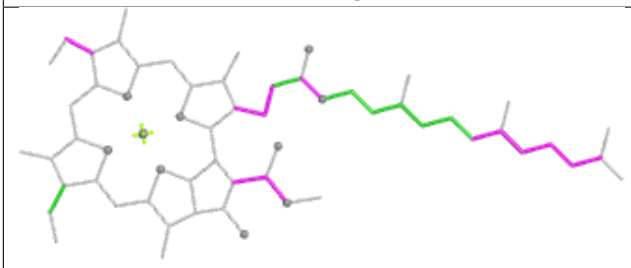

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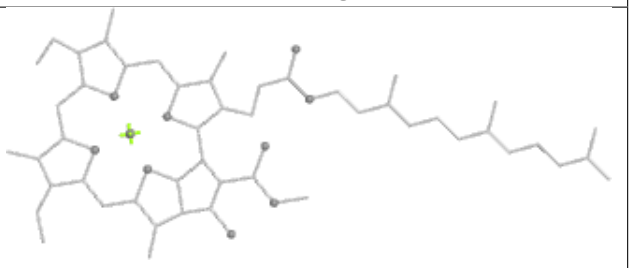
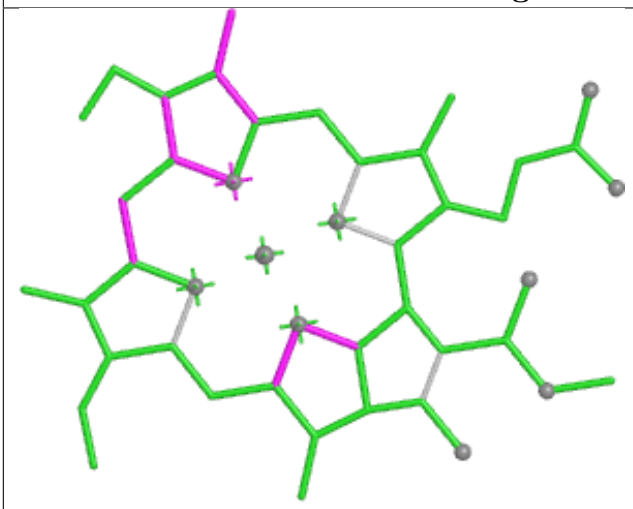


Rings

Ligand CLA AE 611



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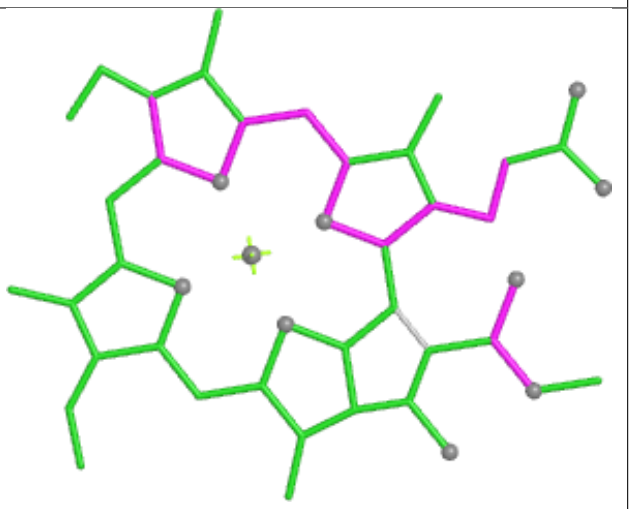
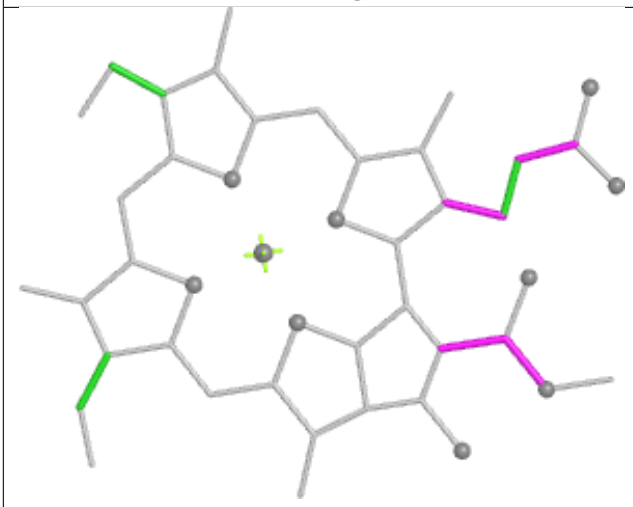


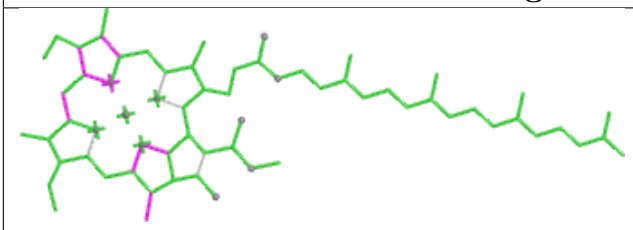
Bond angles



Torsions

Rings

Ligand CLA P 507



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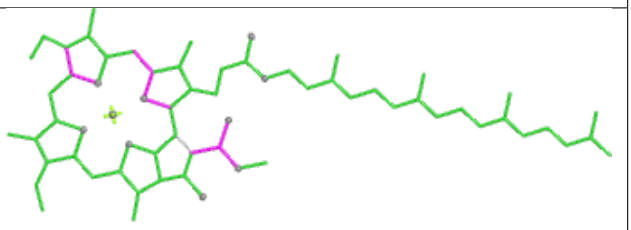
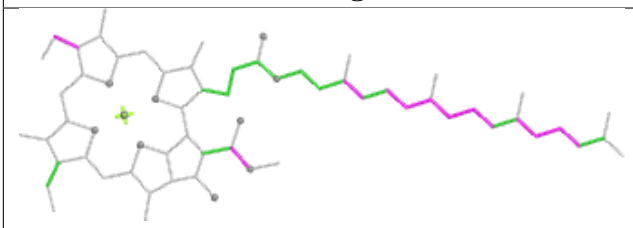


Bond angles



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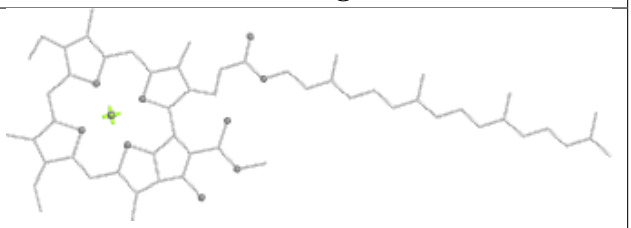
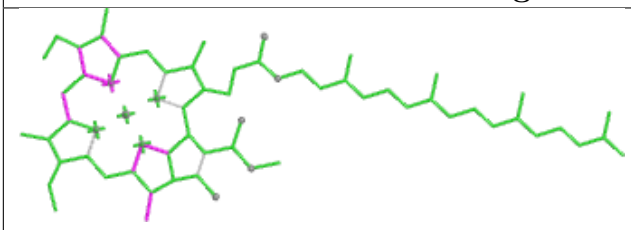


Rings

Ligand CLA AL 508



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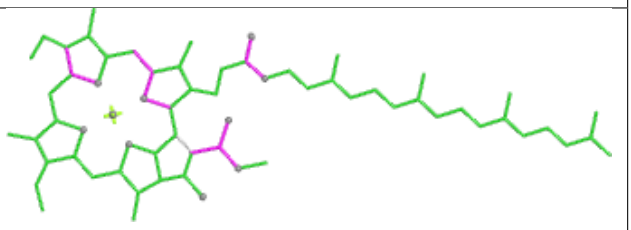
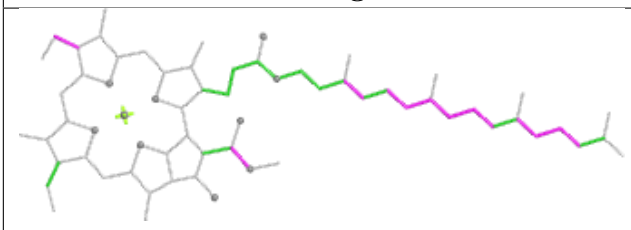


Bond angles



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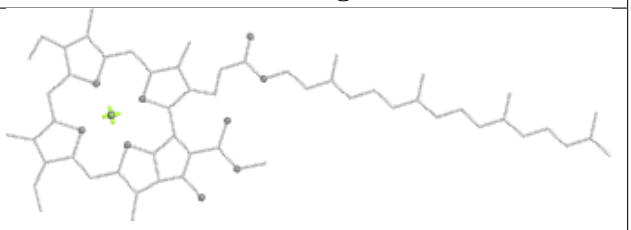
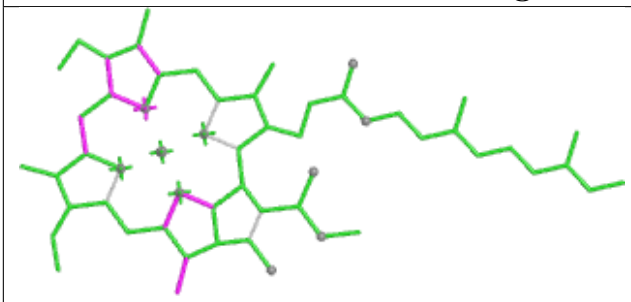
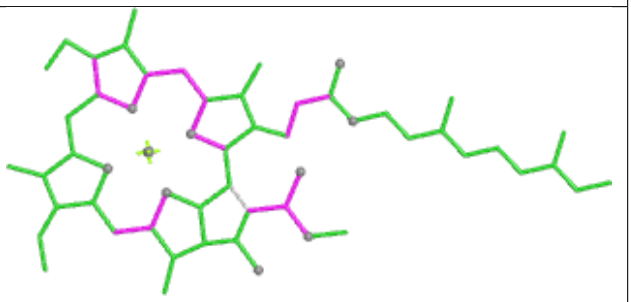


Rings

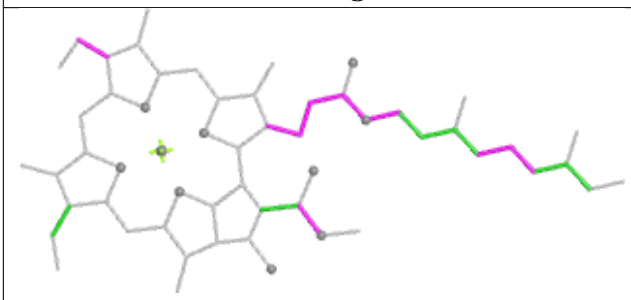
Ligand CLA AS 311



Bond lengths



Bond angles



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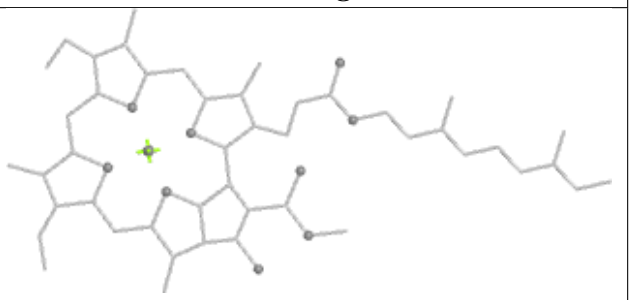
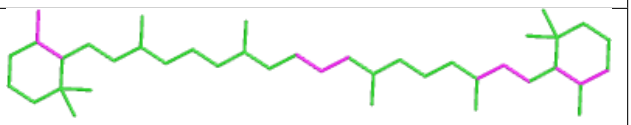


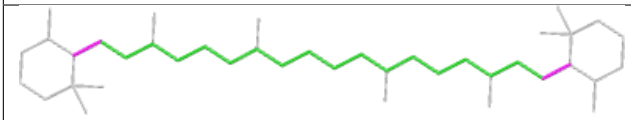
Rings

Ligand BCR AL 515

Bond lengths



Bond angles



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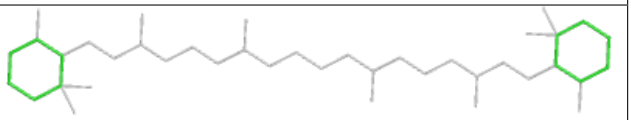
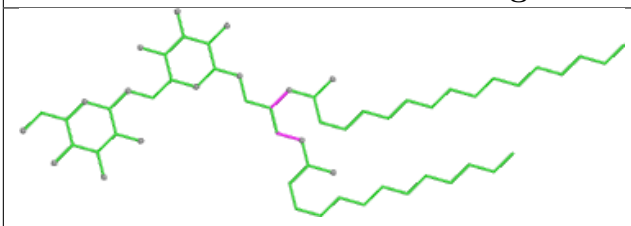
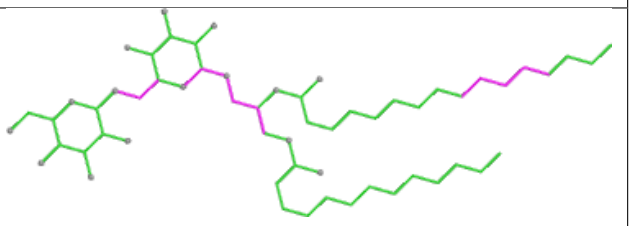
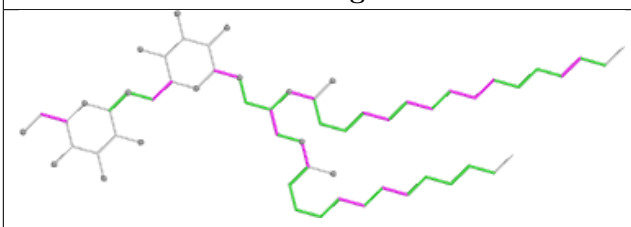
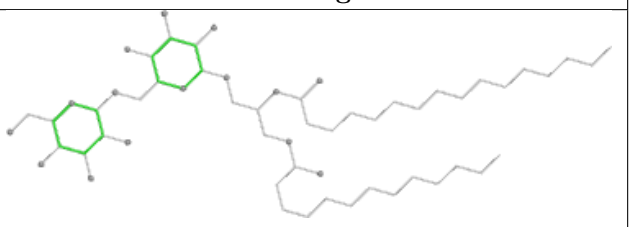
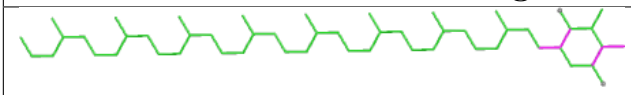
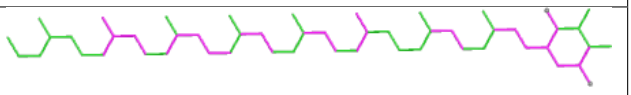
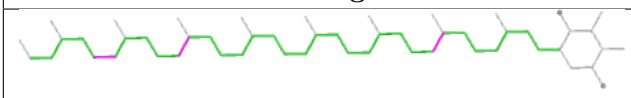
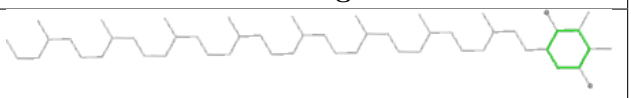
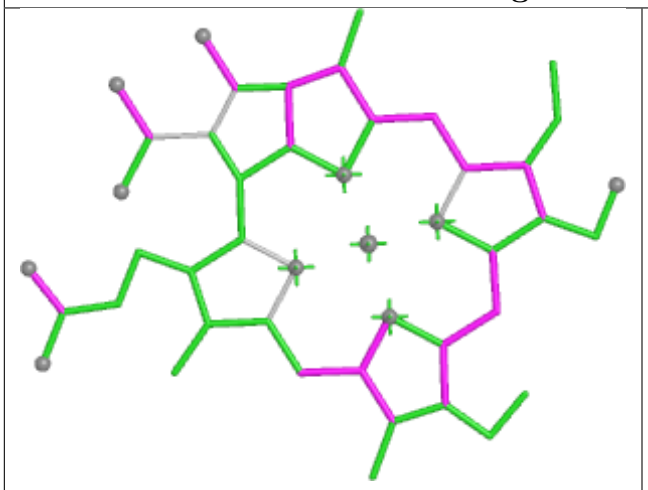


Rings

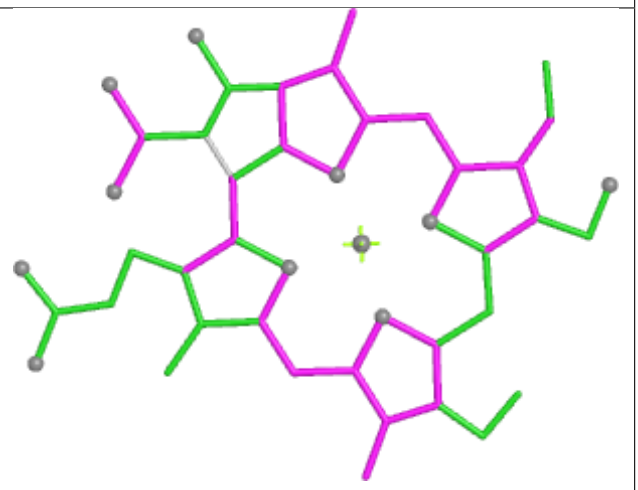
Ligand DGD AJ 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 AM 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

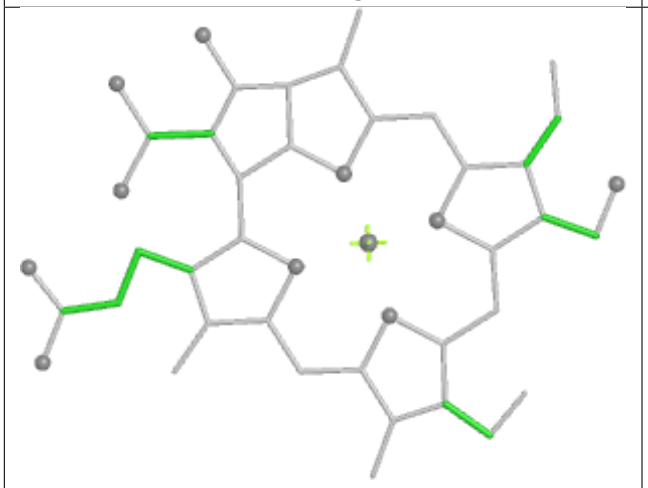
Ligand CHL AB 601



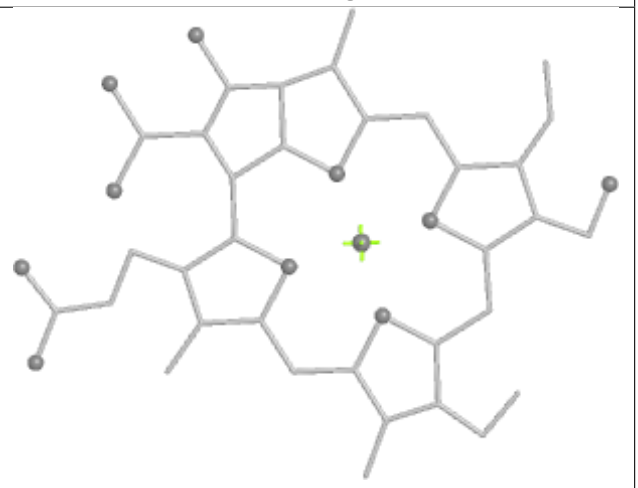
Bond lengths



Bond angles

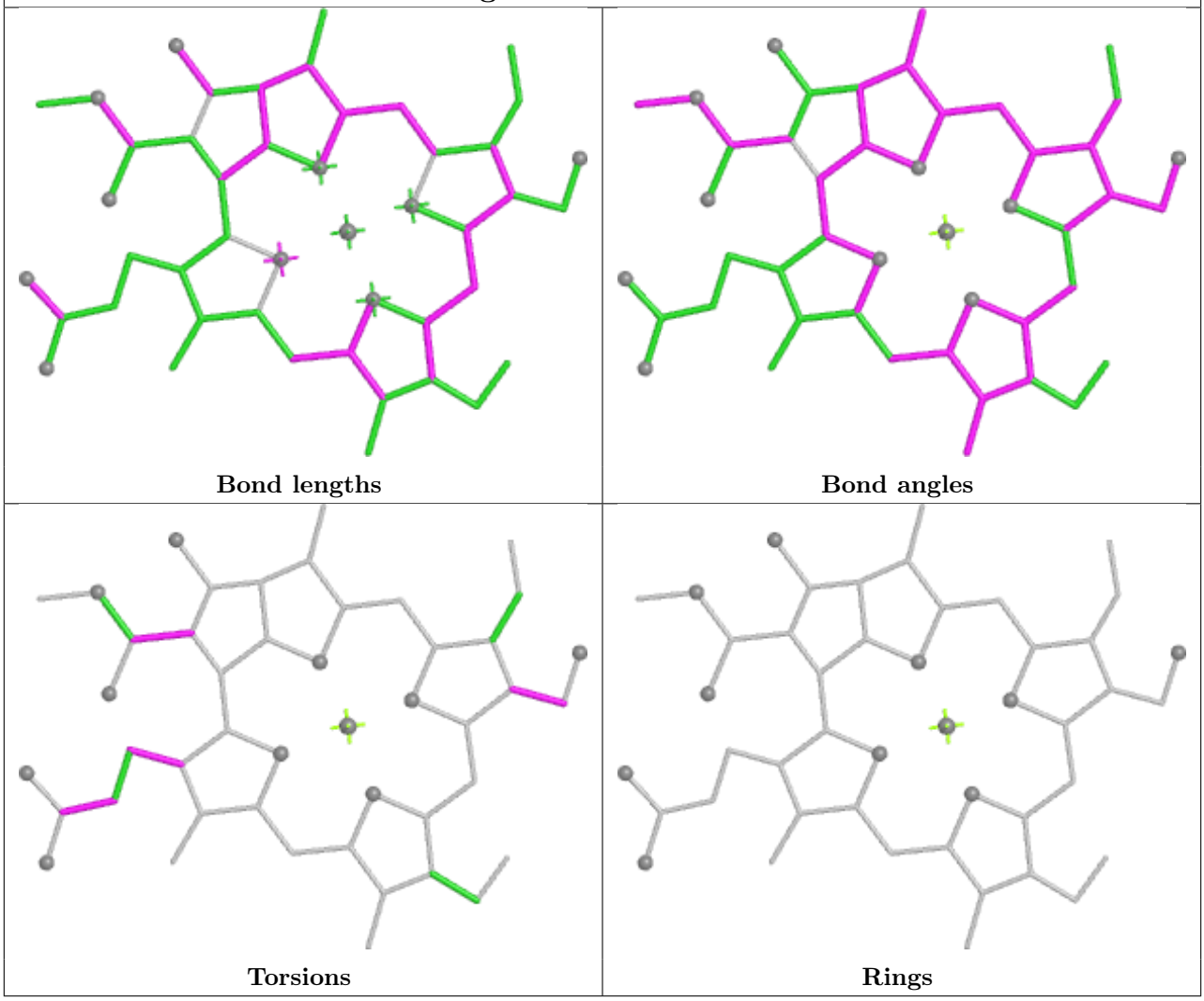


Torsions

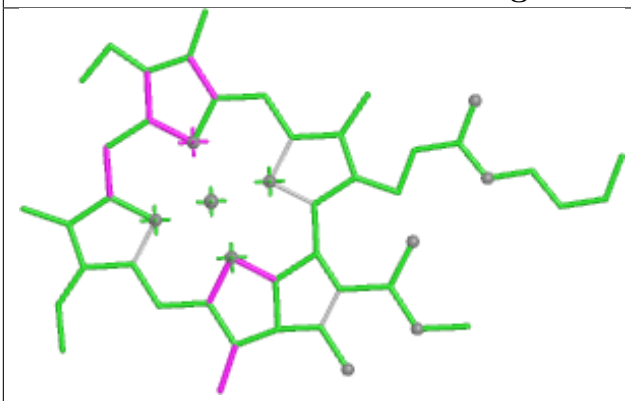


Rings

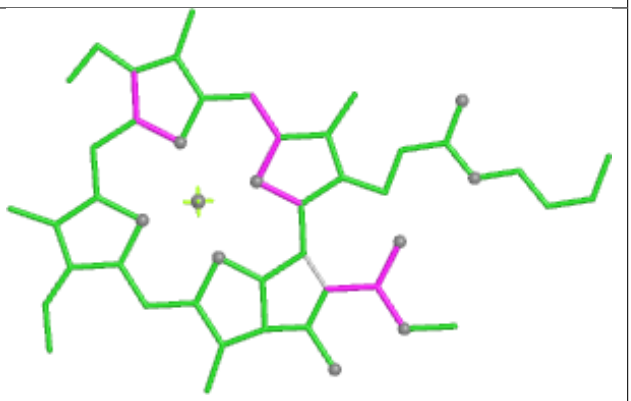
Ligand CHL AB 607



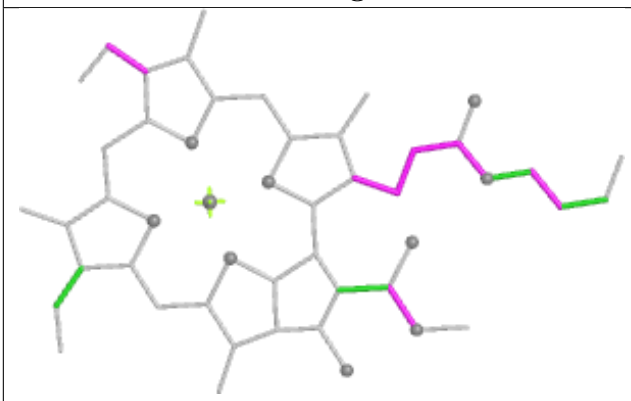
Ligand CLA AR 610



Bond lengths



Bond angles



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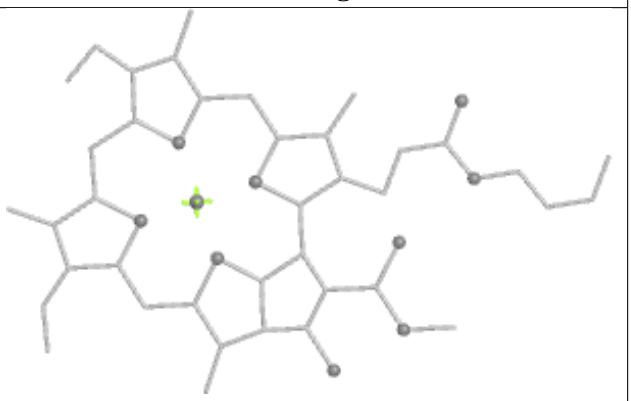
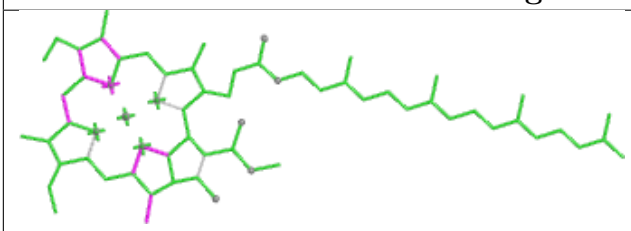
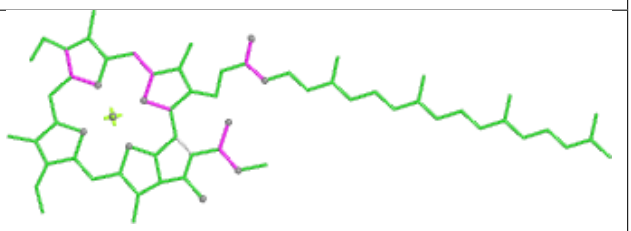


Rings

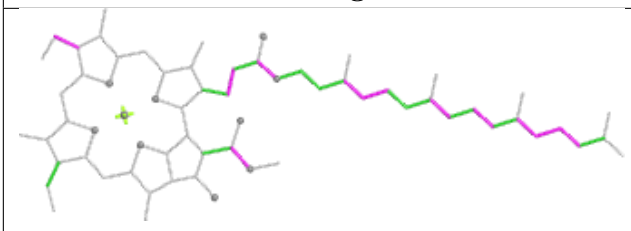
Ligand CLA P 510



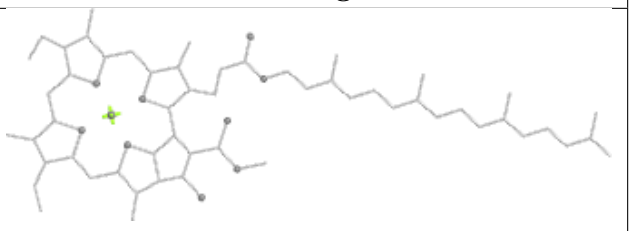
Bond lengths



Bond angles

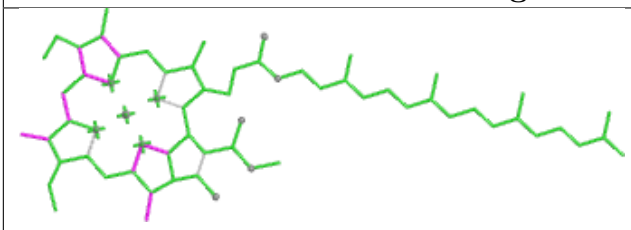


Torsions



Rings

Ligand CLA AK 607



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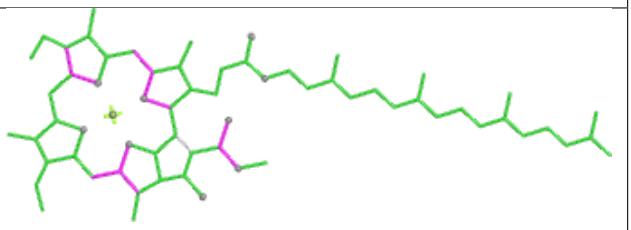

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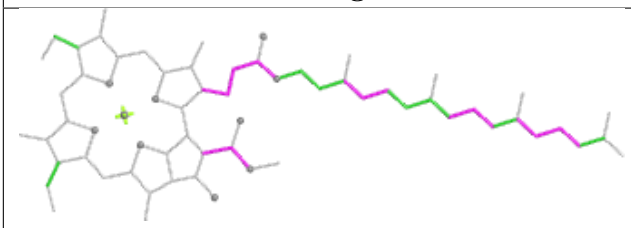

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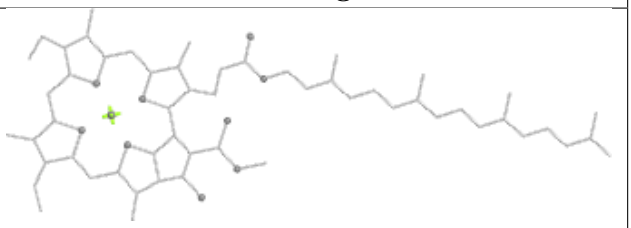
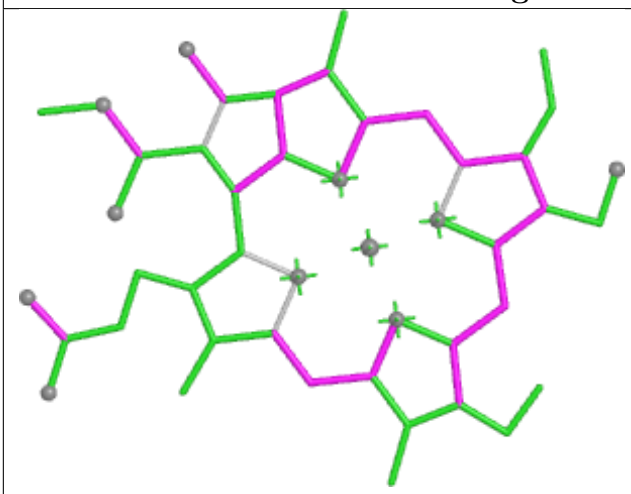


Rings

Ligand CHL AE 617



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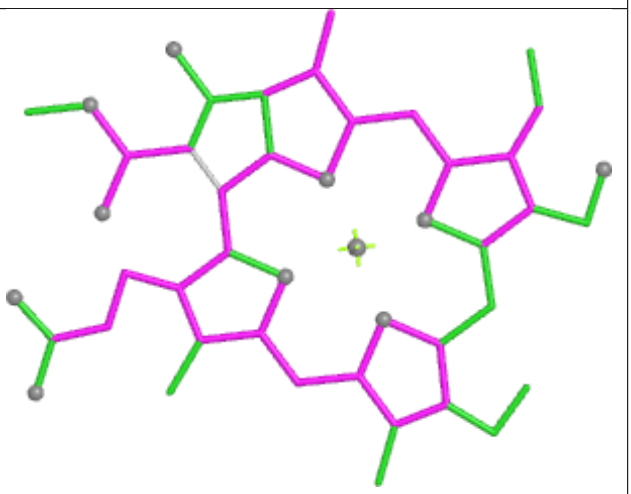
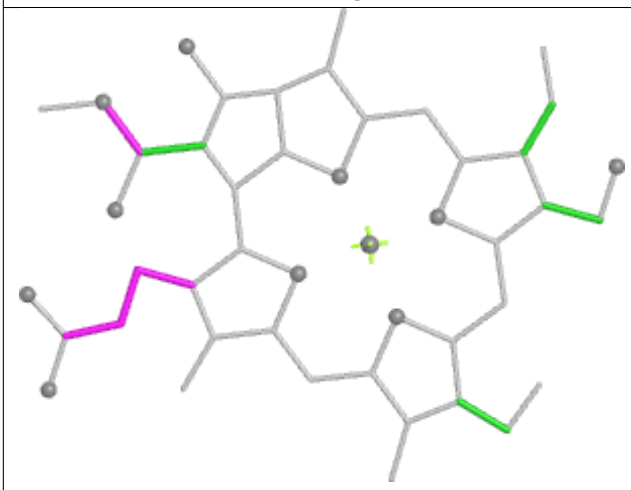


Bond angles



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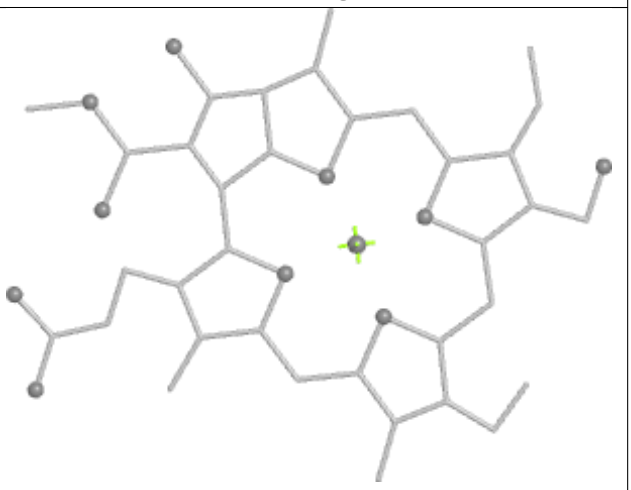
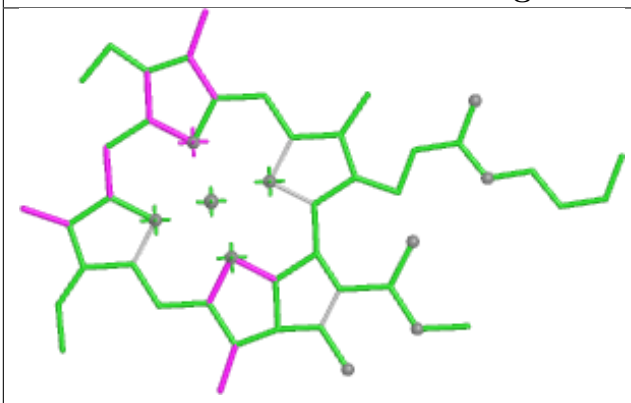
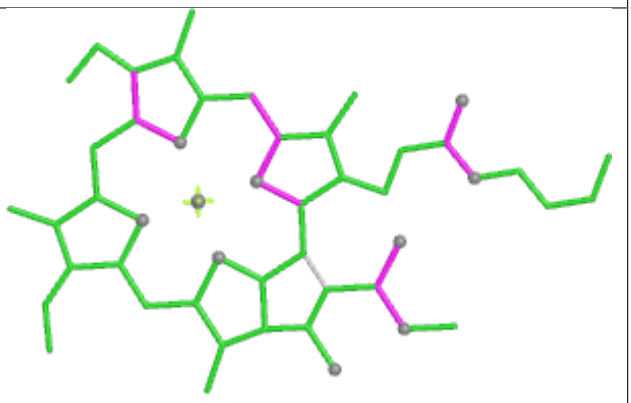
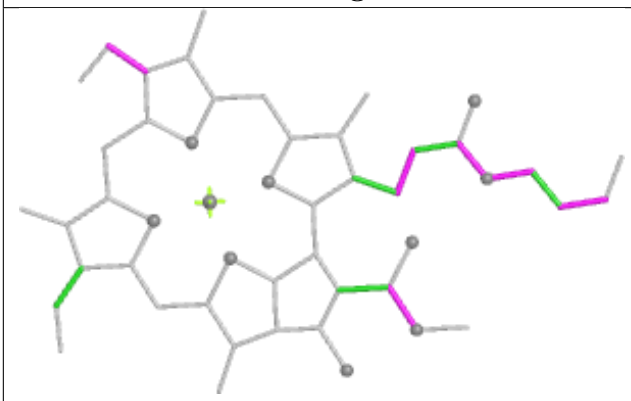
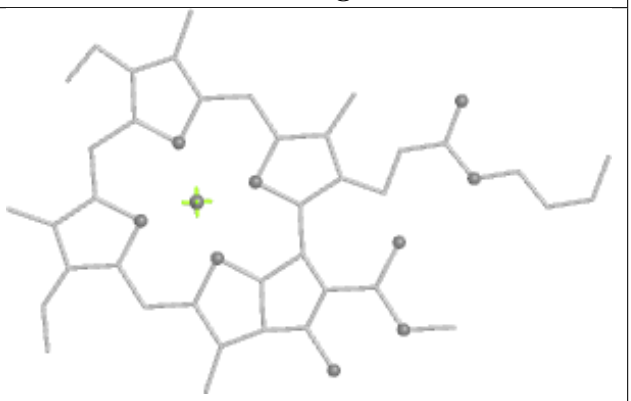


Rings

Ligand CLA AS 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

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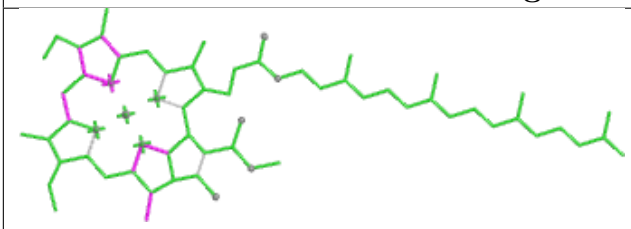
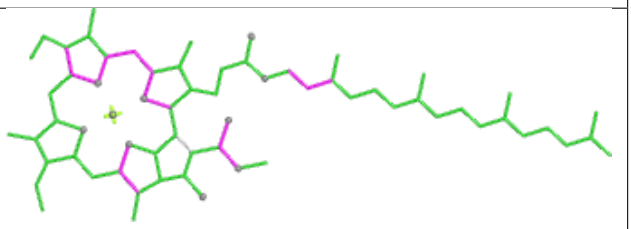
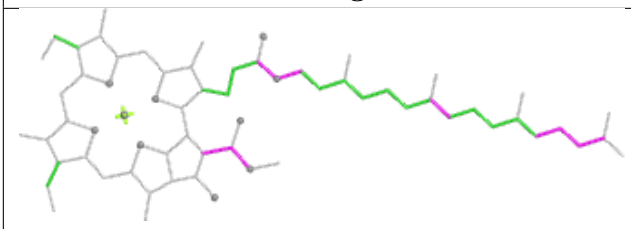
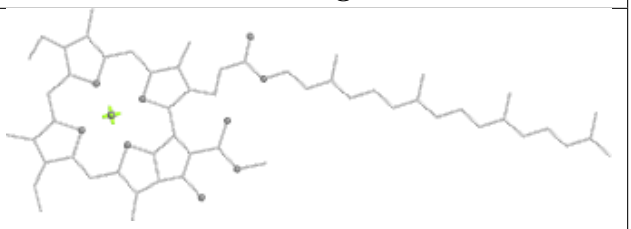
 Bond lengths	 Bond angles
 Torsions	 Rings

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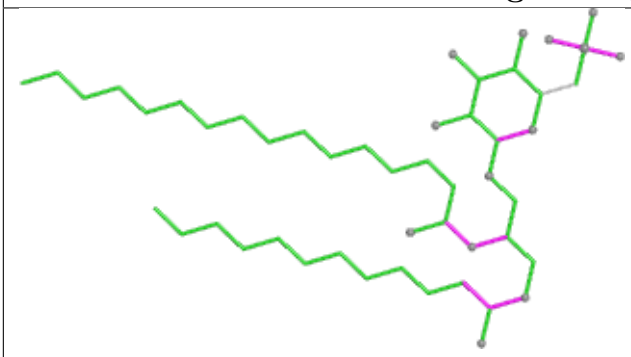
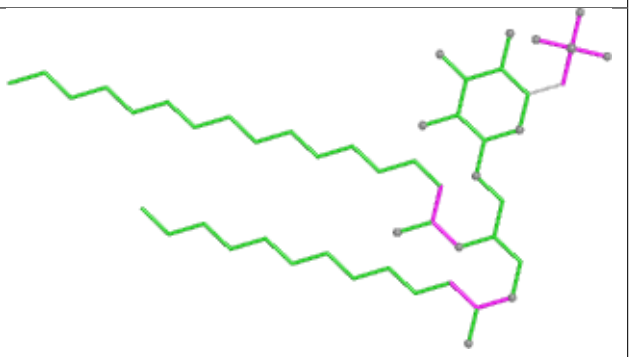
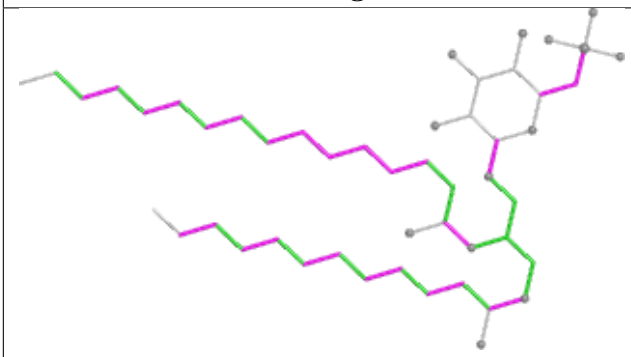
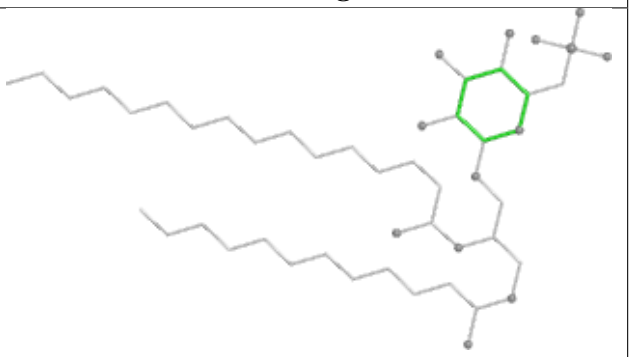
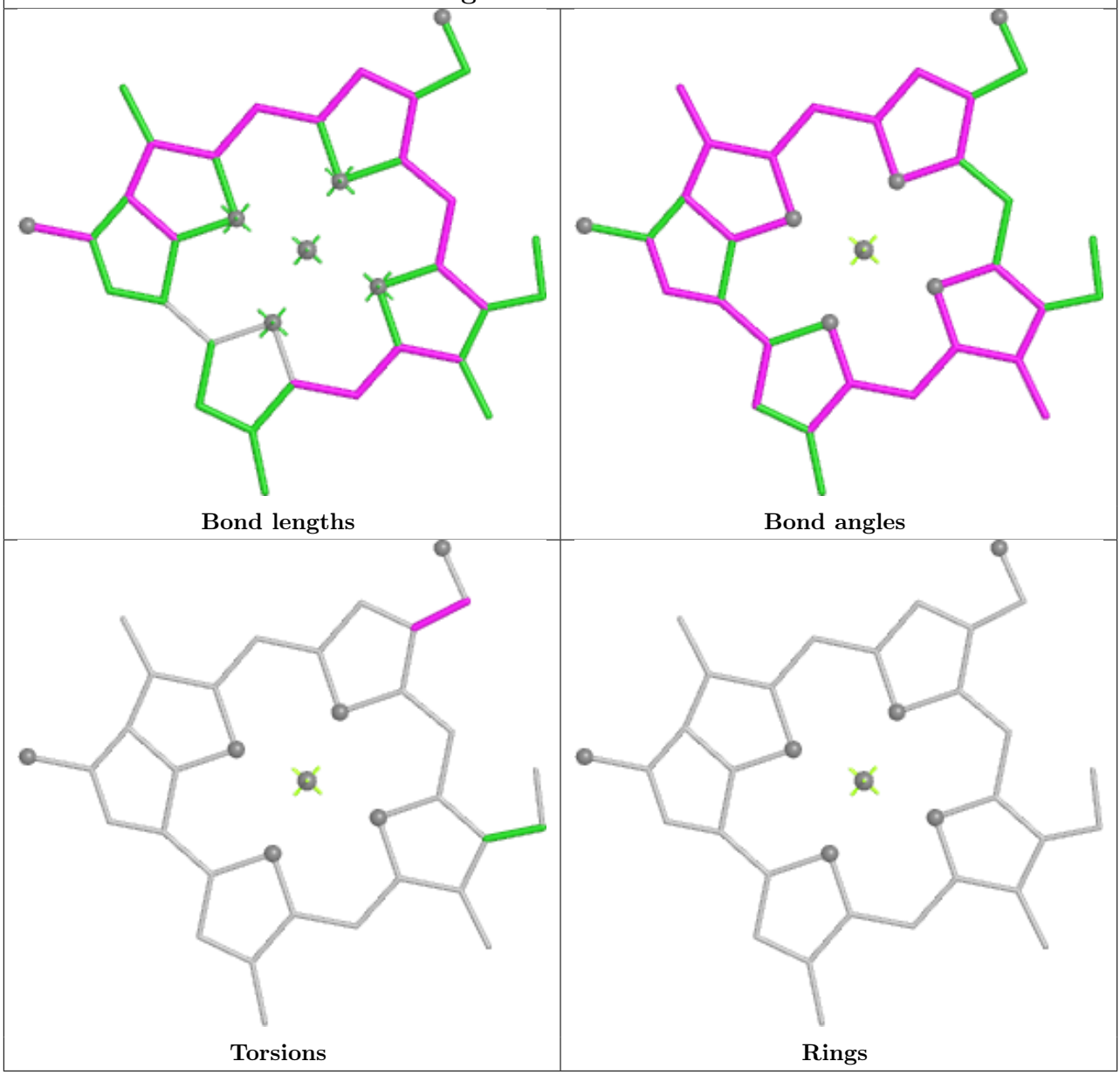
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL v 306



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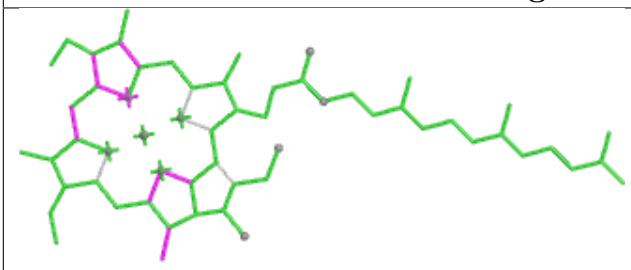
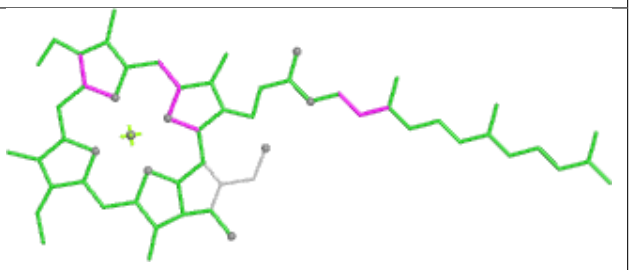
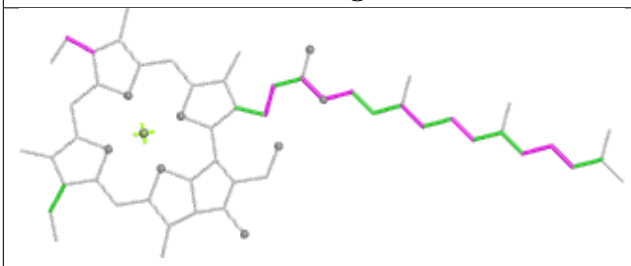
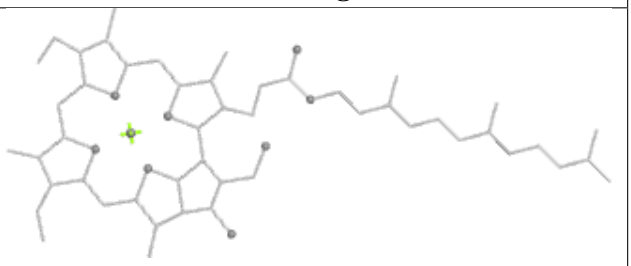
 Bond lengths	 Bond angles
 Torsions	 Rings

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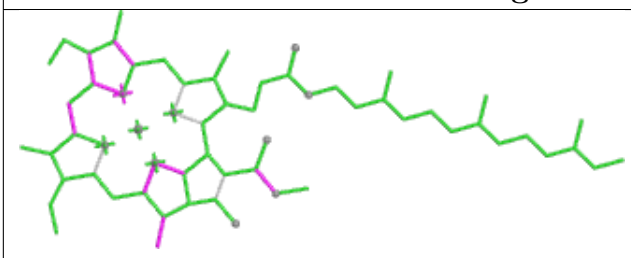
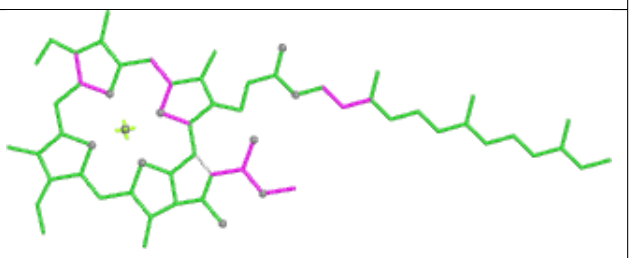
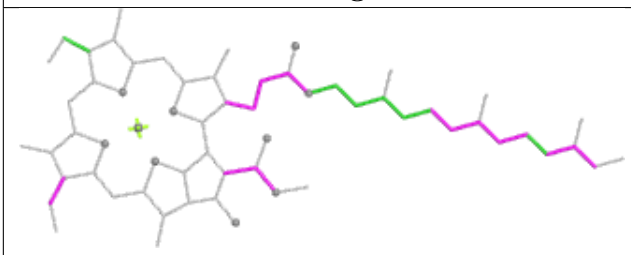
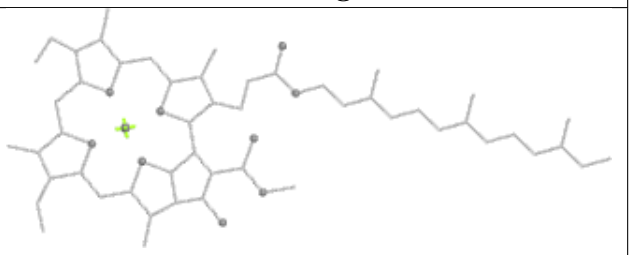
 Bond lengths	 Bond angles
 Torsions	 Rings

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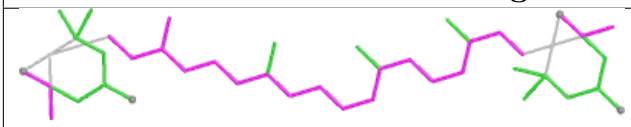
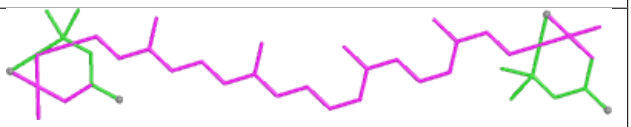
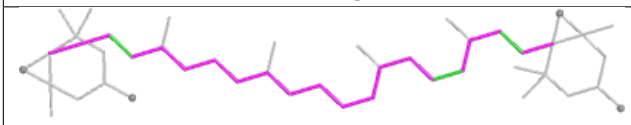
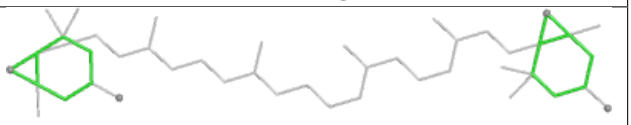
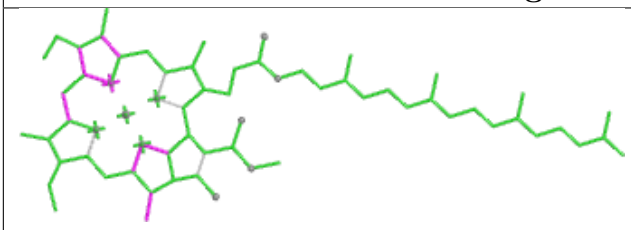
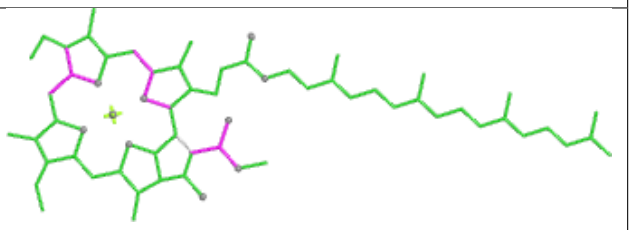
 Bond lengths	 Bond angles
 Torsions	 Rings

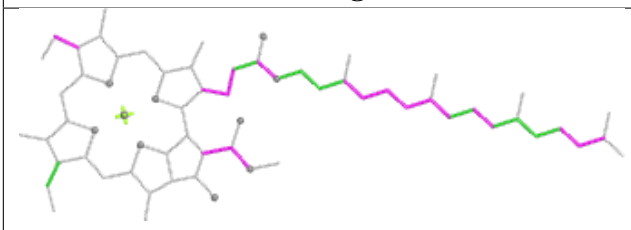
Ligand CLA P 505



Bond lengths



Bond angles



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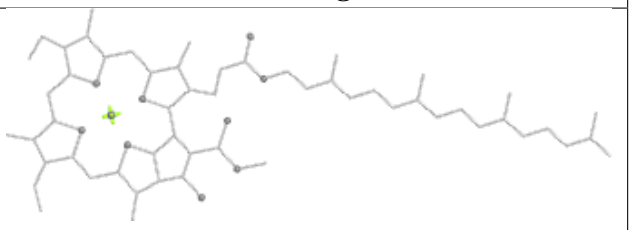
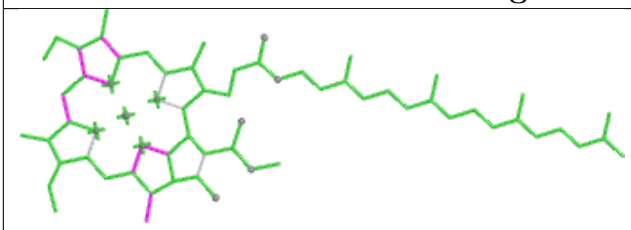


Rings

Ligand CLA AK 603



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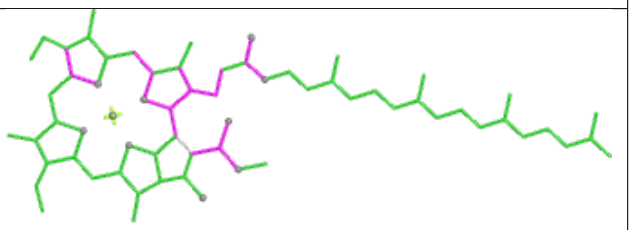

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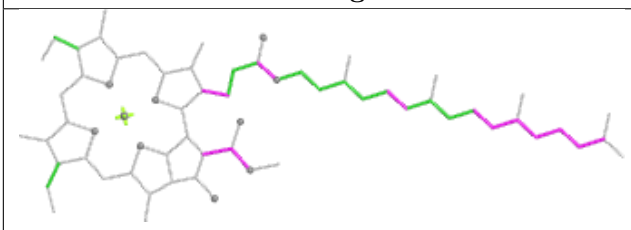

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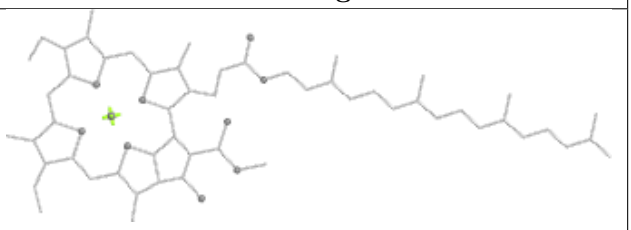
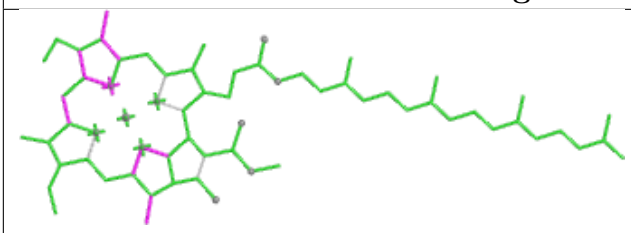


Rings

Ligand CLA AL 510



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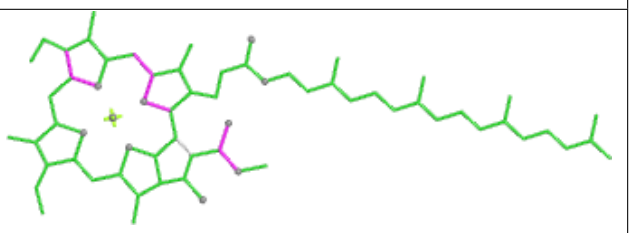
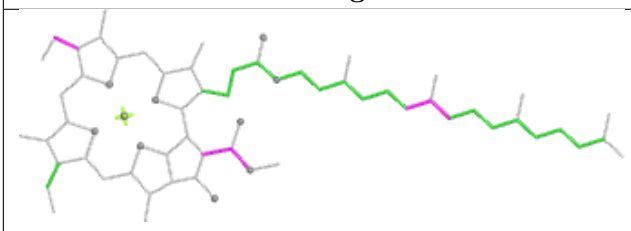


Bond angles



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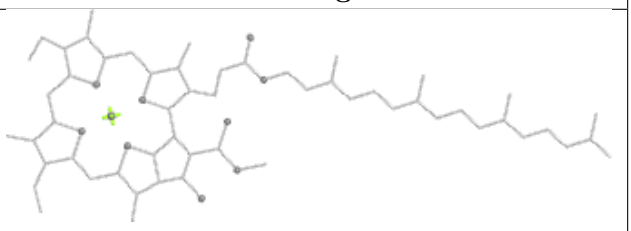
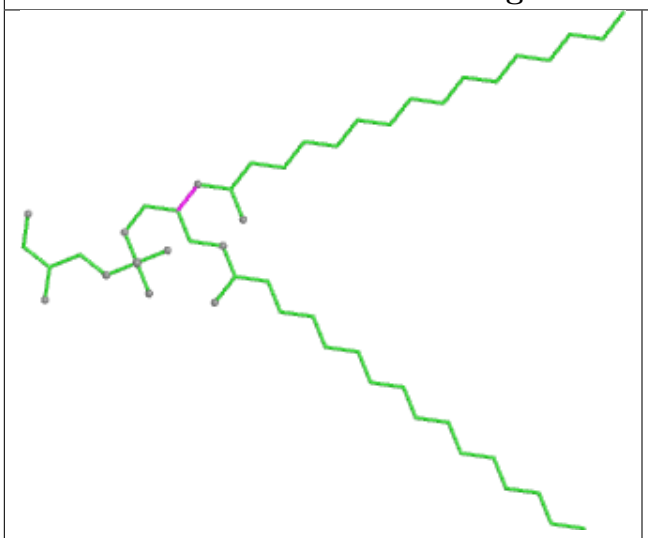


Rings

Ligand LHG AM 406



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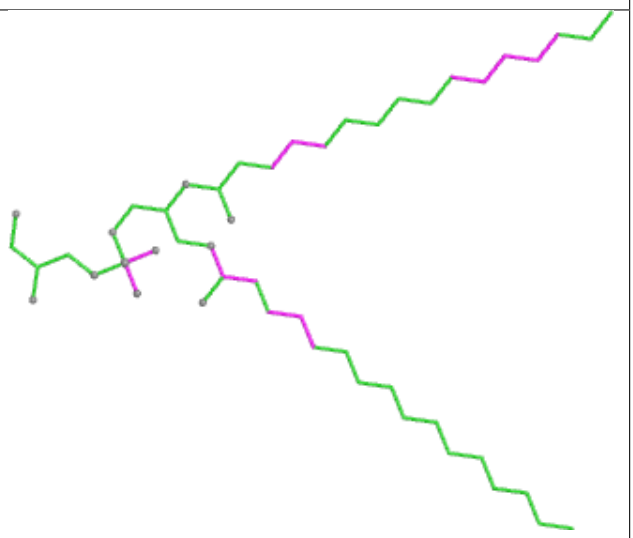
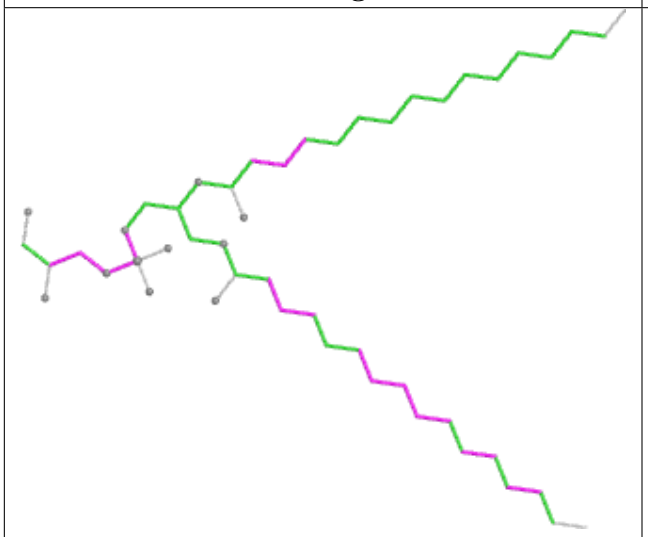


Bond angles



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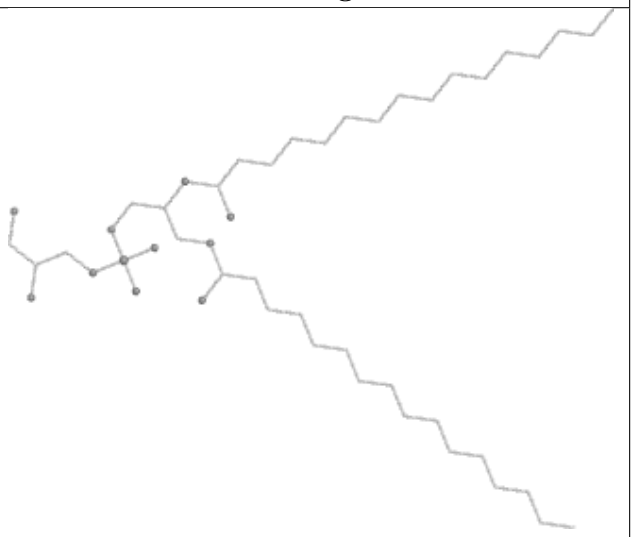
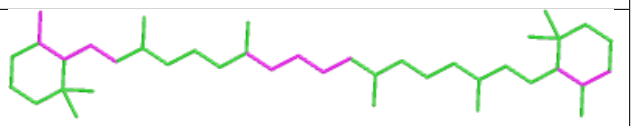


Rings

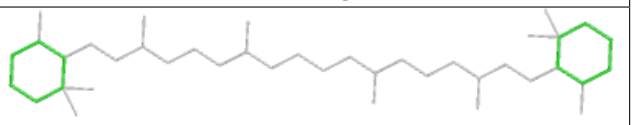
Ligand BCR O 618

Bond lengths



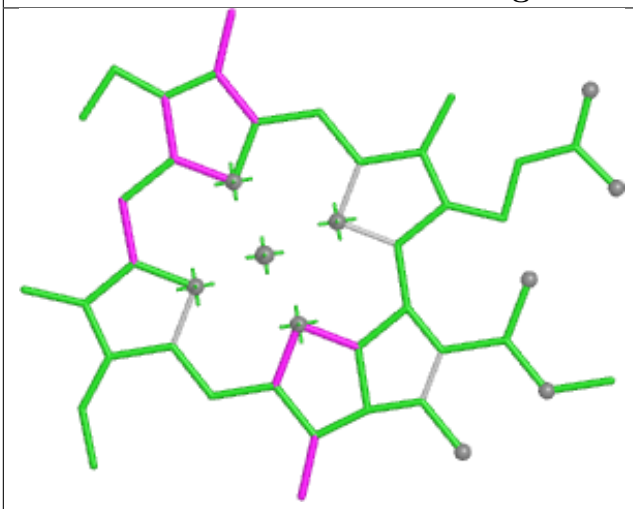
Bond angles

Torsions

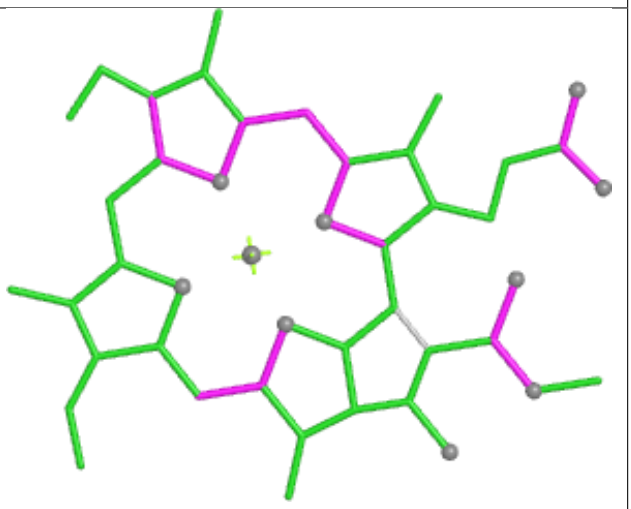


Rings

Ligand CLA AF 603



Bond lengths



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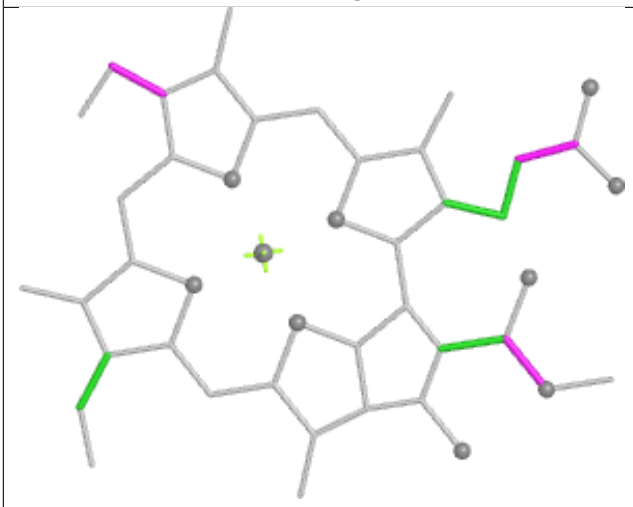
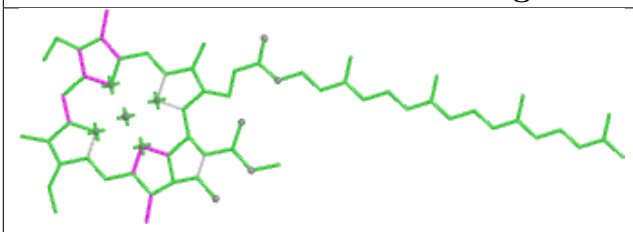


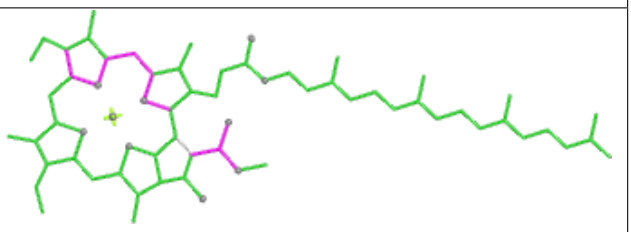
Torsions

Rings

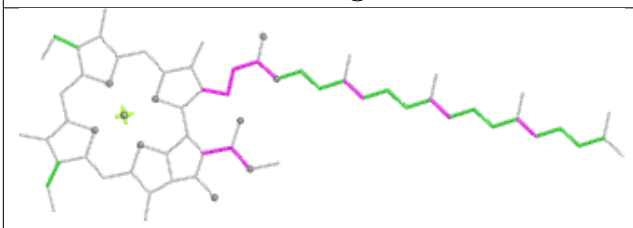
Ligand CLA AL 502



Bond lengths



Bond angles



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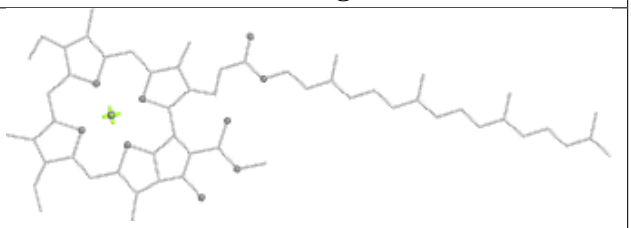
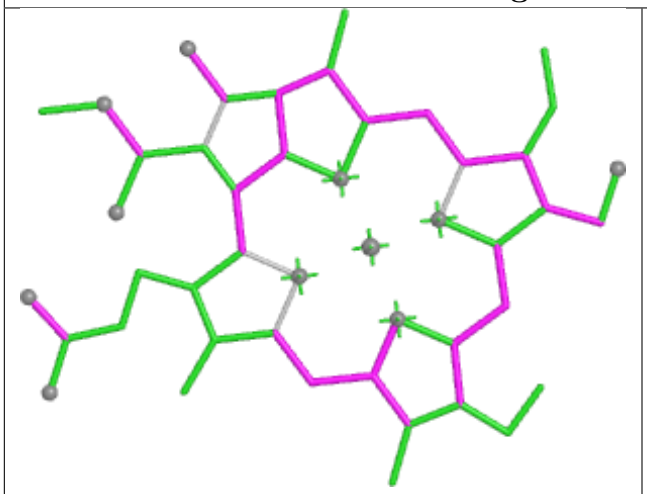


Rings

Ligand CHL AA 617



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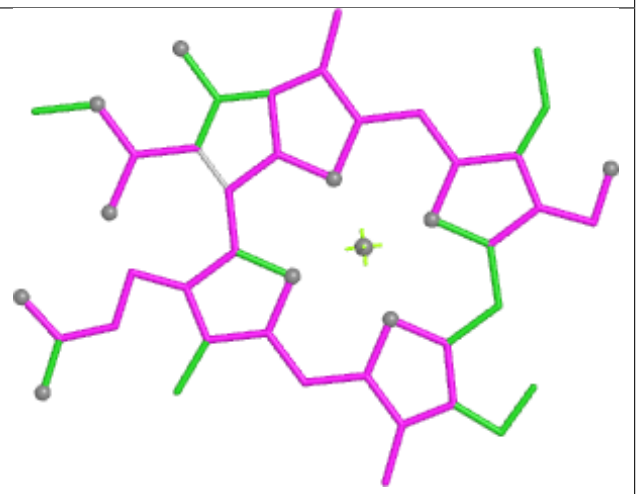

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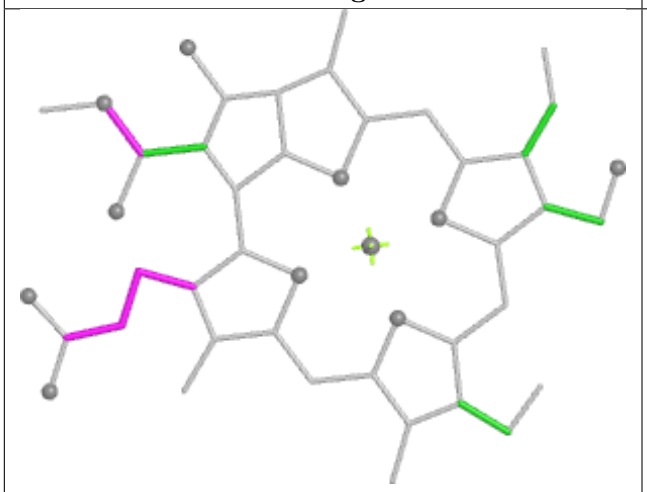

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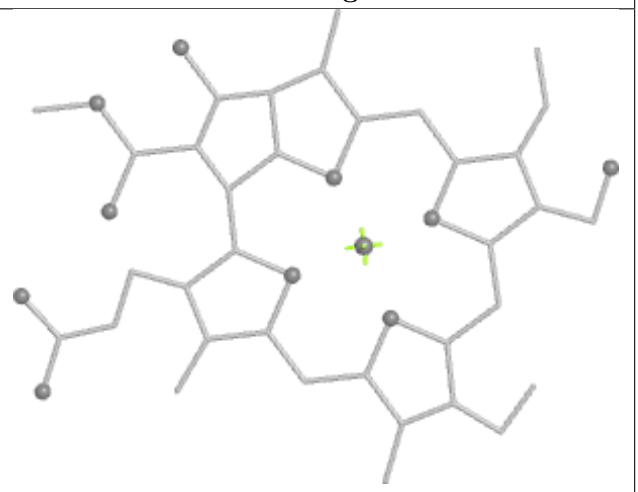
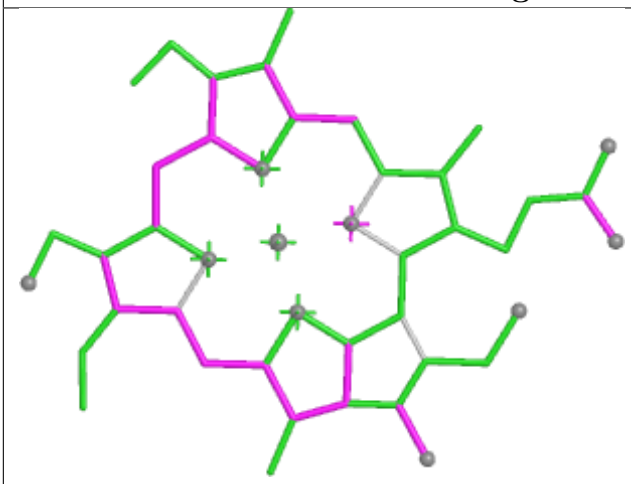


Rings

Ligand CHL AF 608



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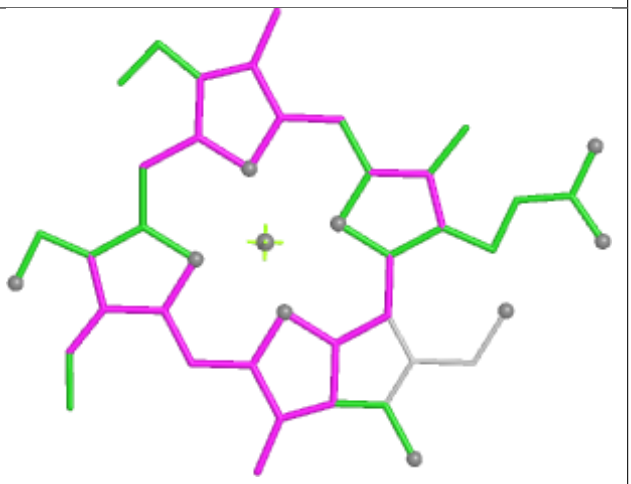

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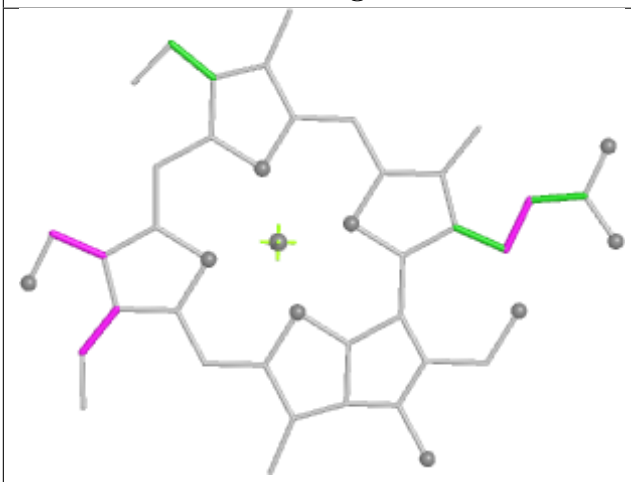

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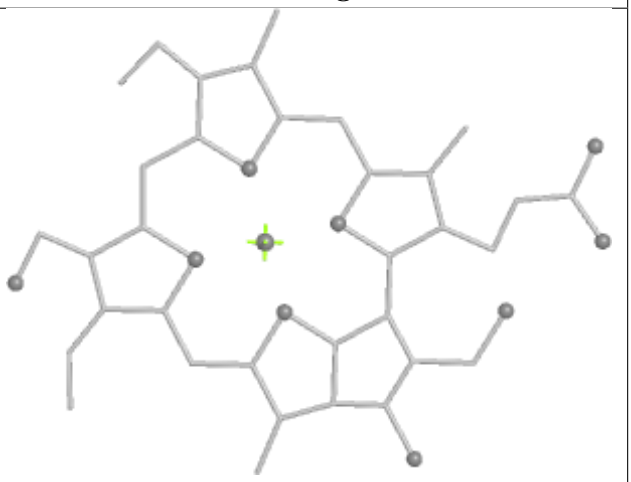
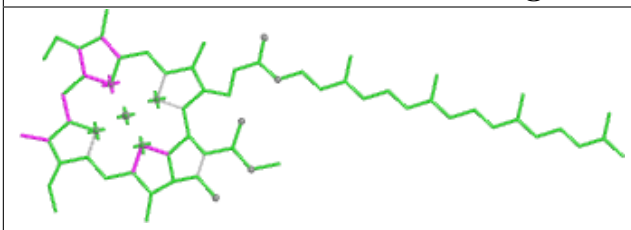


Rings

Ligand CLA P 508



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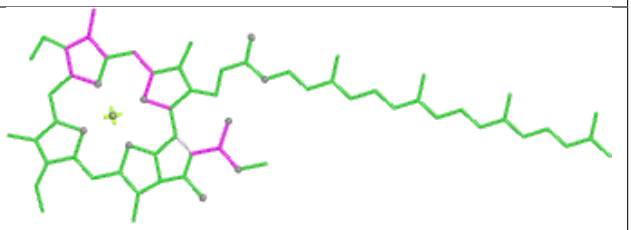
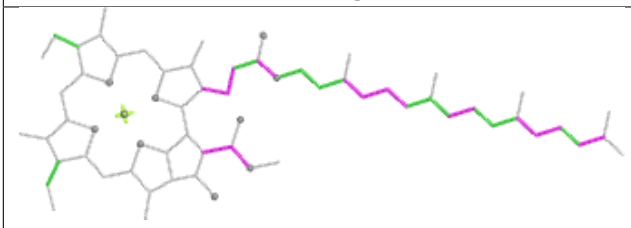


Bond angles



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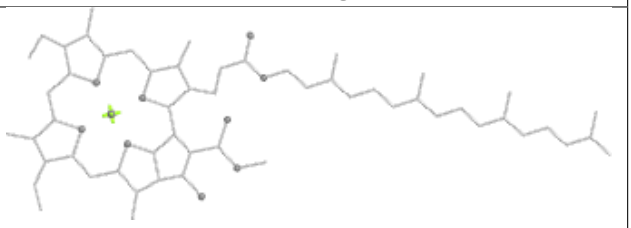
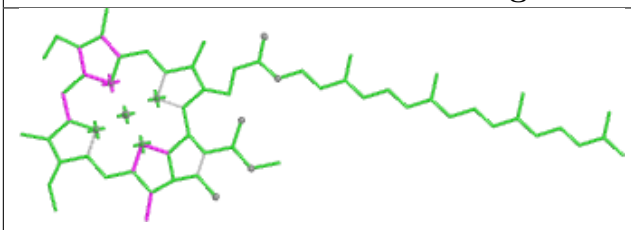
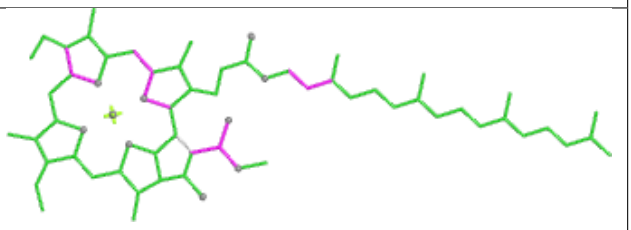
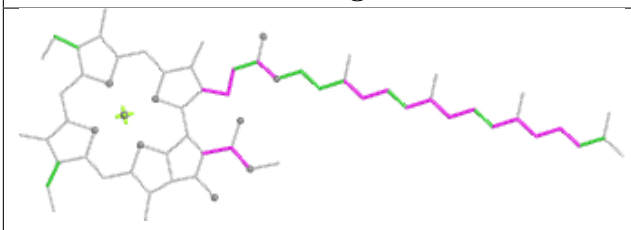
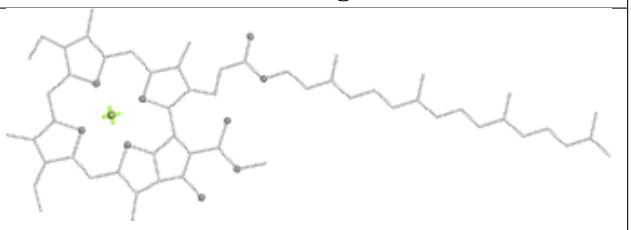


Rings

Ligand CLA AH 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

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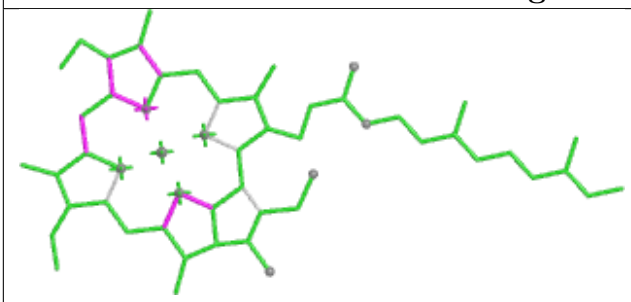
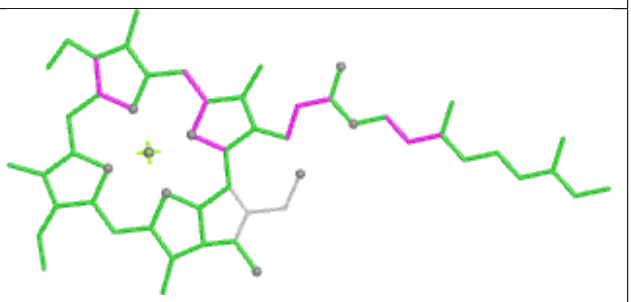
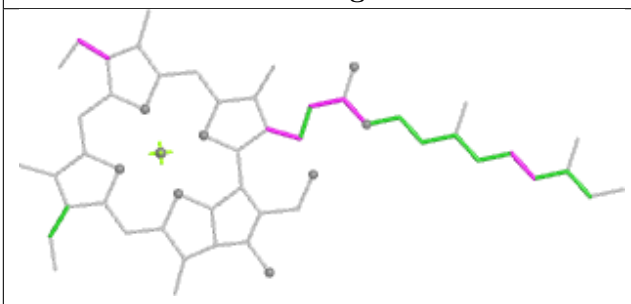
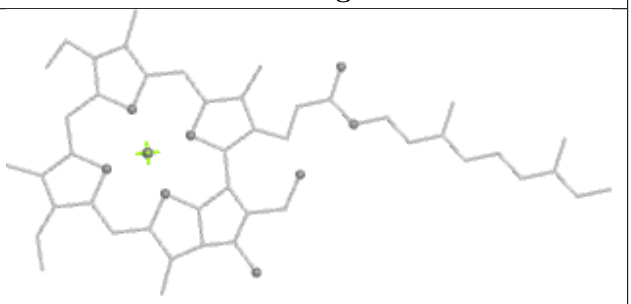
 Bond lengths	 Bond angles
 Torsions	 Rings

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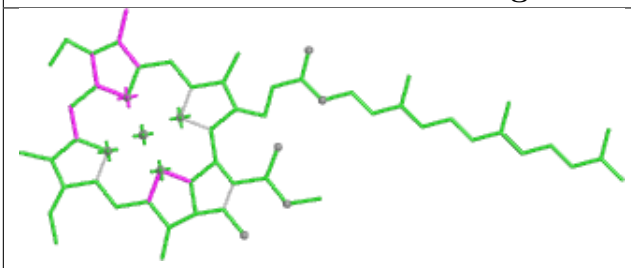
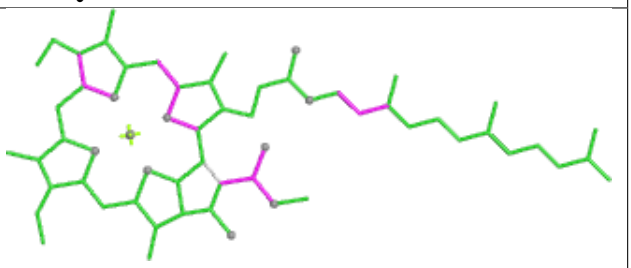
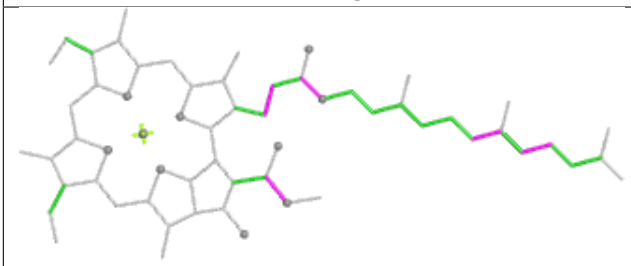
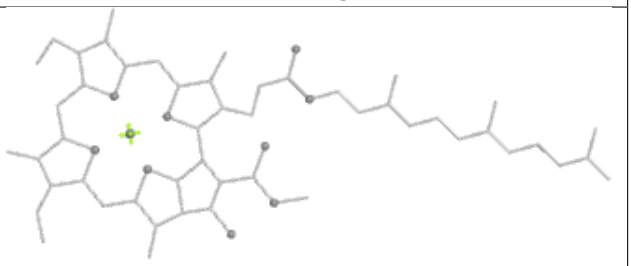
 Bond lengths	 Bond angles
 Torsions	 Rings

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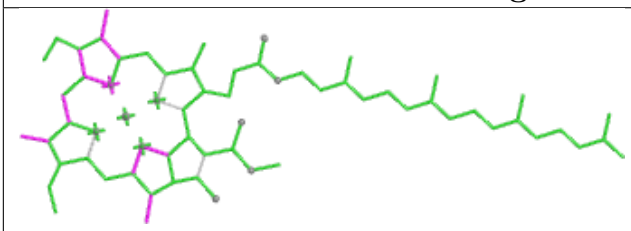
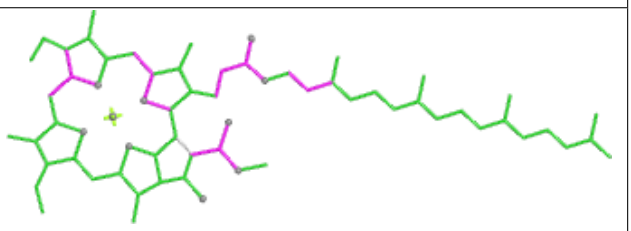
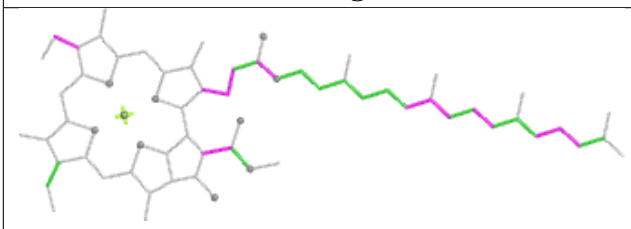
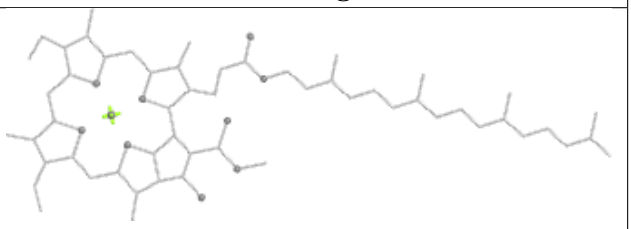
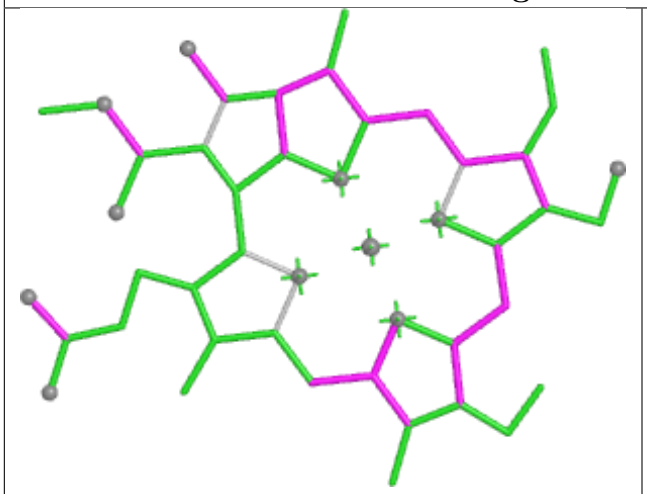
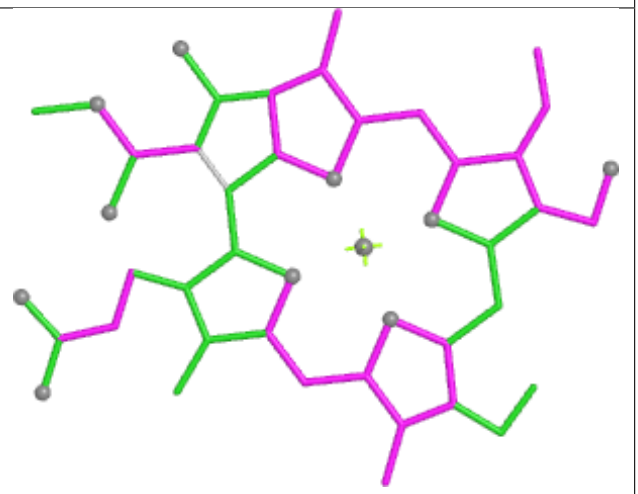
 Bond lengths	 Bond angles
 Torsions	 Rings

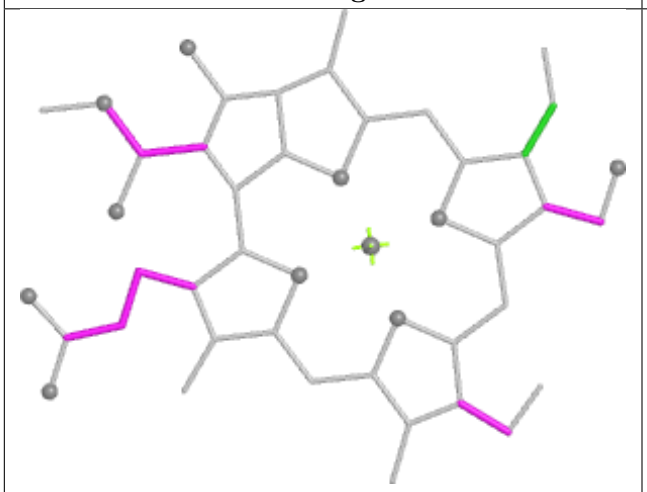
Ligand CHL AE 606



Bond lengths



Bond angles



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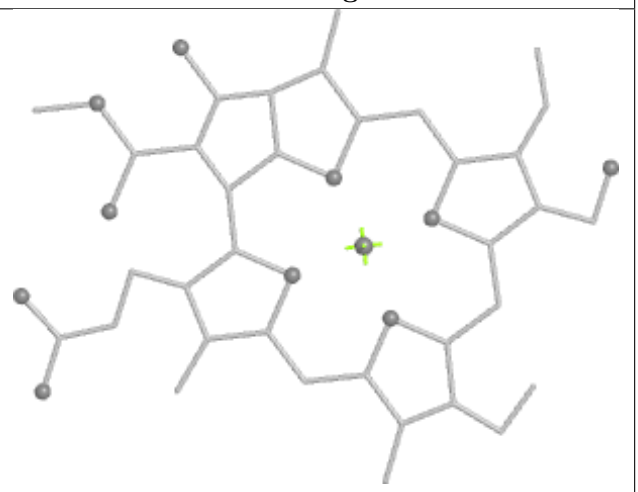
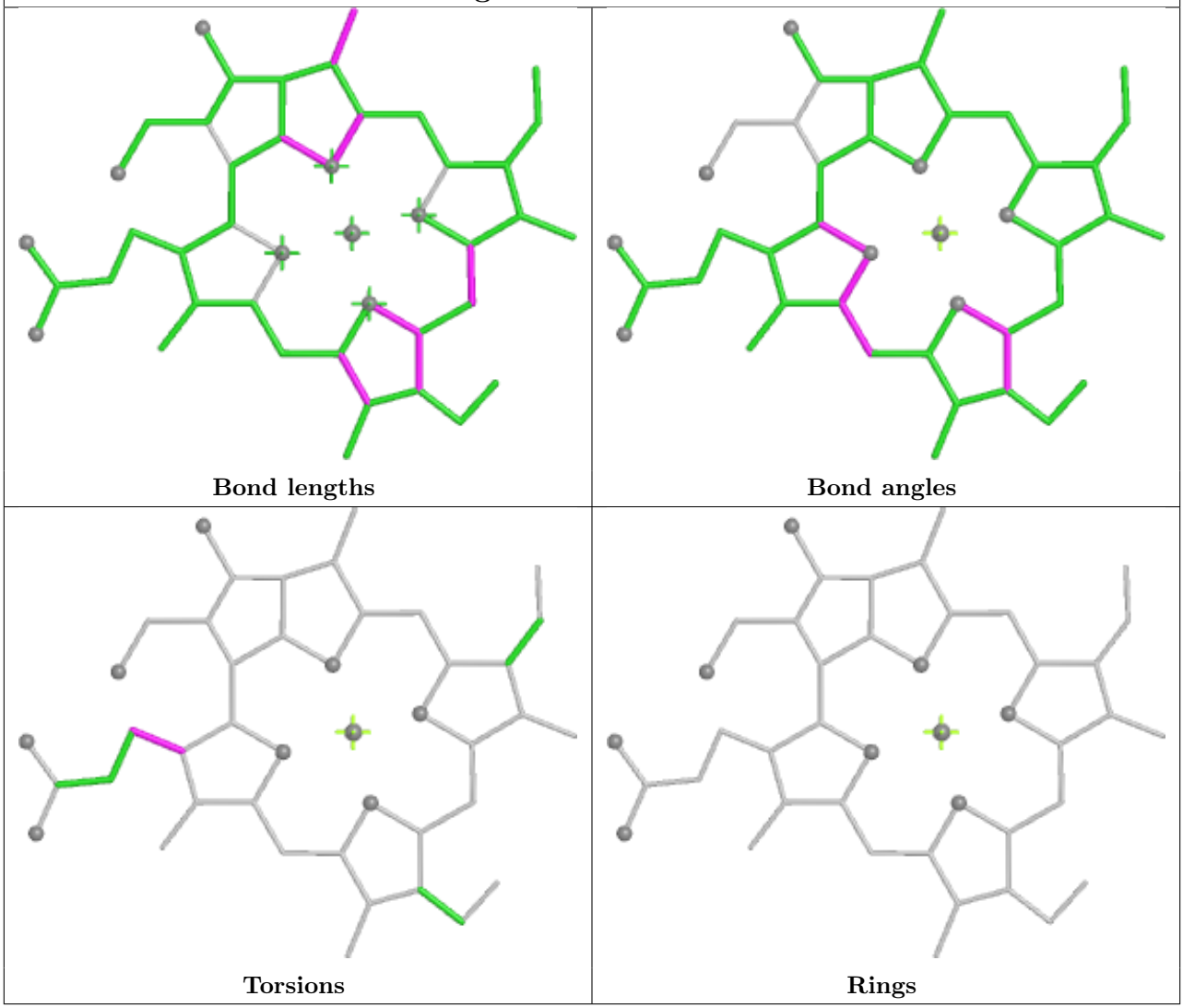


Rings

Ligand CLA AS 309



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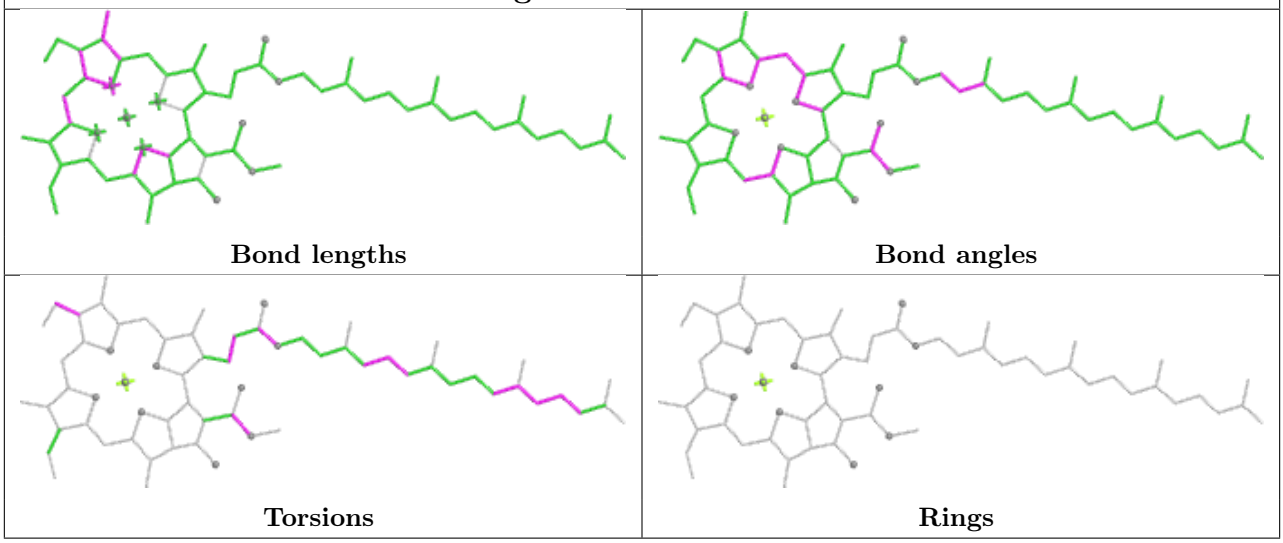

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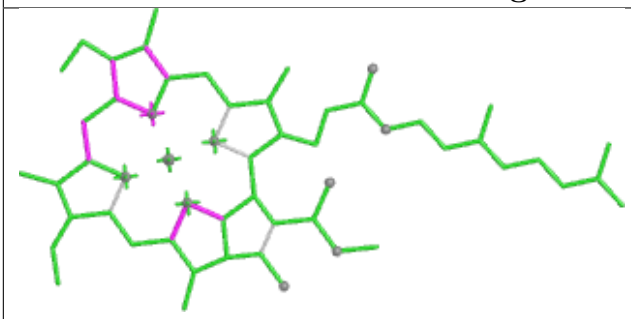
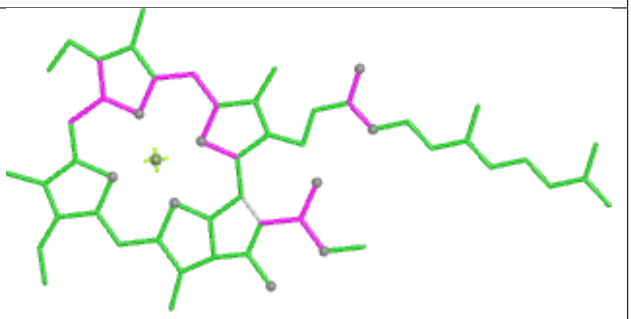
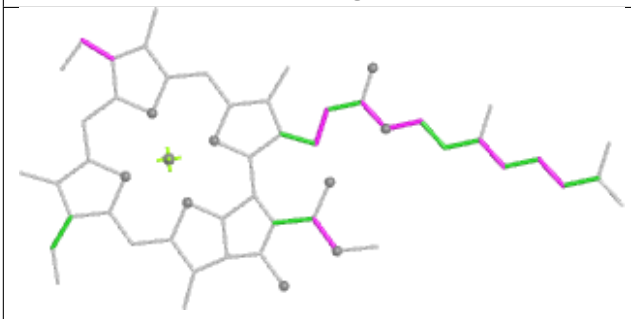
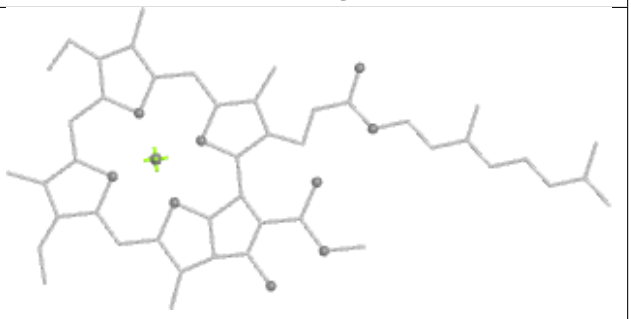
 Bond lengths	 Bond angles
 Torsions	 Rings

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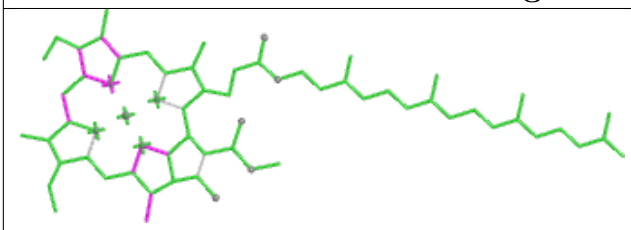
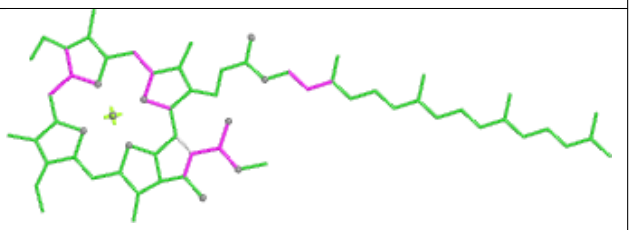
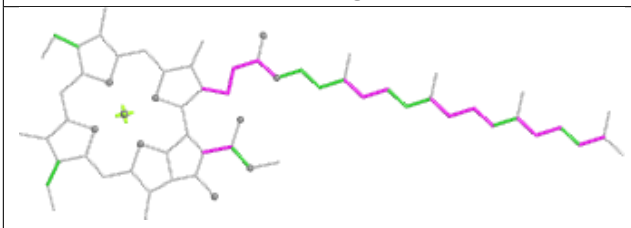
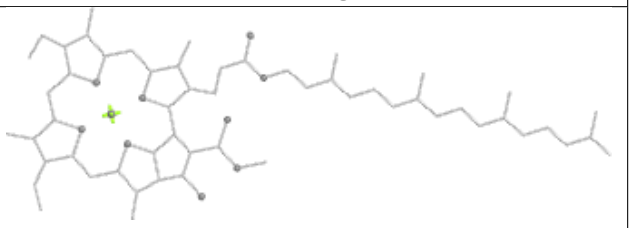
 Bond lengths	 Bond angles
 Torsions	 Rings

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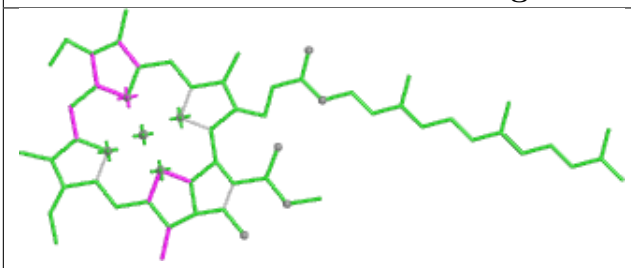
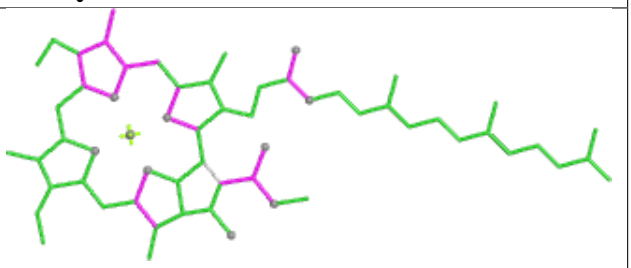
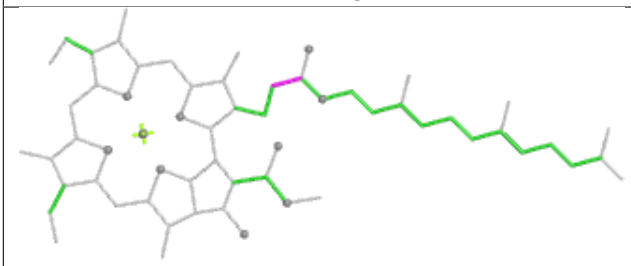
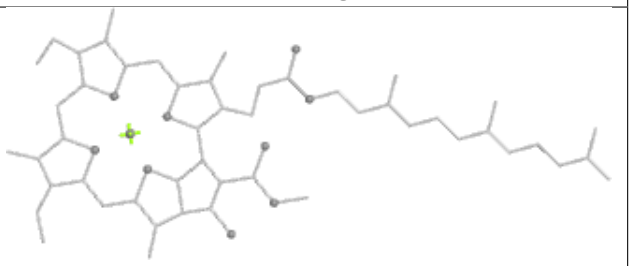
 Bond lengths	 Bond angles
 Torsions	 Rings

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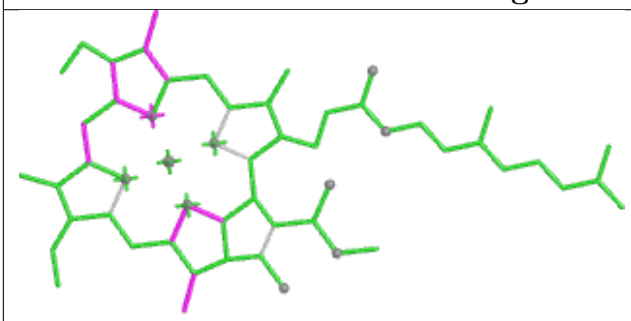
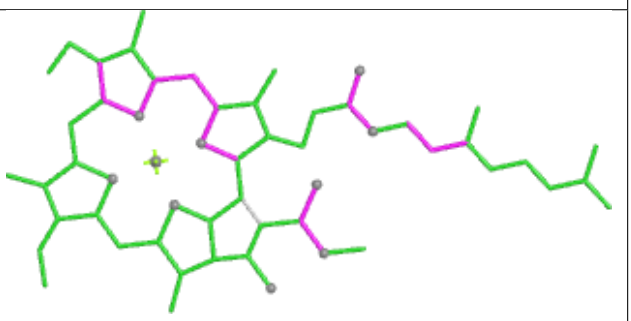
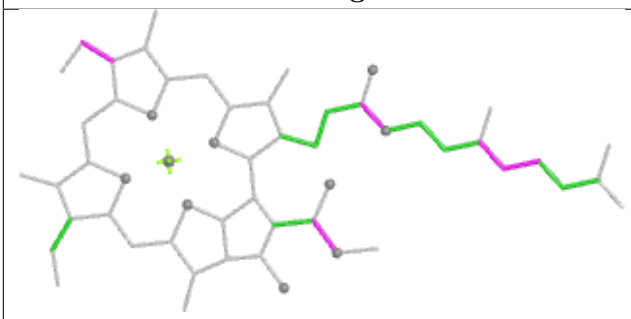
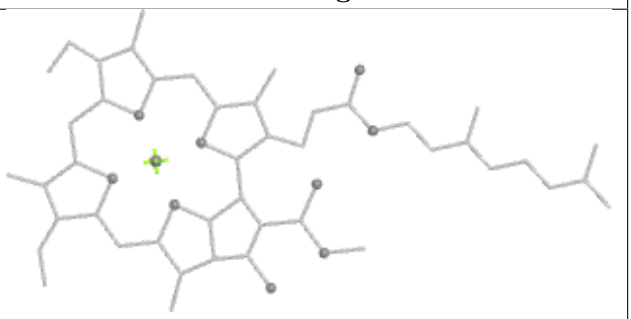
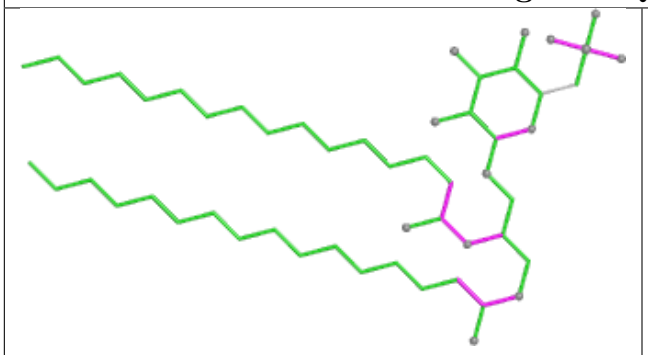
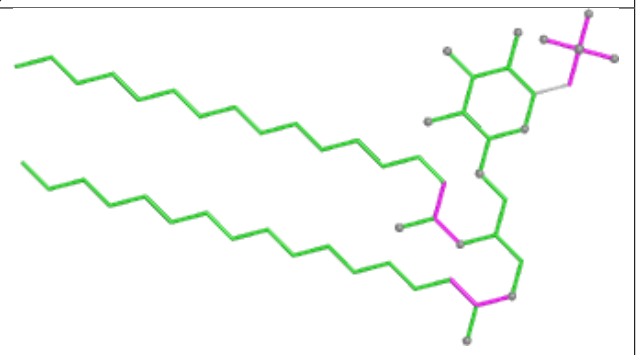
 Bond lengths	 Bond angles
 Torsions	 Rings

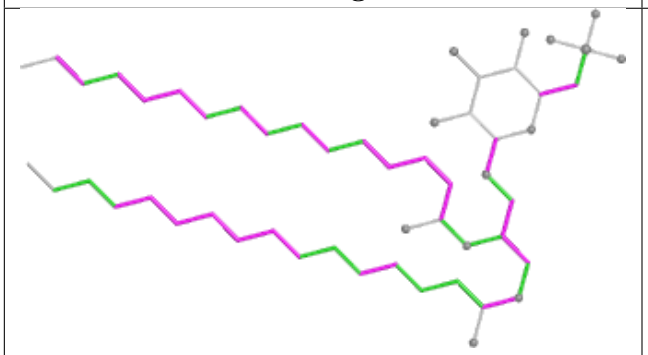
Ligand SQD AJ 411



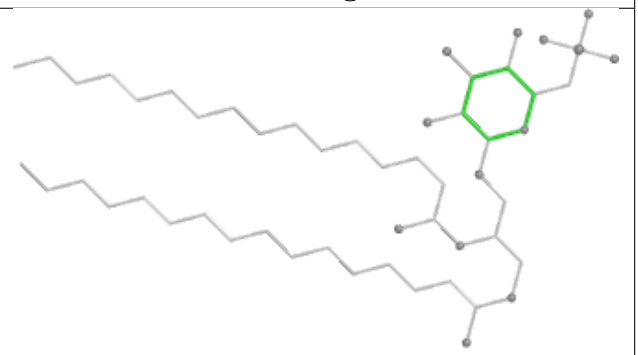
Bond lengths



Bond angles



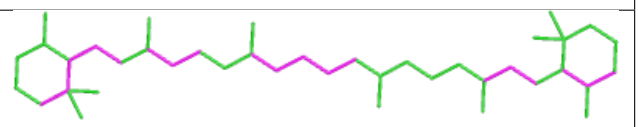
Torsions



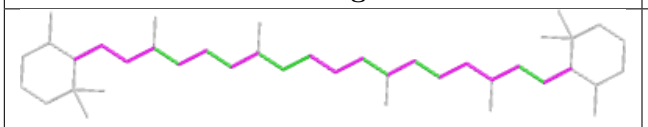
Rings

Ligand BCR O 625

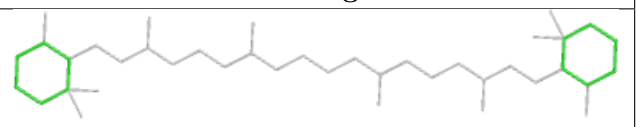
Bond lengths



Bond angles

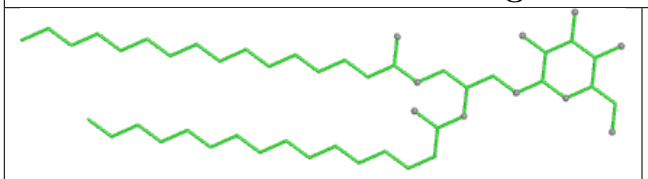


Torsions



Rings

Ligand LMG AK 622



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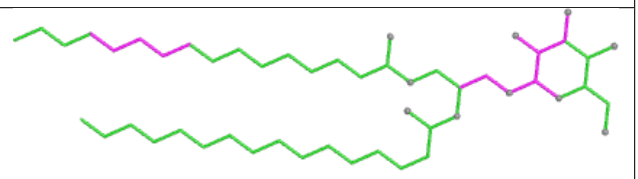
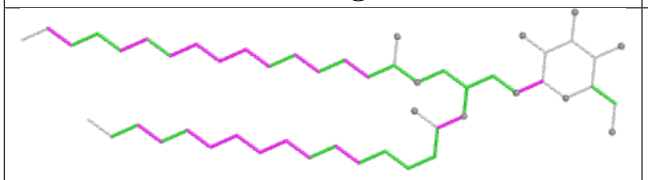


Bond angles



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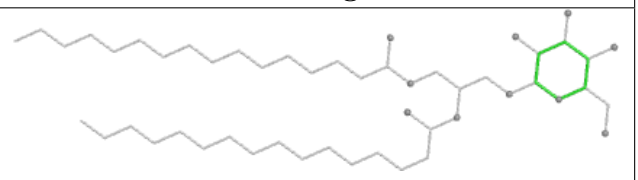
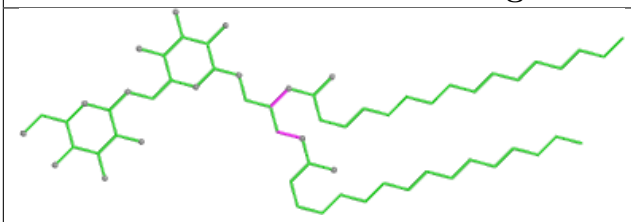
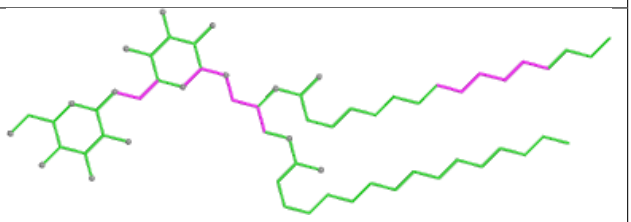


Rings

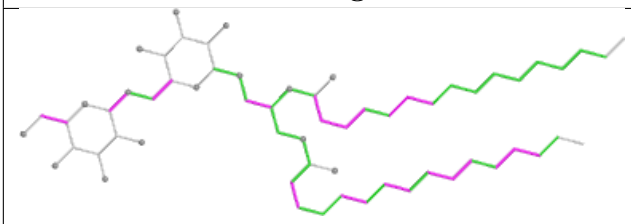
Ligand DGD AO 102



Bond lengths



Bond angles



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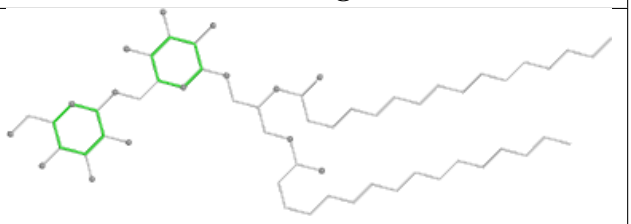
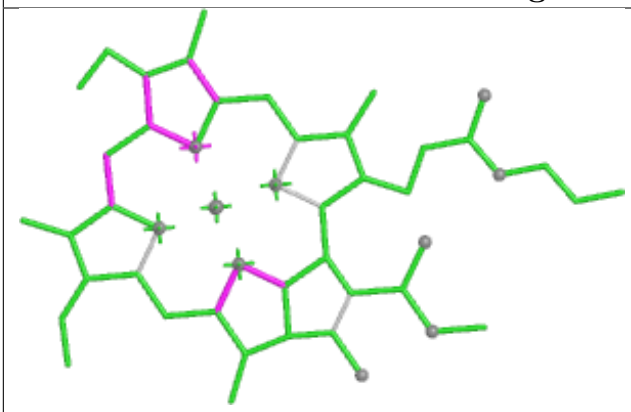


Rings

Ligand CLA 0 613



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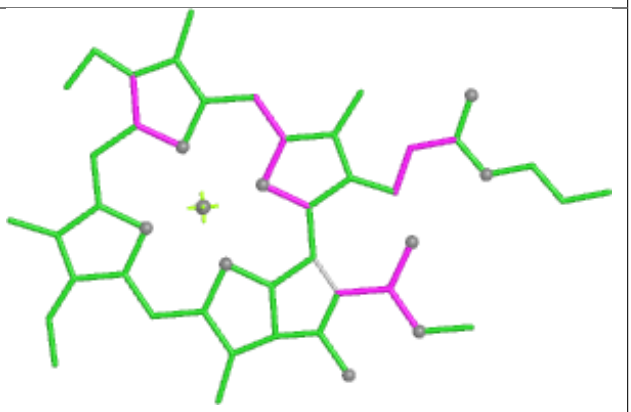
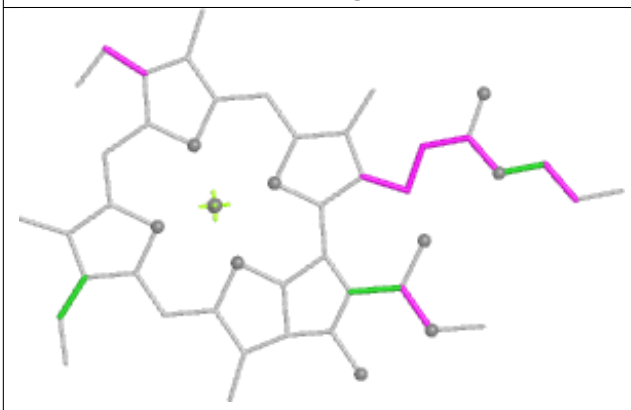


Bond angles



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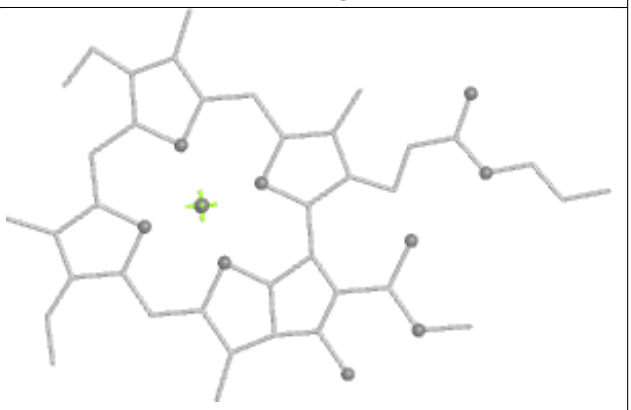
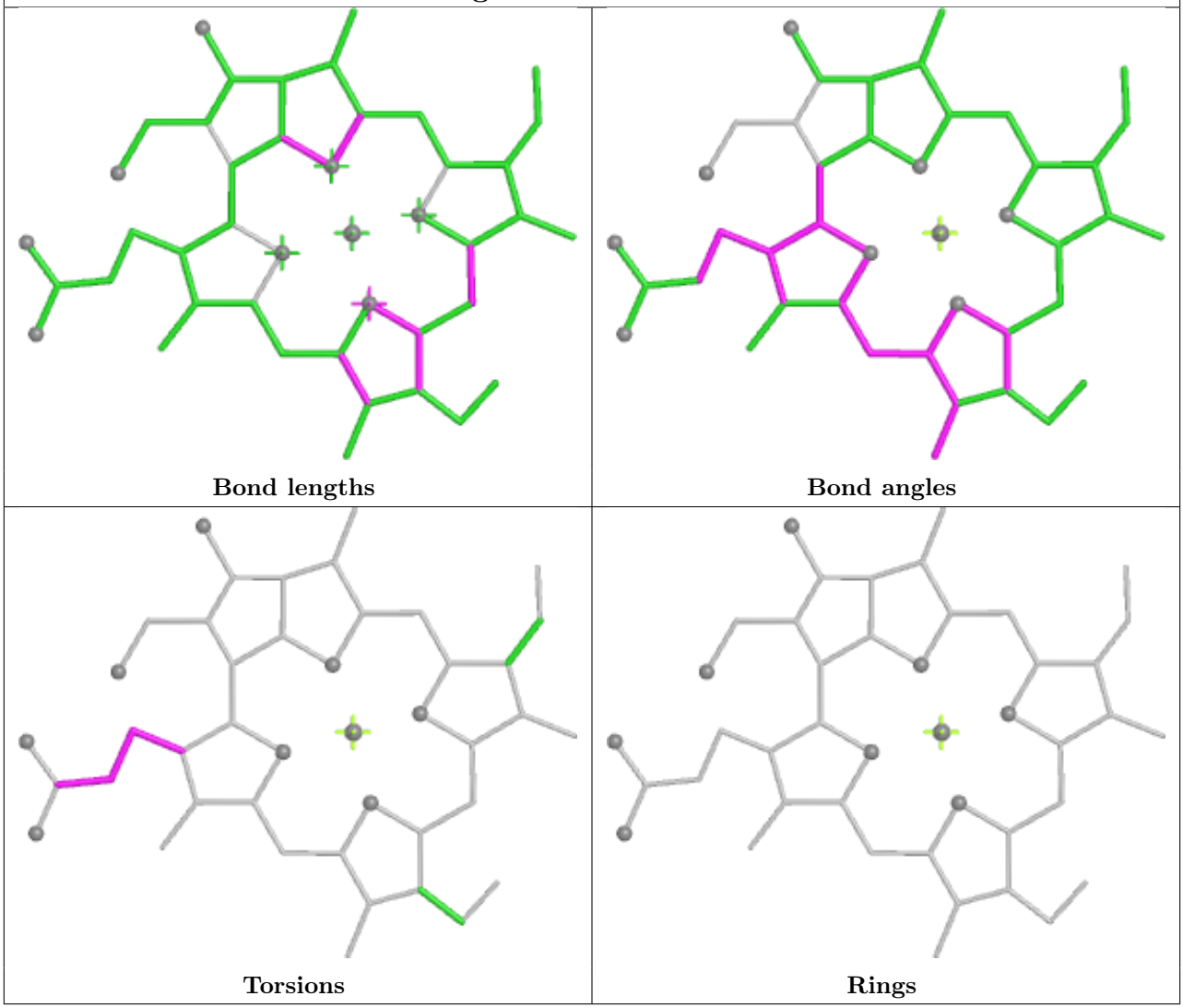
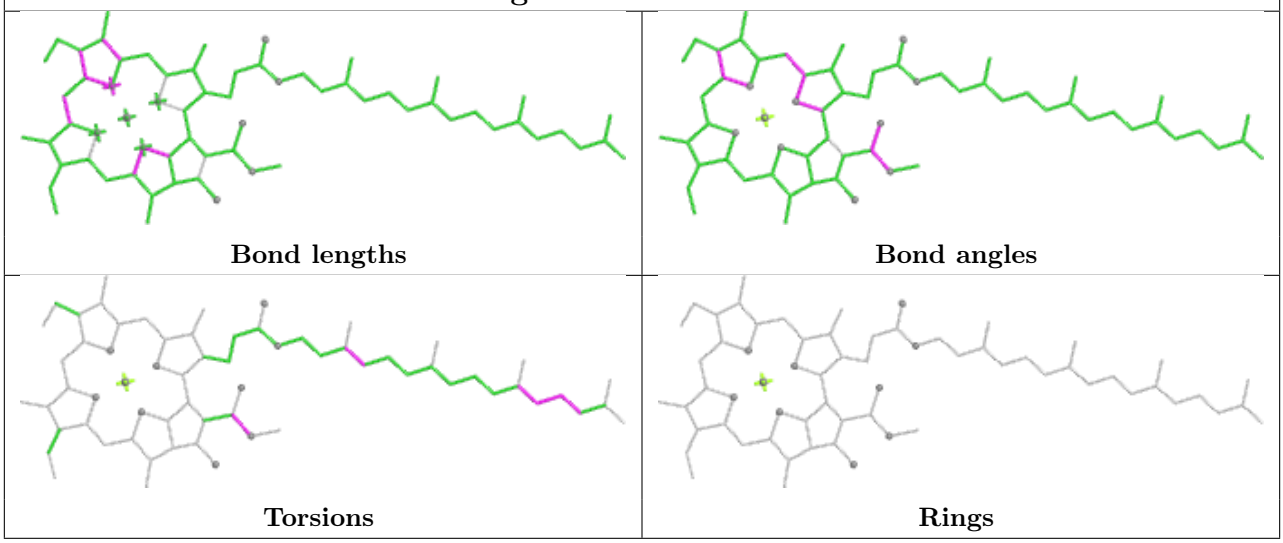


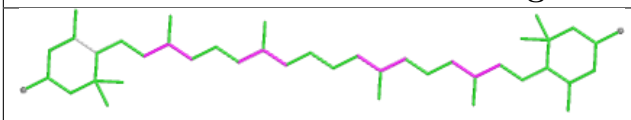
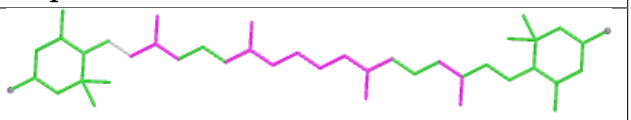
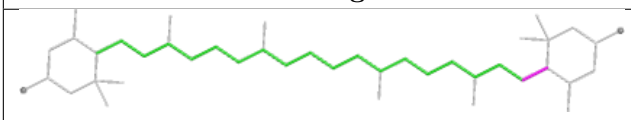
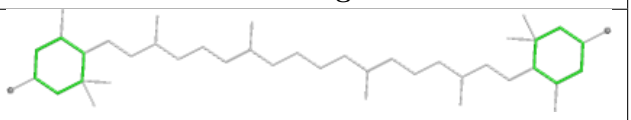
Rings

Ligand CLA AC 613



Ligand CLA AK 605



Ligand LUT p 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

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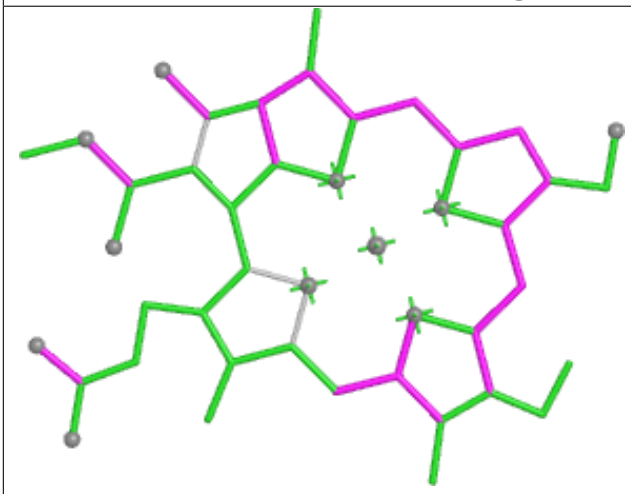
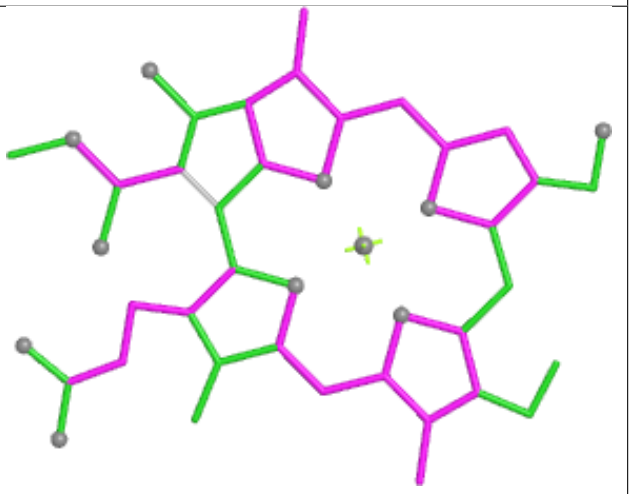
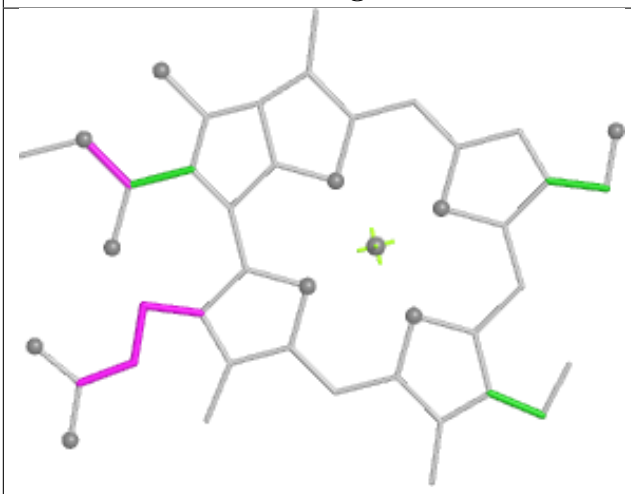
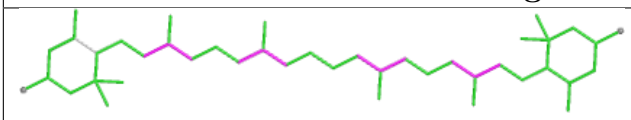
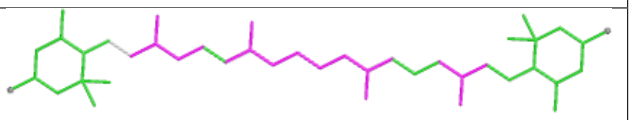
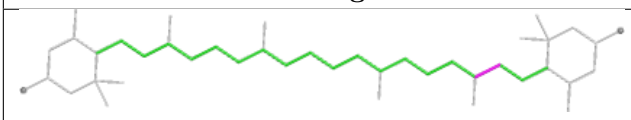
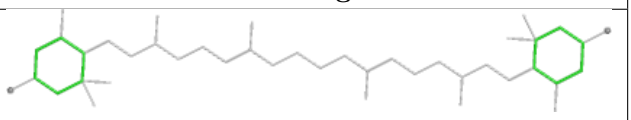
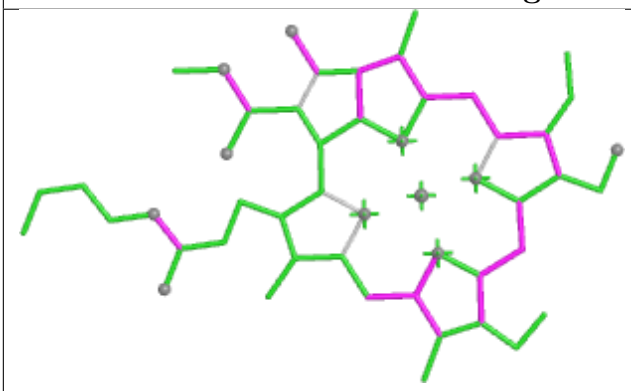
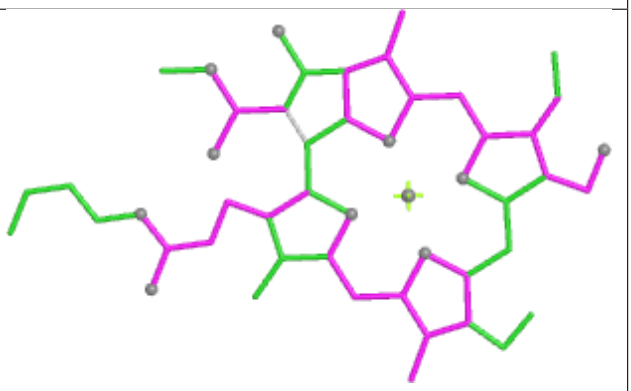
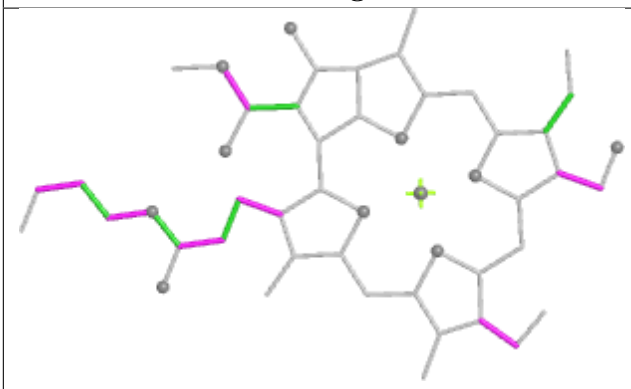
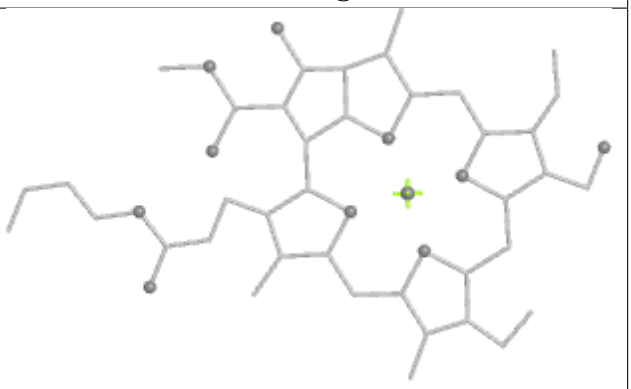
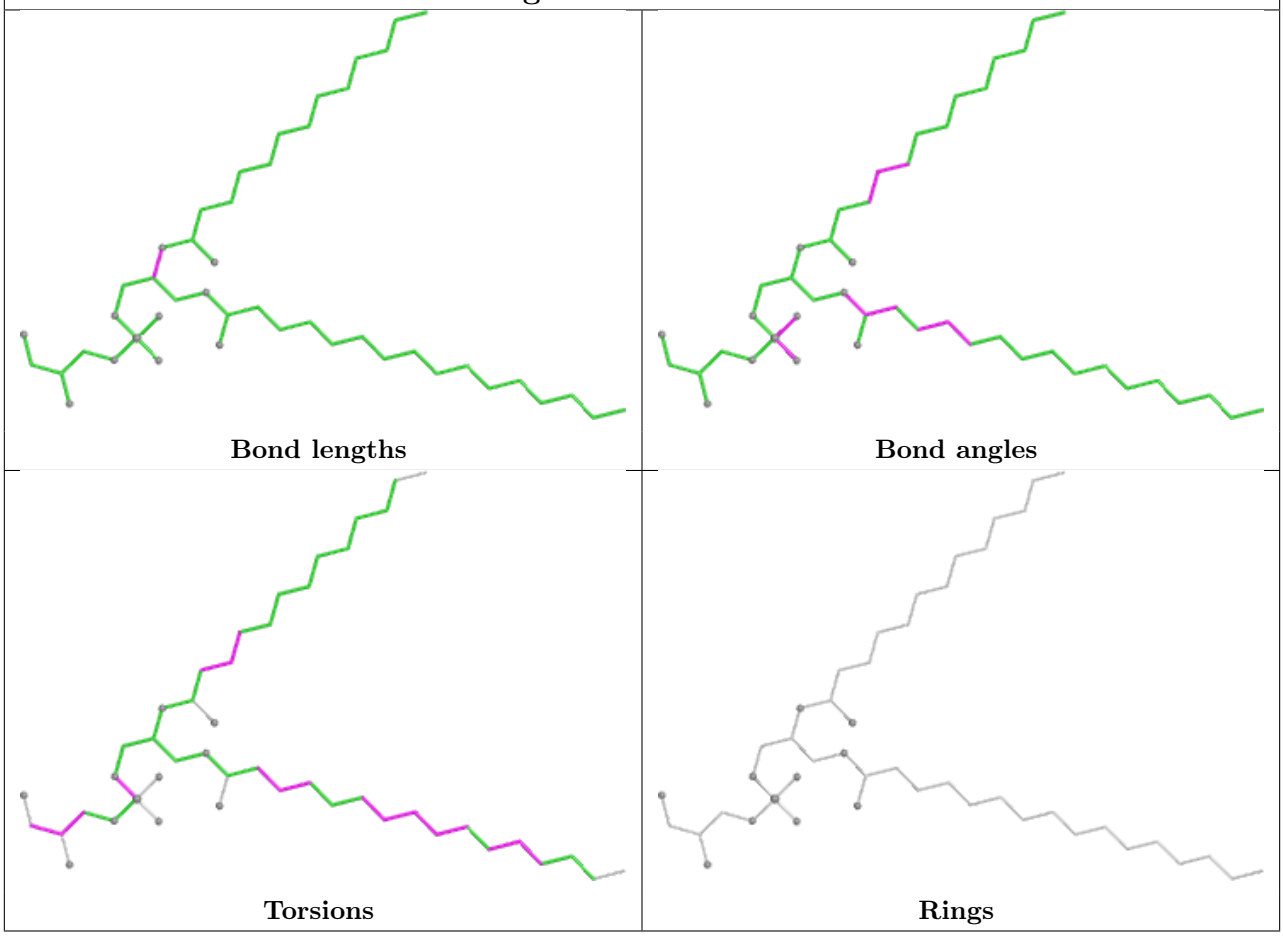
 Bond lengths	 Bond angles
 Torsions	Rings

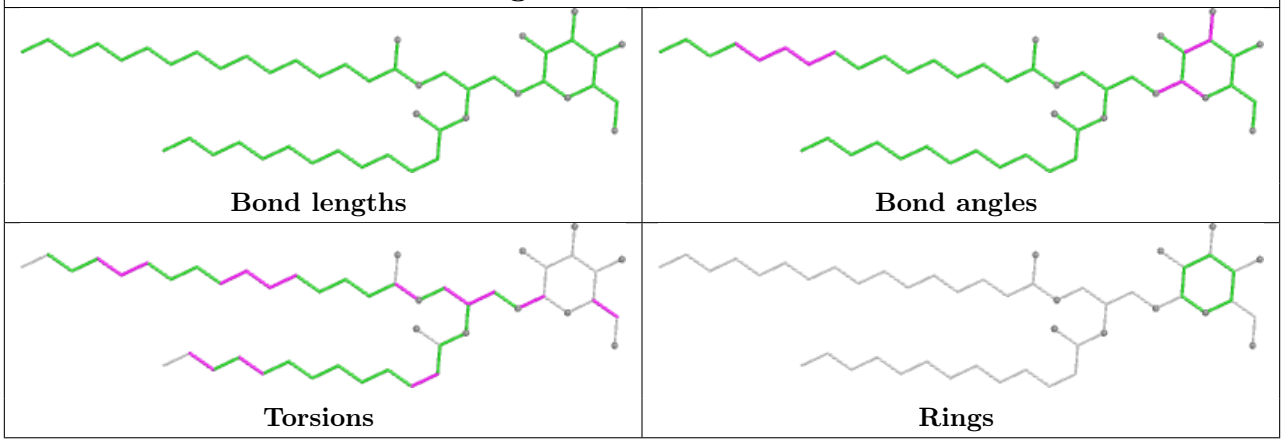
Ligand LUT V 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL V 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

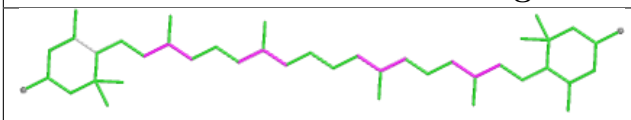
Ligand LHG O 622



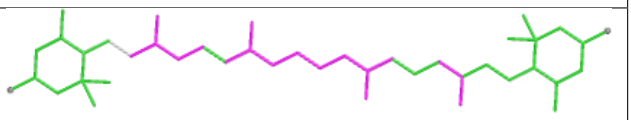
Ligand LMG AL 501



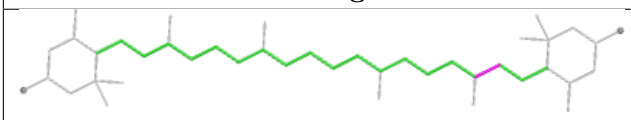
Ligand LUT AS 315



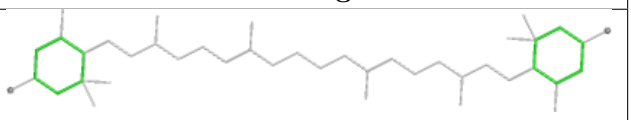
Bond lengths



Bond angles

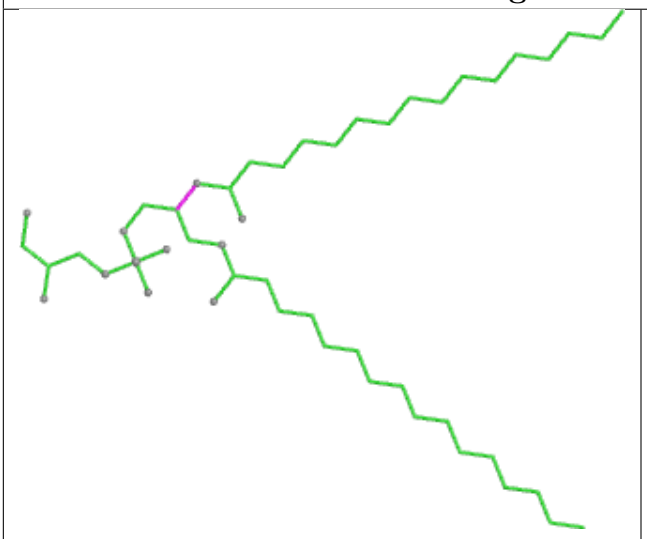


Torsions



Rings

Ligand LHG AQ 618



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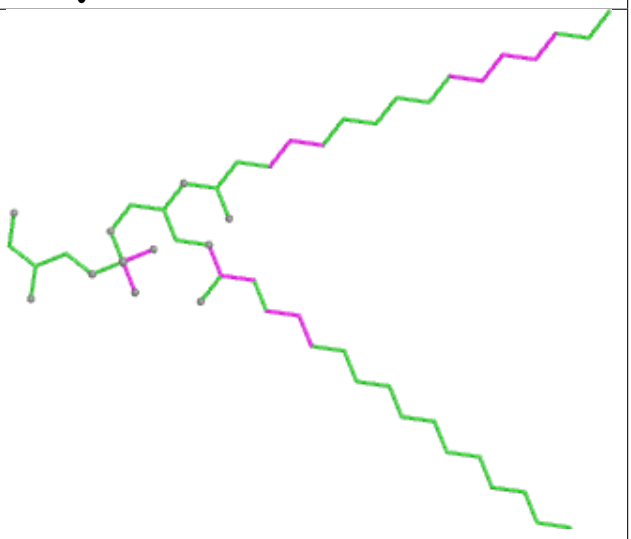
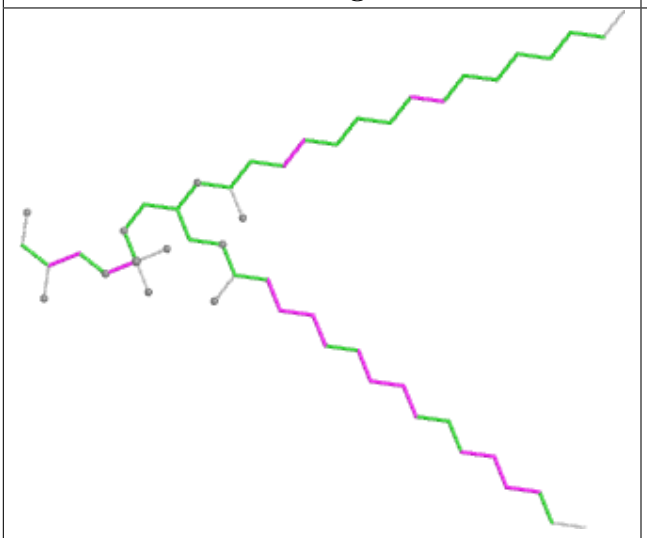


Bond angles



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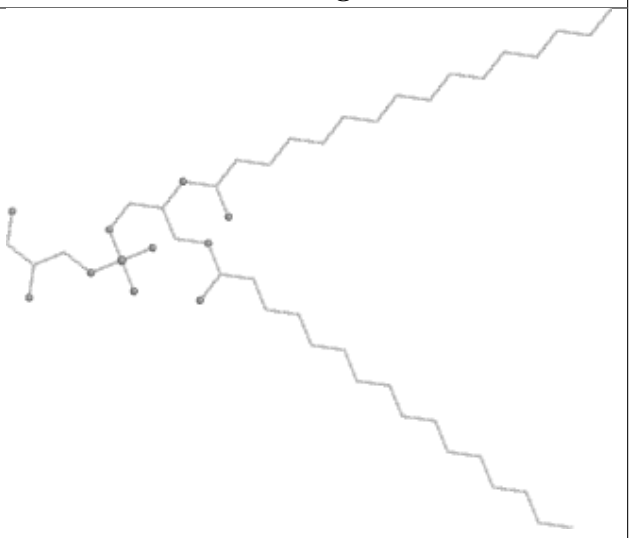
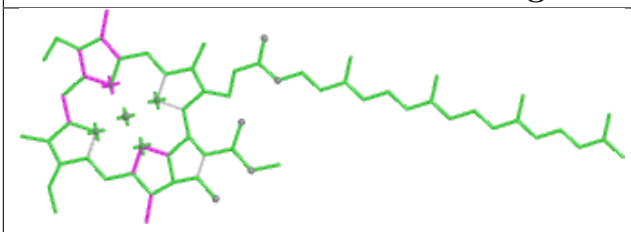
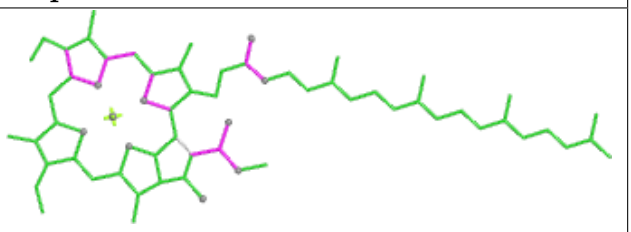
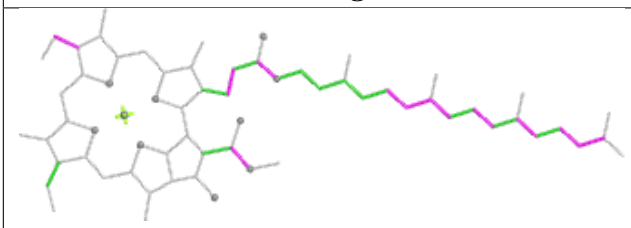
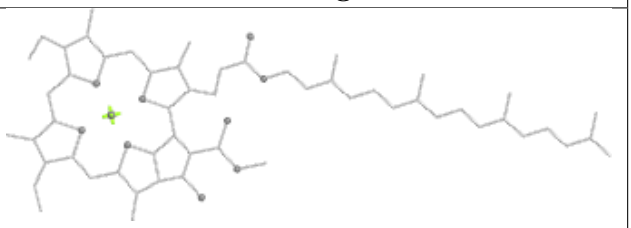
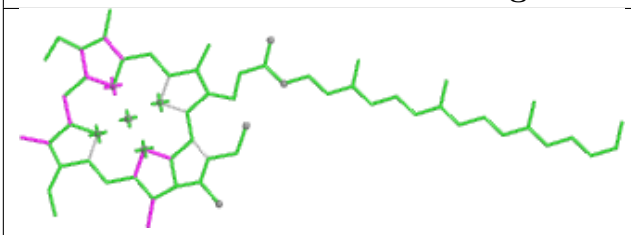
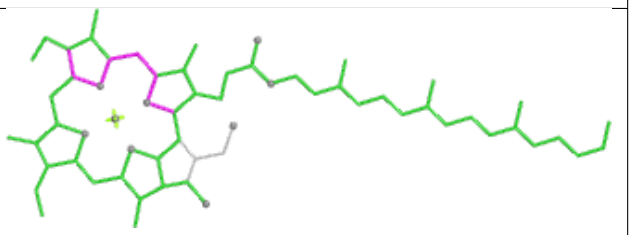
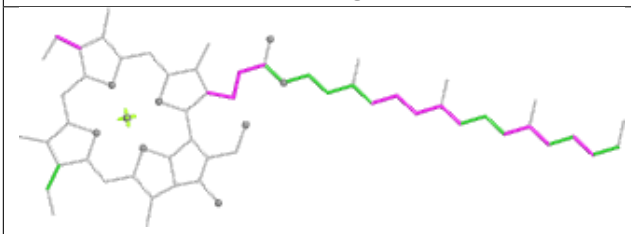
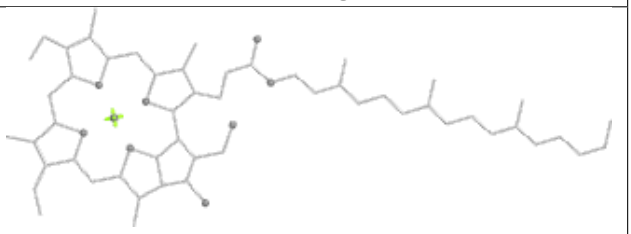
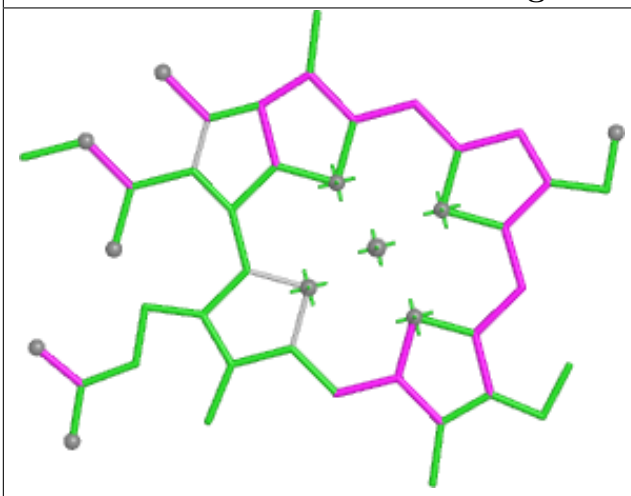


Rings

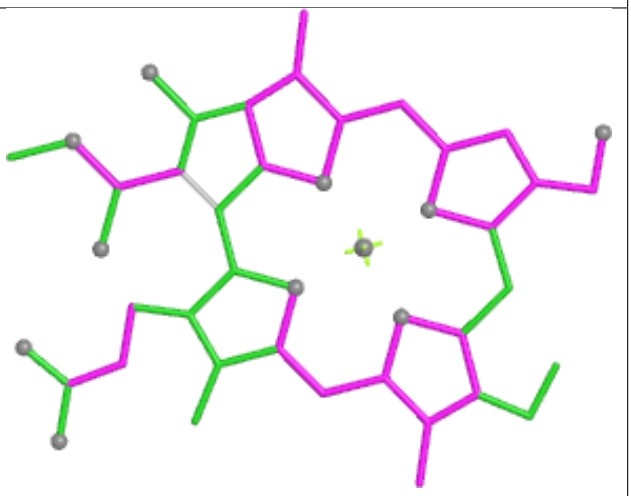
Ligand CLA p 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AN 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

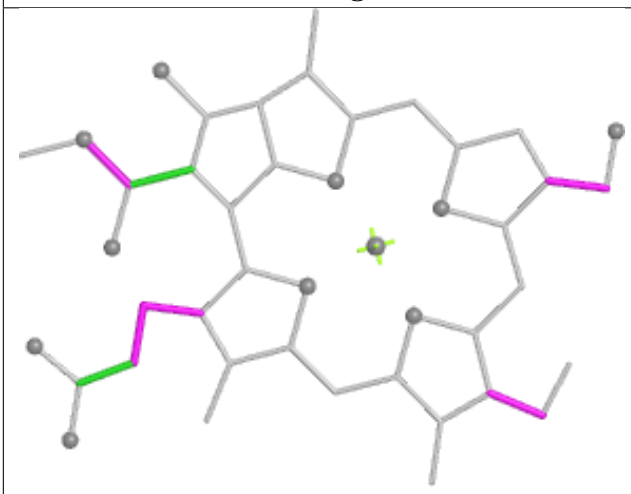
Ligand CHL 9 608



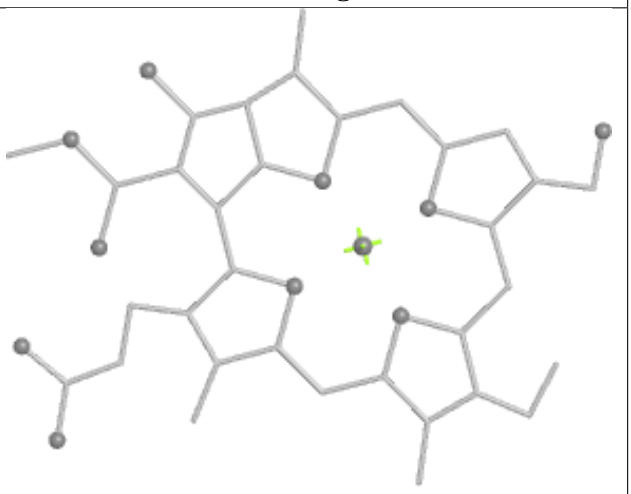
Bond lengths



Bond angles

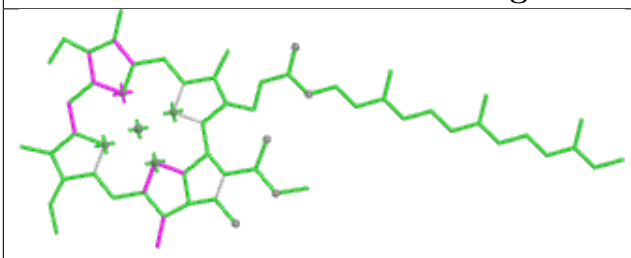


Torsions

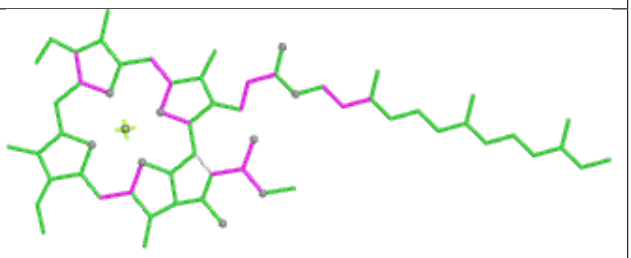


Rings

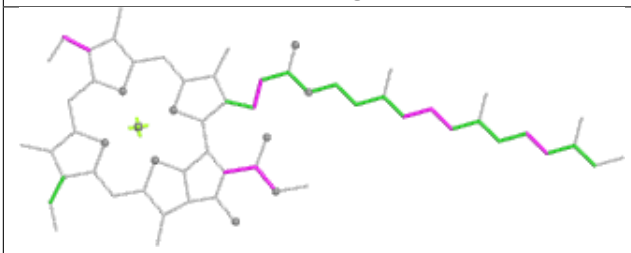
Ligand CLA AA 602



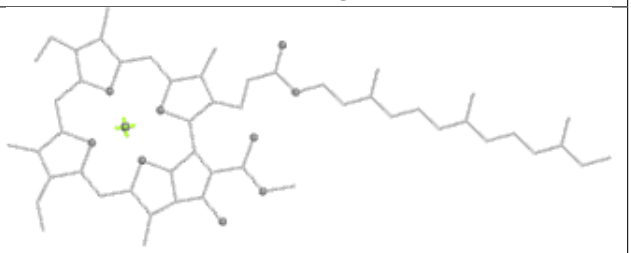
Bond lengths



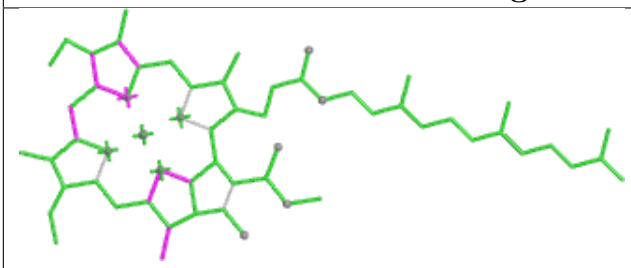
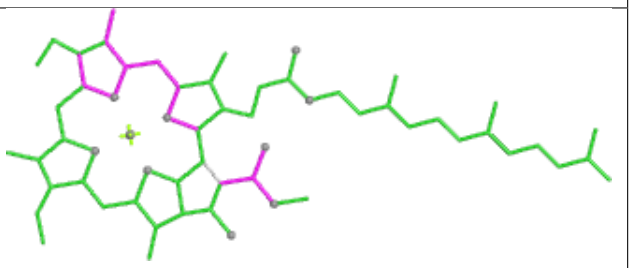
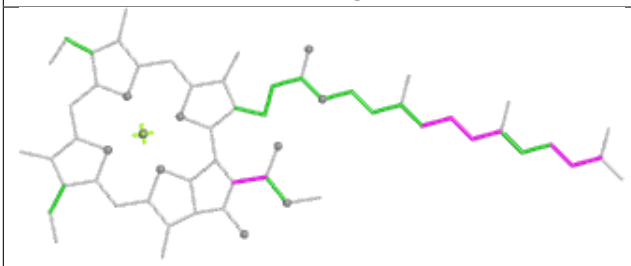
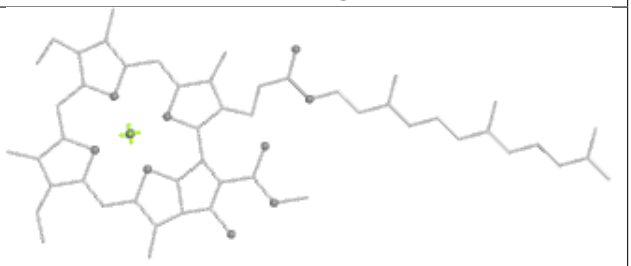
Bond angles



Torsions



Rings

Ligand CLA AR 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

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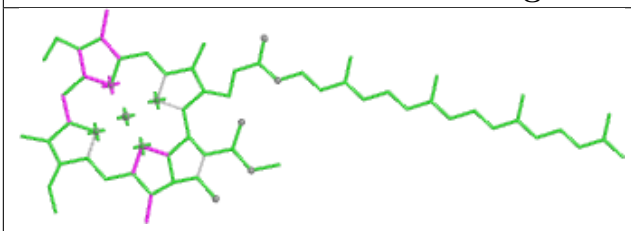
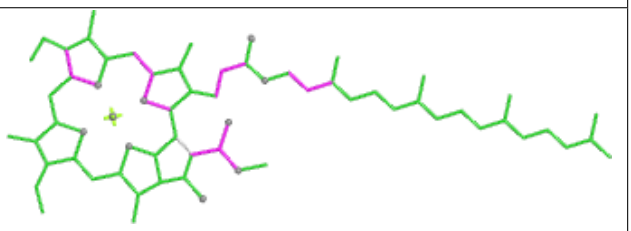
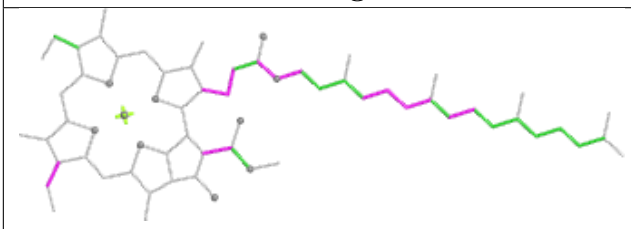
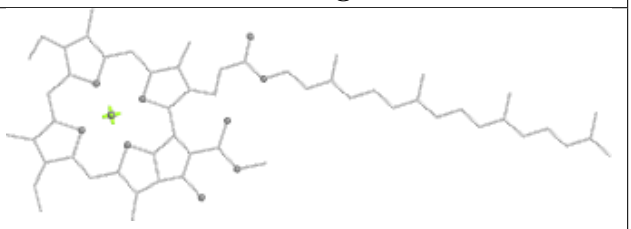
 Bond lengths	 Bond angles
 Torsions	 Rings

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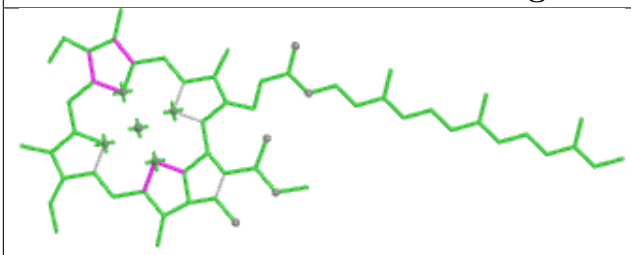
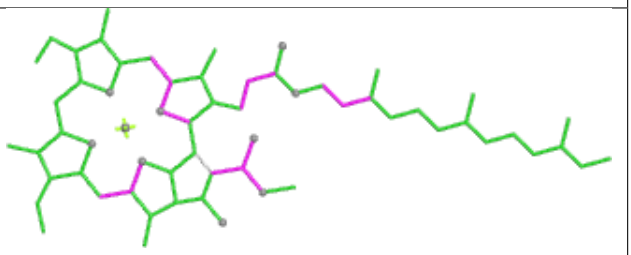
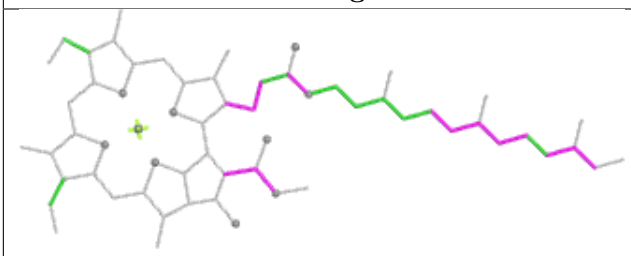
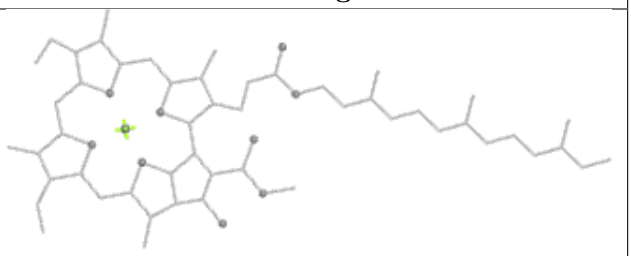
 Bond lengths	 Bond angles
 Torsions	 Rings

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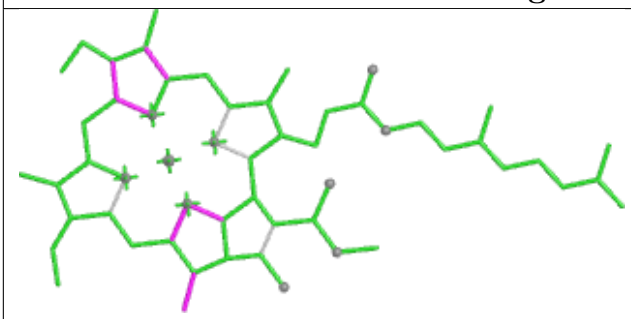
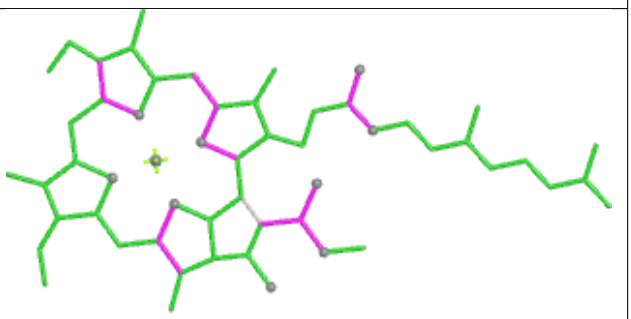
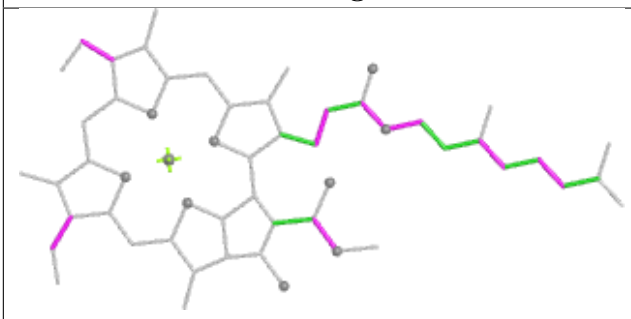
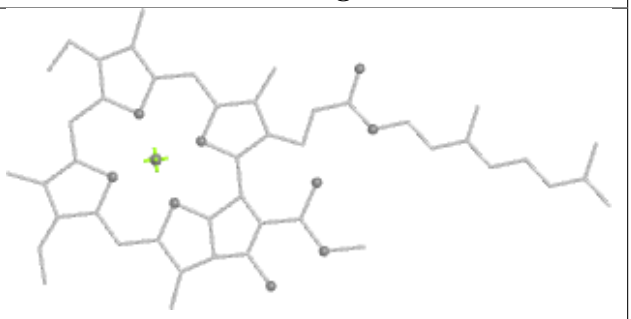
 Bond lengths	 Bond angles
 Torsions	 Rings

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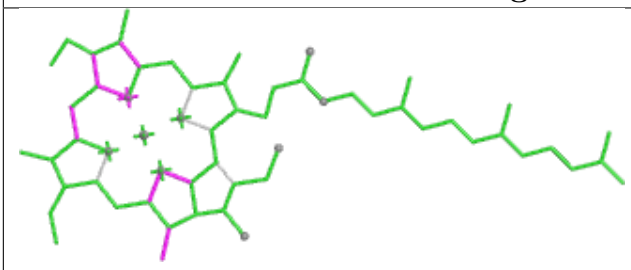
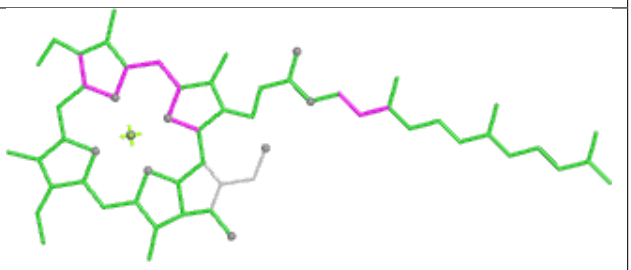
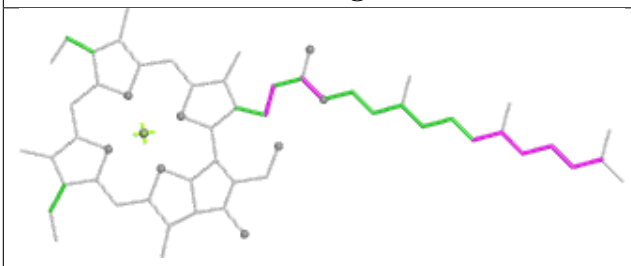
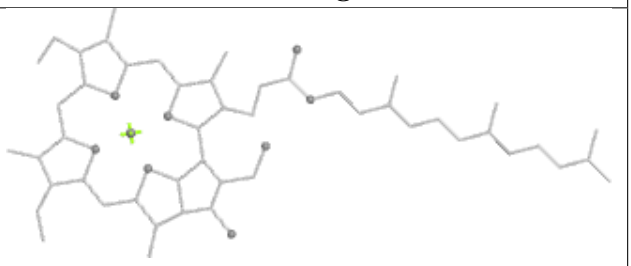
 Bond lengths	 Bond angles
 Torsions	 Rings

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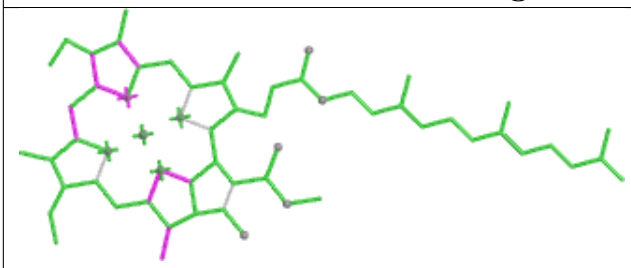
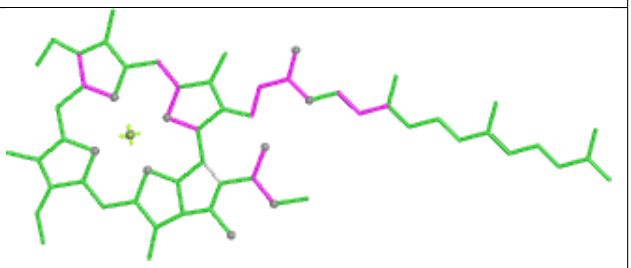
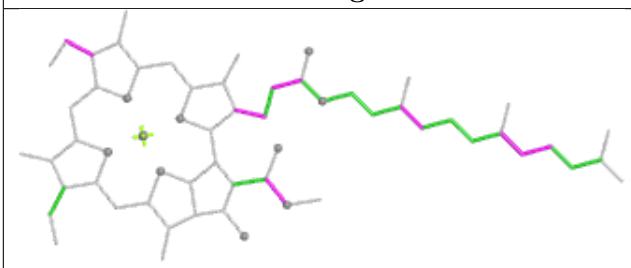
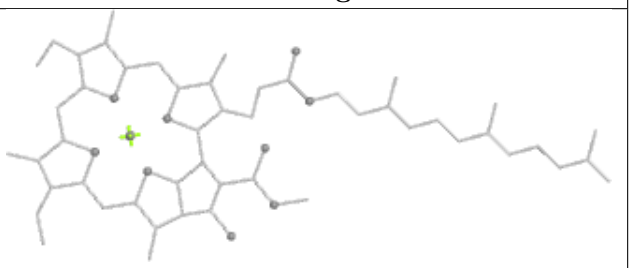
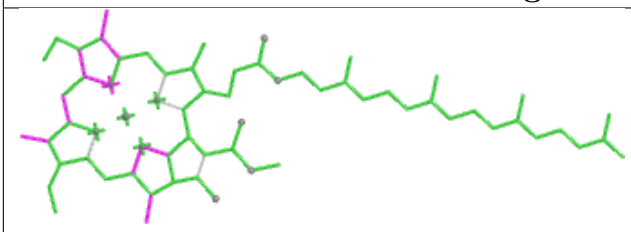
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA O 612



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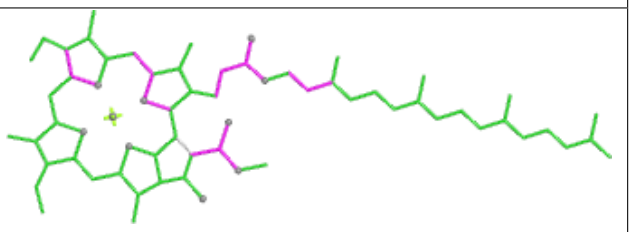

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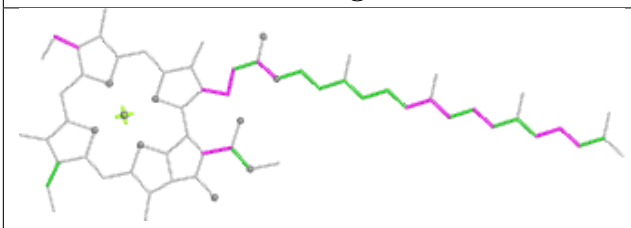

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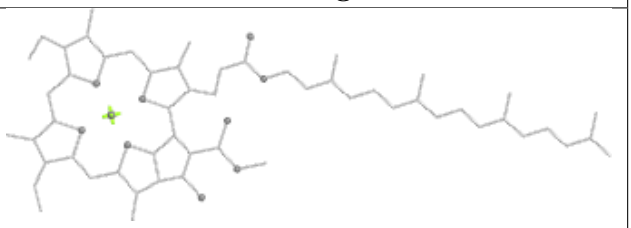
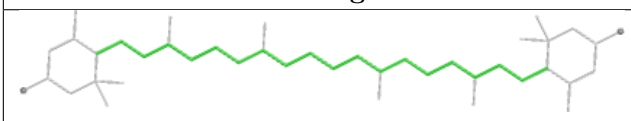


Rings

Ligand LUT AD 314

Bond lengths

Bond angles



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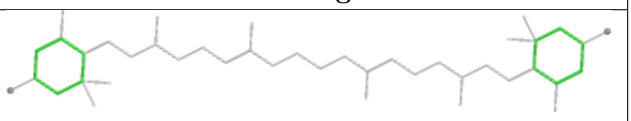
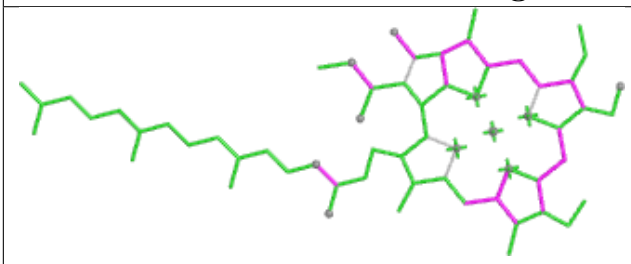


Rings

Ligand CHL AA 606



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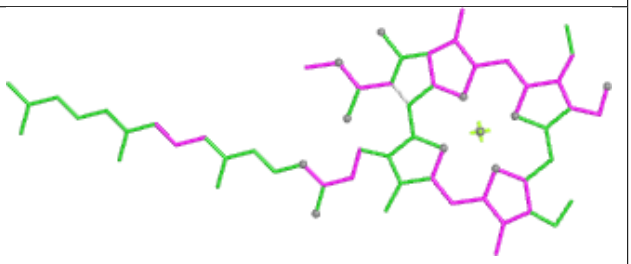

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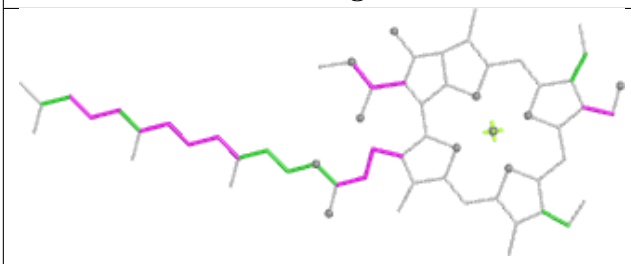

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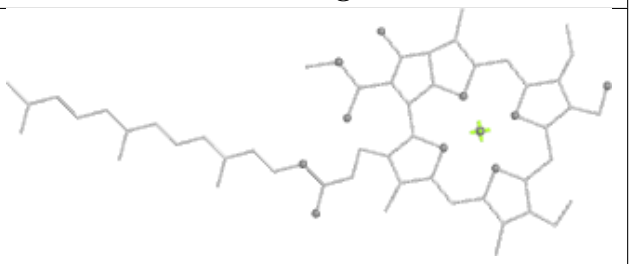
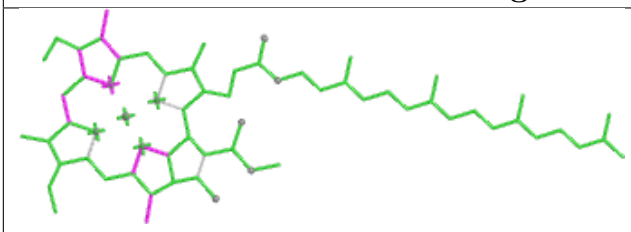
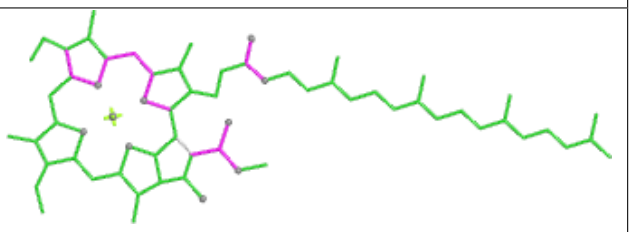
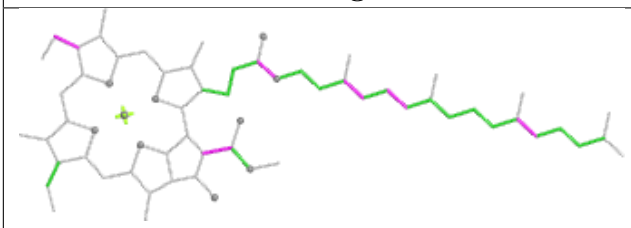
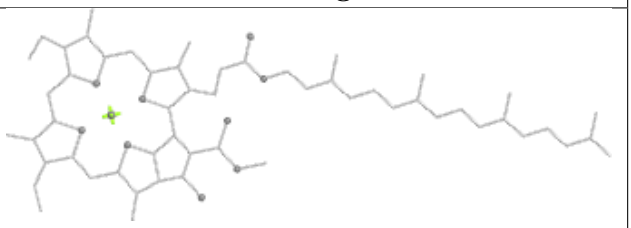


Rings

Ligand CLA AU 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

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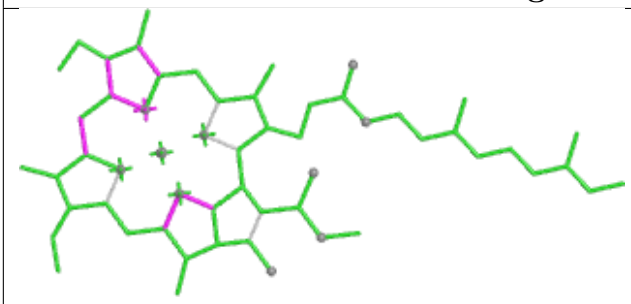
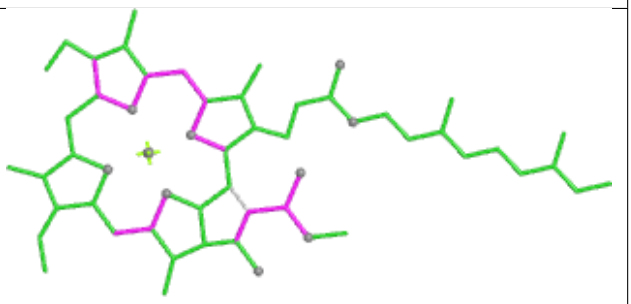
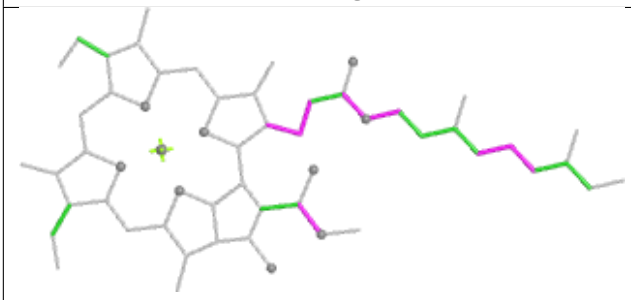
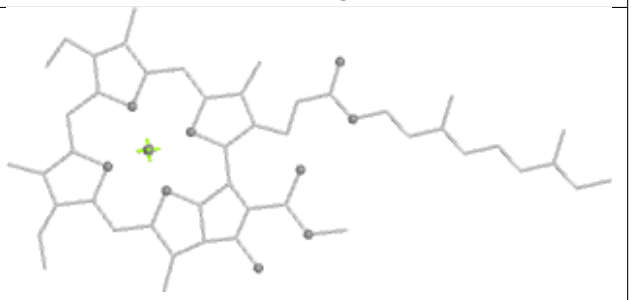
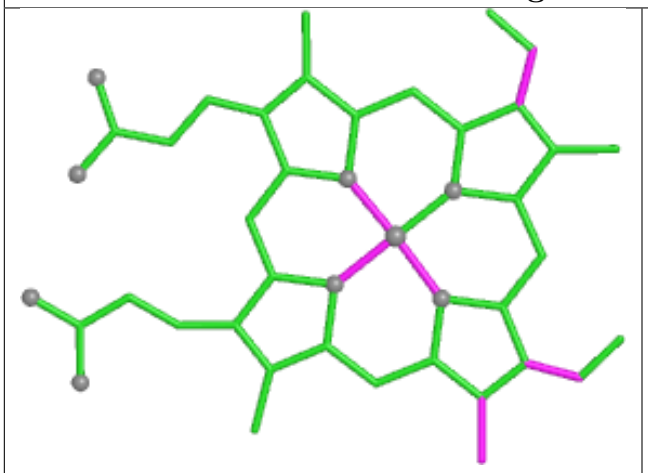
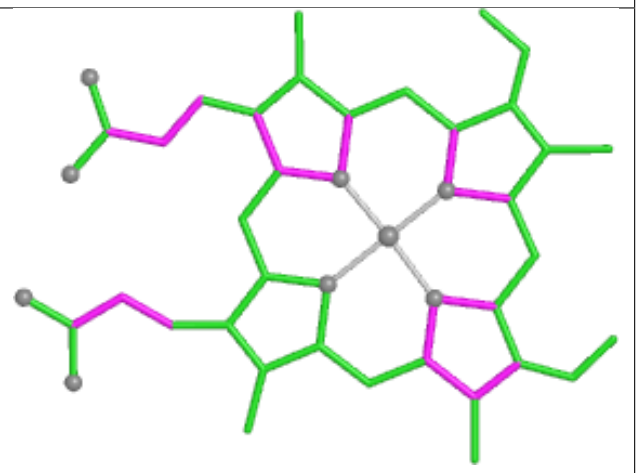
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM f 102



Bond lengths



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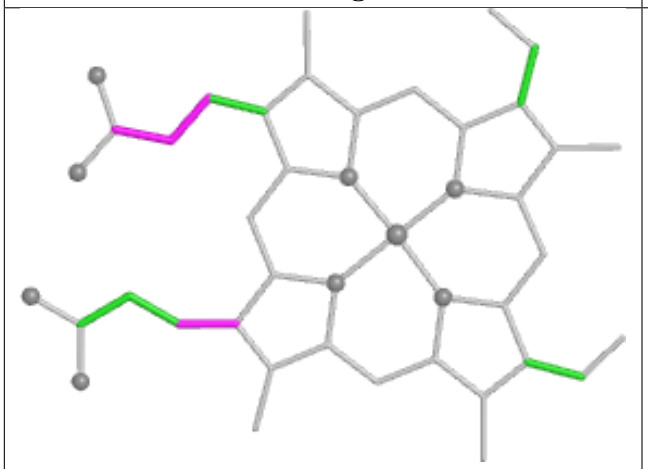

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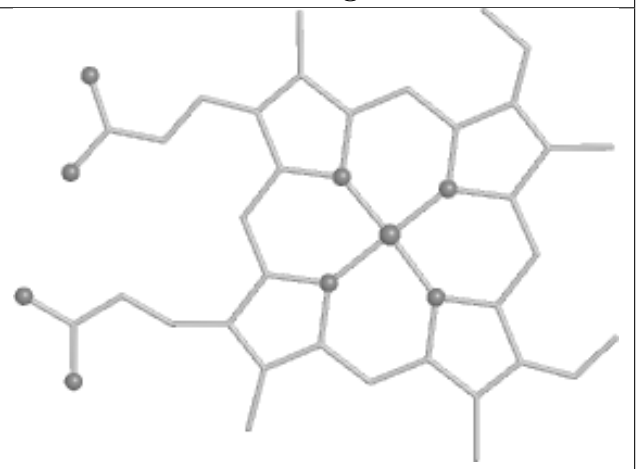
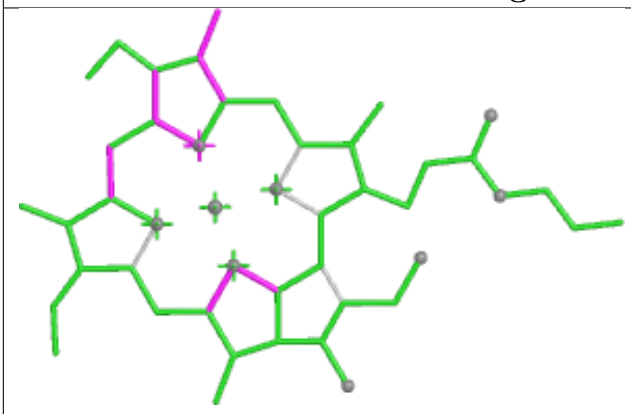
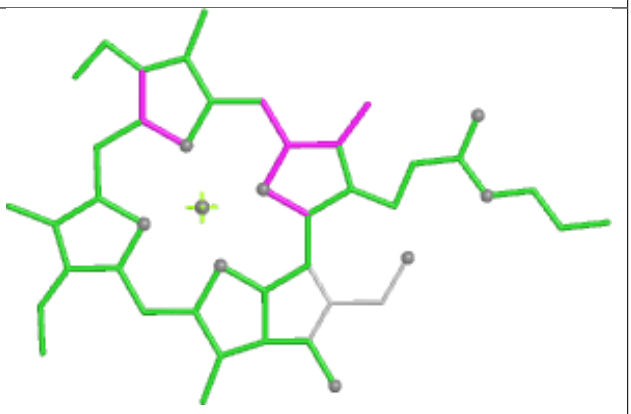
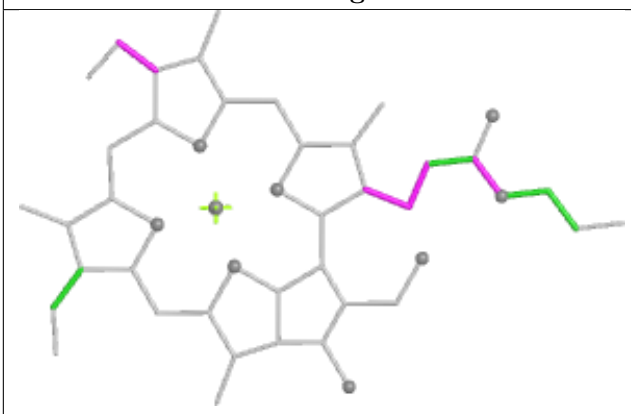
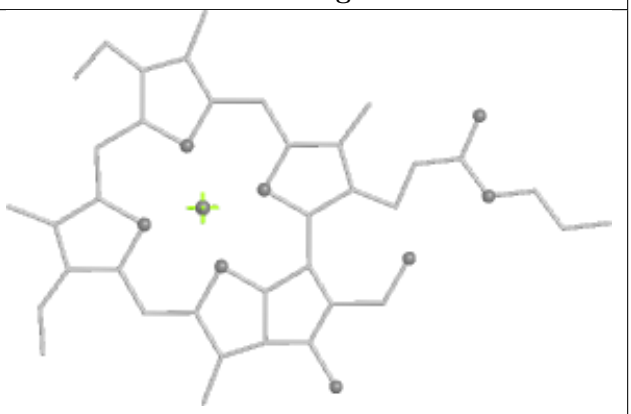
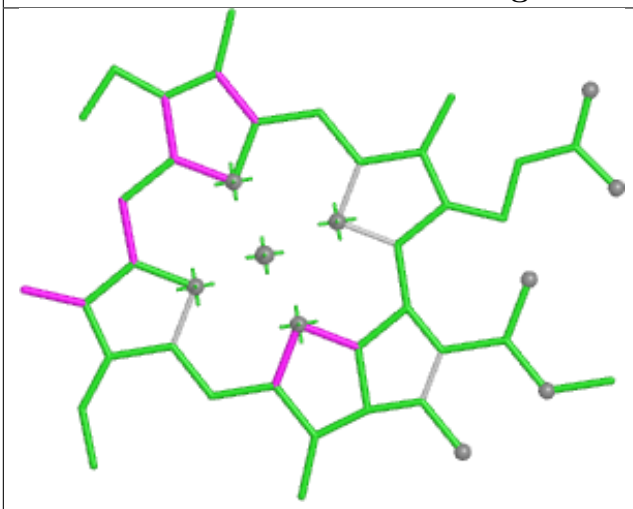


Rings

Ligand CLA AH 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AB 610



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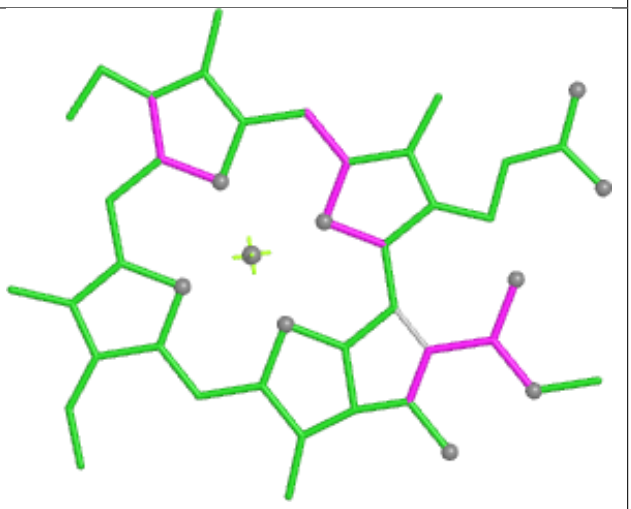

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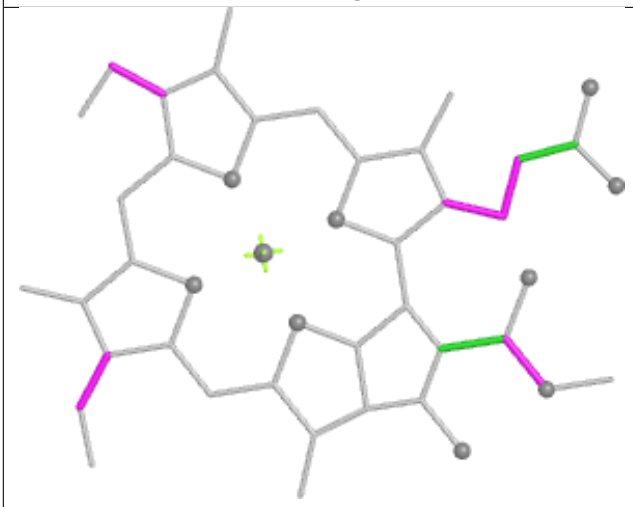
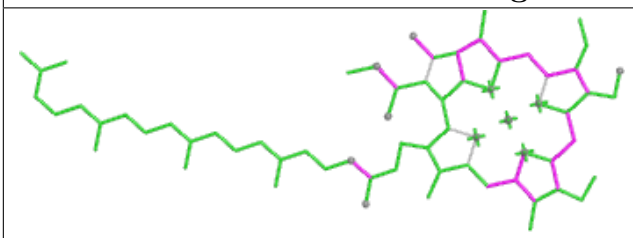


Torsions

Rings

Ligand CHL AQ 609



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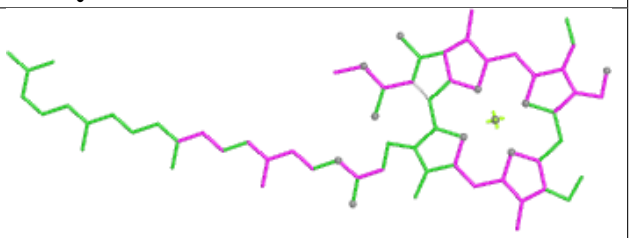

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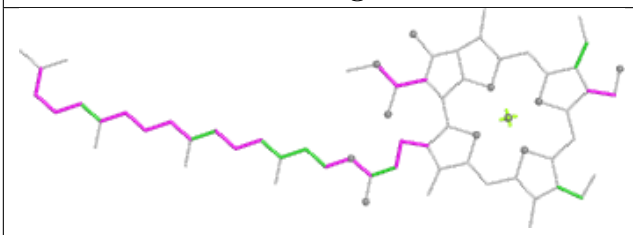

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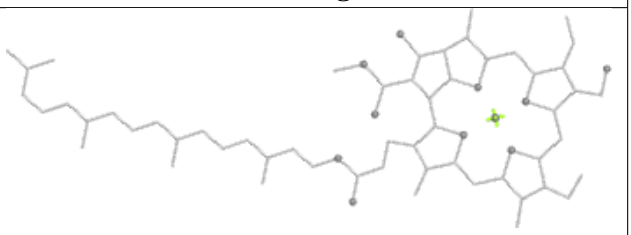
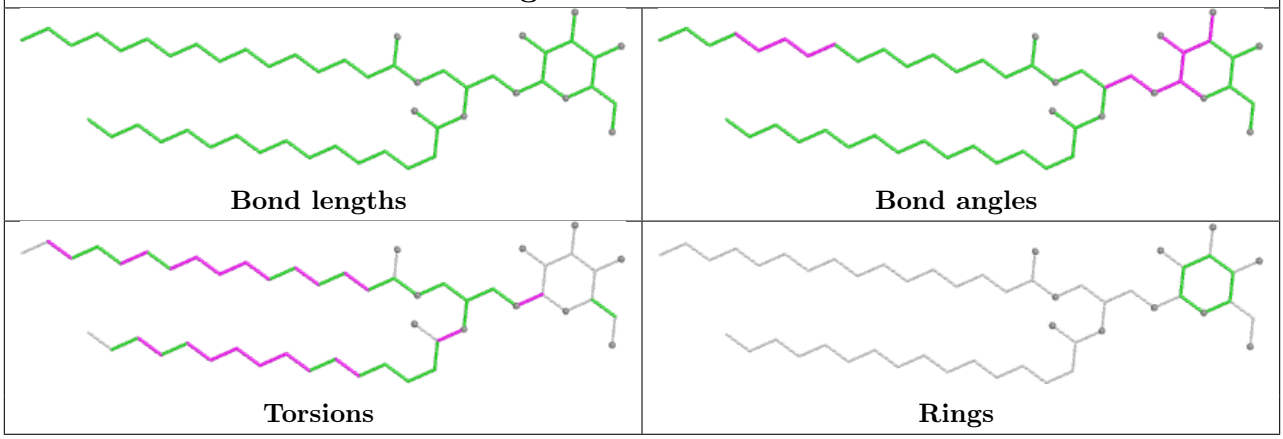
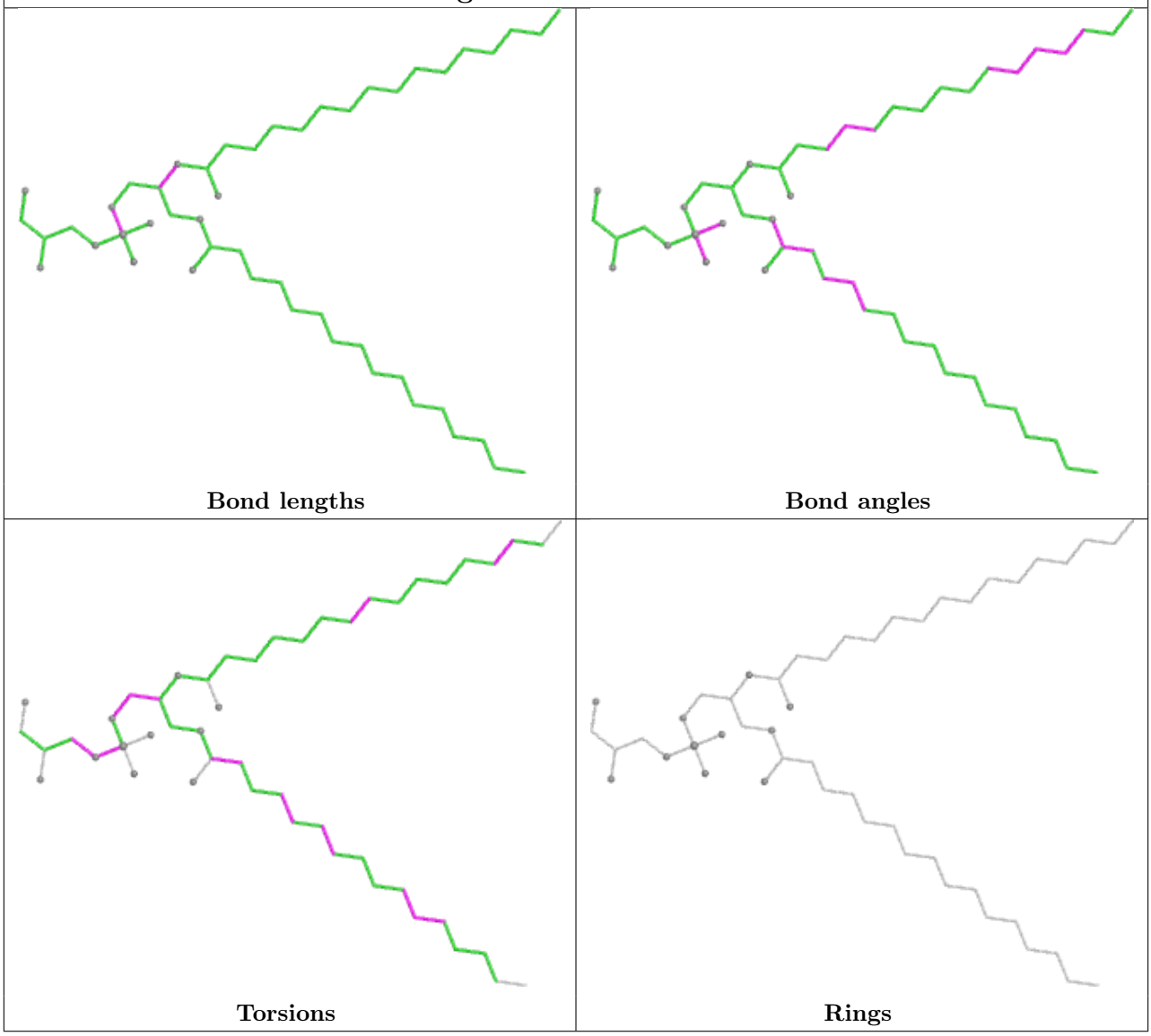


Rings

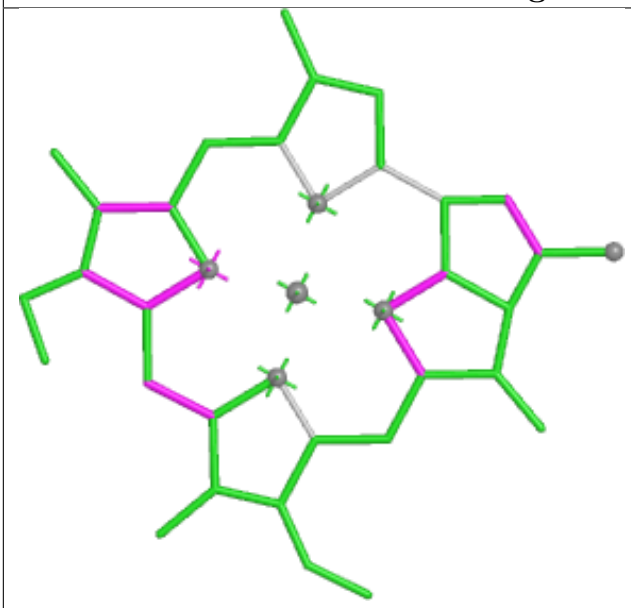
Ligand LMG O 620



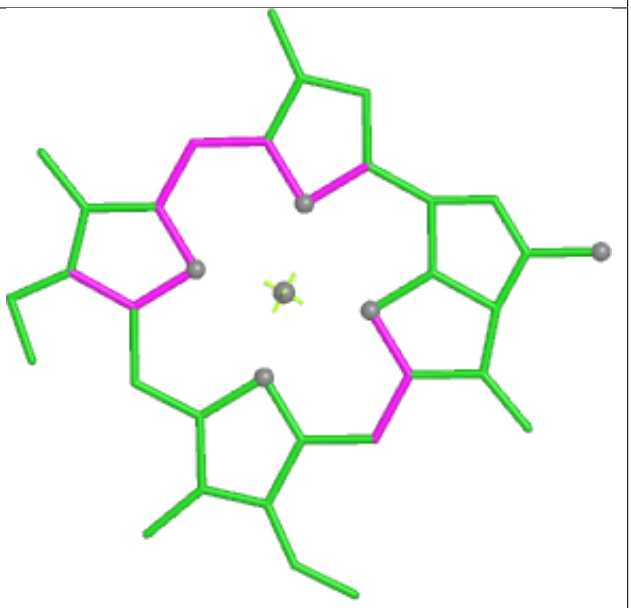
Ligand LHG AU 617



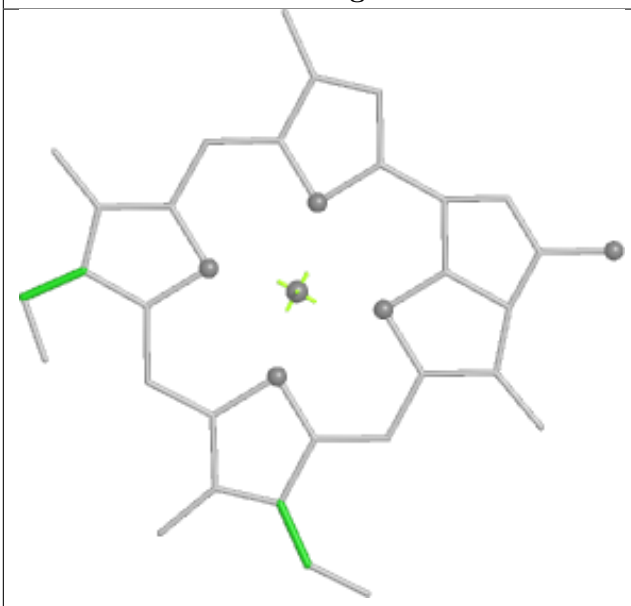
Ligand CLA 9 614



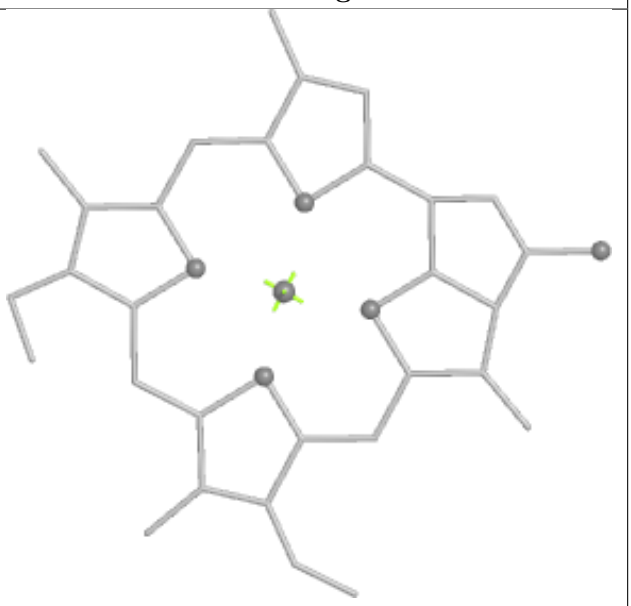
Bond lengths



Bond angles

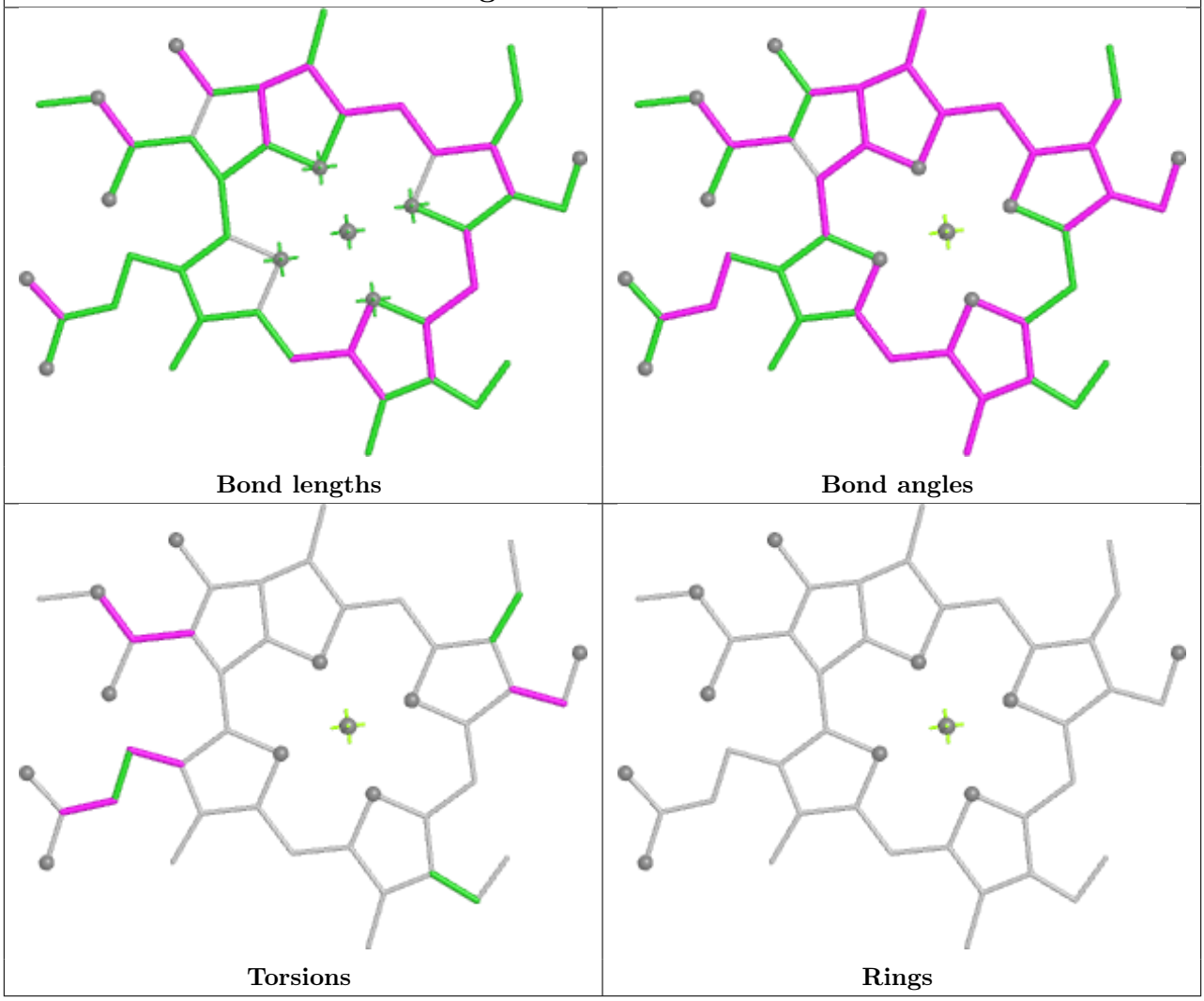


Torsions

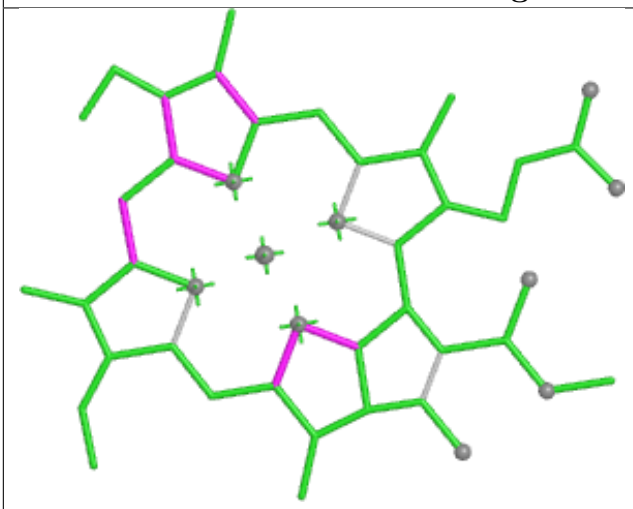


Rings

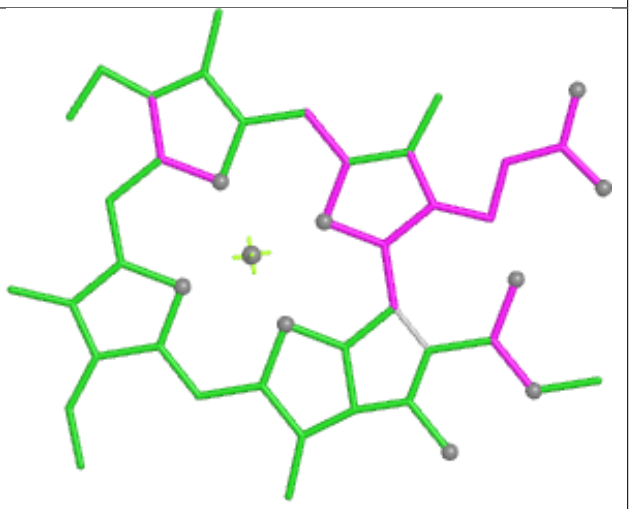
Ligand CHL AA 605



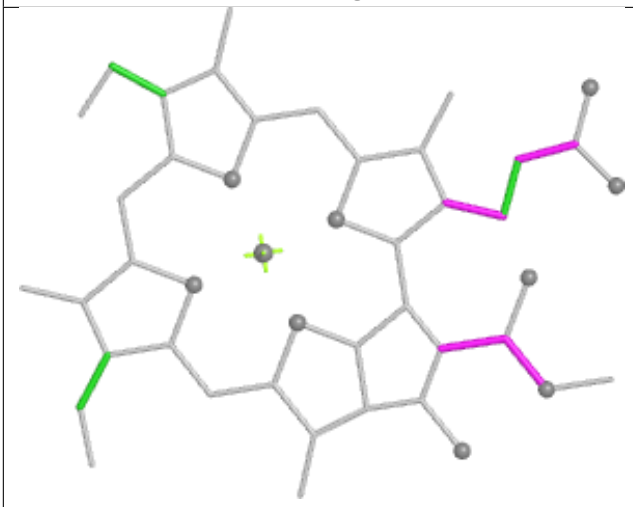
Ligand CLA AB 611



Bond lengths



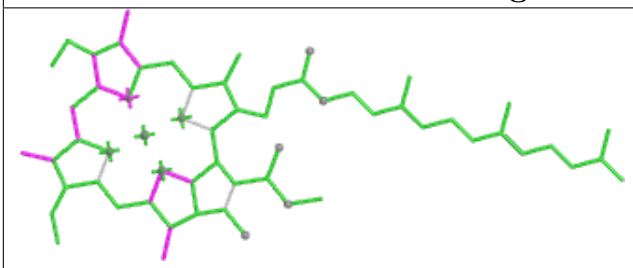
Bond angles



Torsions

Rings

Ligand CLA AH 611



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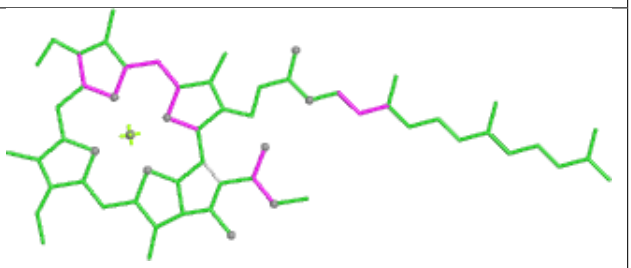
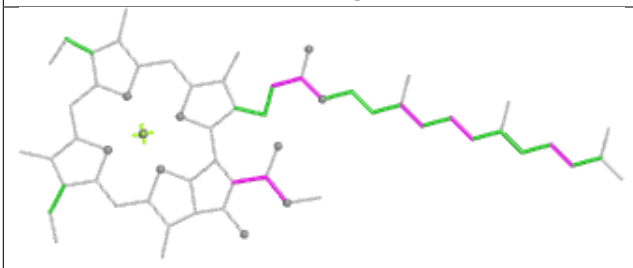


Bond angles



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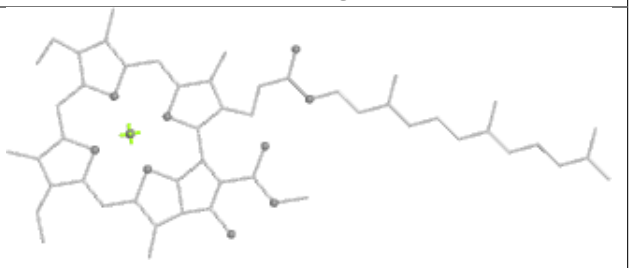
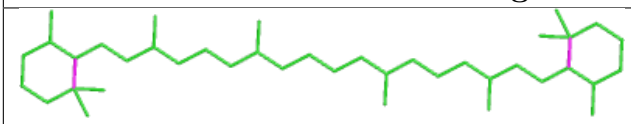
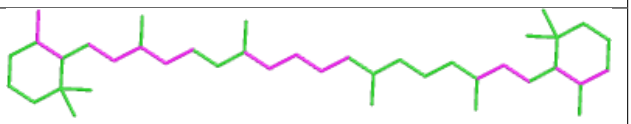


Rings

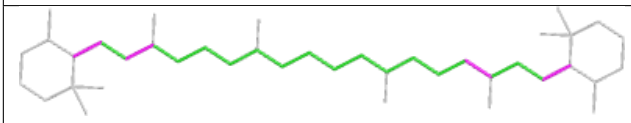
Ligand BCR AL 516



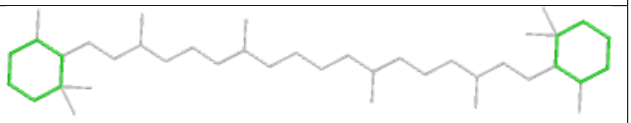
Bond lengths



Bond angles



Torsions

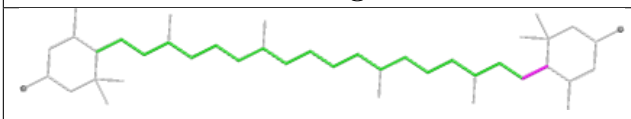


Rings

Ligand LUT p 615

Bond lengths

Bond angles



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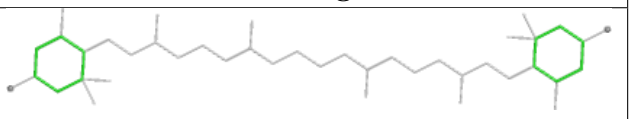
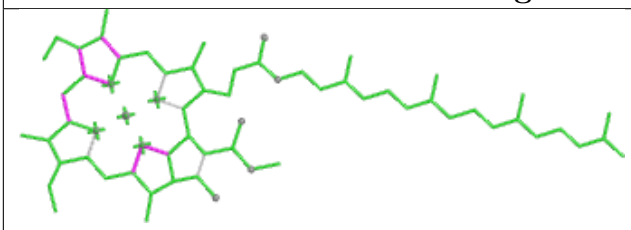


Rings

Ligand CLA AJ 404



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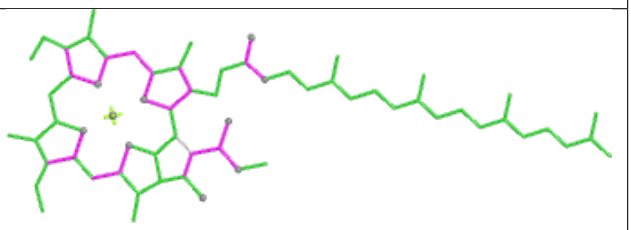
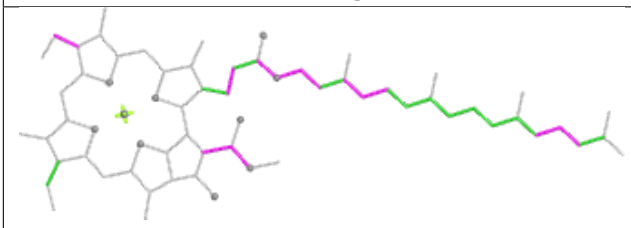


Bond angles



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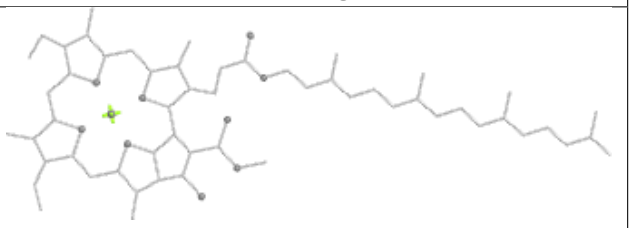
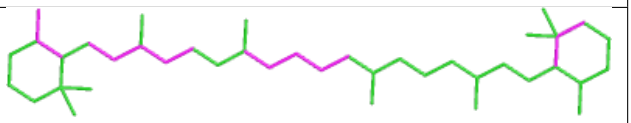


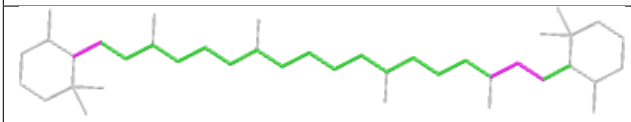
Rings

Ligand BCR AK 619

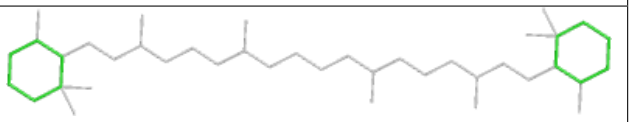
Bond lengths



Bond angles

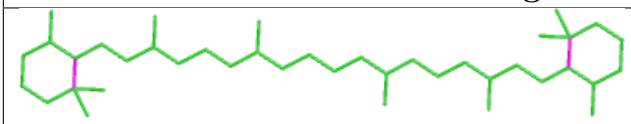


Torsions

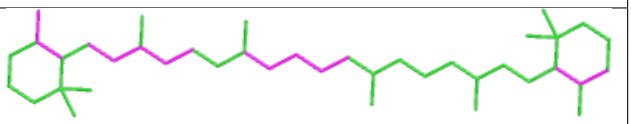


Rings

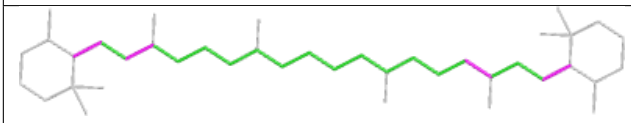
Ligand BCR P 514



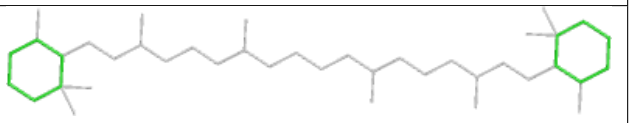
Bond lengths



Bond angles

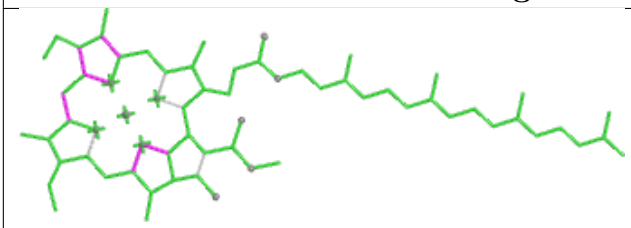


Torsions

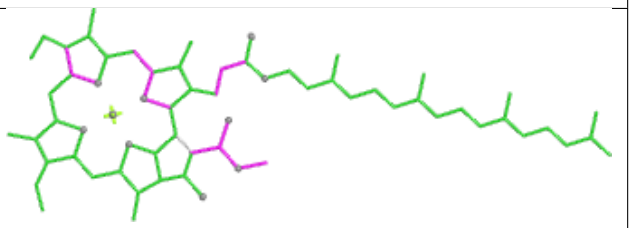


Rings

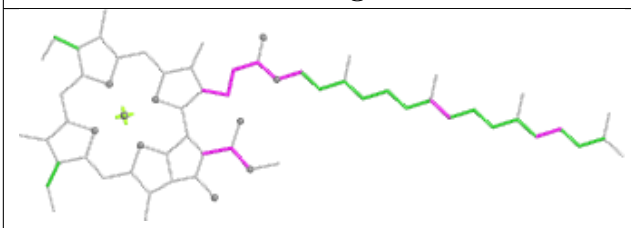
Ligand CLA AL 505



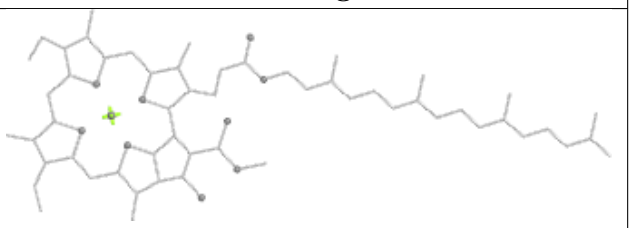
Bond lengths



Bond angles

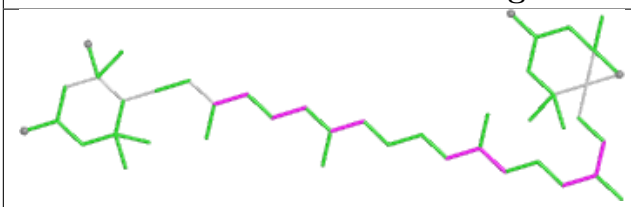


Torsions

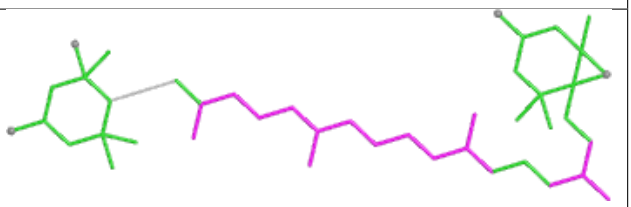


Rings

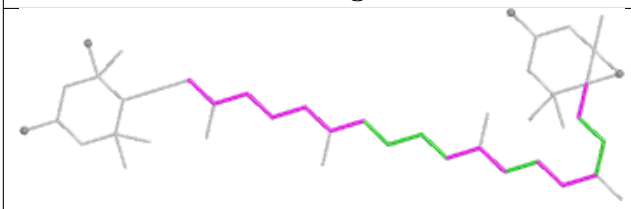
Ligand NEX AA 616



Bond lengths



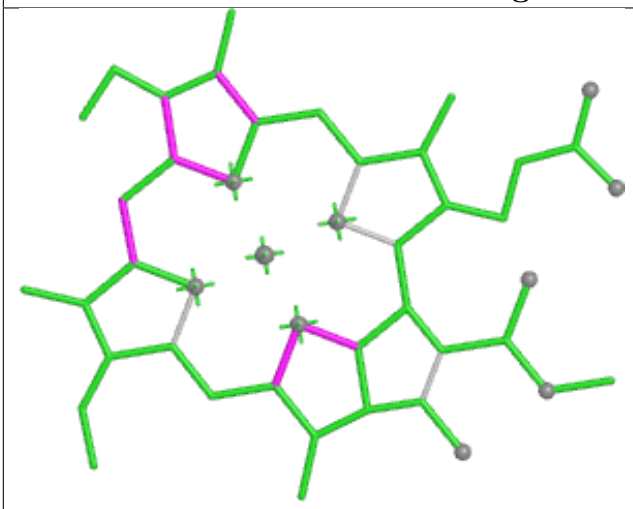
Bond angles



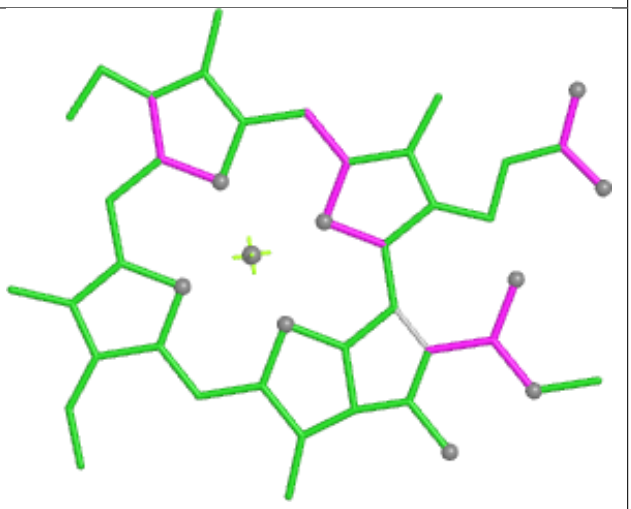
Torsions

Rings

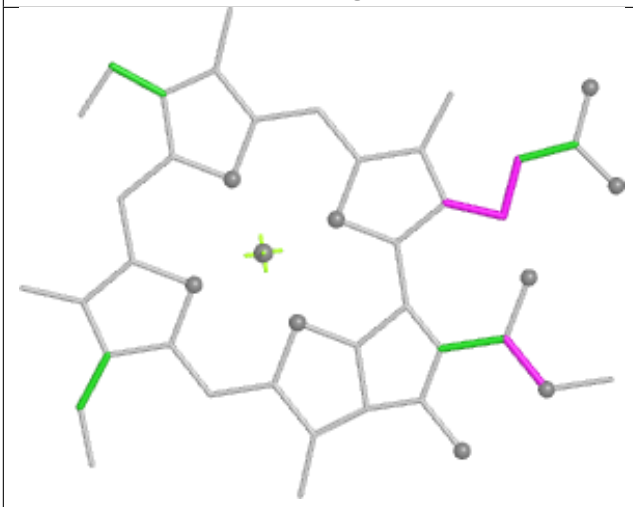
Ligand CLA AE 612



Bond lengths



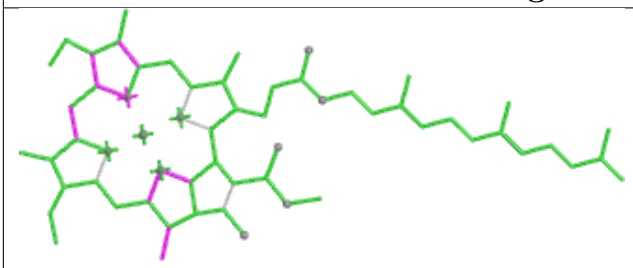
Bond angles



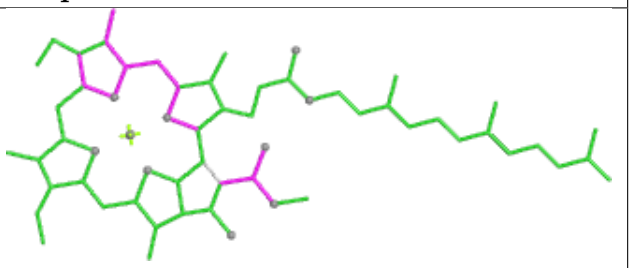
Torsions

Rings

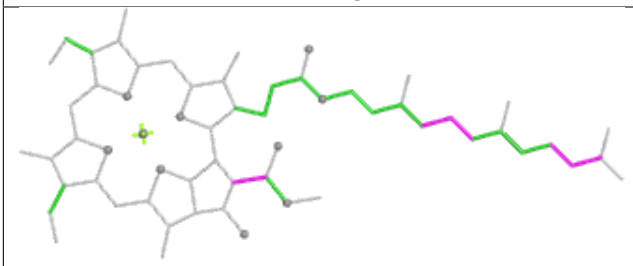
Ligand CLA q 603



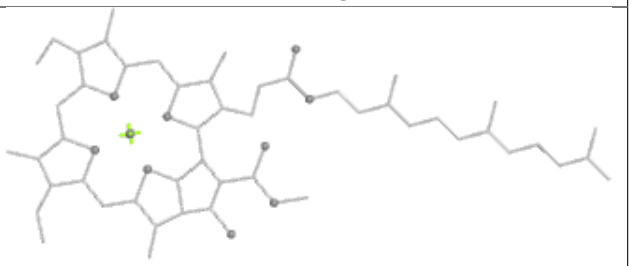
Bond lengths



Bond angles

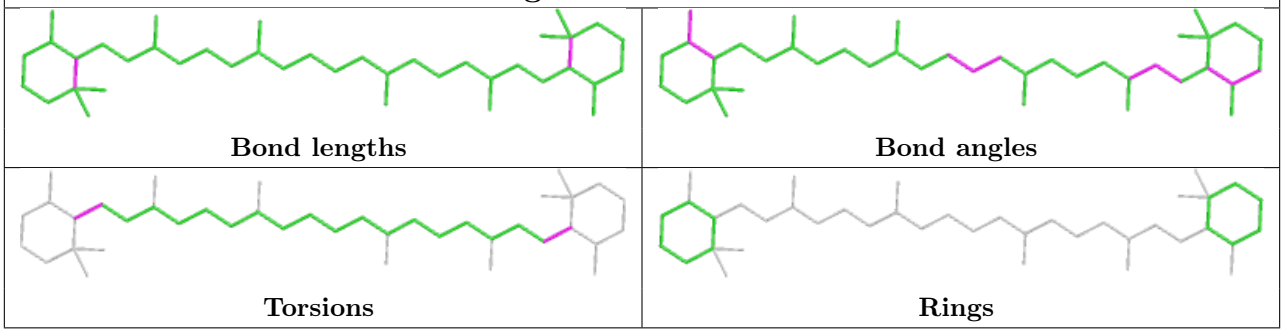


Torsions

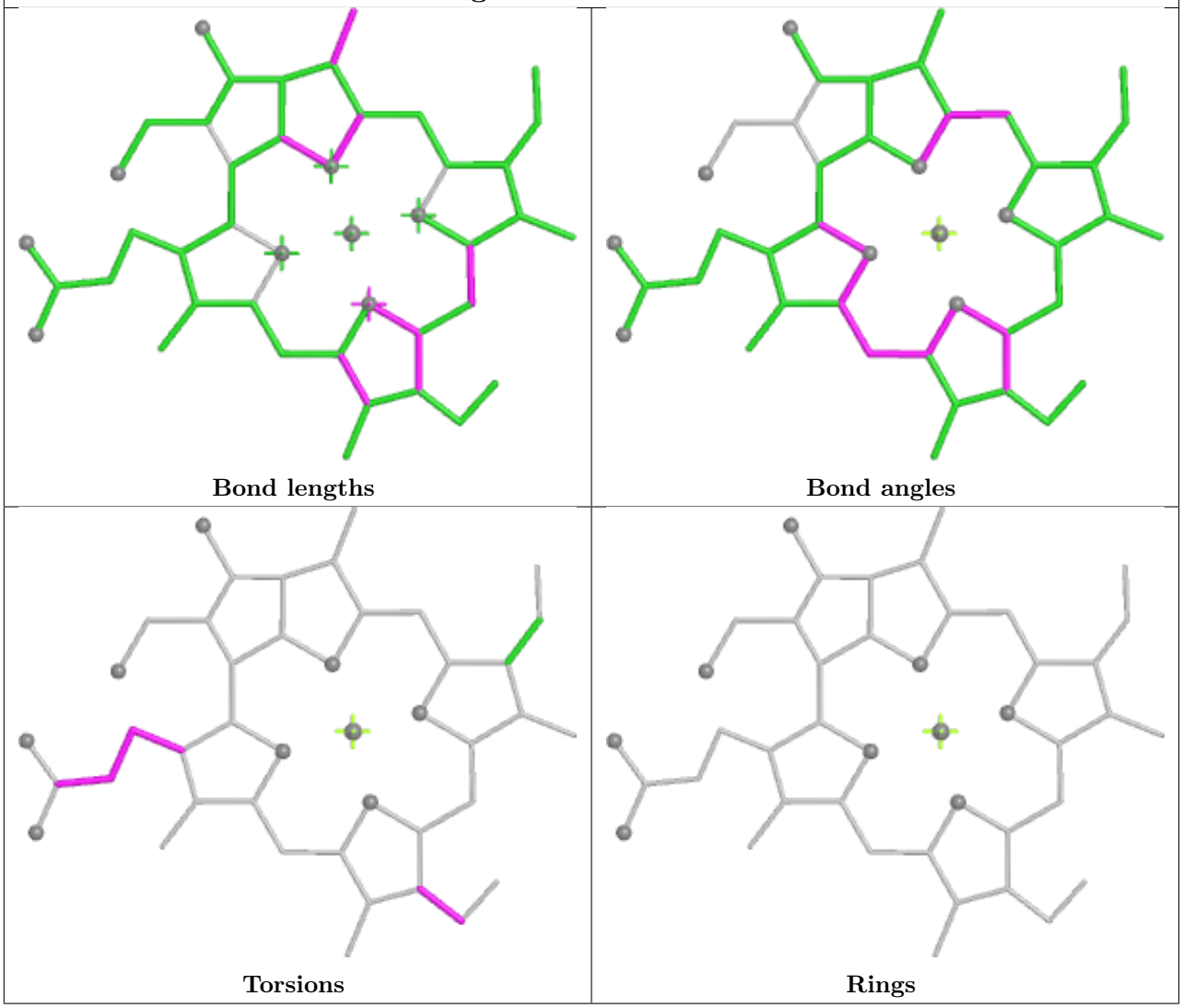


Rings

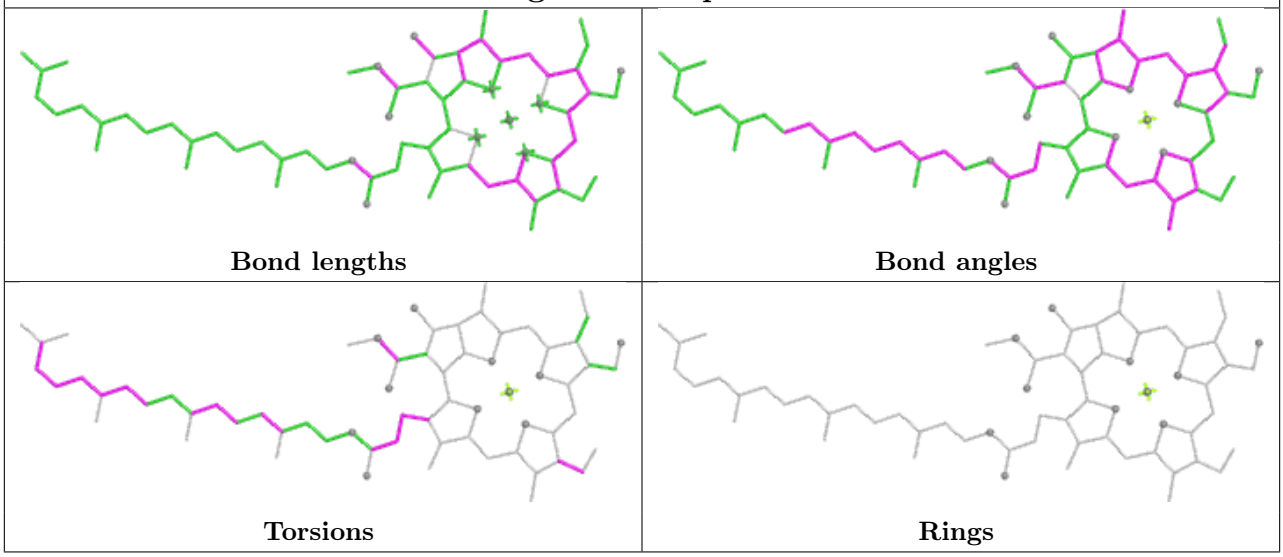
Ligand BCR P 513



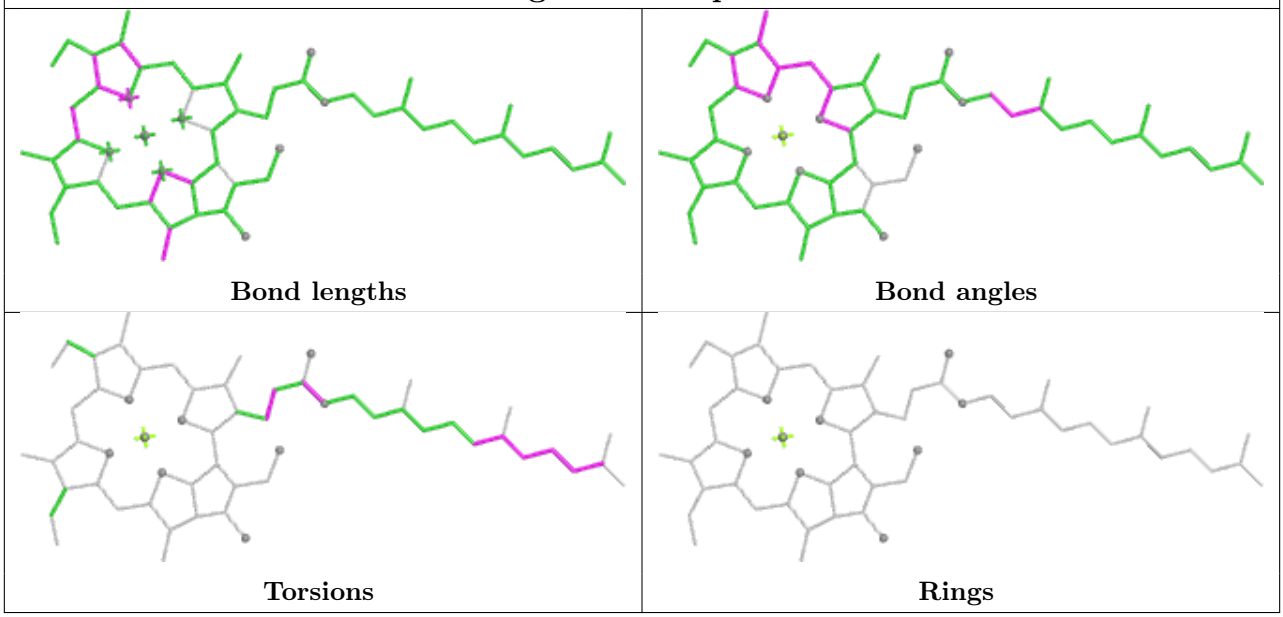
Ligand CLA AA 610



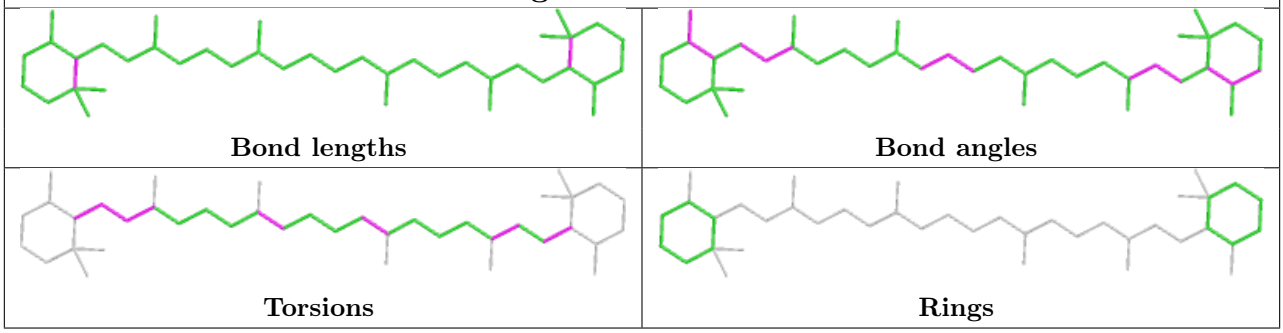
Ligand CHL p 607



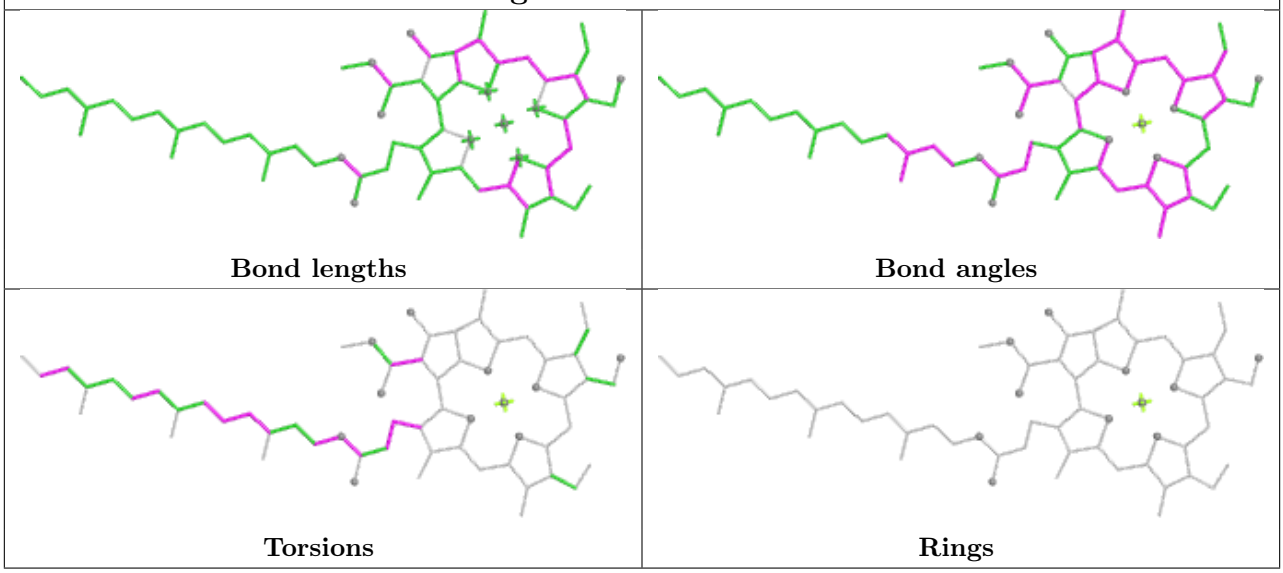
Ligand CLA q 602



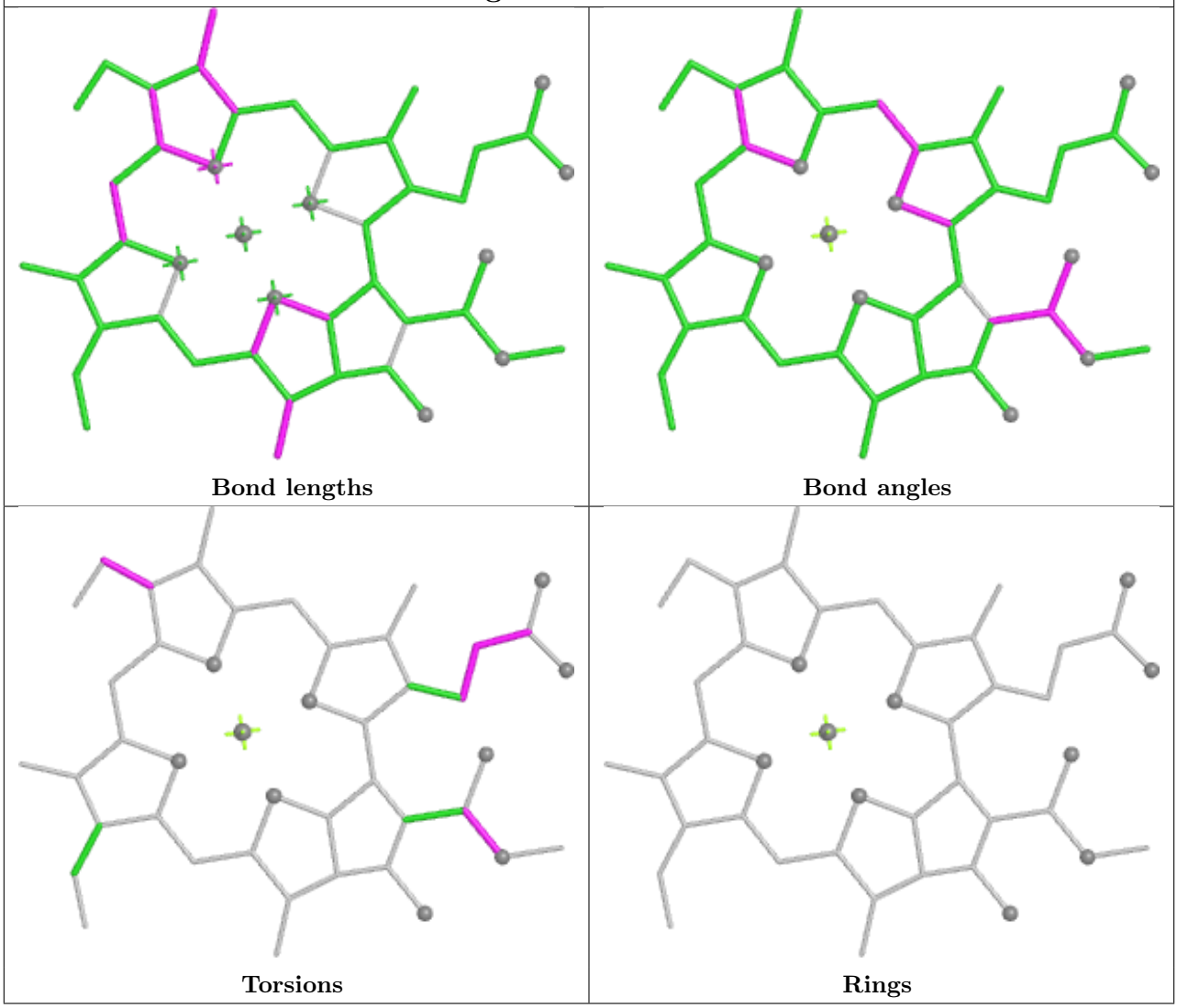
Ligand BCR f 101



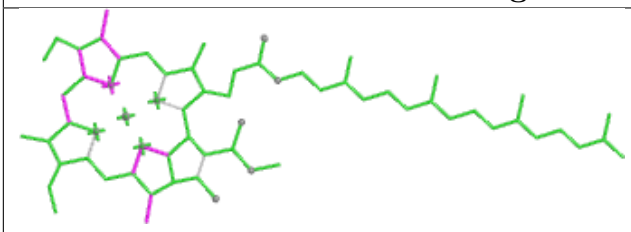
Ligand CHL AD 301



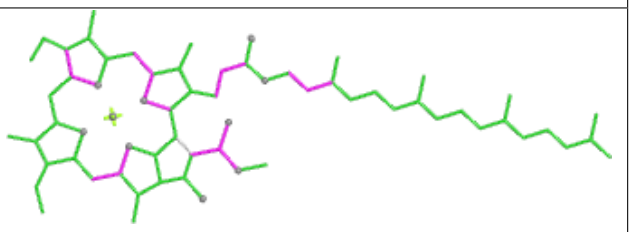
Ligand CLA 9 612



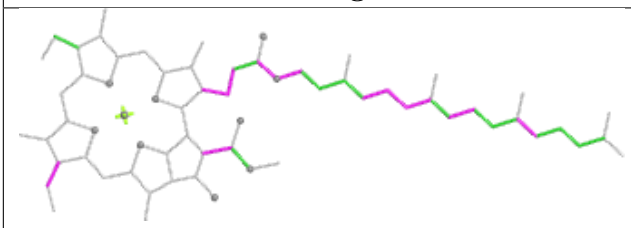
Ligand CLA AK 606



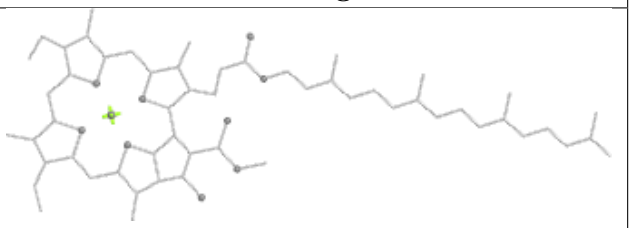
Bond lengths



Bond angles

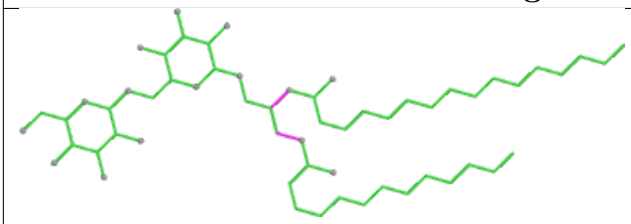


Torsions

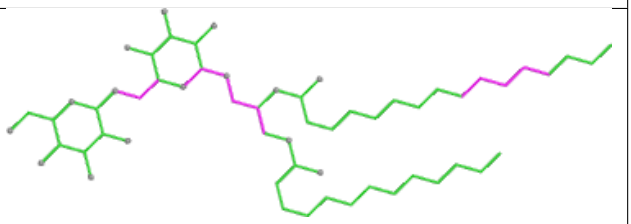


Rings

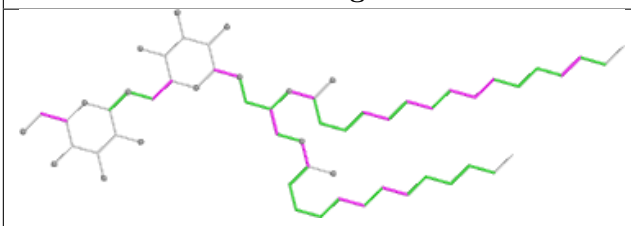
Ligand DGD J 413



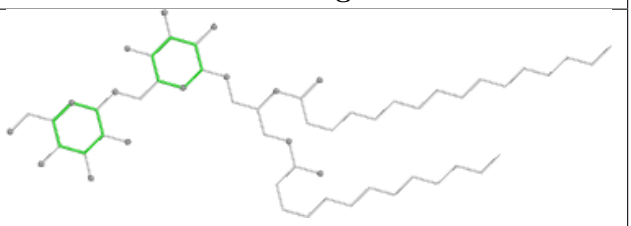
Bond lengths



Bond angles



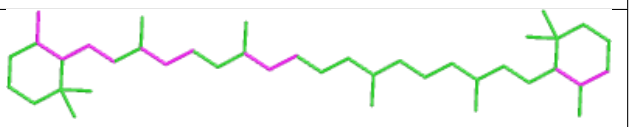
Torsions



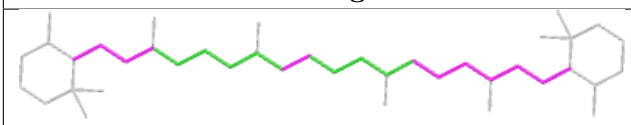
Rings

Ligand BCR AF 612

Bond lengths



Bond angles



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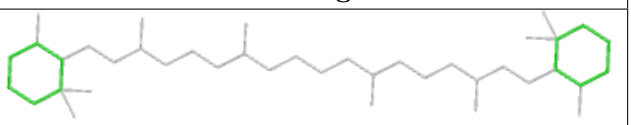
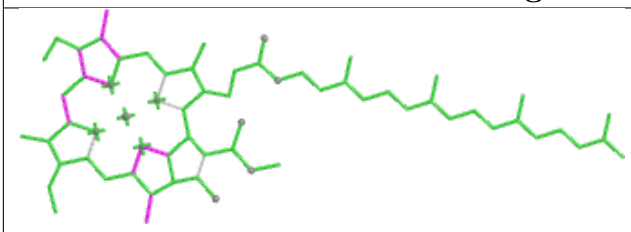
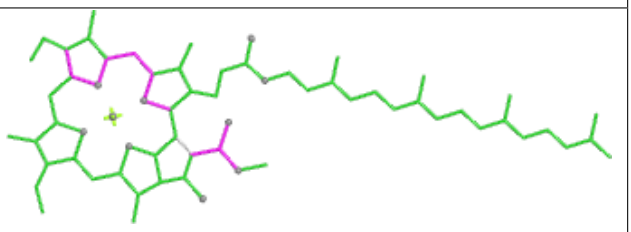
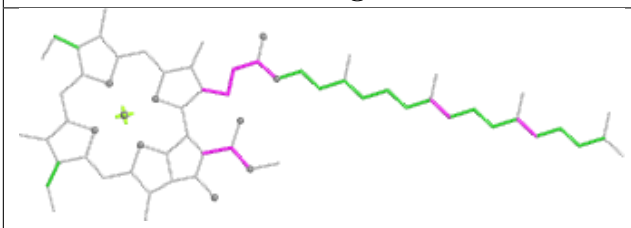
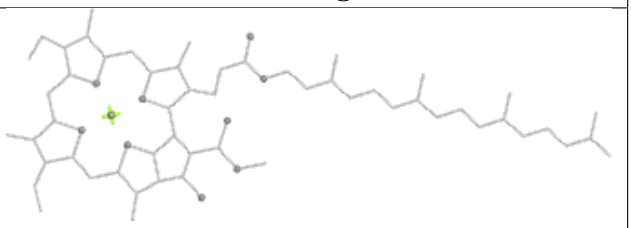


Rings

Ligand CLA P 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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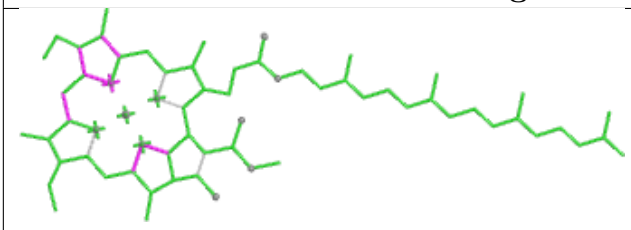
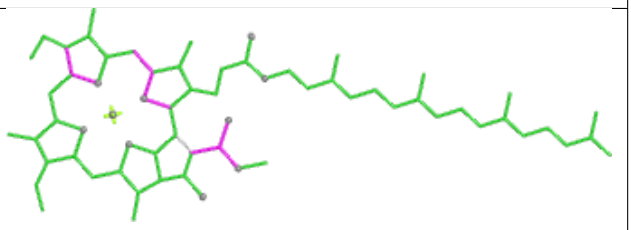
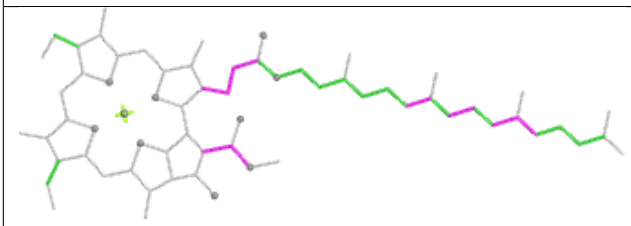
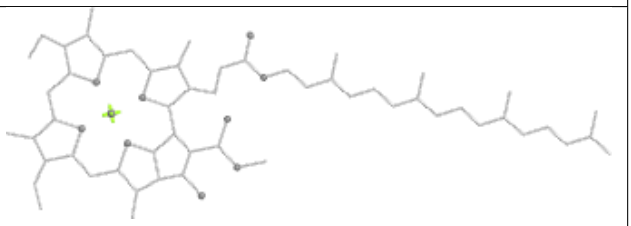
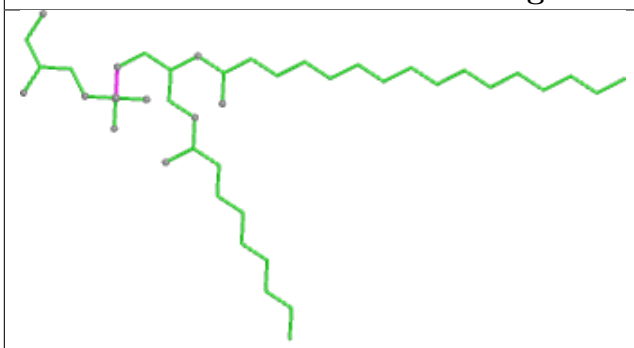
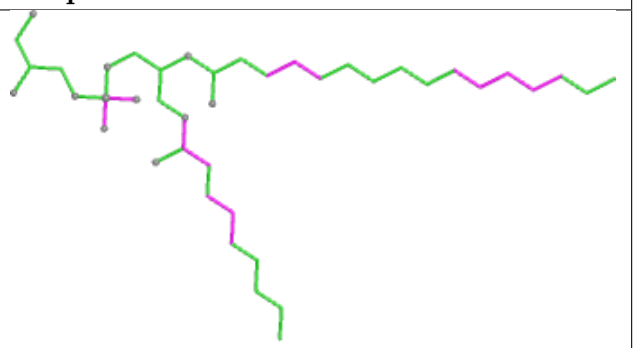
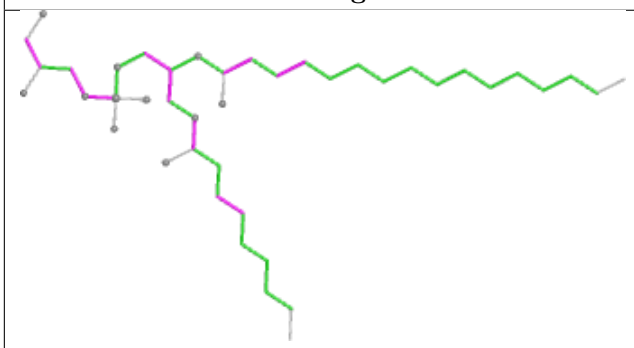
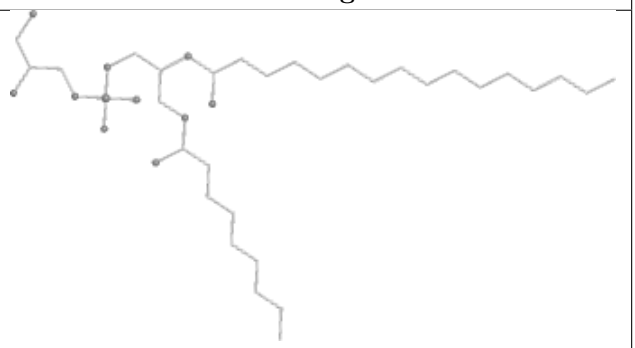
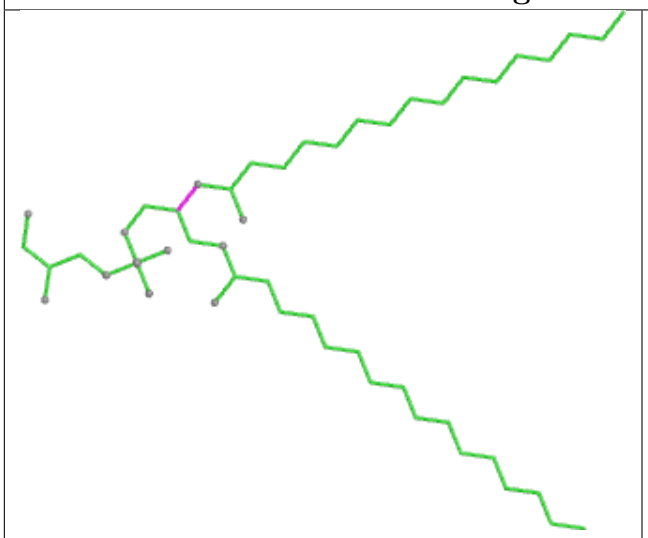
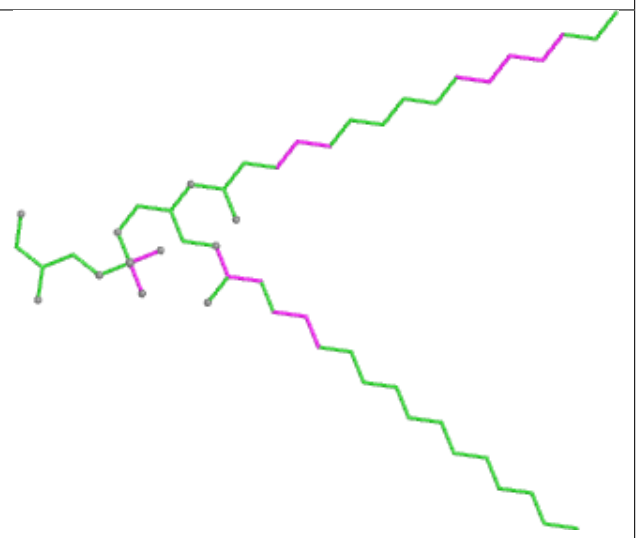
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG q 616	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

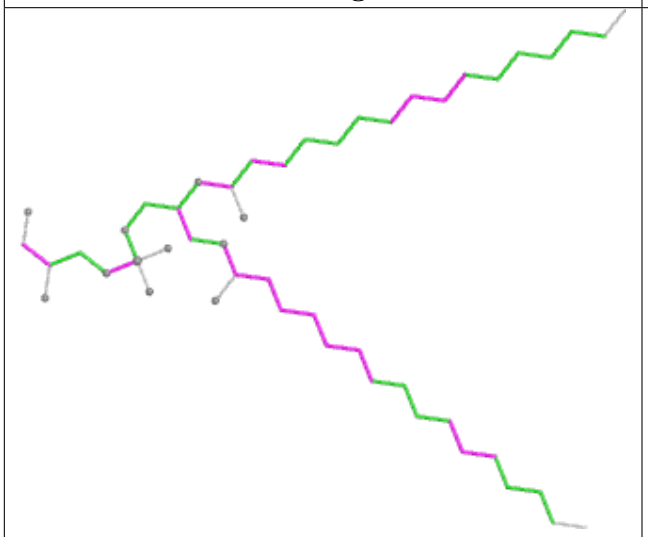
Ligand LHG AS 301



Bond lengths



Bond angles



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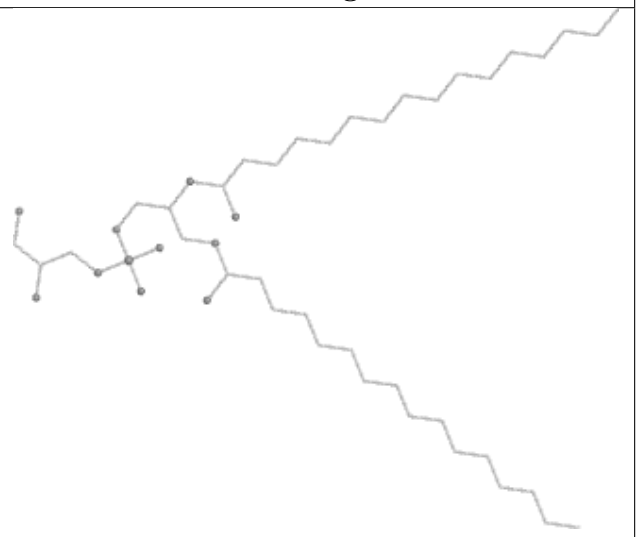
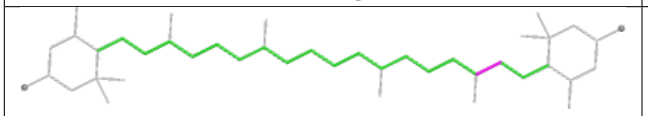


Rings

Ligand LUT v 315

Bond lengths

Bond angles



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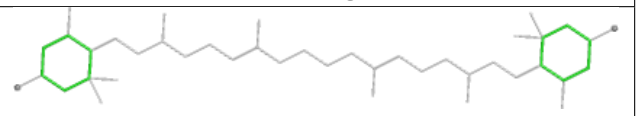
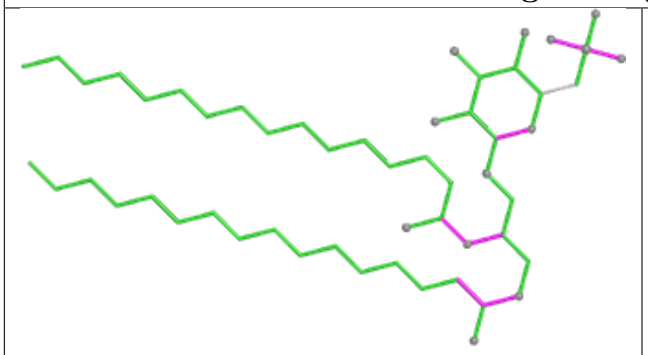
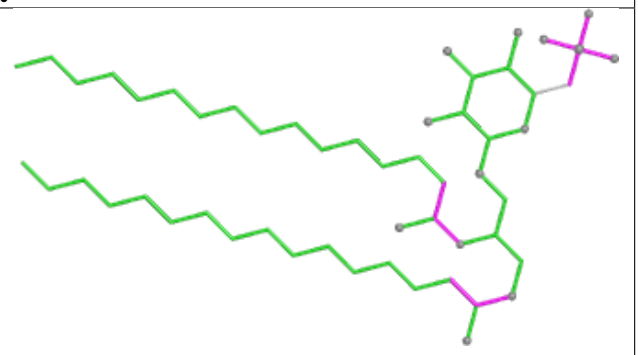


Rings

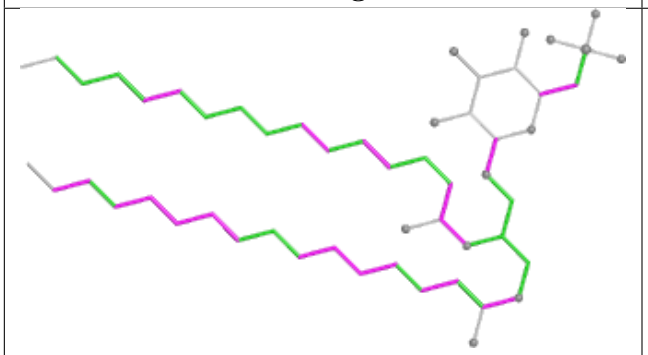
Ligand SQD M 101



Bond lengths



Bond angles



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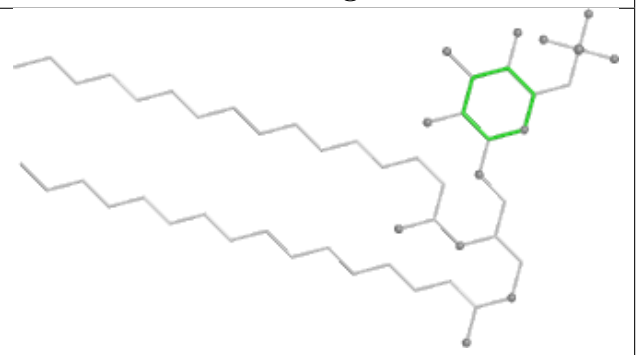
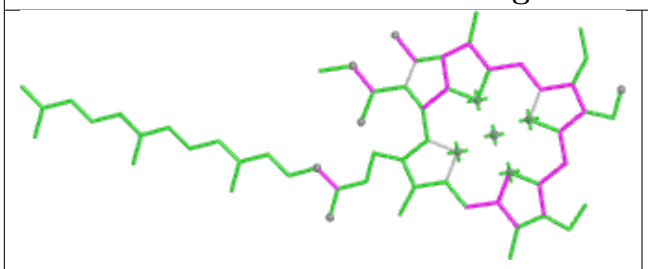


Rings

Ligand CHL AE 607



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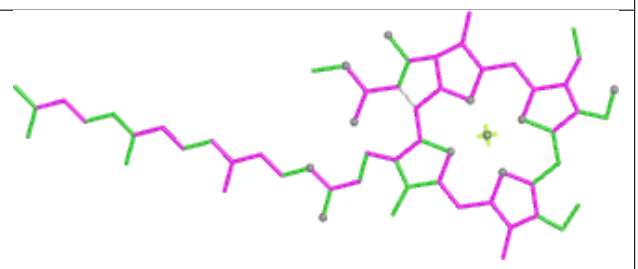
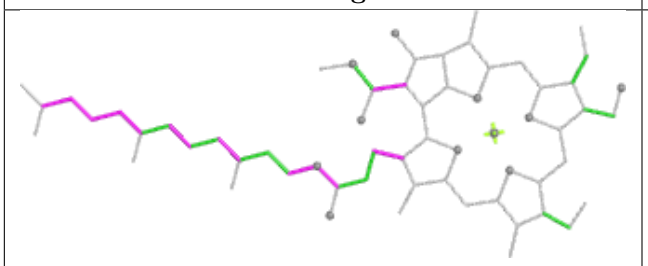


Bond angles



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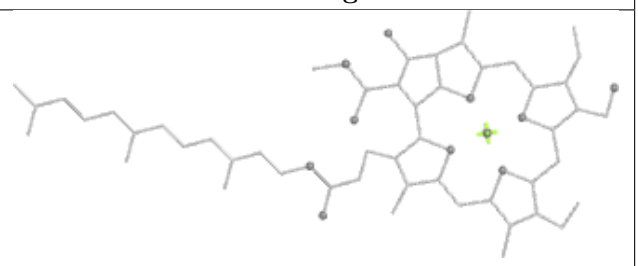
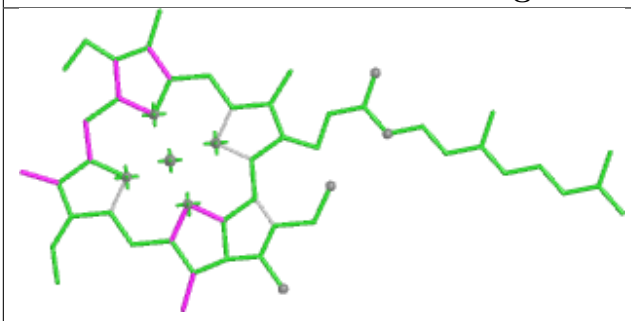
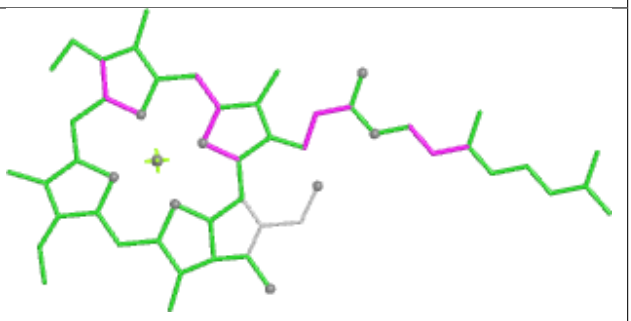
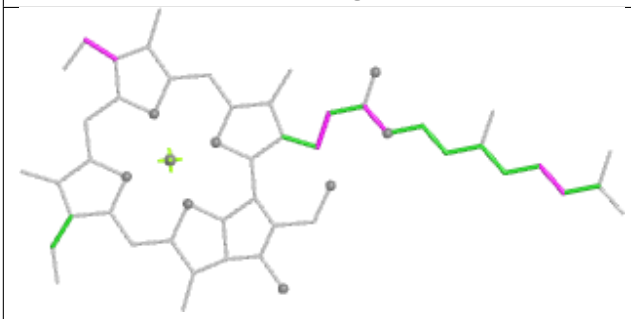
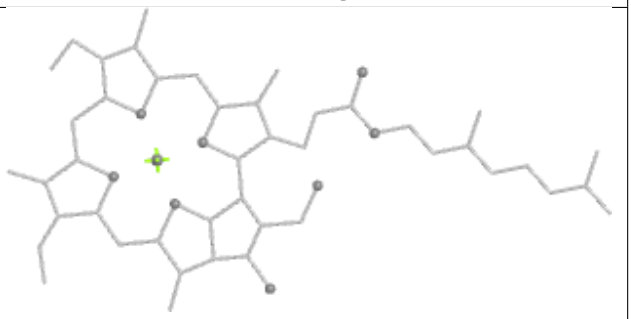
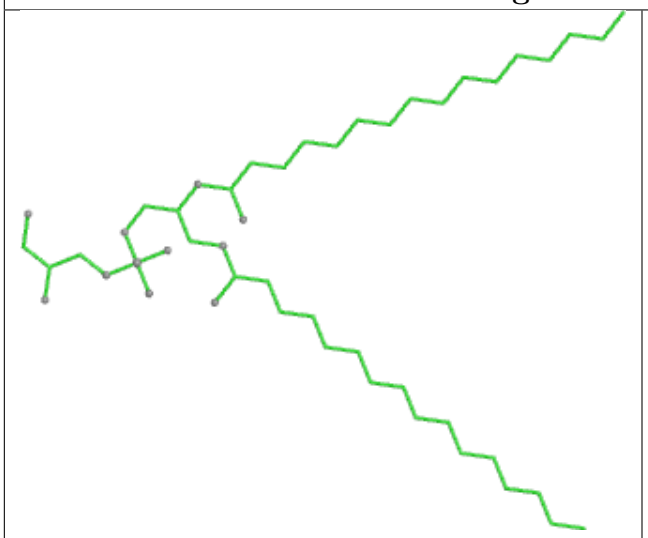


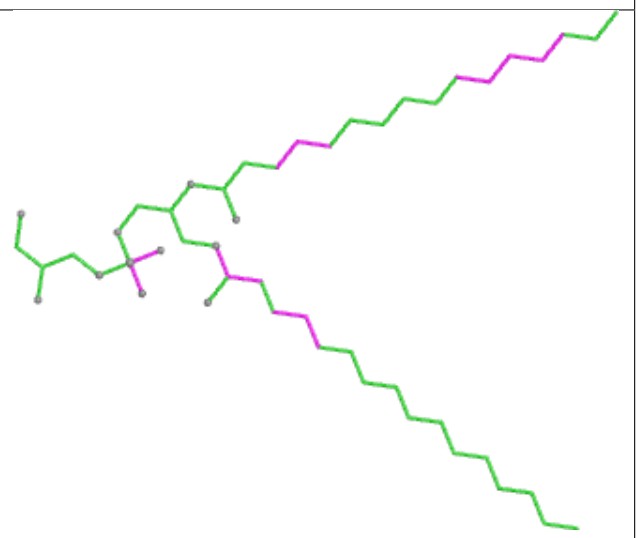
Rings

Ligand CLA AS 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

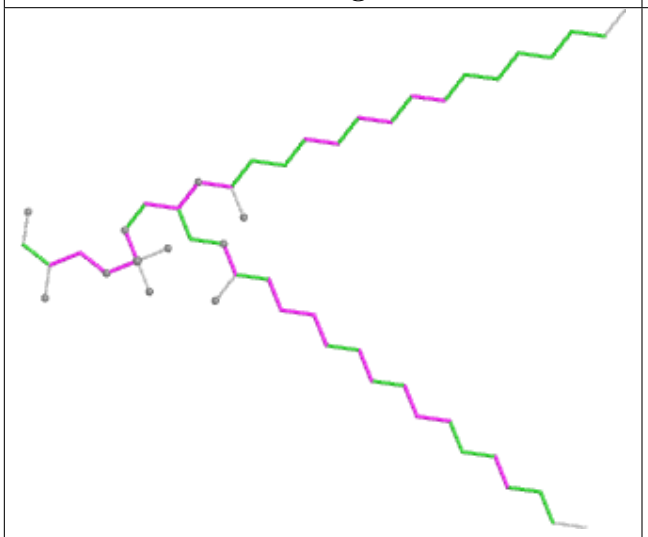
Ligand LHG AL 519



Bond lengths



Bond angles



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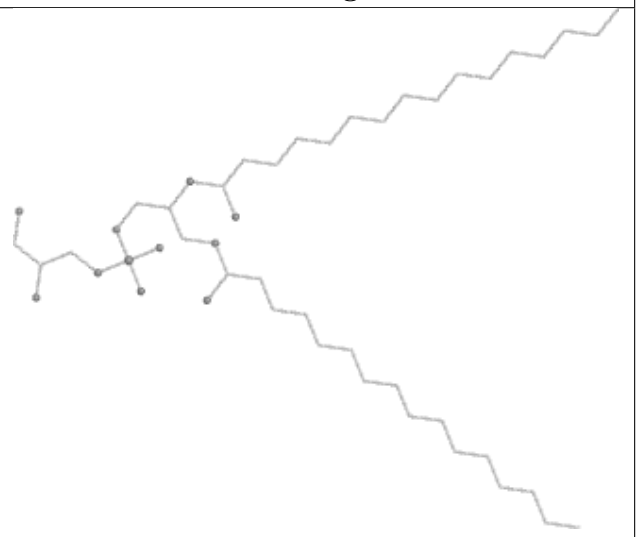
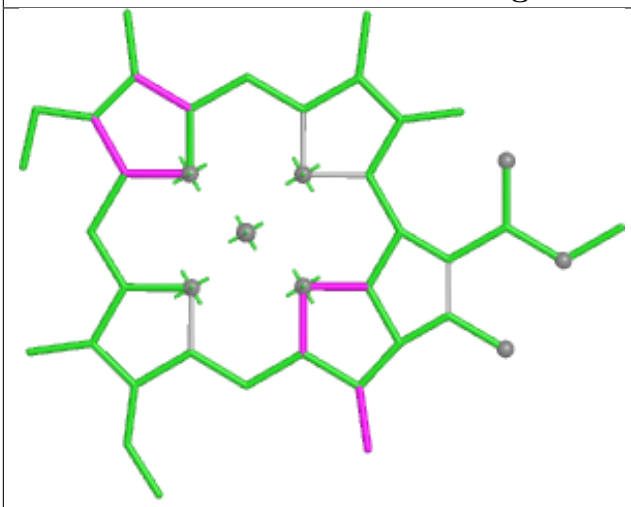


Rings

Ligand CLA AC 612



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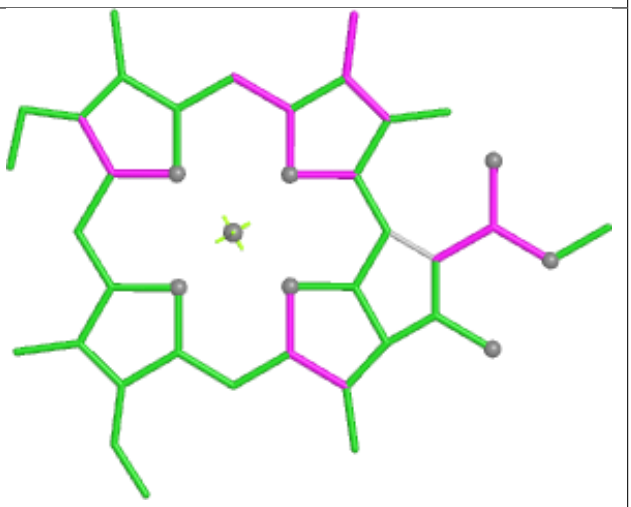
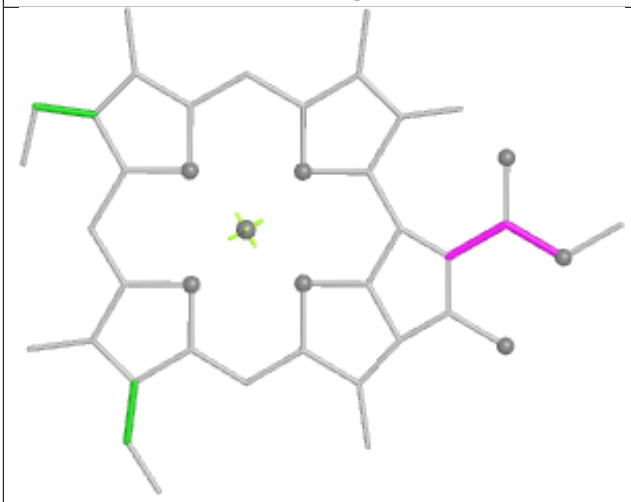


Bond angles



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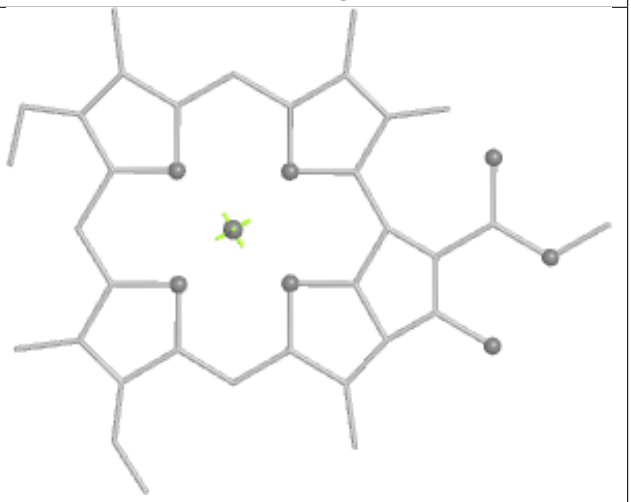
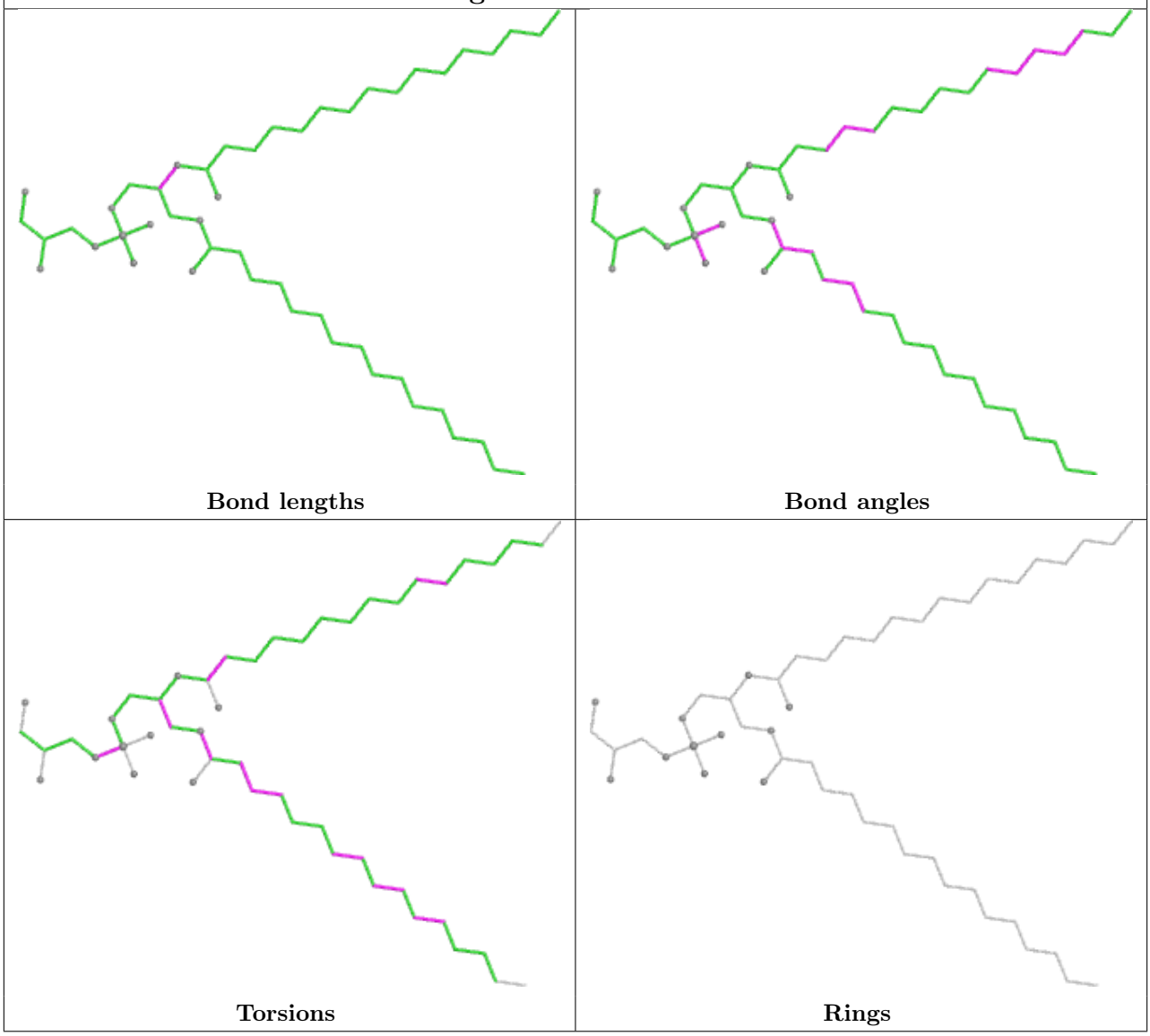
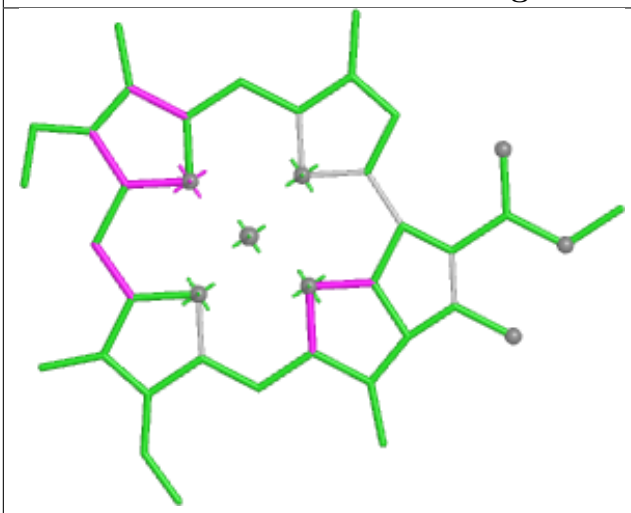


Rings

Ligand LHG w 201



Ligand CLA AB 609



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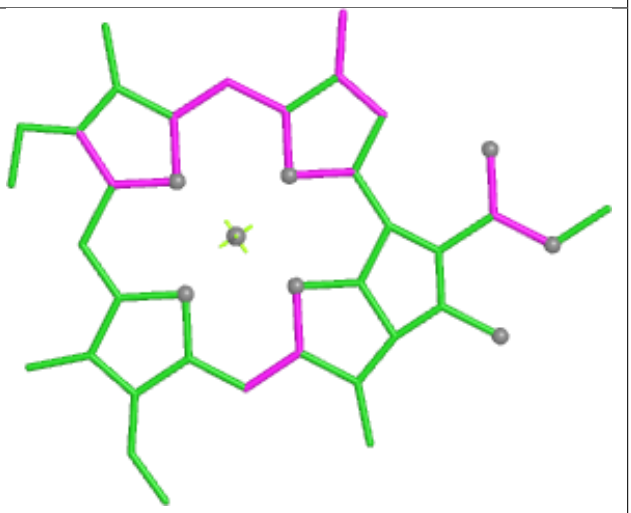
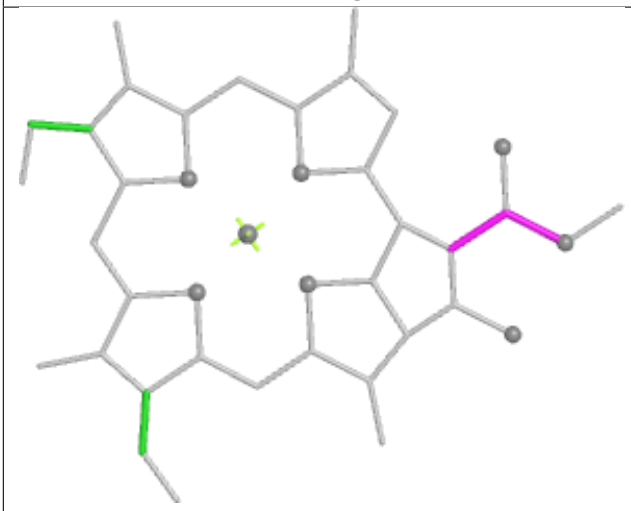


Bond angles



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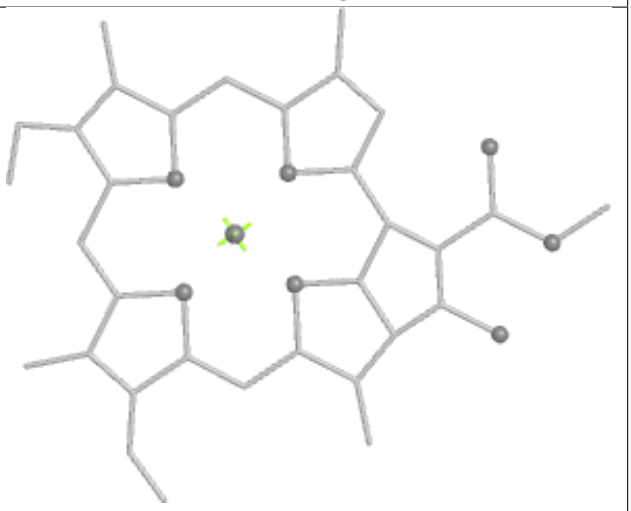
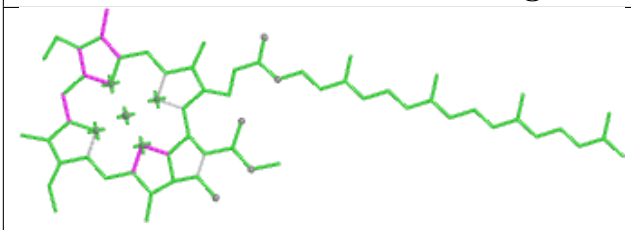
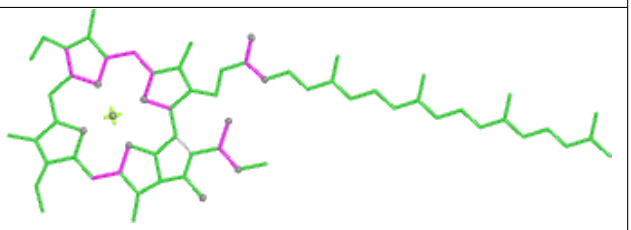


Rings

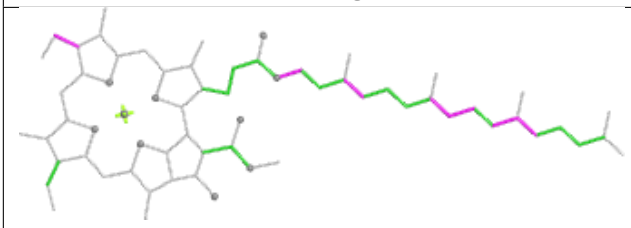
Ligand CLA O 615



Bond lengths



Bond angles



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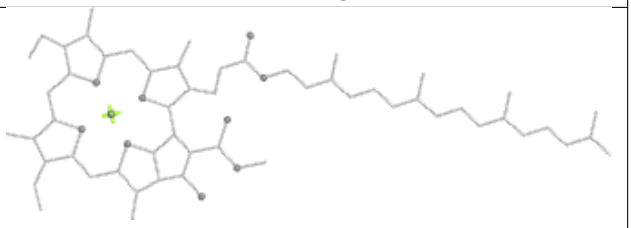
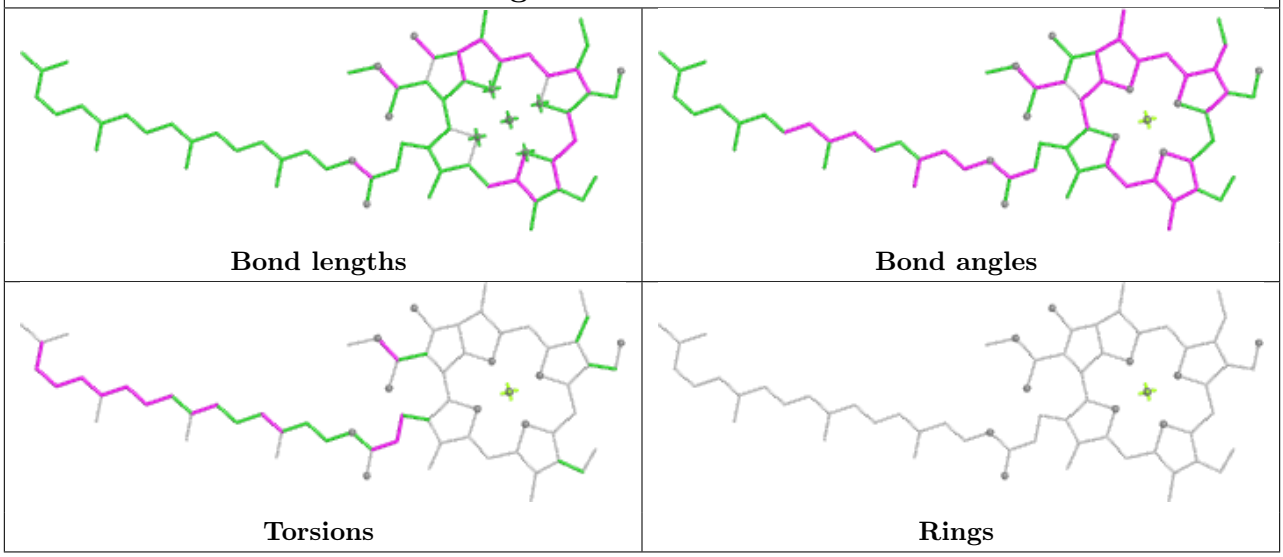
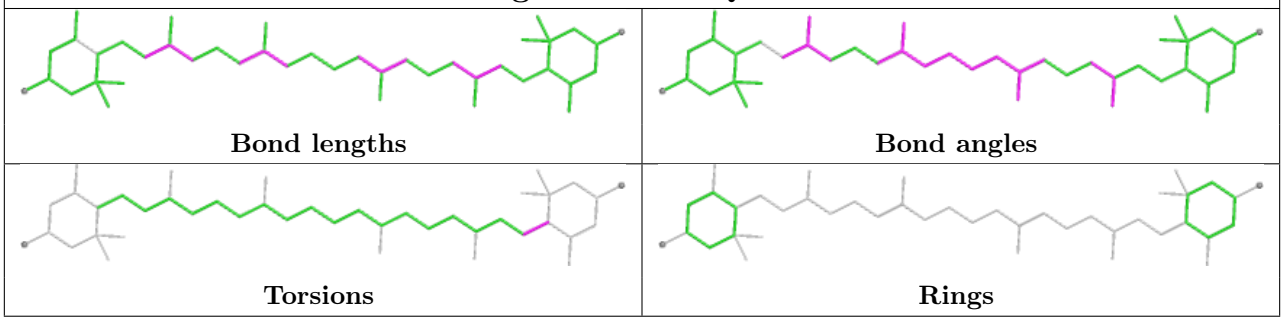


Rings

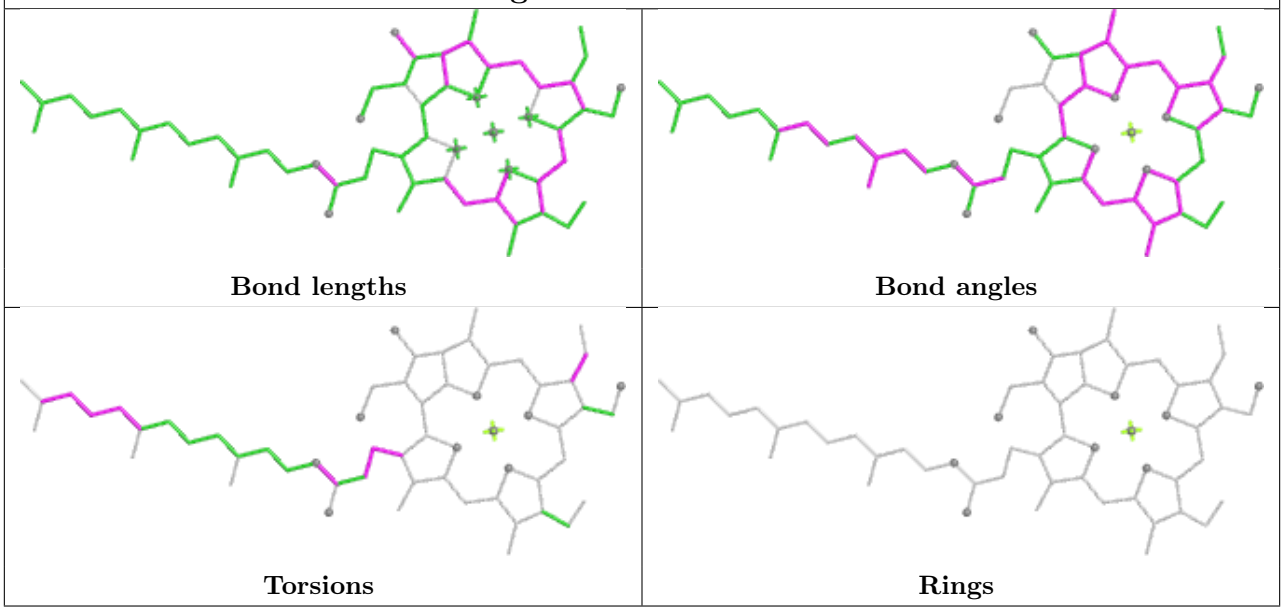
Ligand CHL AH 607

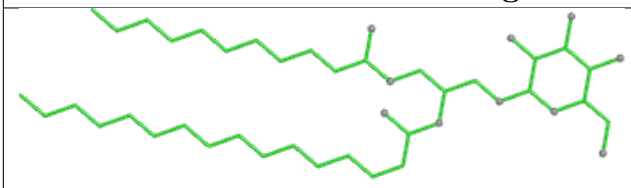
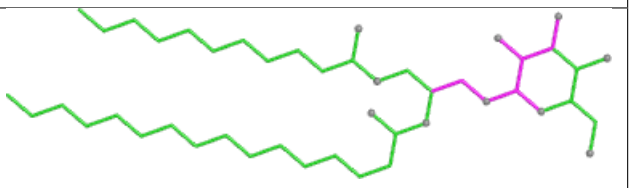
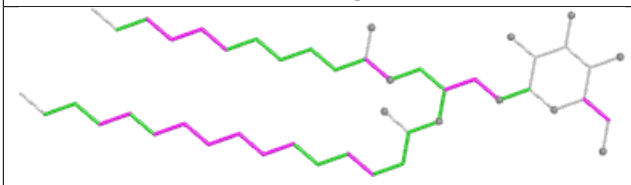
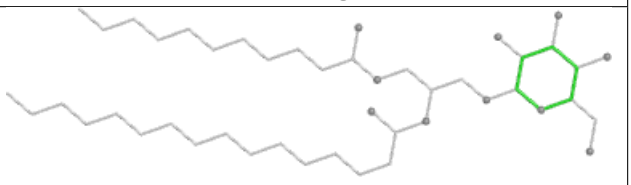


Ligand LUT AQ 615



Ligand CHL AD 308



Ligand LMG AM 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

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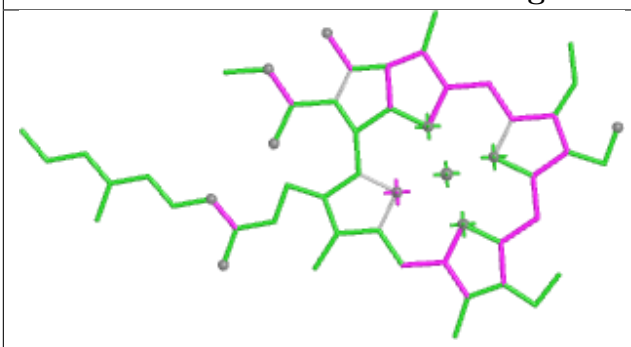
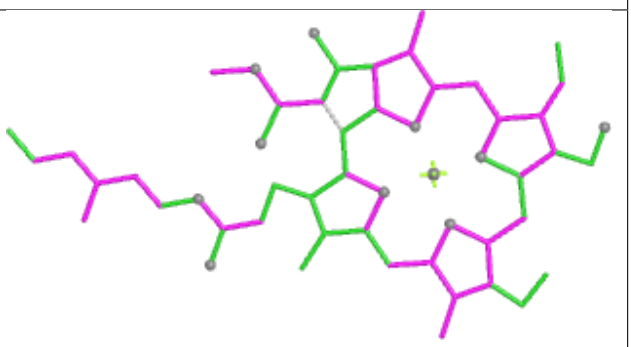
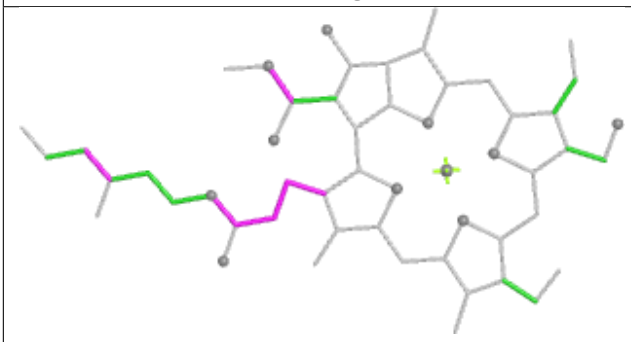
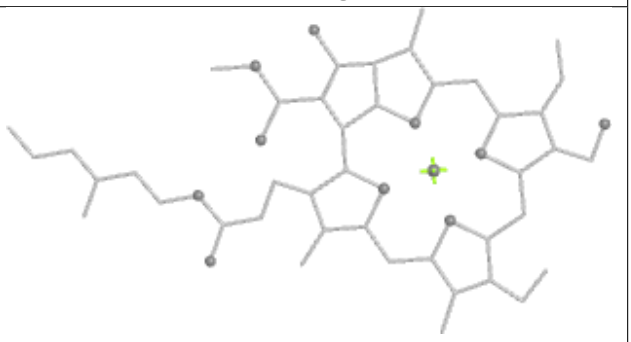
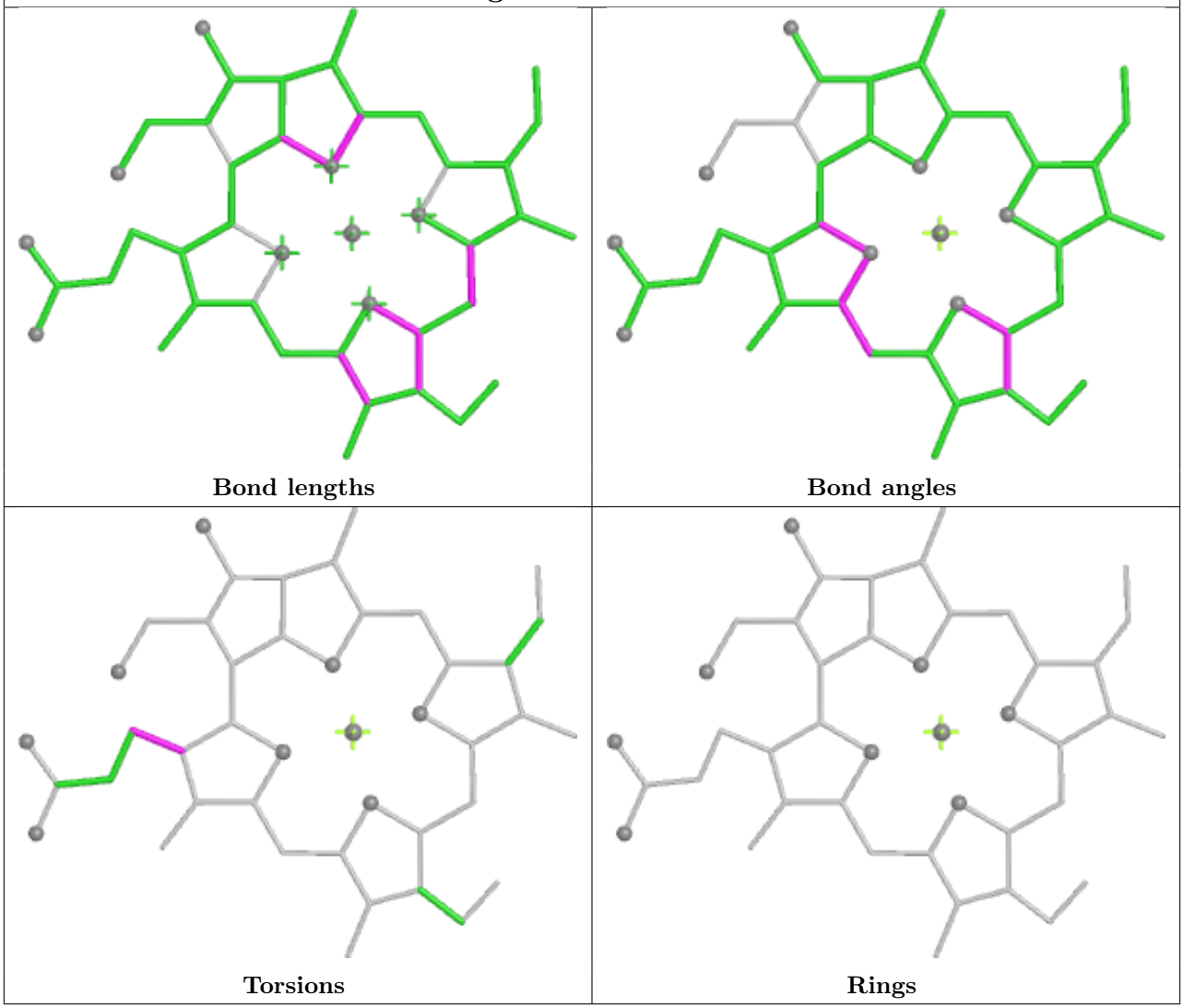
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA v 309



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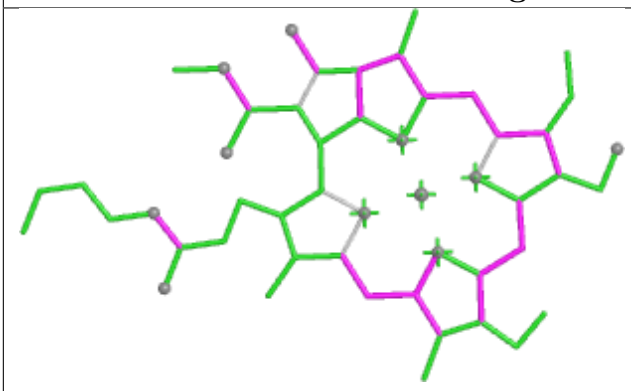
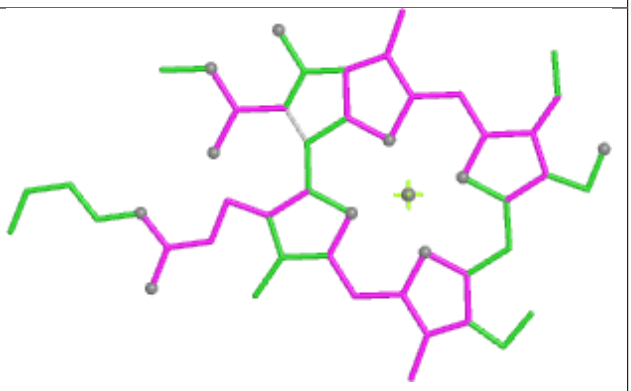
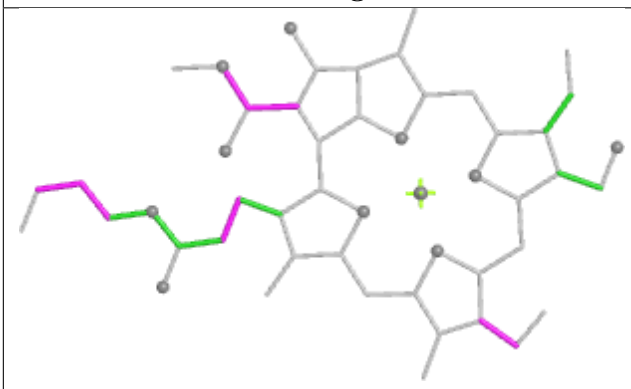
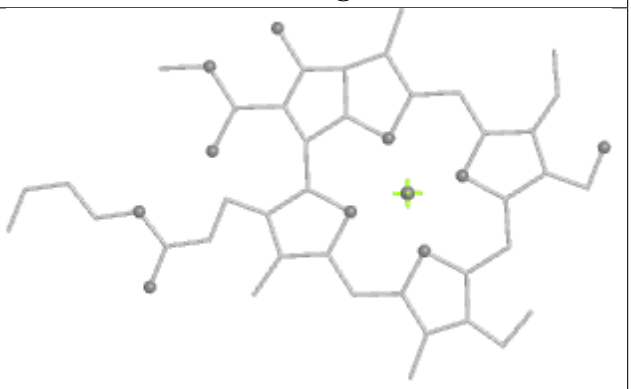
 Bond lengths	 Bond angles
 Torsions	 Rings

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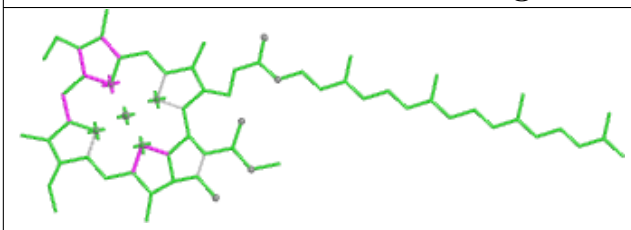
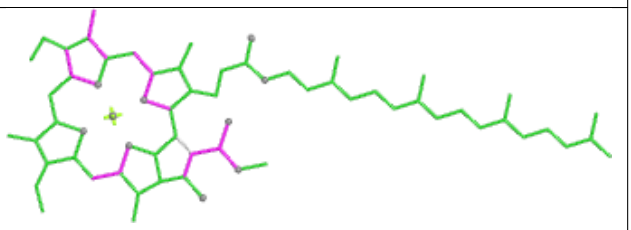
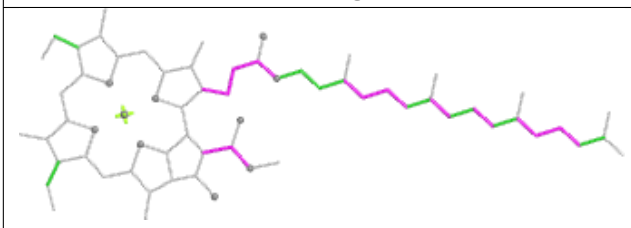
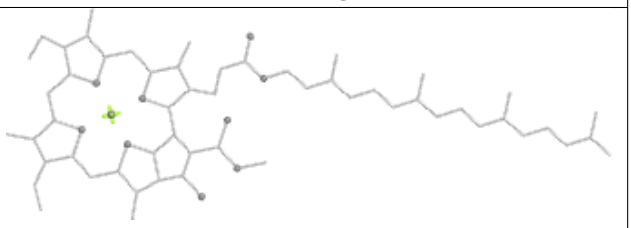
 Bond lengths	 Bond angles
 Torsions	 Rings

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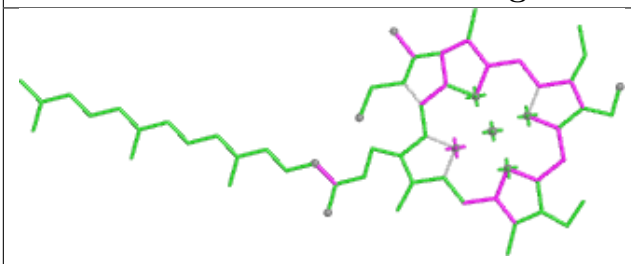
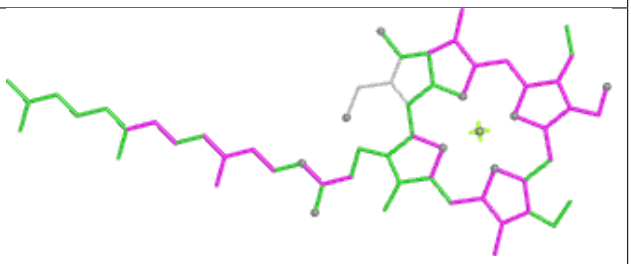
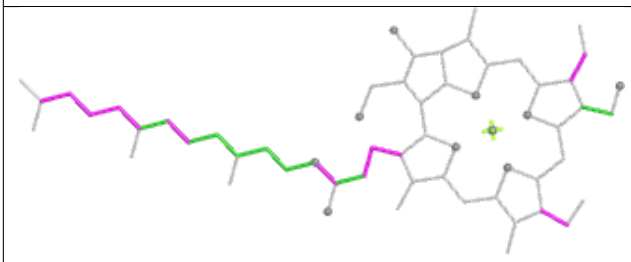
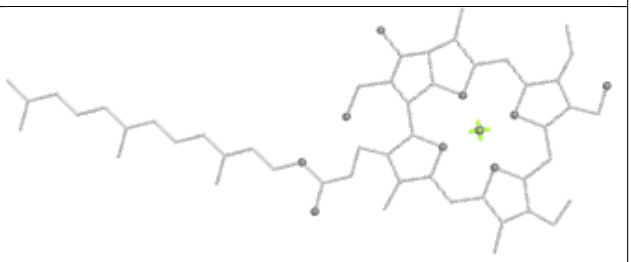
 Bond lengths	 Bond angles
 Torsions	 Rings

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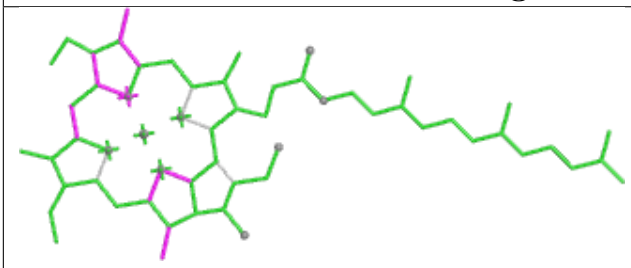
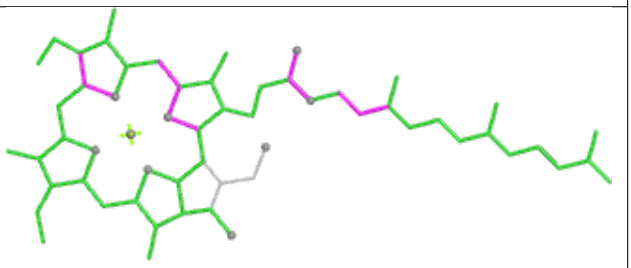
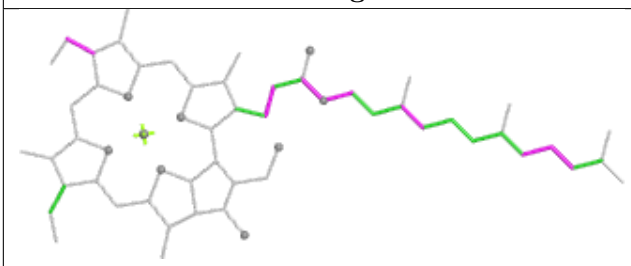
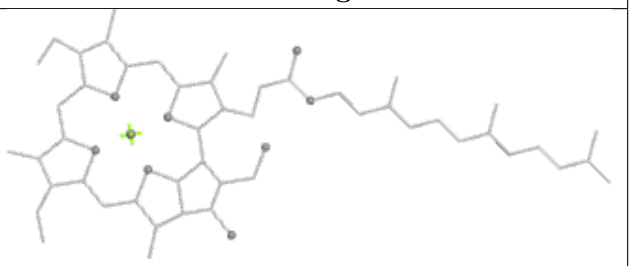
 Bond lengths	 Bond angles
 Torsions	 Rings

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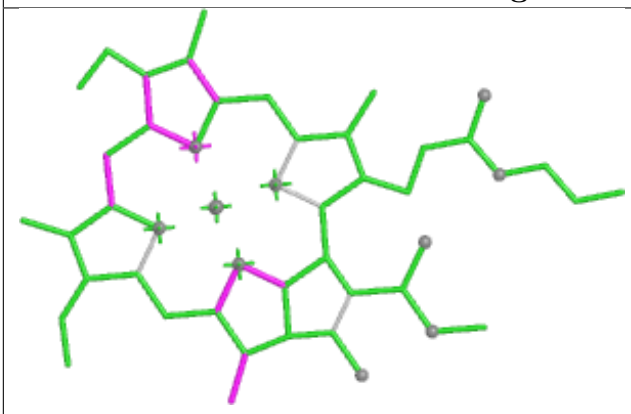
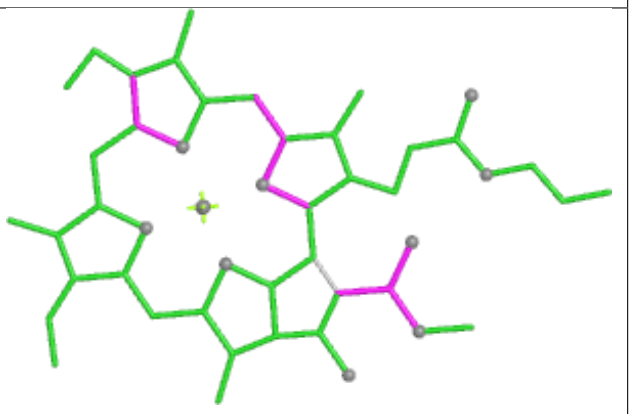
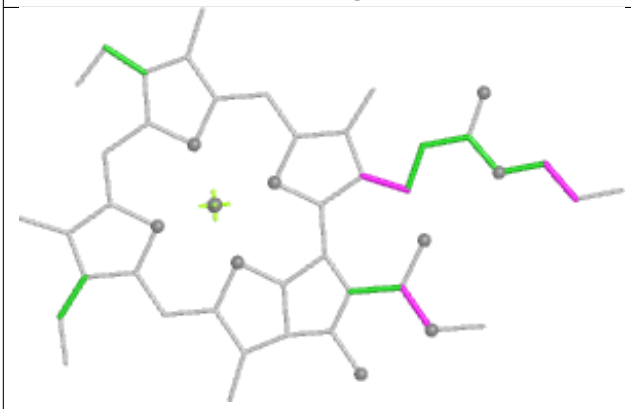
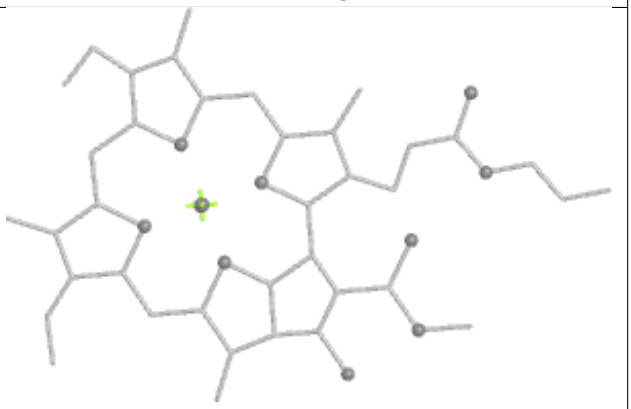
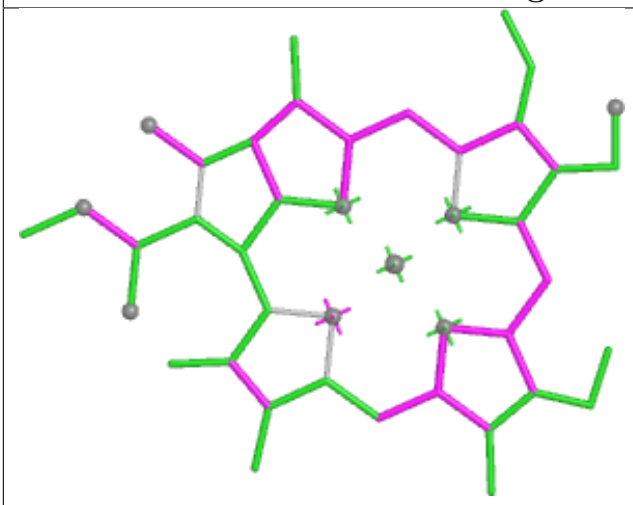
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL q 613



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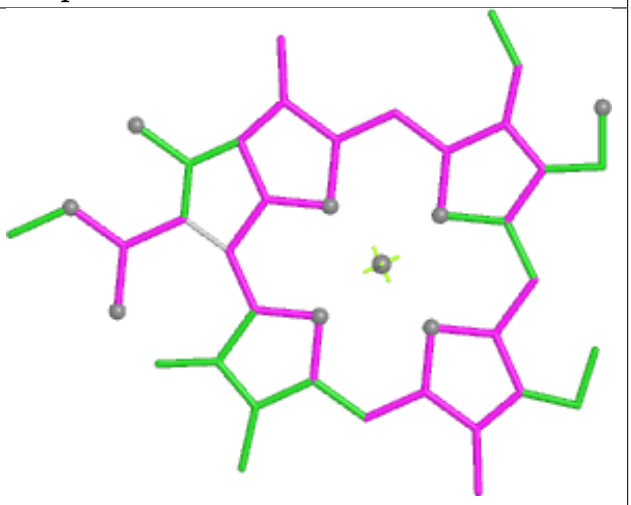
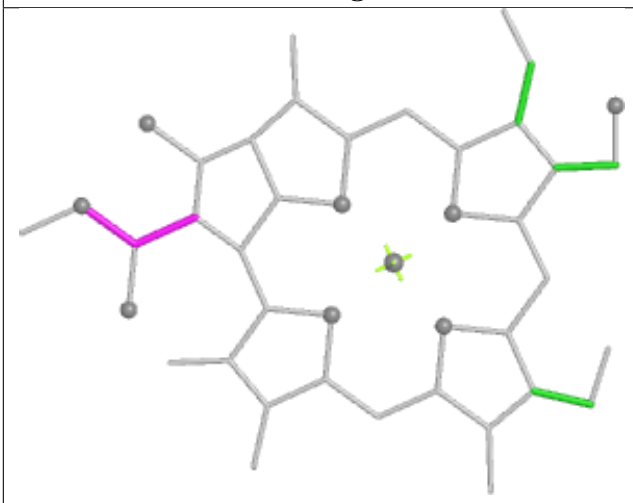


Bond angles



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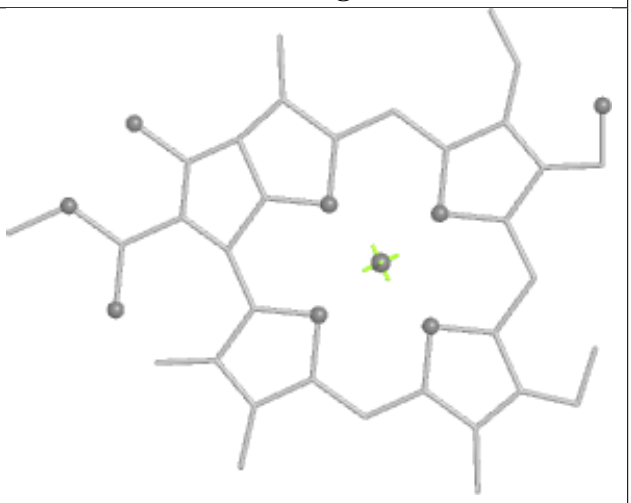
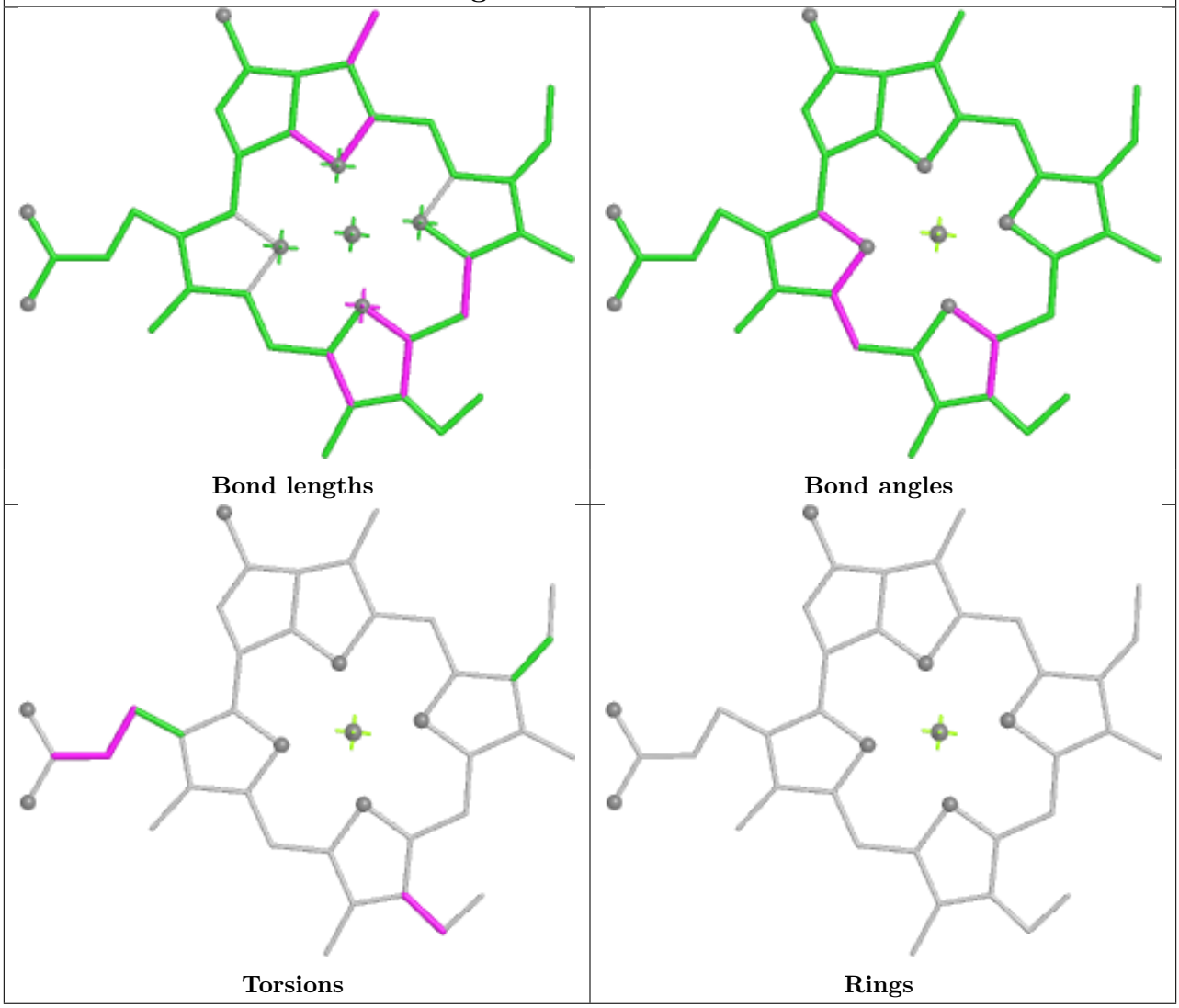
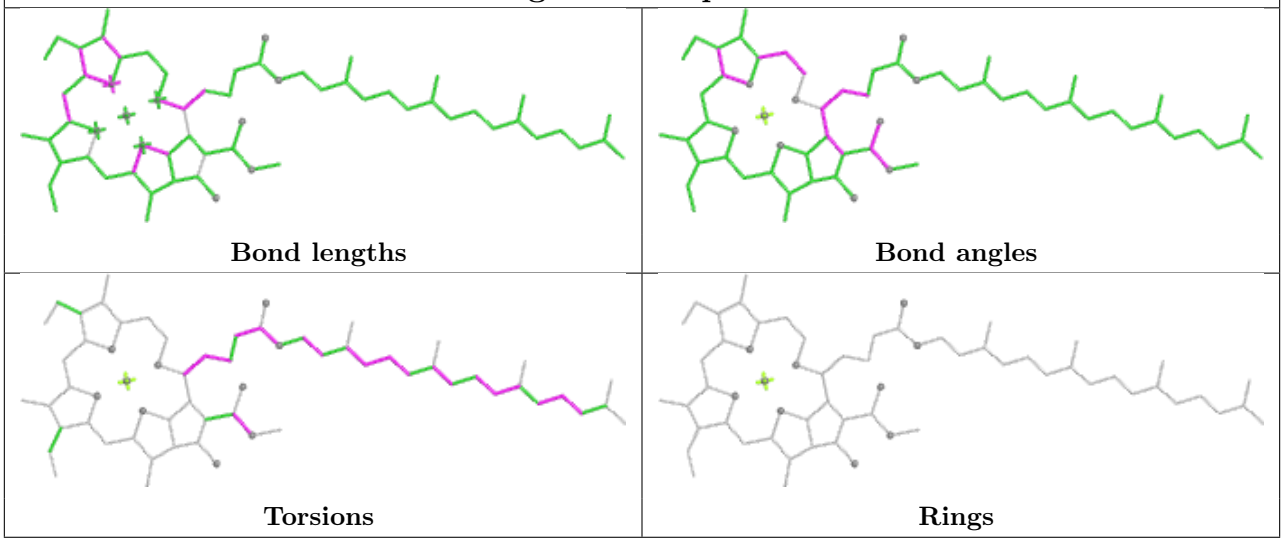


Rings

Ligand CLA AC 611



Ligand CLA p 610



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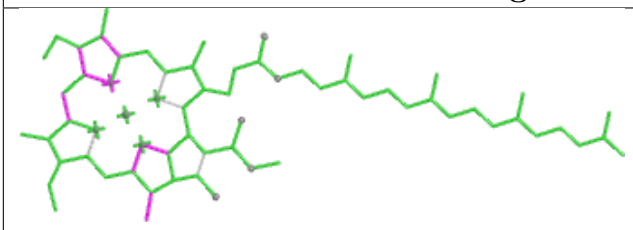

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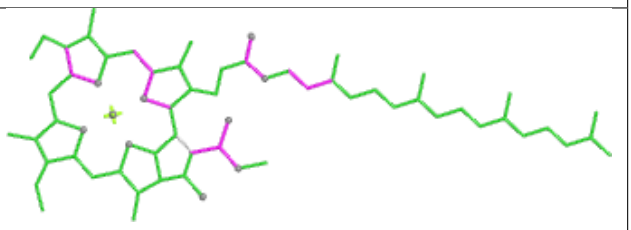

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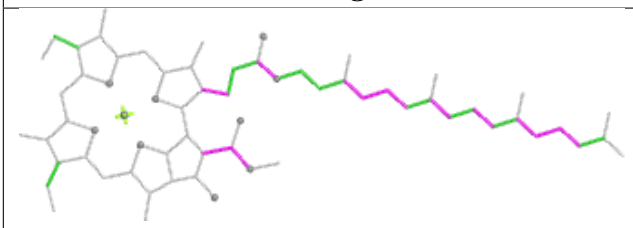

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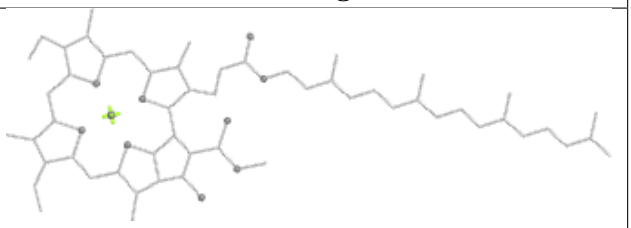
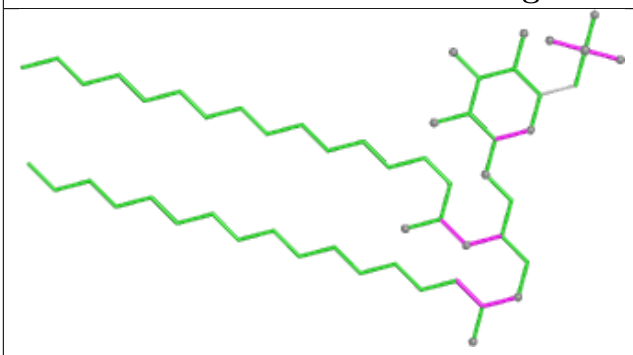


Rings

Ligand SQD m 101



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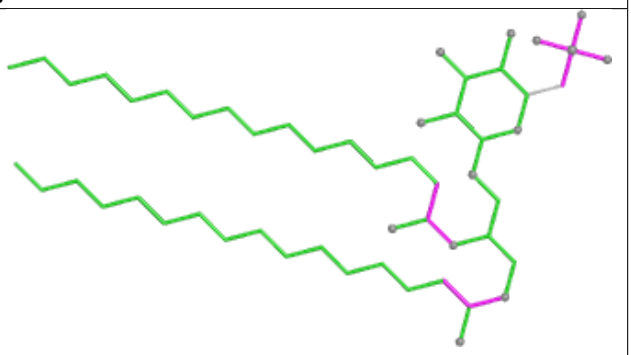

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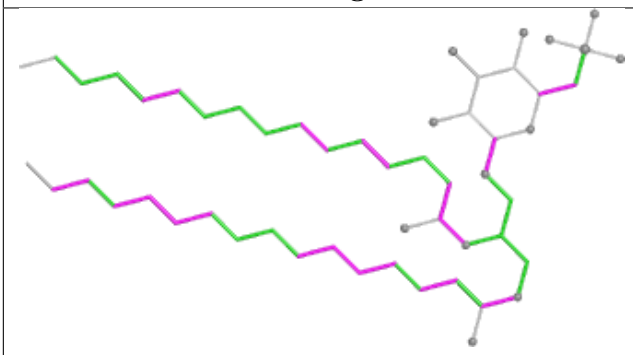

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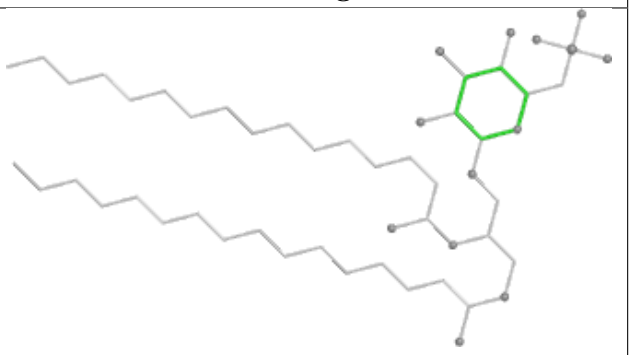
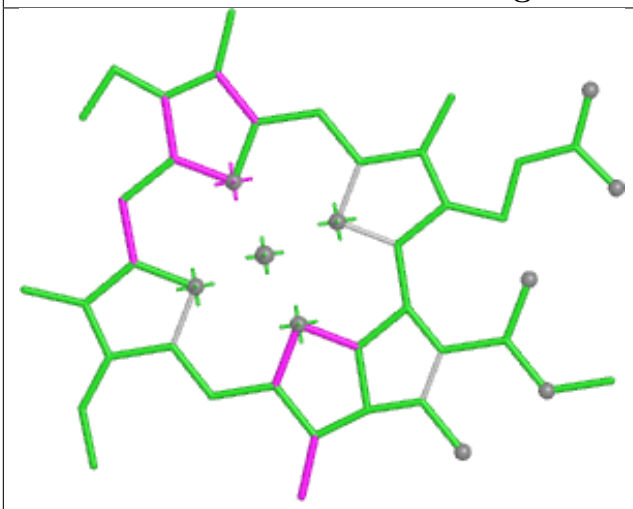


Rings

Ligand CLA AS 304



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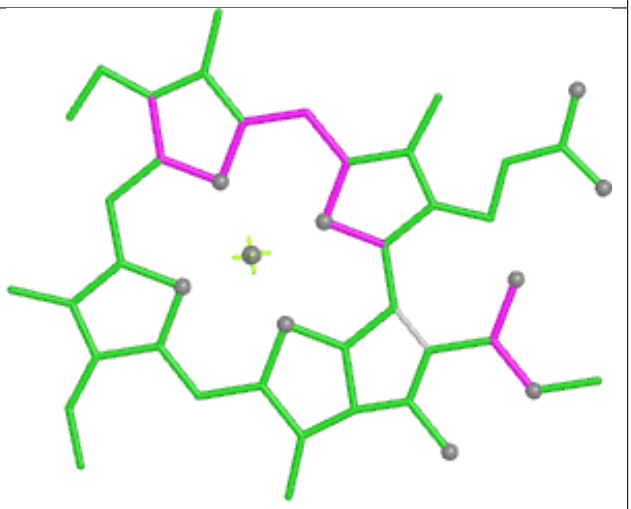

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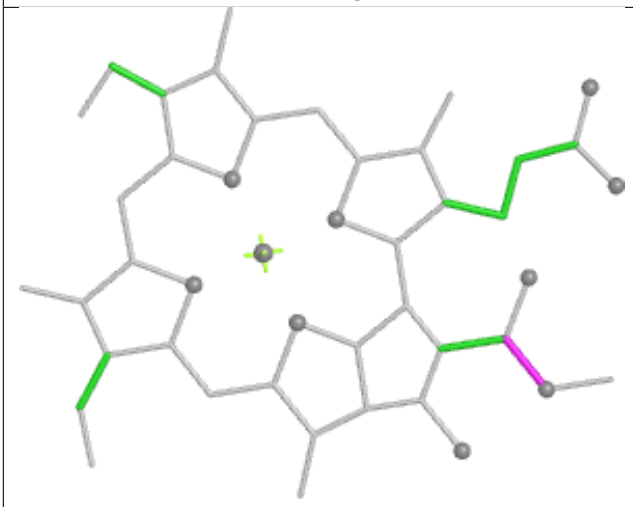
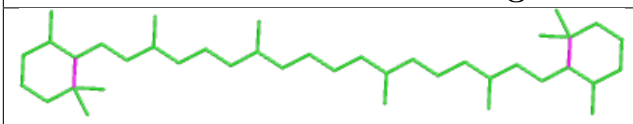


Torsions

Rings

Ligand BCR AK 620



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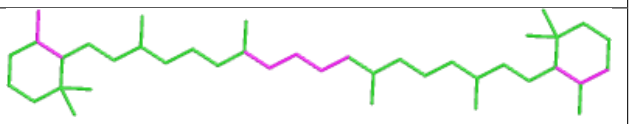

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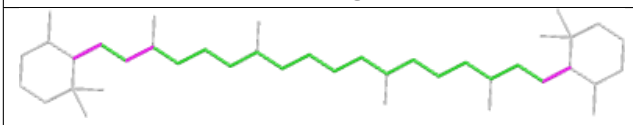

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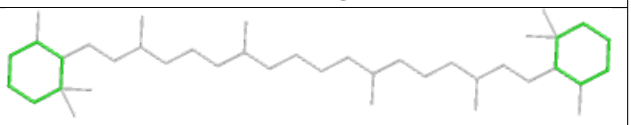
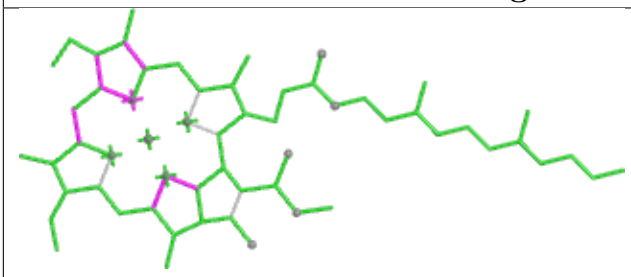


Rings

Ligand CLA AD 312



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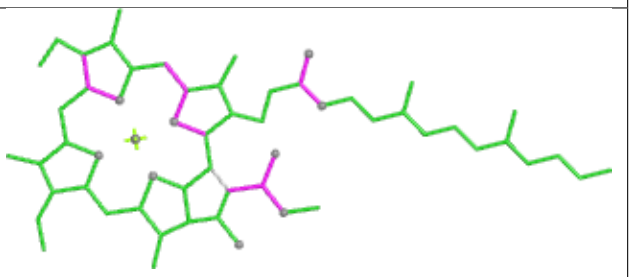

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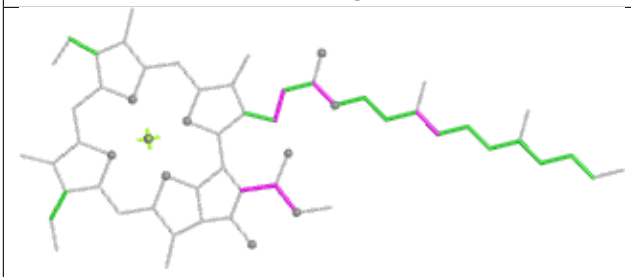

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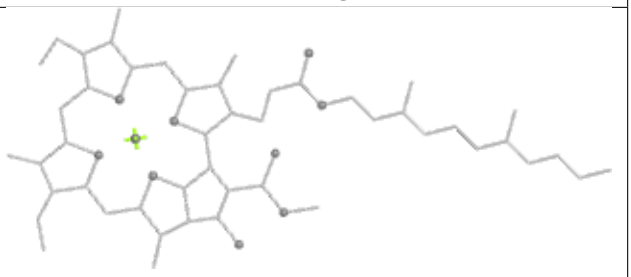

Rings

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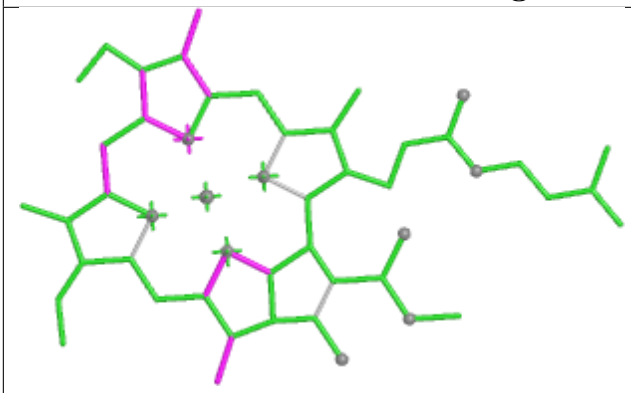

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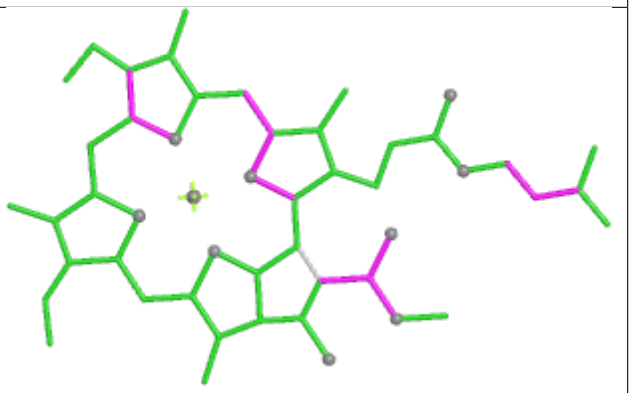
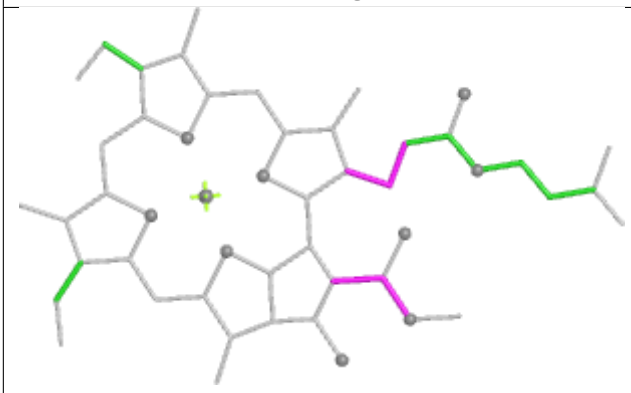
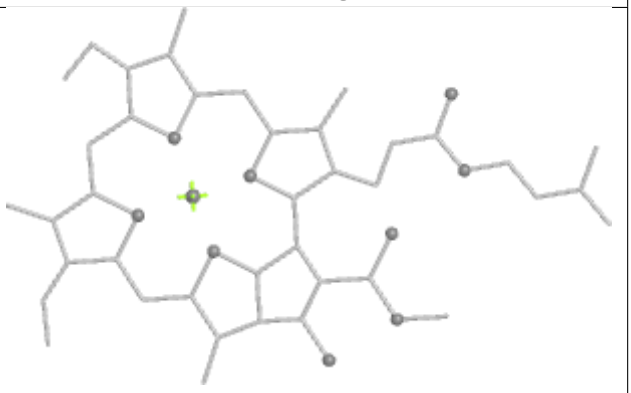


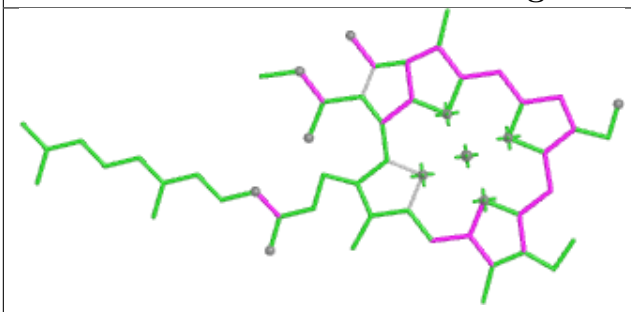
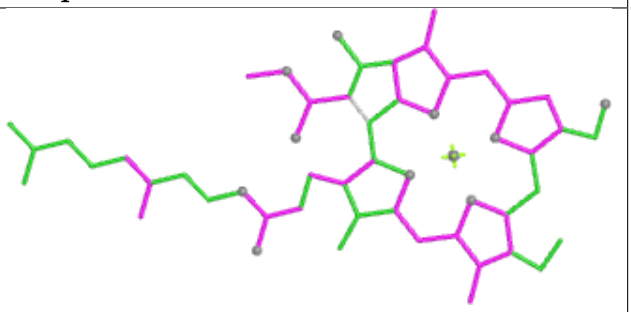
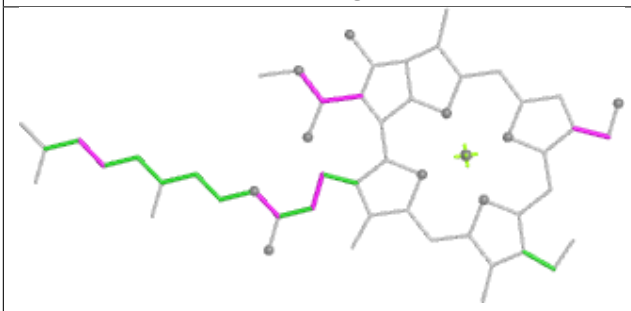
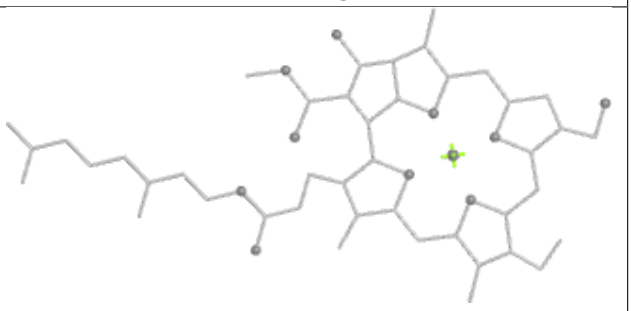
Bond angles



Torsions



Rings

Ligand CHL q 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

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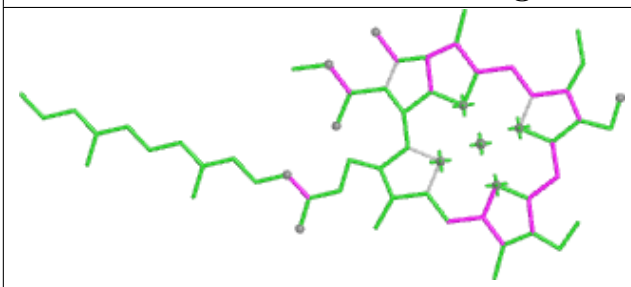
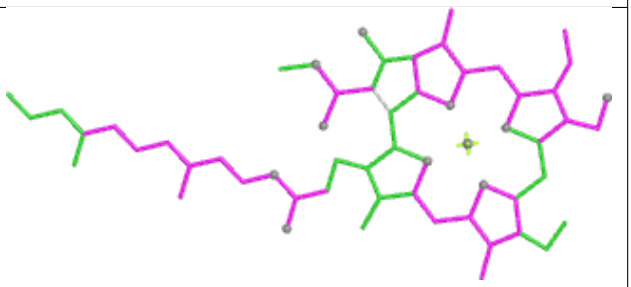
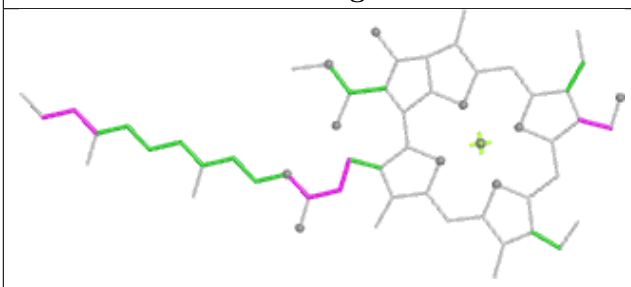
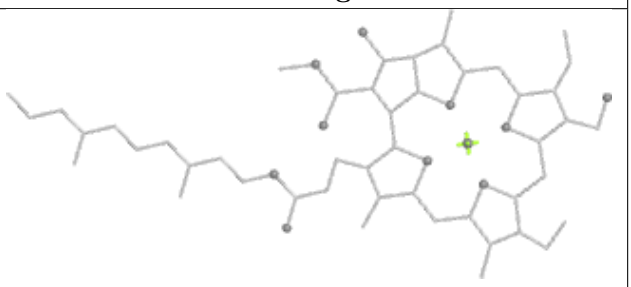
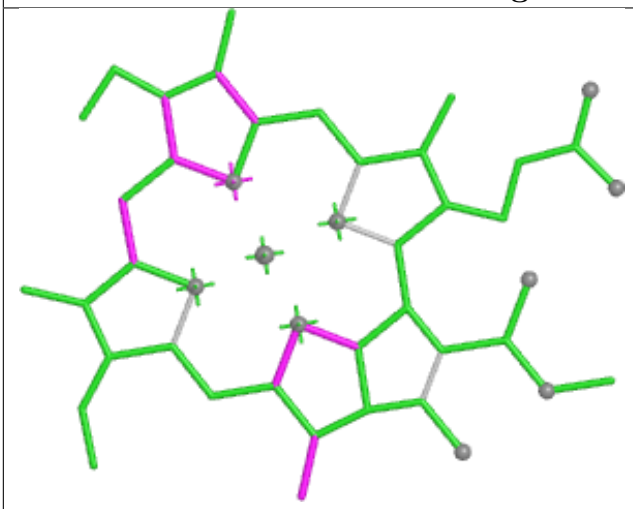
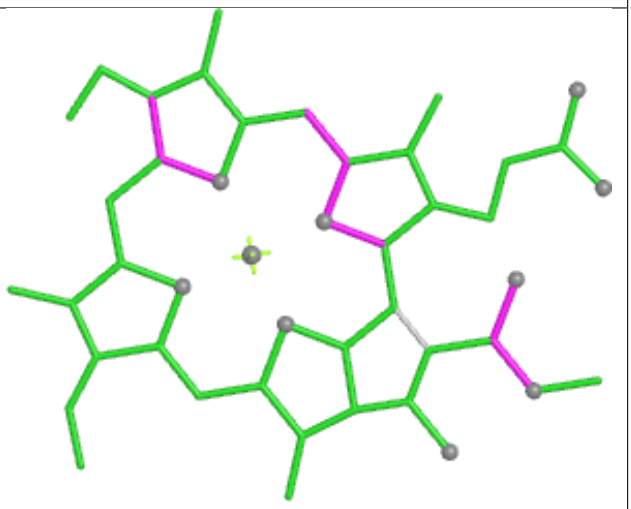
 Bond lengths	 Bond angles
 Torsions	 Rings

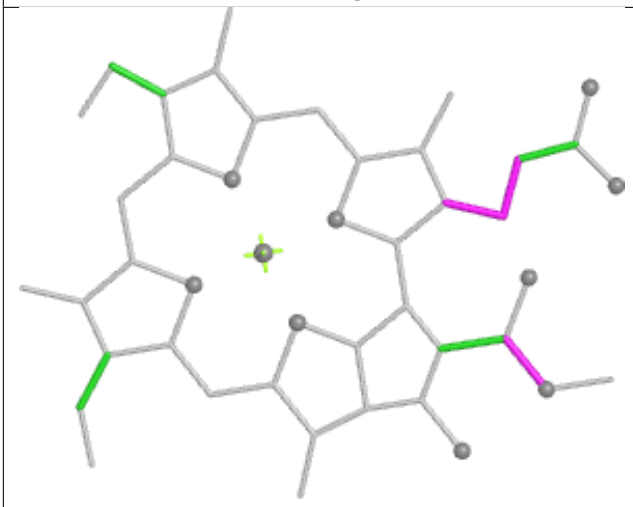
Ligand CLA AB 604



Bond lengths



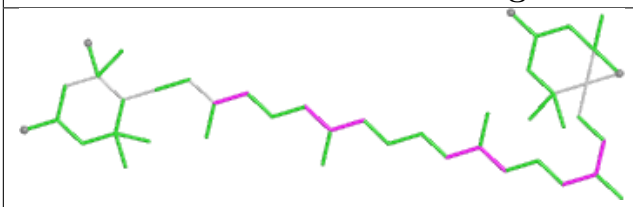
Bond angles



Torsions

Rings

Ligand NEX AQ 617



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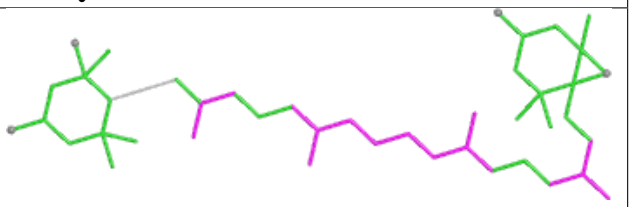

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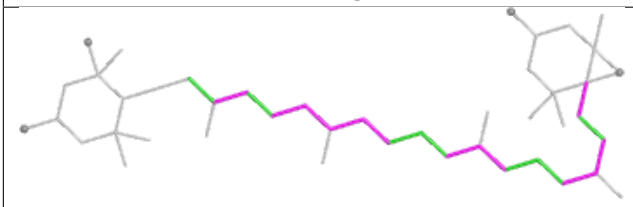

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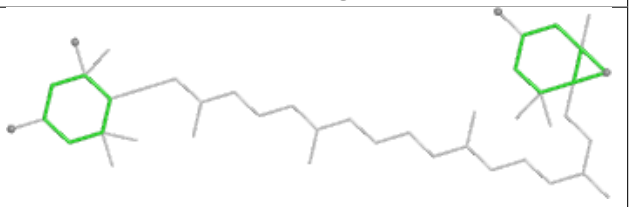
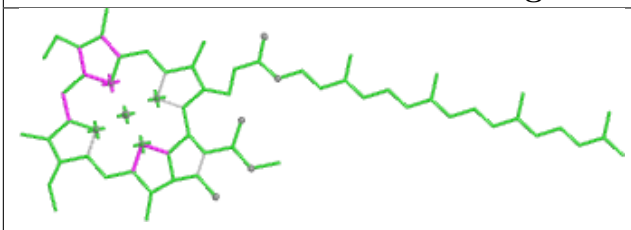
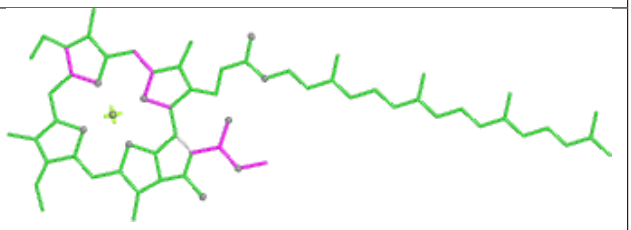
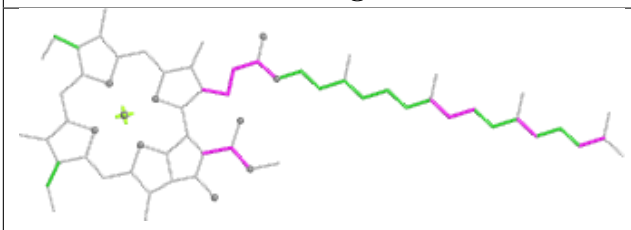
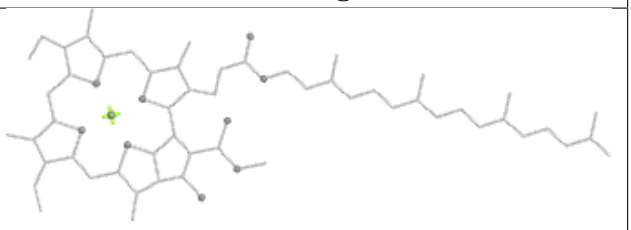


Rings

Ligand CLA P 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

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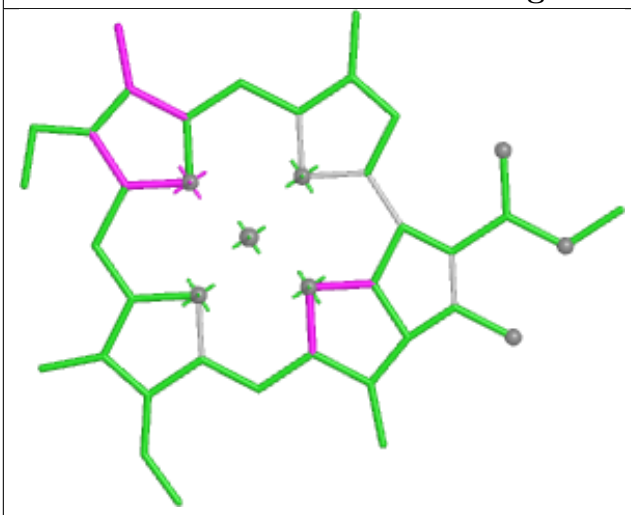
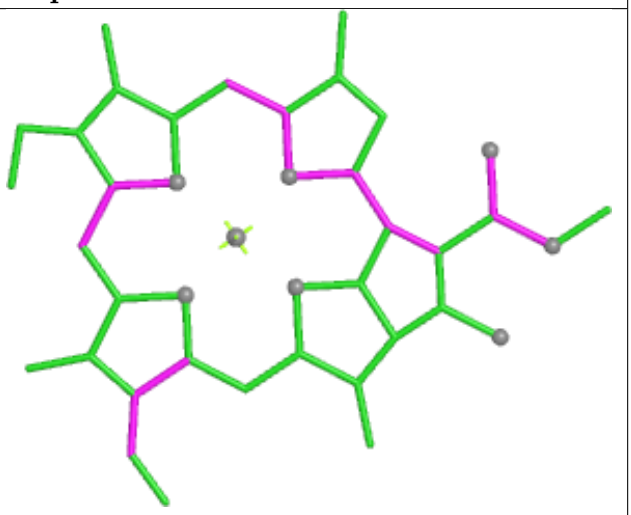
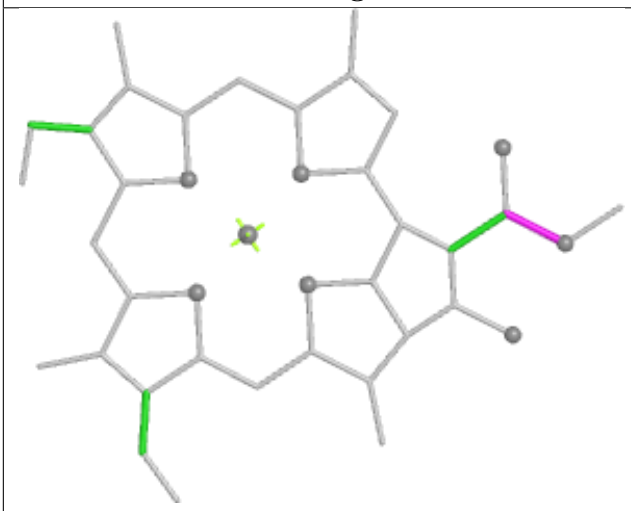
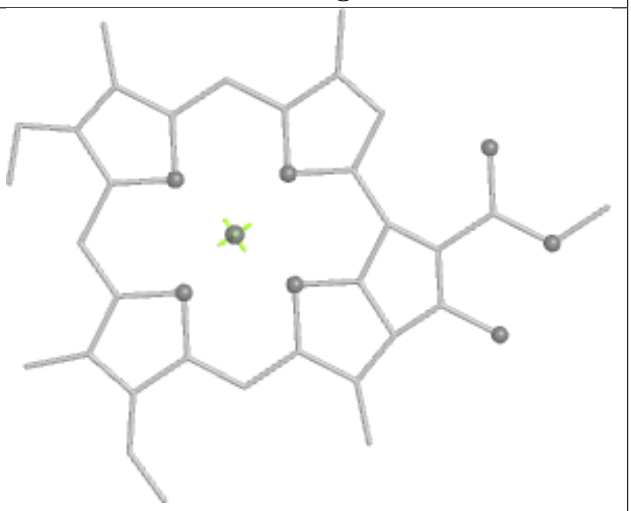
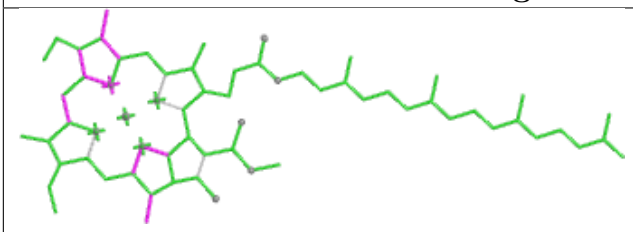
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AL 511



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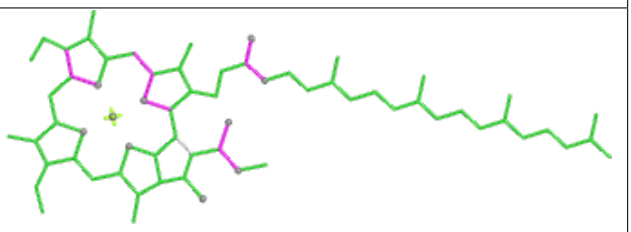
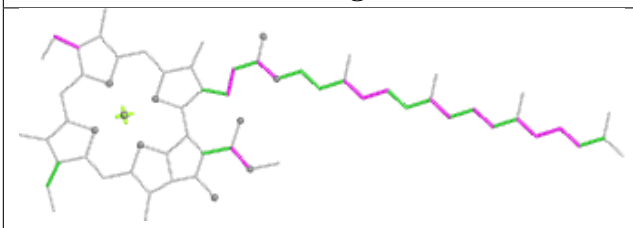


Bond angles



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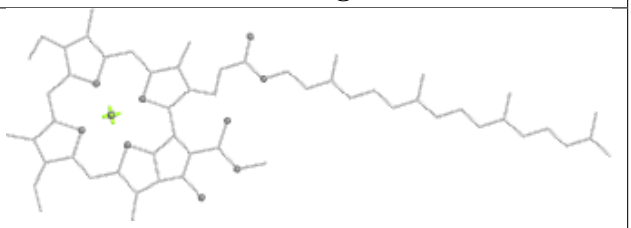
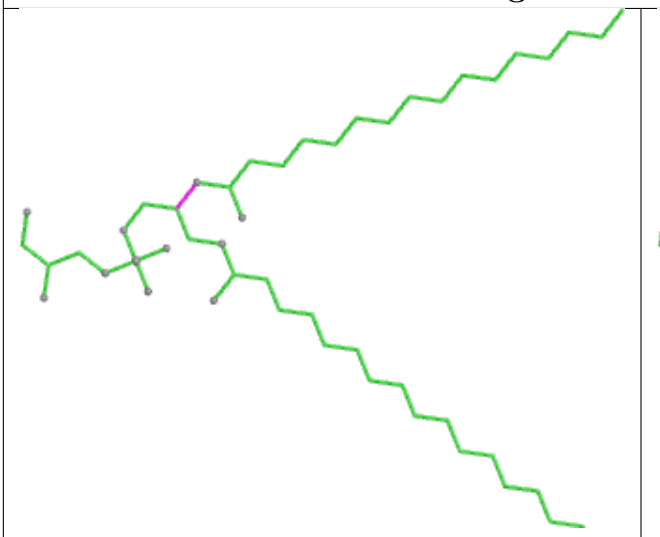


Rings

Ligand LHG AH 616



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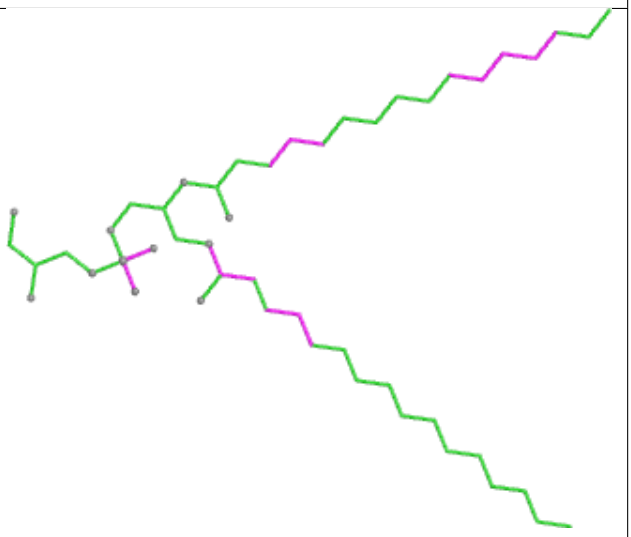
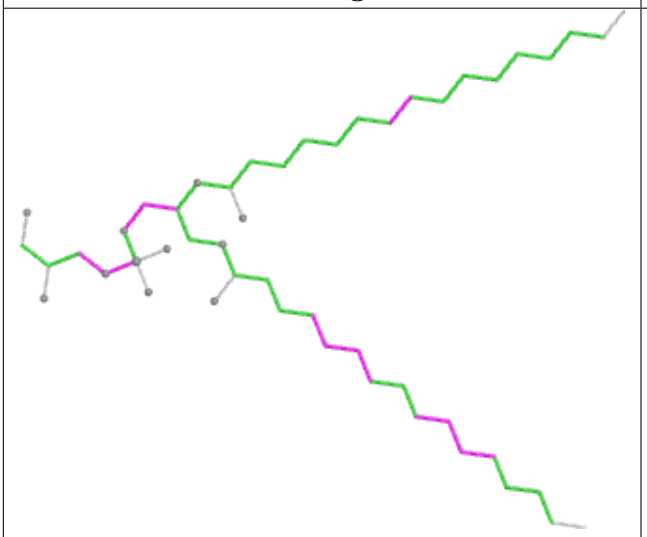


Bond angles



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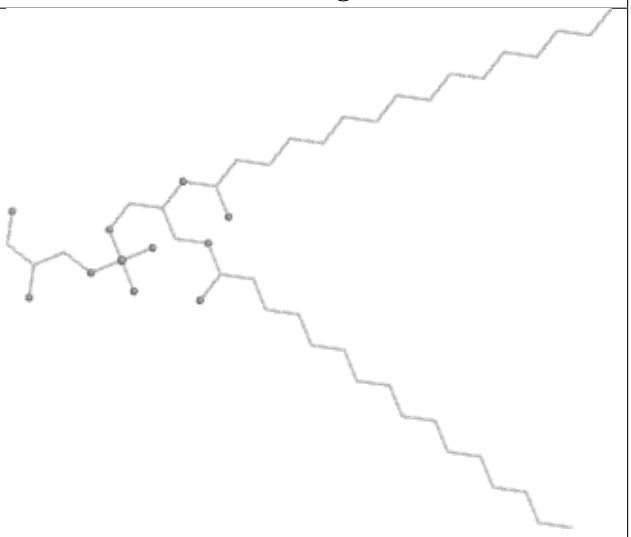
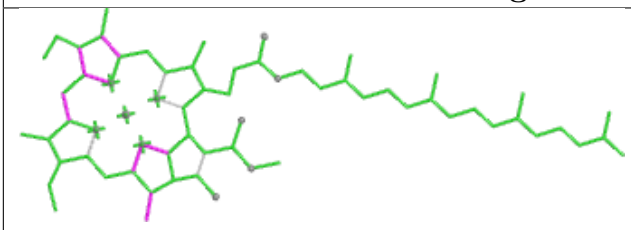
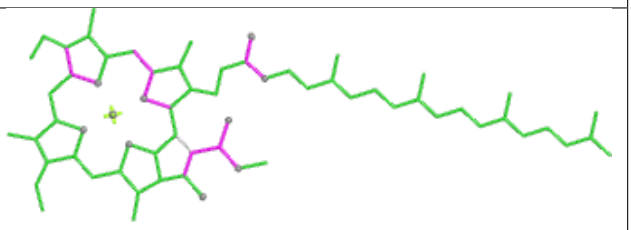
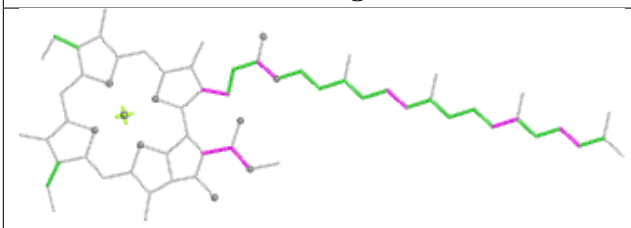
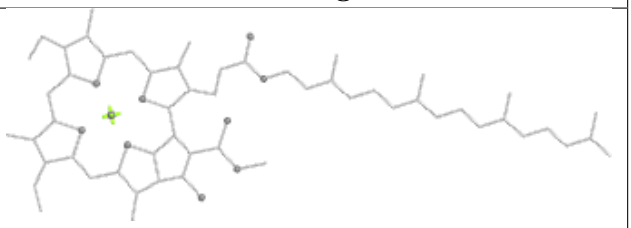


Rings

Ligand CLA AK 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

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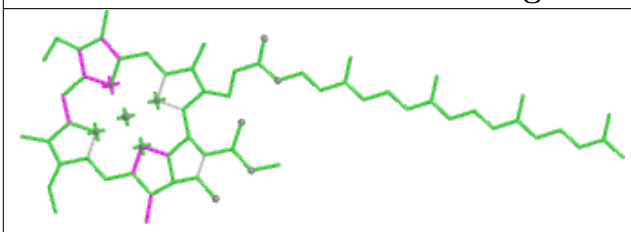
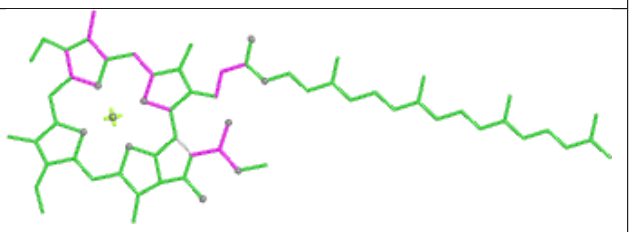
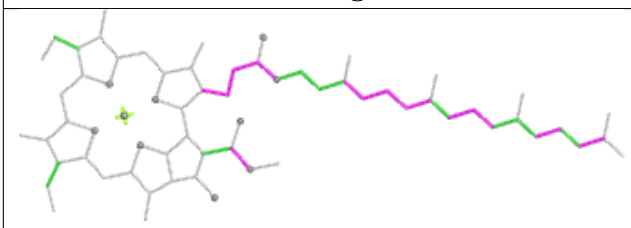
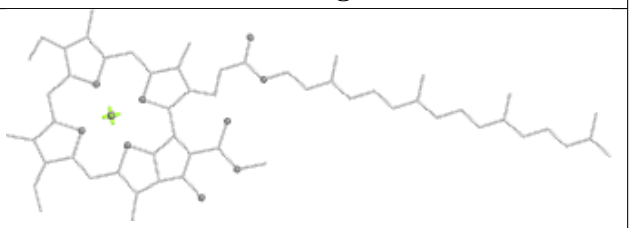
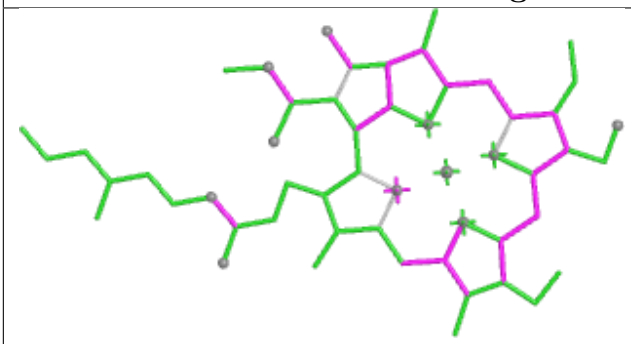
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL AR 607



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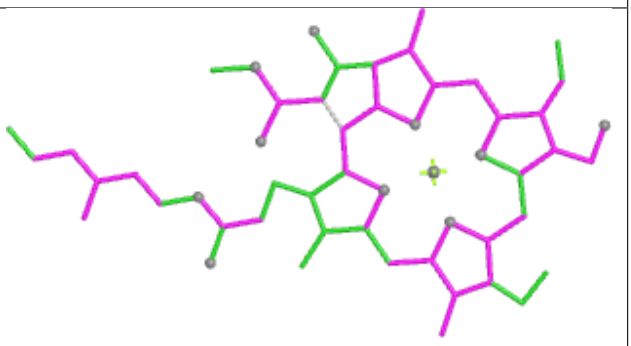

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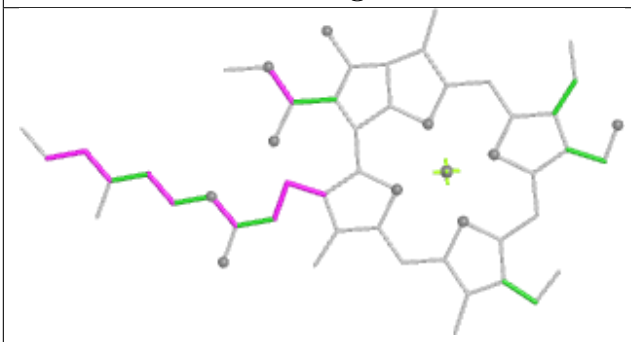

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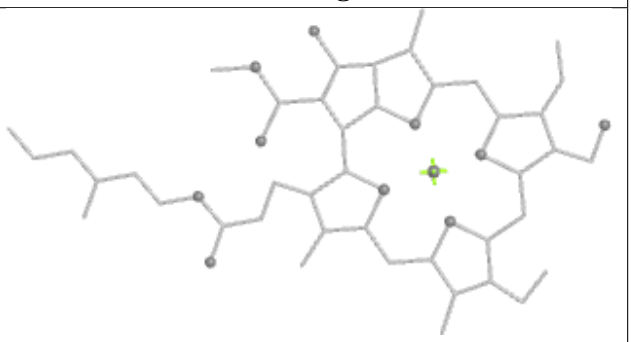
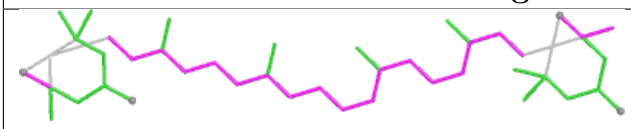


Rings

Ligand XAT AF 613



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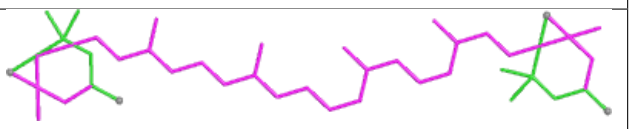

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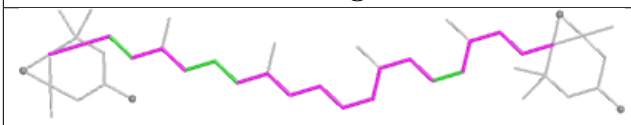

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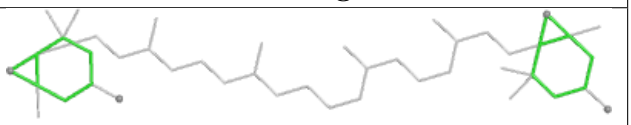
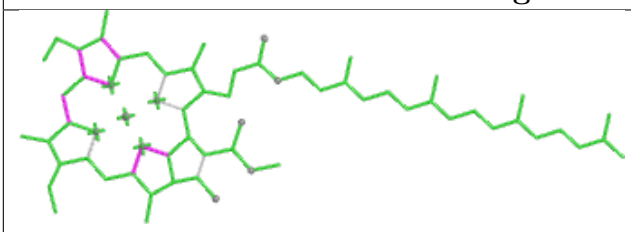


Rings

Ligand CLA AL 512



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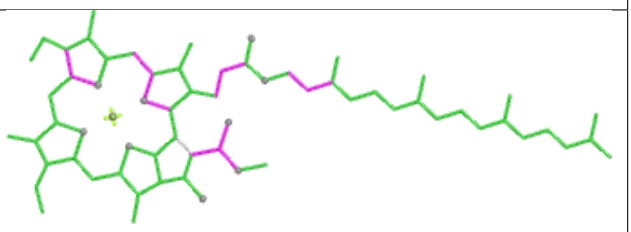
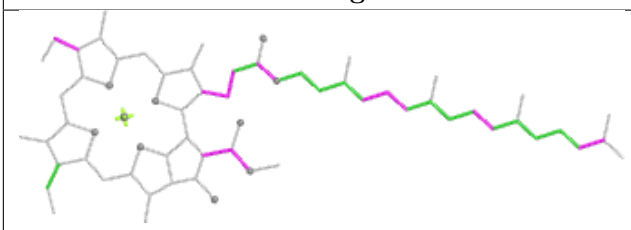


Bond angles



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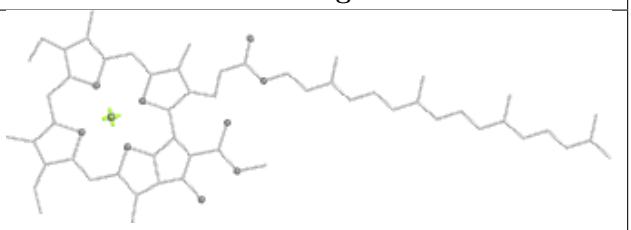
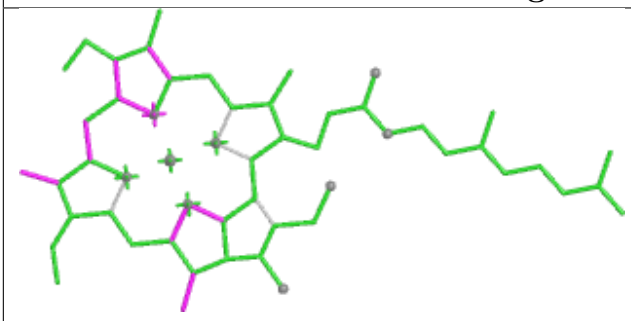
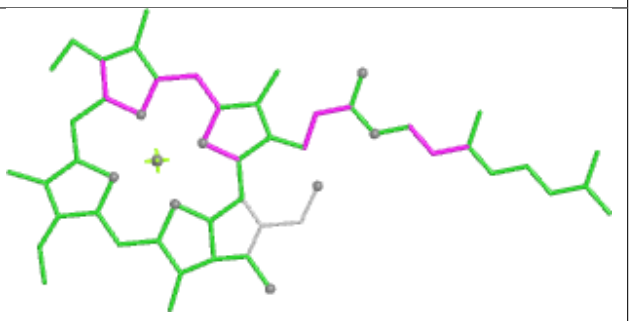
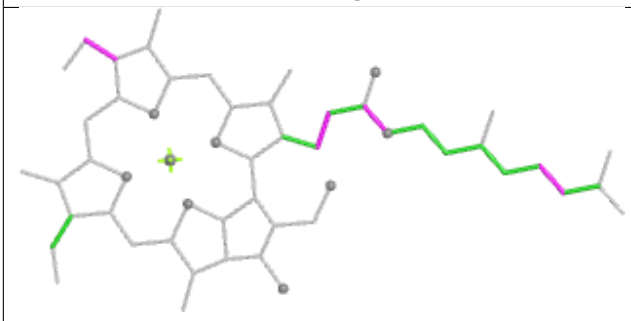
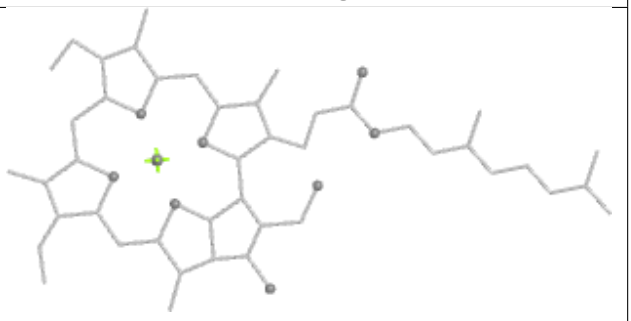
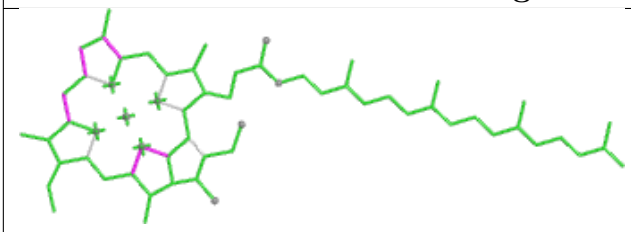
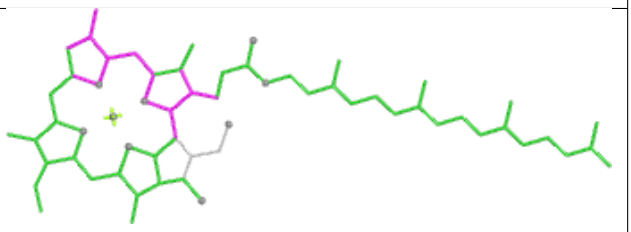
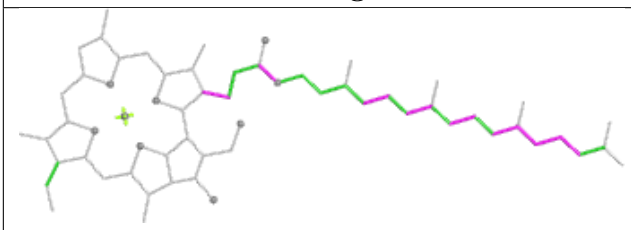
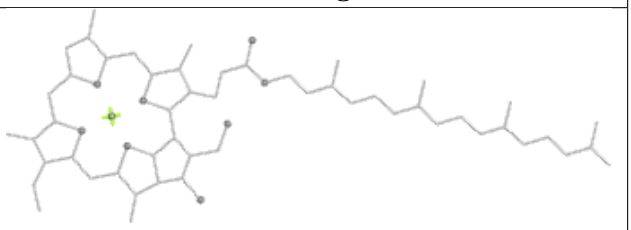


Rings

Ligand CLA v 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AL 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

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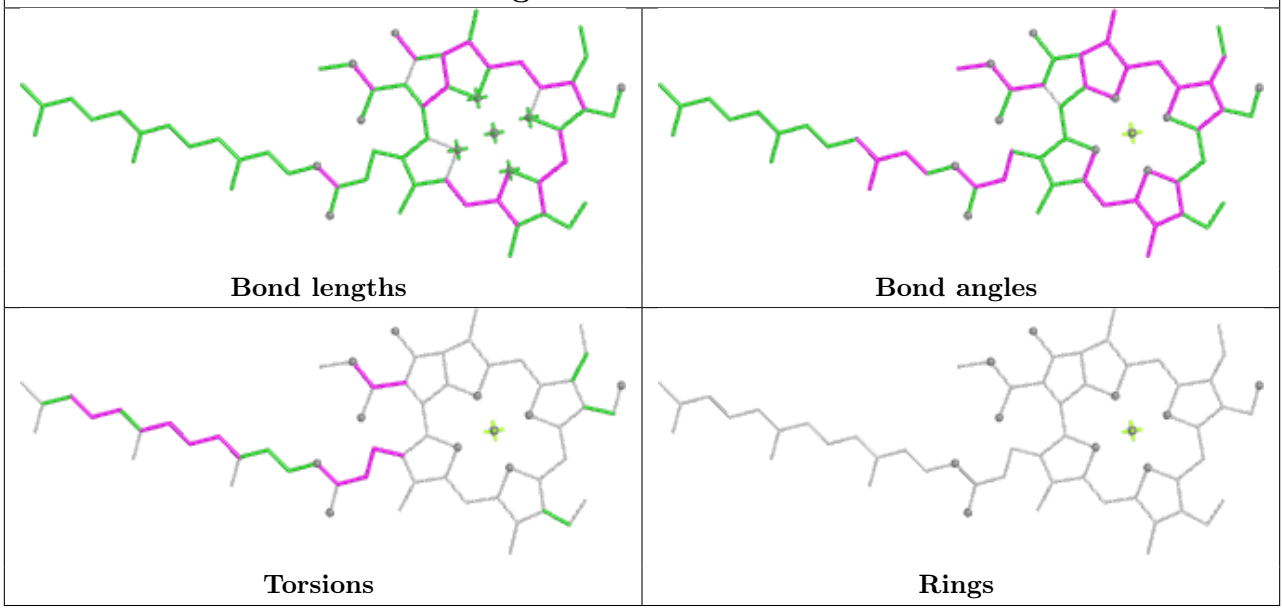

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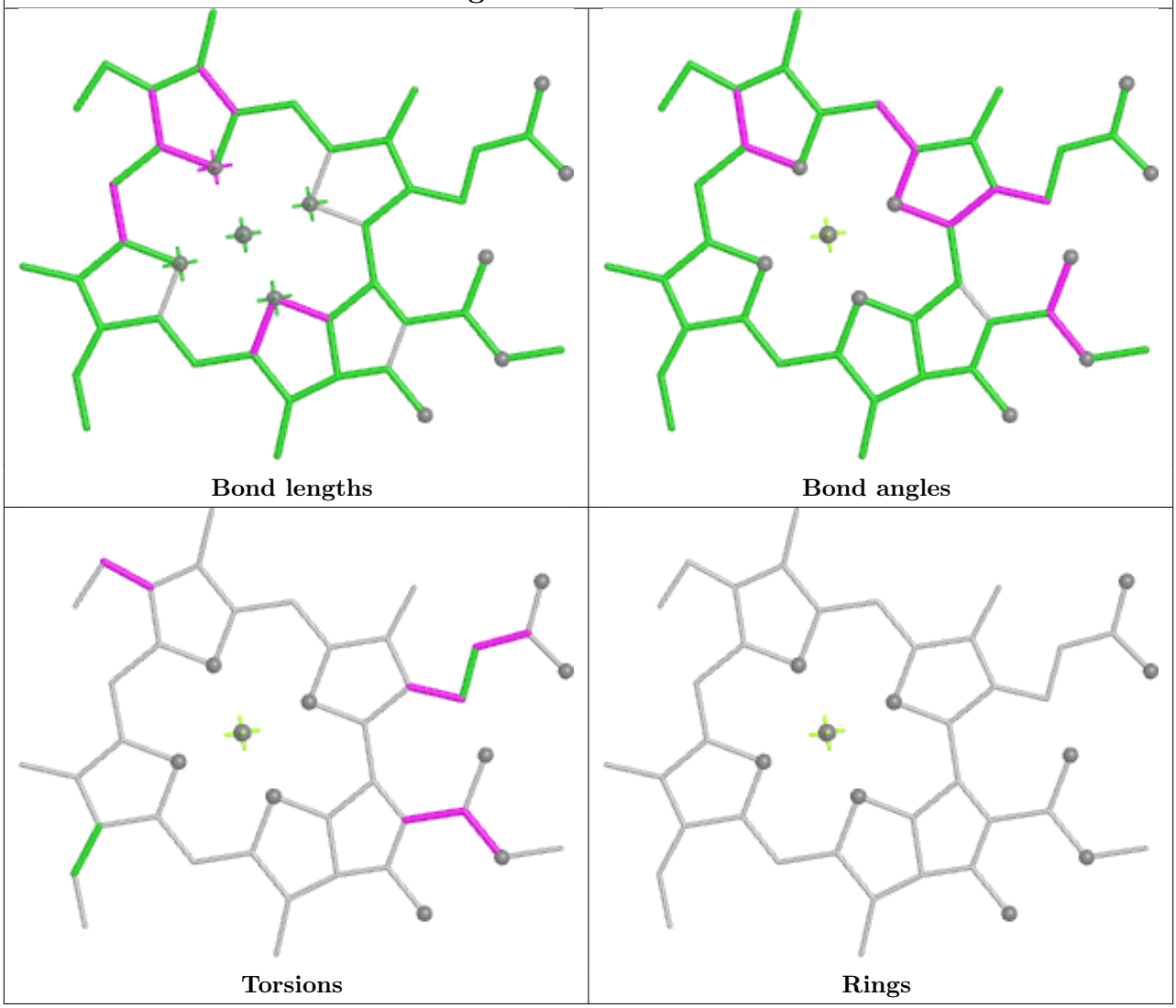

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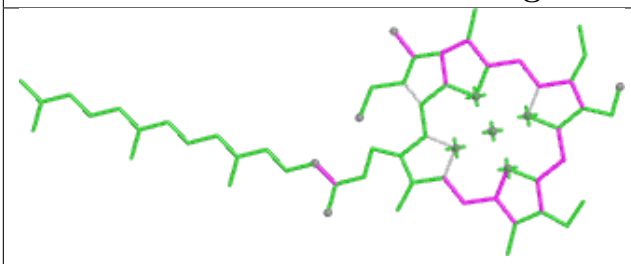
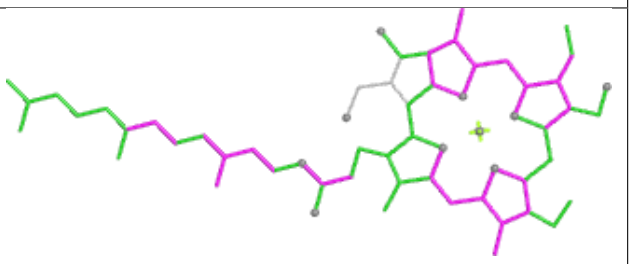
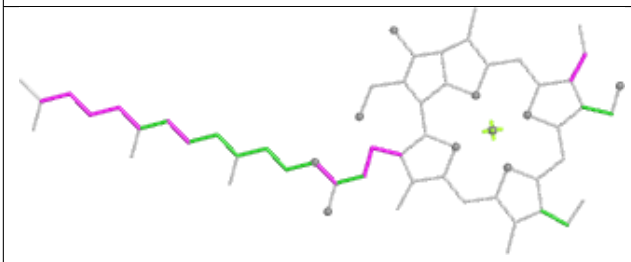
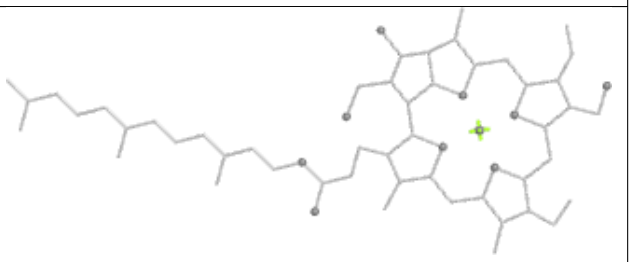
 Bond lengths	 Bond angles
 Torsions	 Rings

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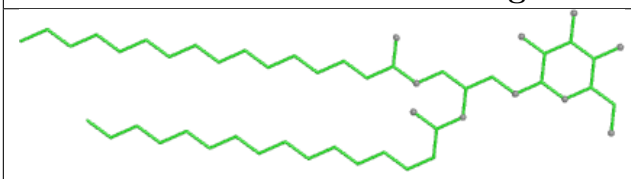
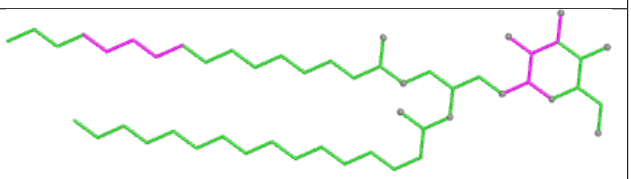
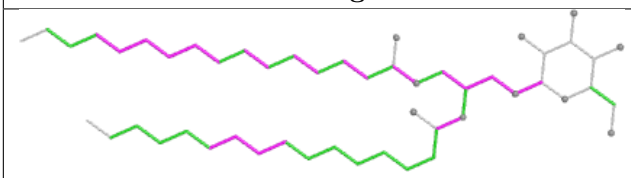
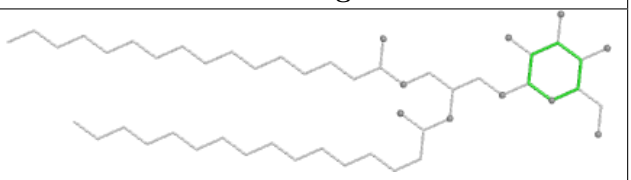
 Bond lengths	 Bond angles
 Torsions	 Rings

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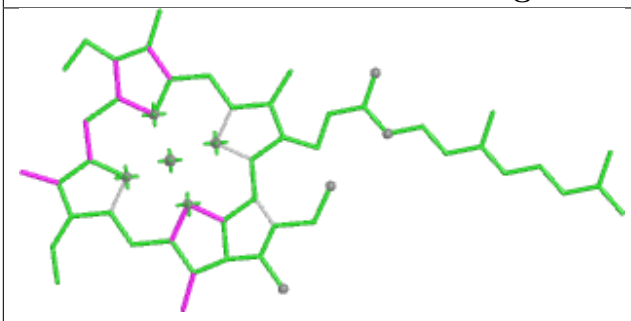
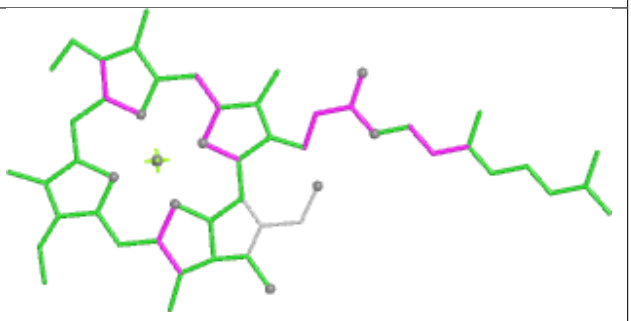
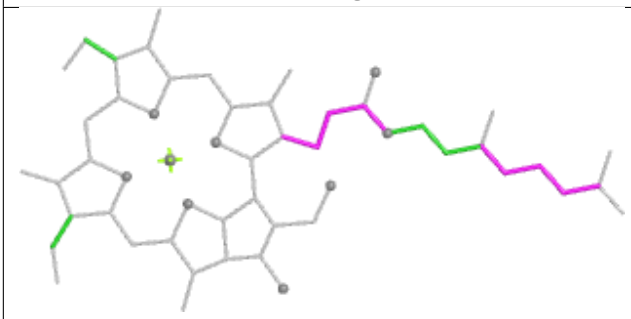
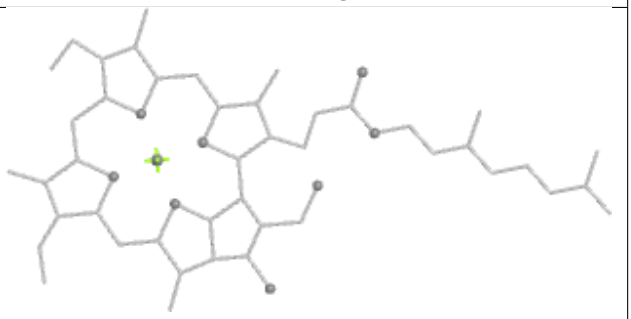
 Bond lengths	 Bond angles
 Torsions	 Rings

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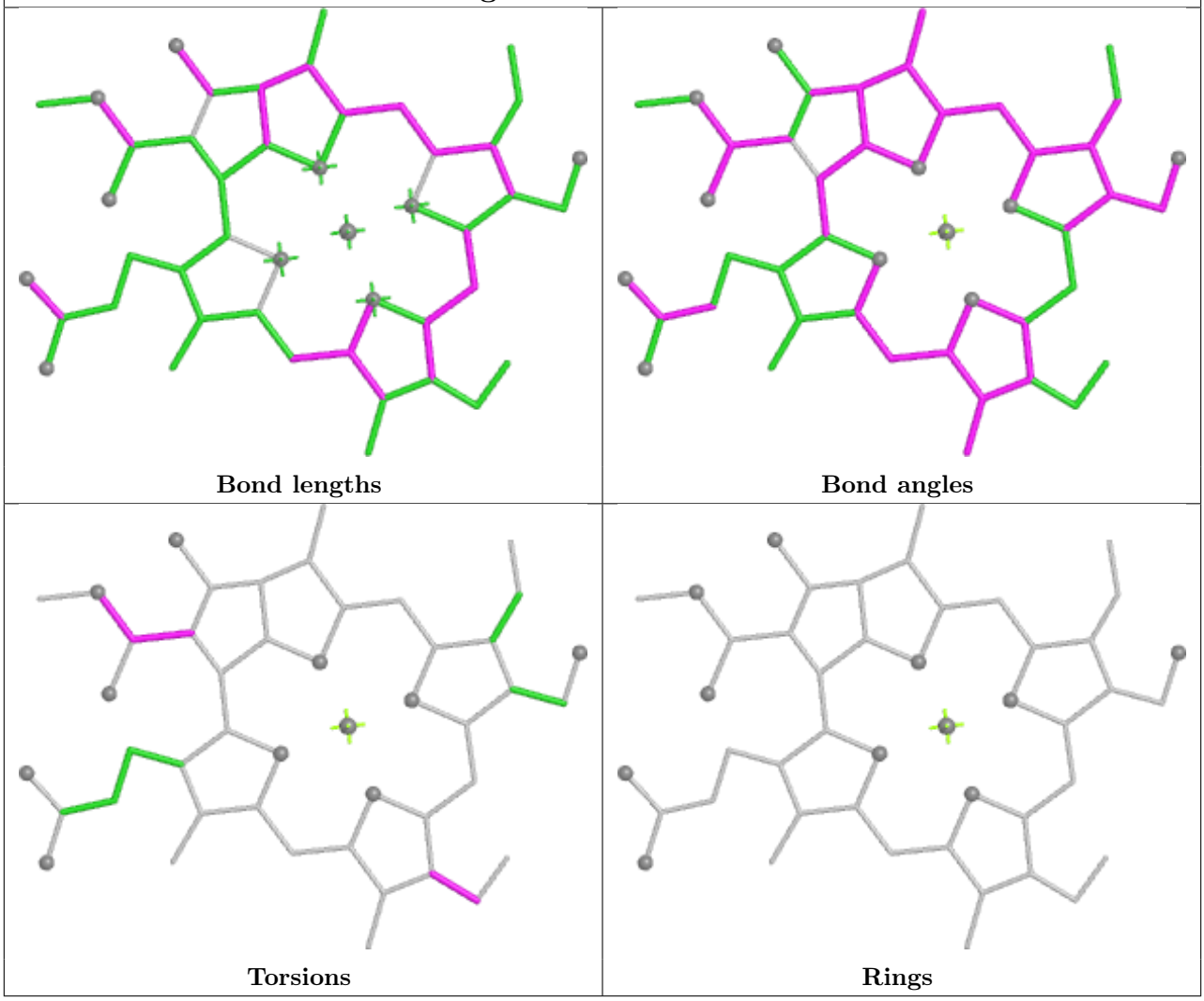

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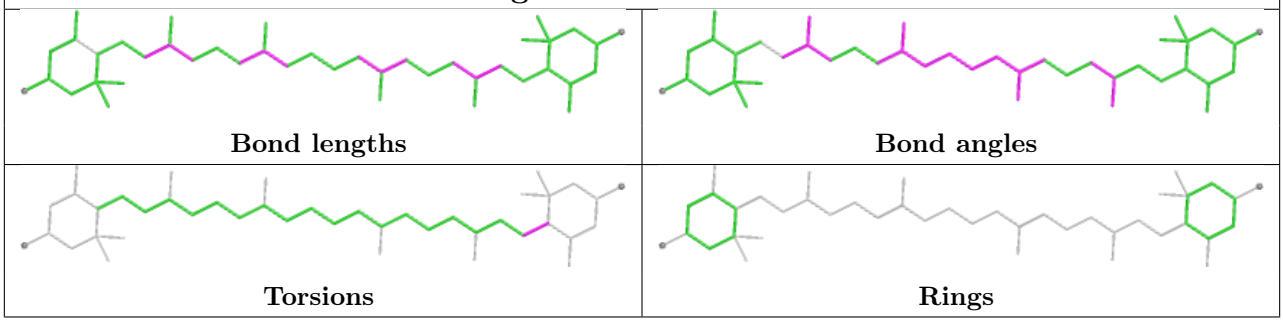

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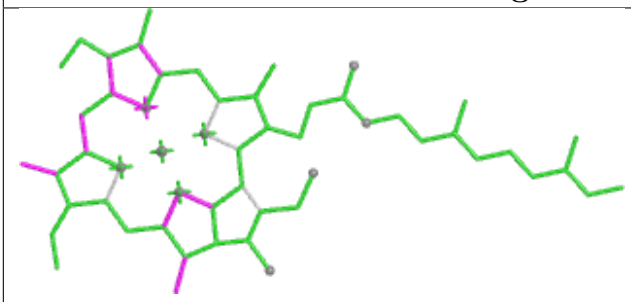
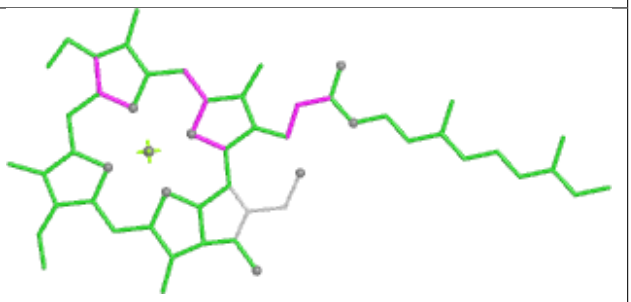
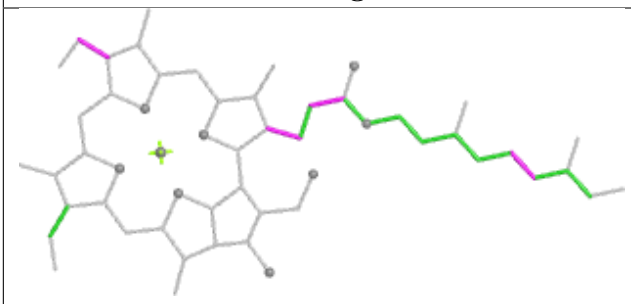
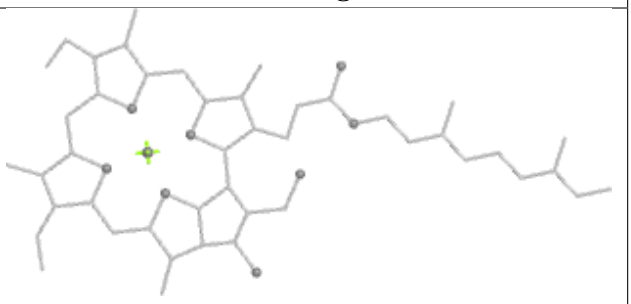
 Bond lengths	 Bond angles
 Torsions	 Rings

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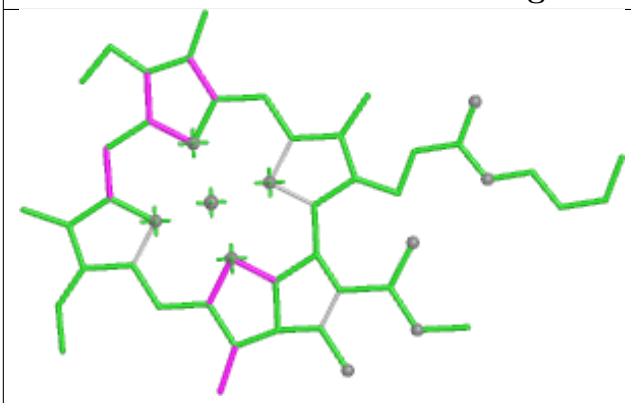
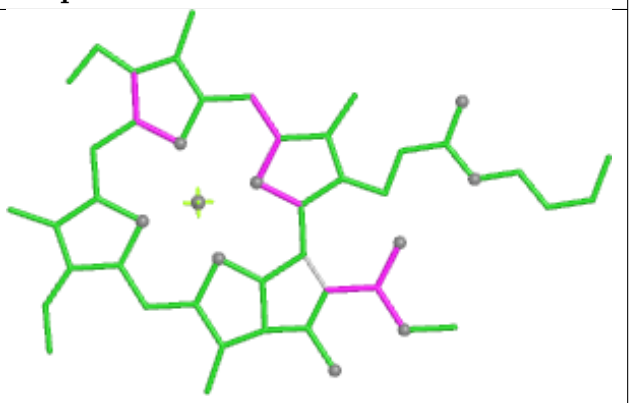
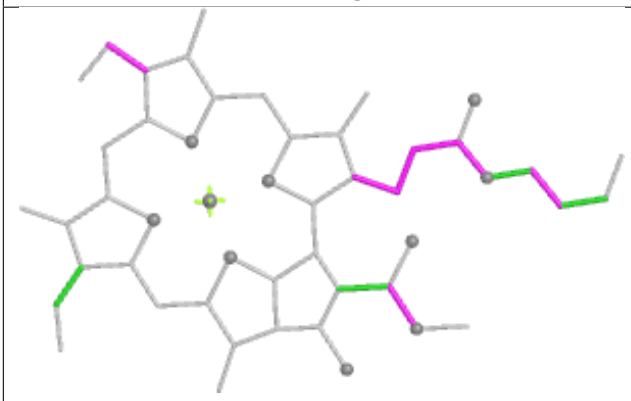
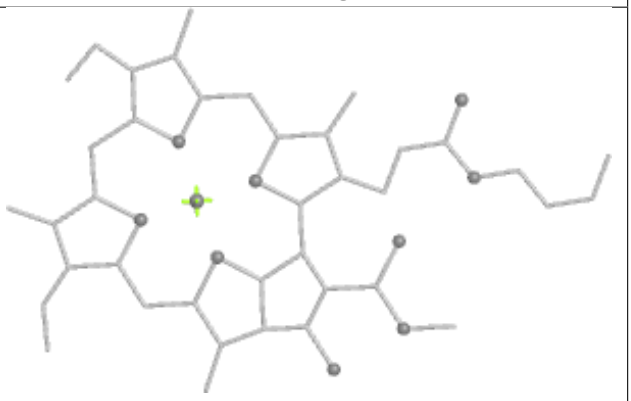
 Bond lengths	 Bond angles
 Torsions	 Rings

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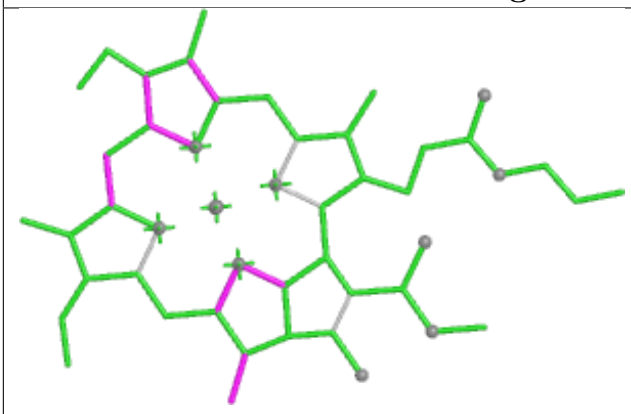
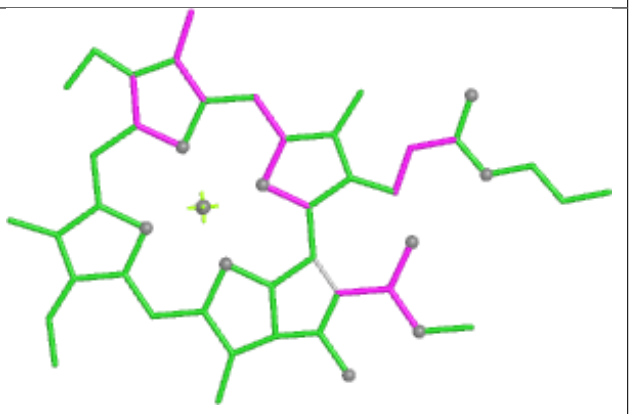
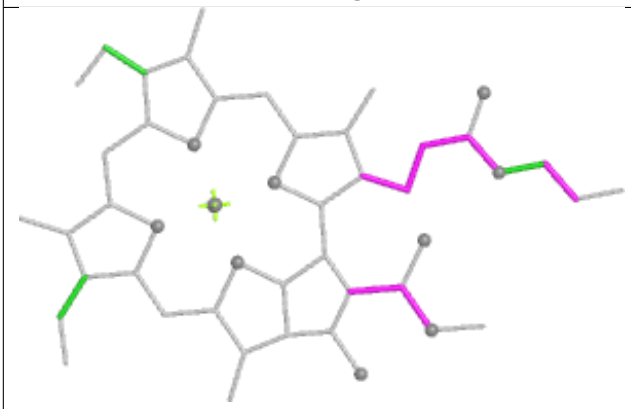
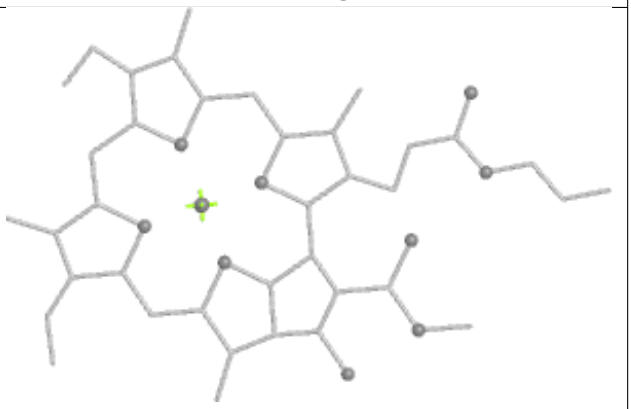
 Bond lengths	 Bond angles
 Torsions	 Rings

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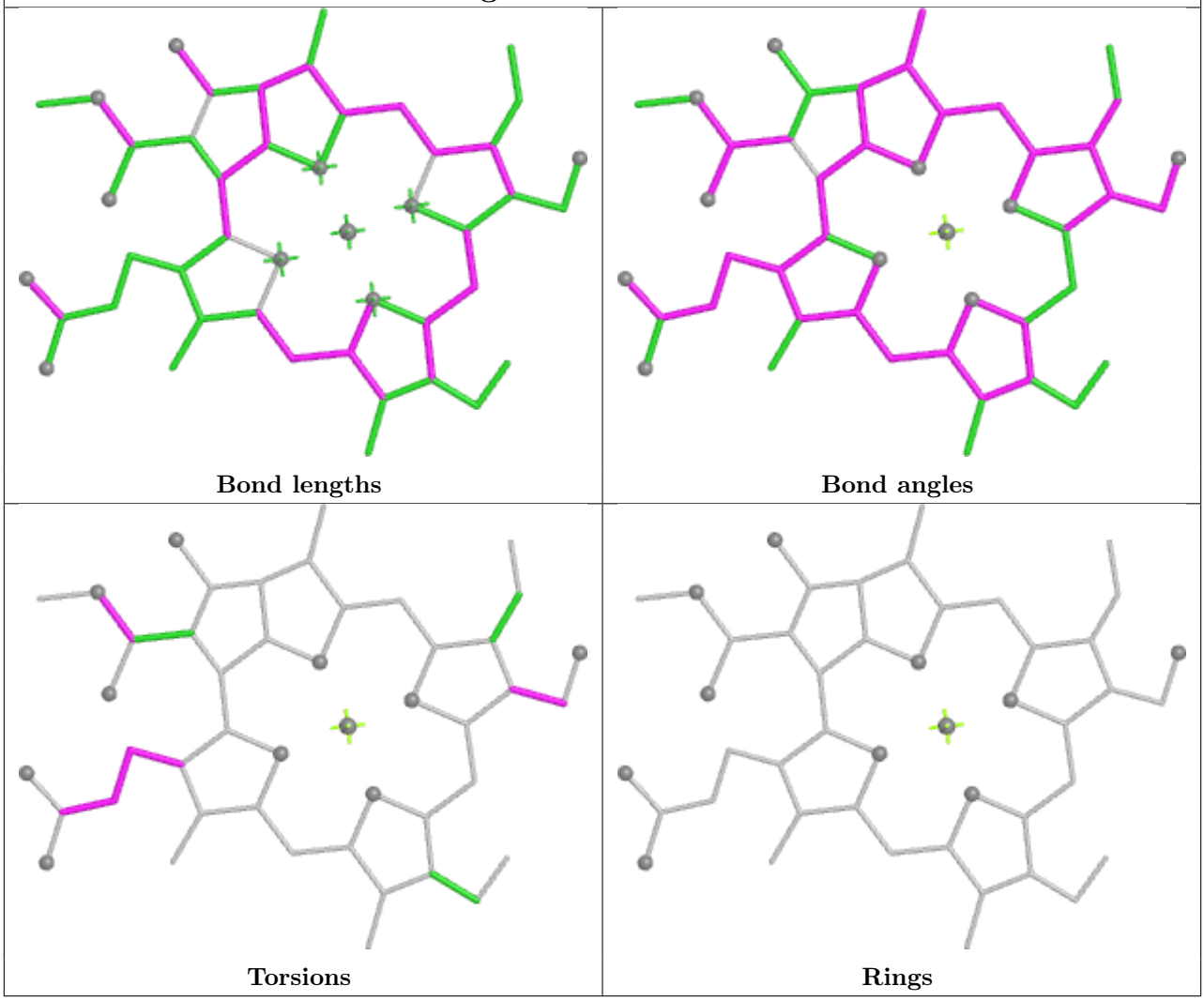

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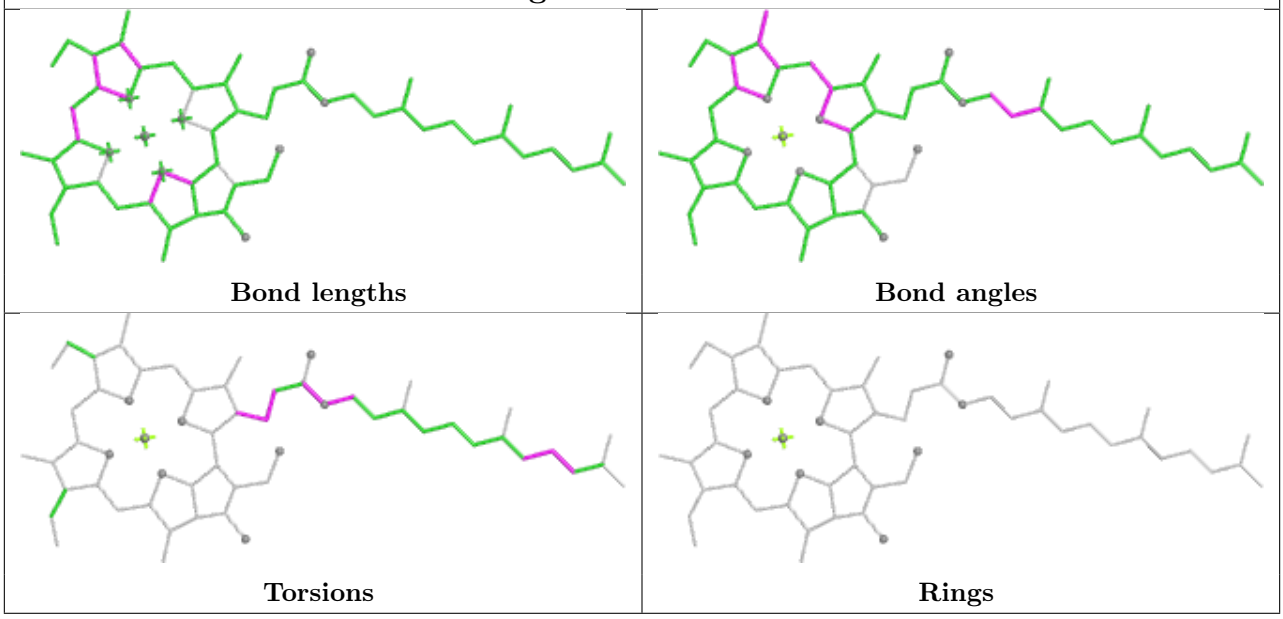

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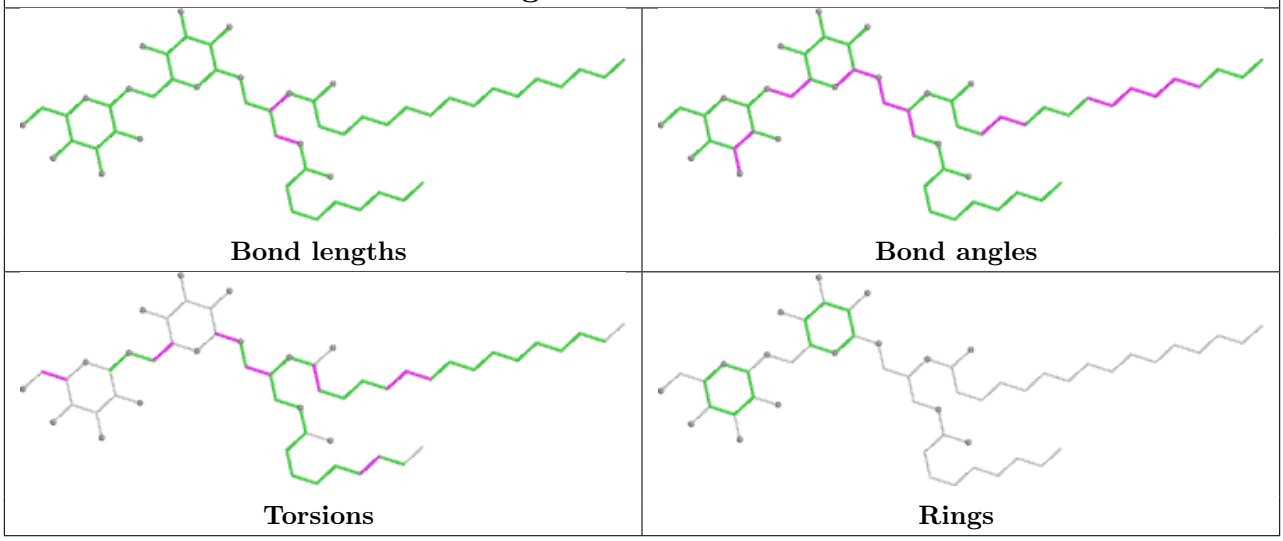

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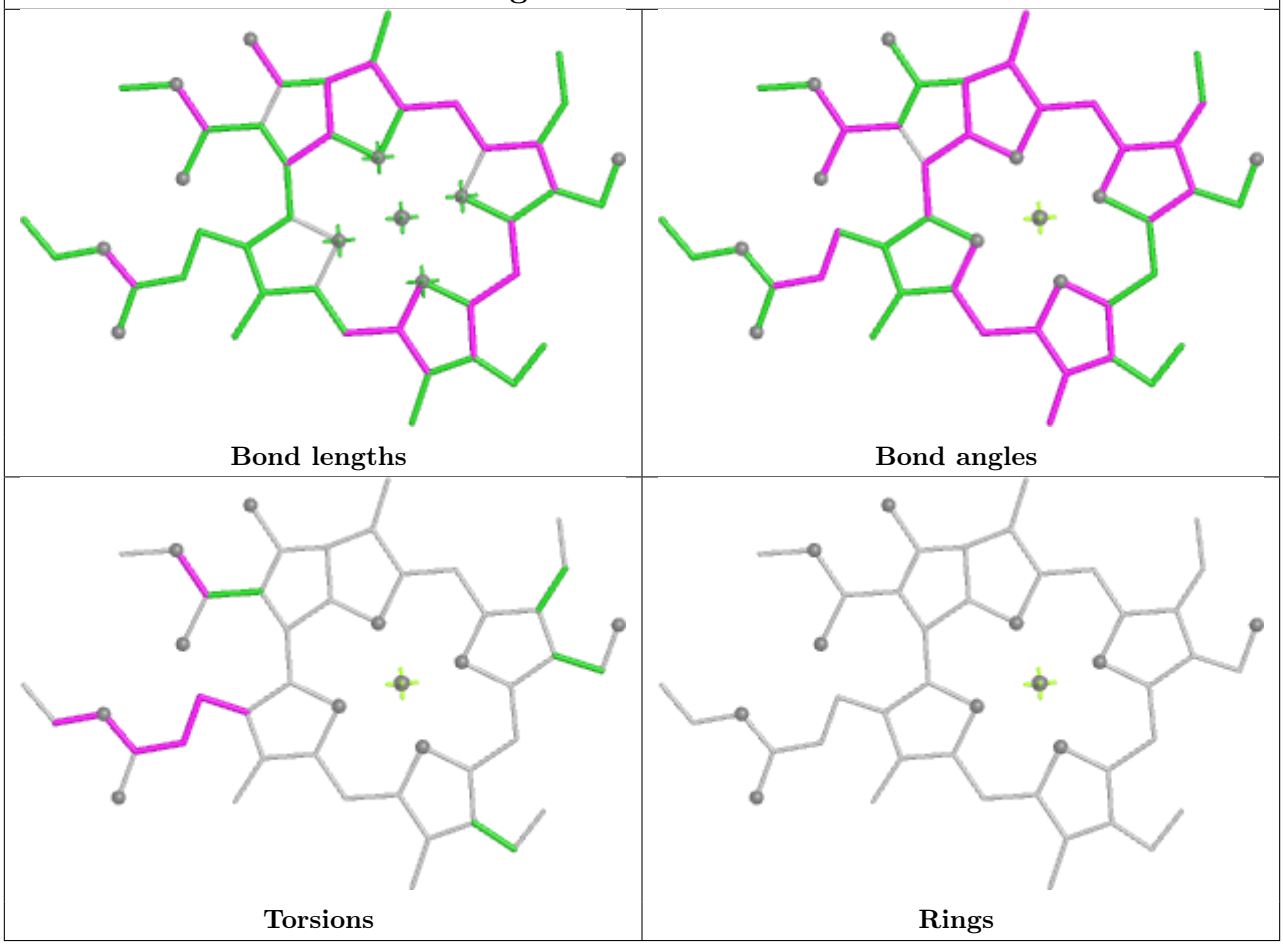

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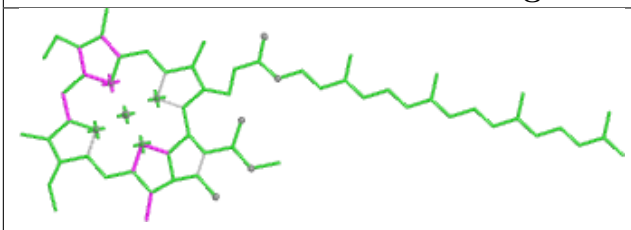
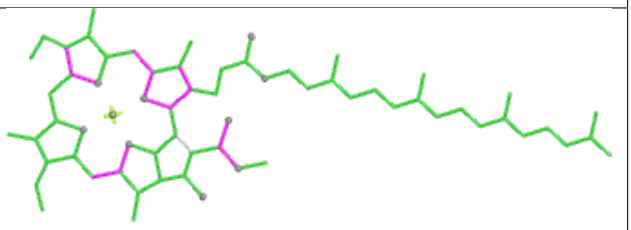
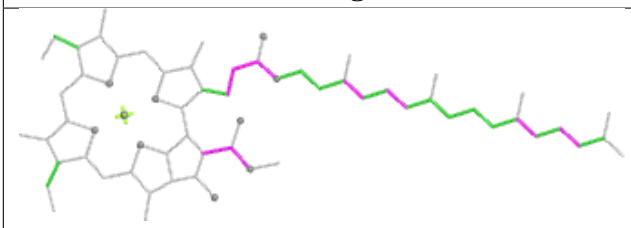
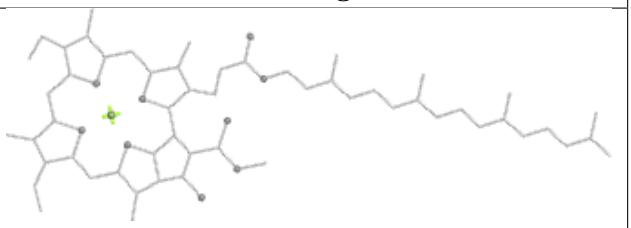
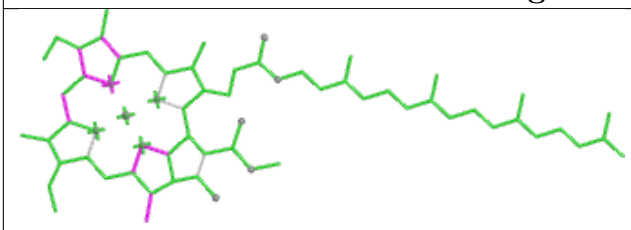
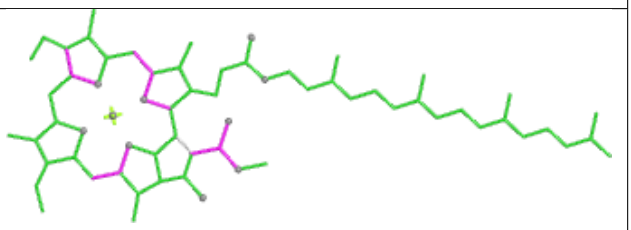
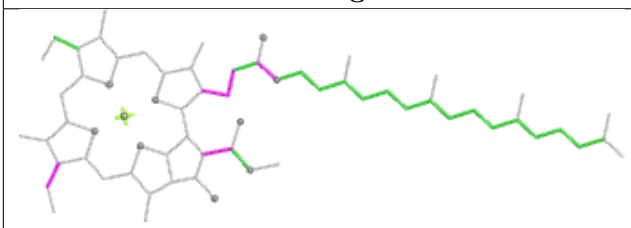
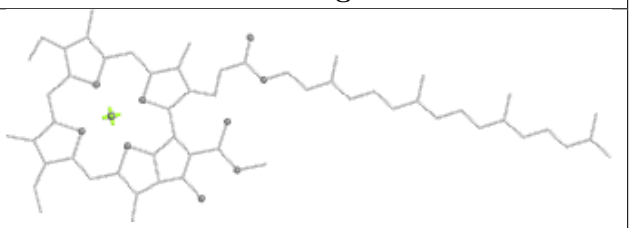
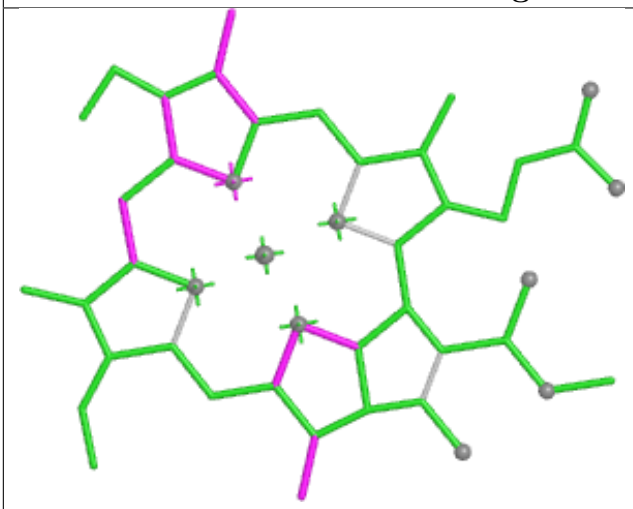
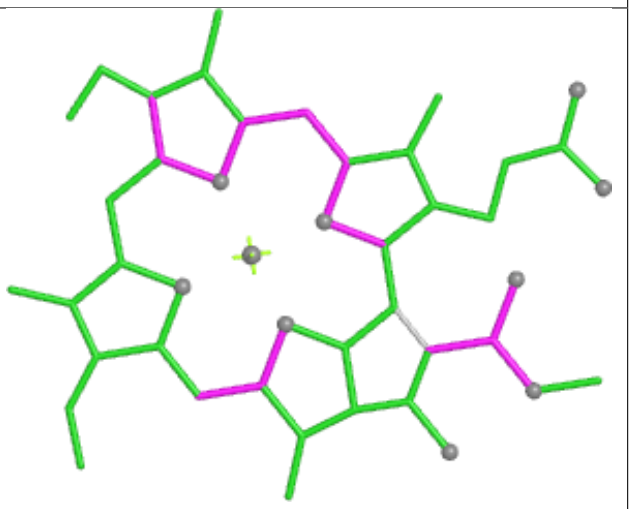
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA J 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AE 609



Bond lengths



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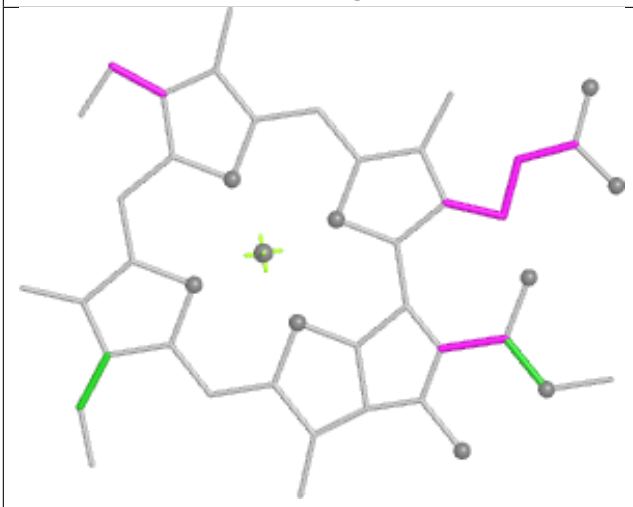
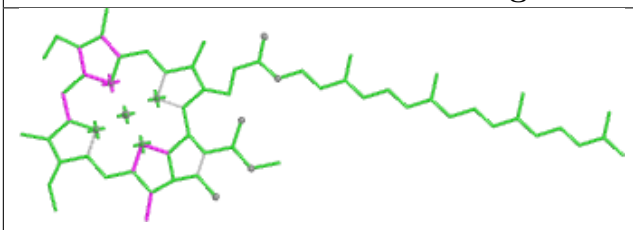


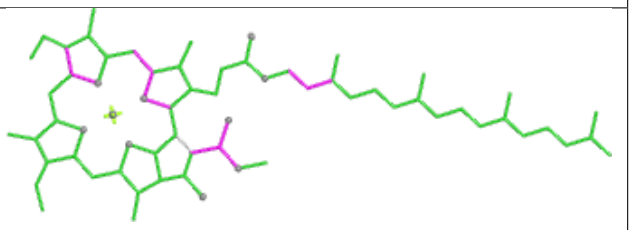
Torsions

Rings

Ligand CLA AK 616



Bond lengths



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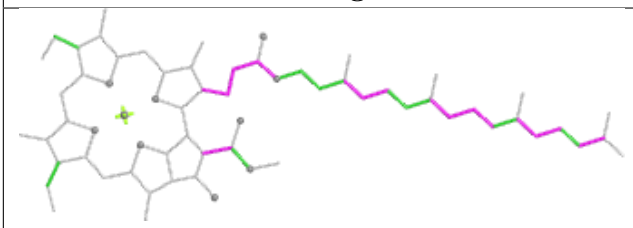

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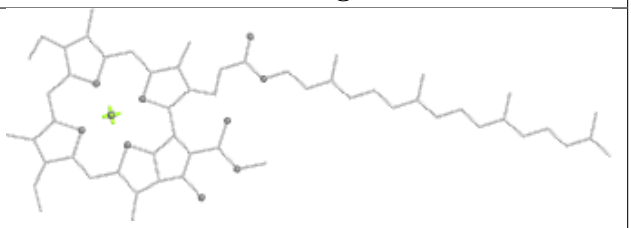
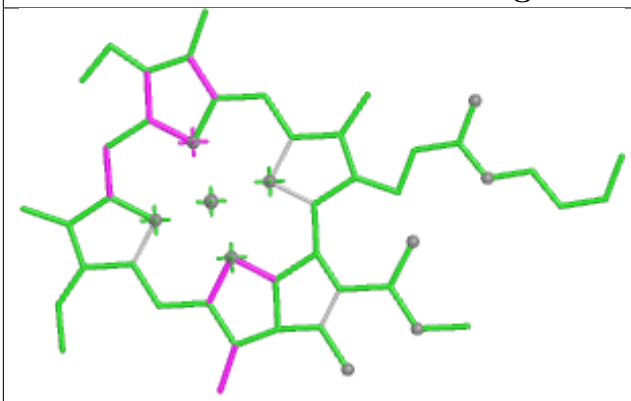


Rings

Ligand CLA AS 314



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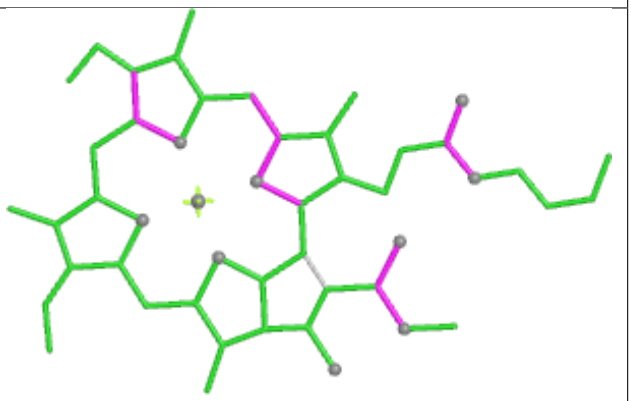

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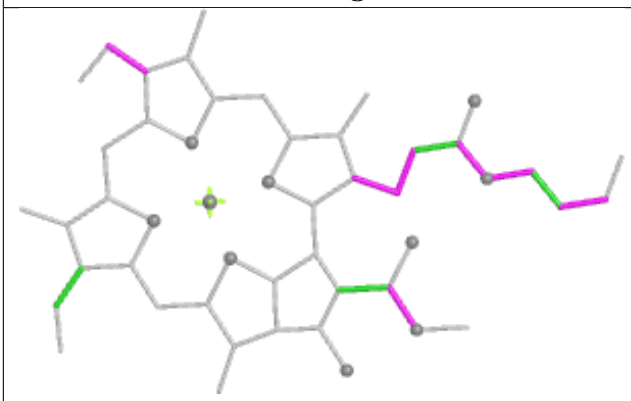

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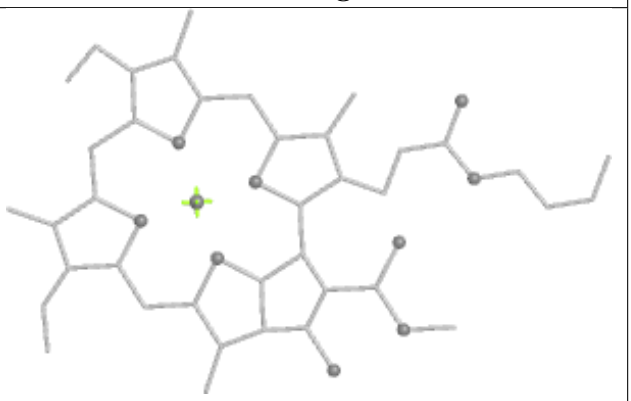
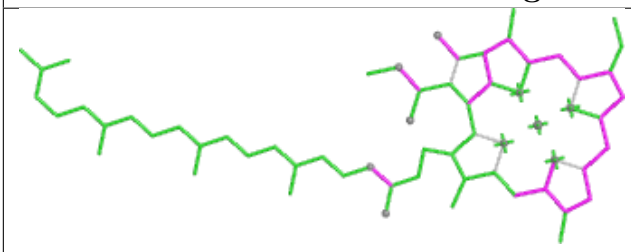


Rings

Ligand CHL V 607



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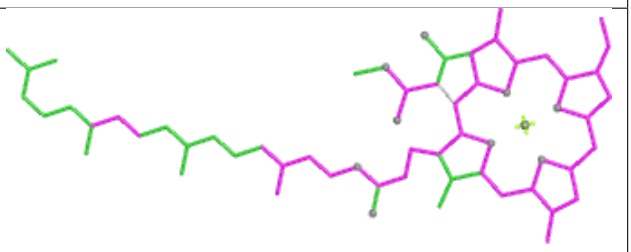
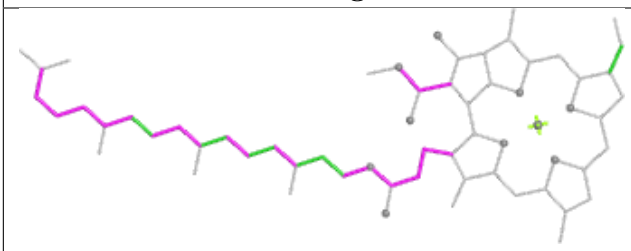
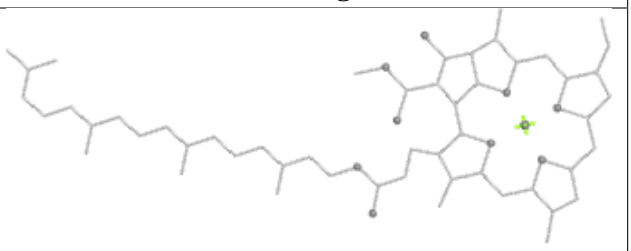


Bond angles

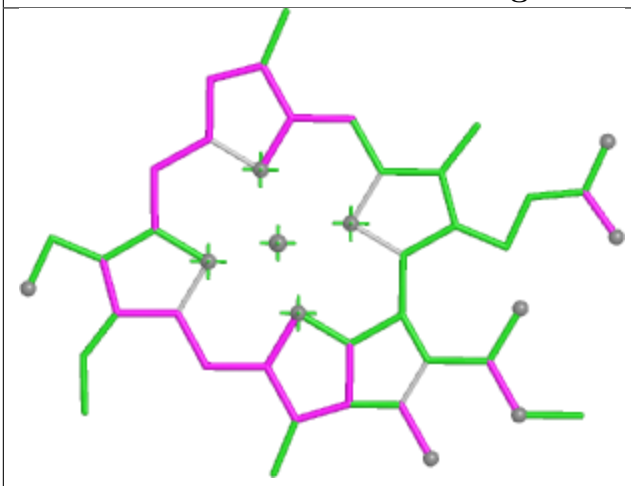


Torsions



Rings

Ligand CHL AC 601



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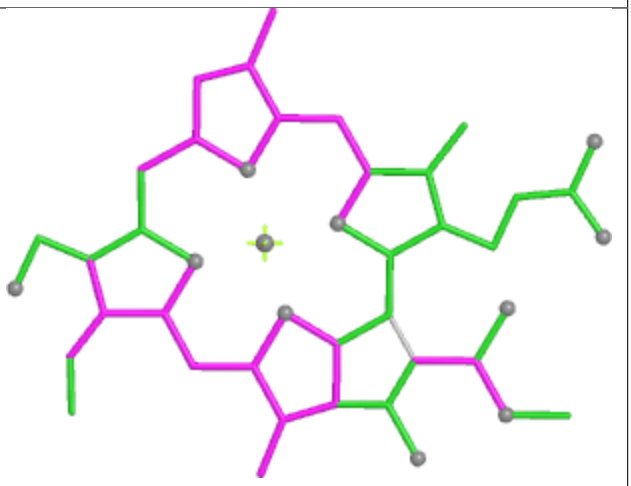

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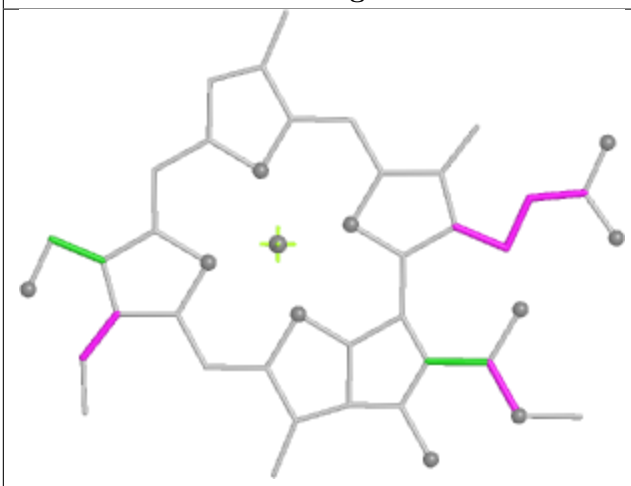
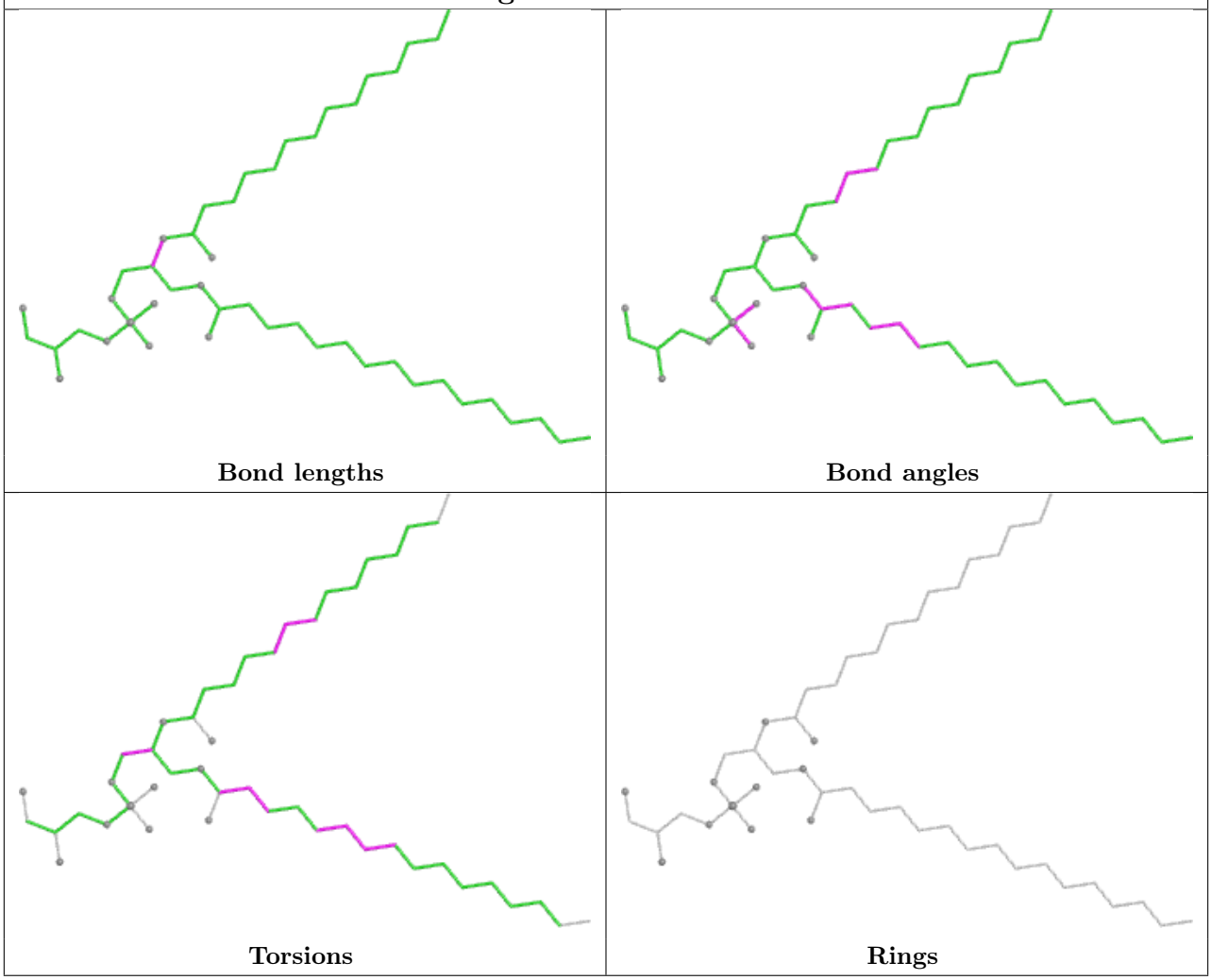


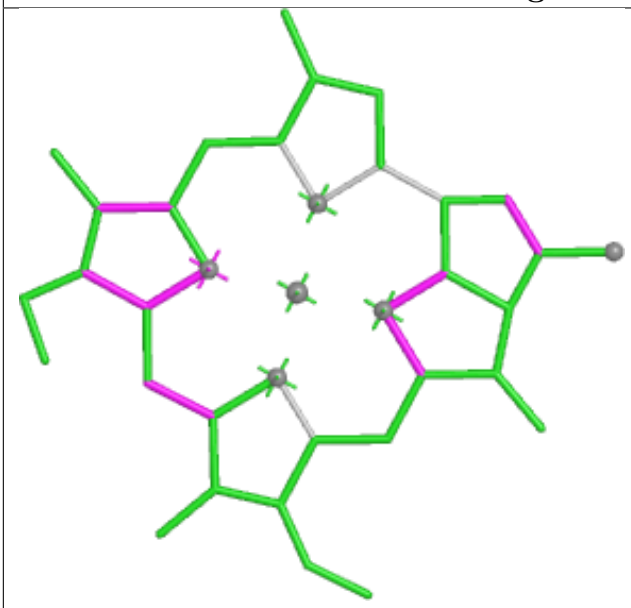
Torsions

Rings

Ligand LHG 0 616



Ligand CLA p 611



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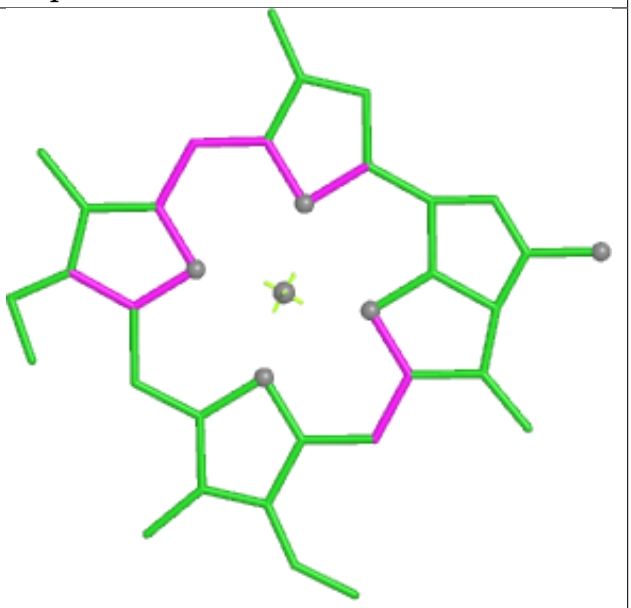

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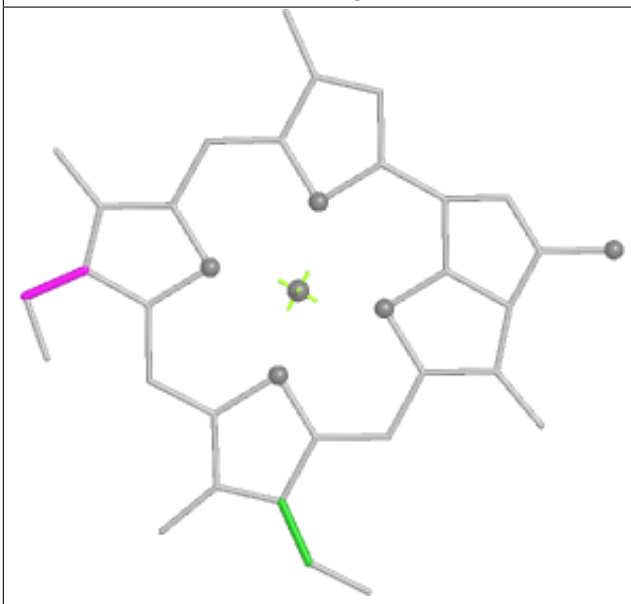

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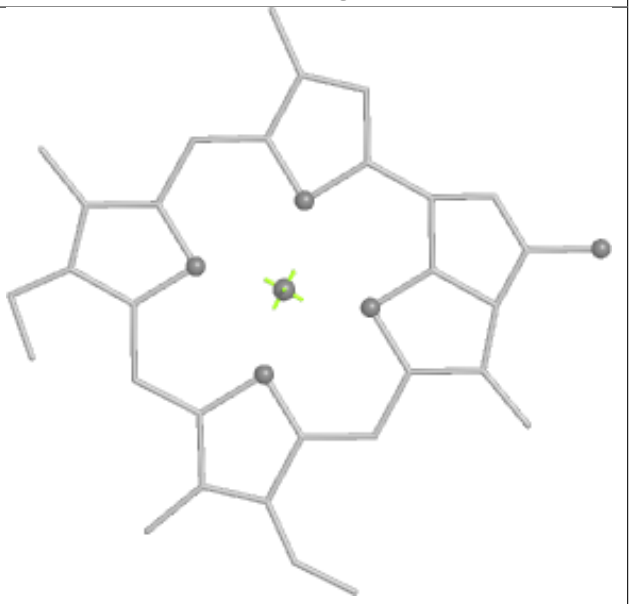
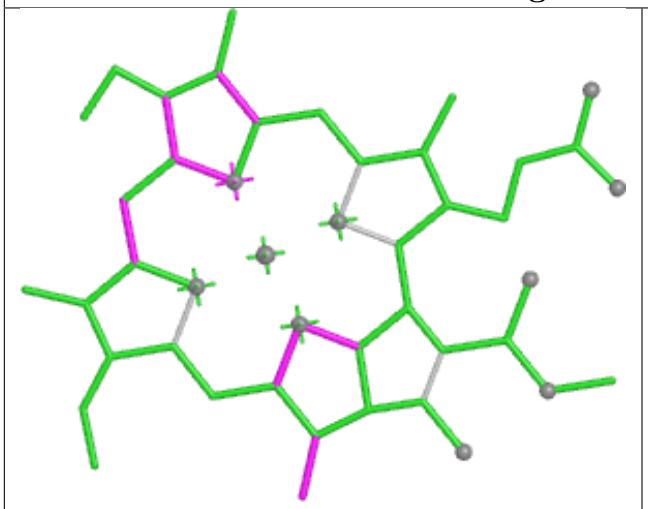


Rings

Ligand CLA v 304



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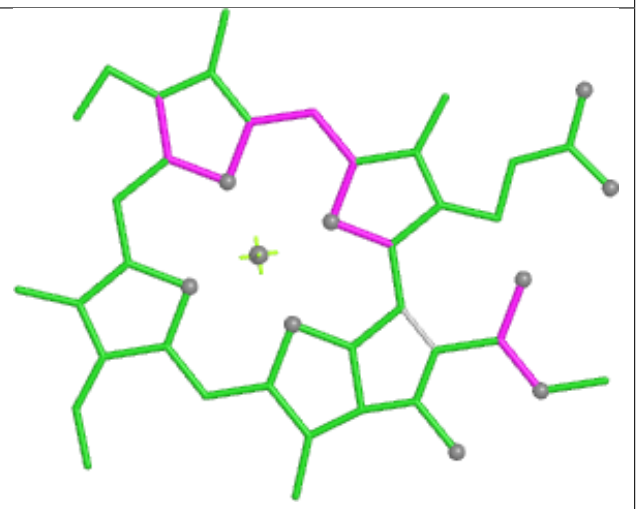

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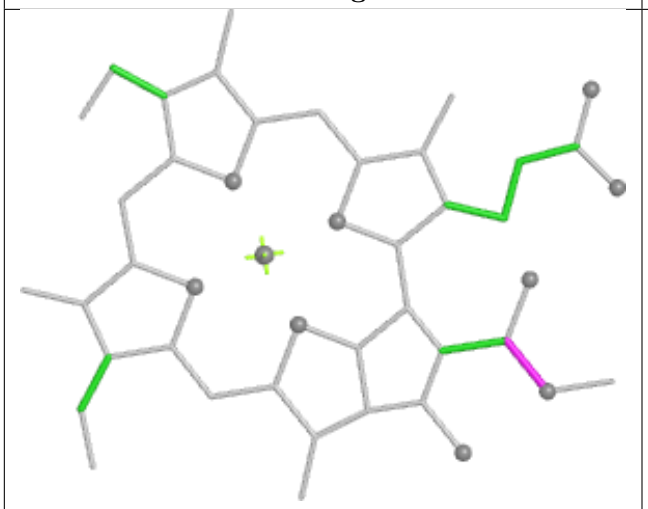
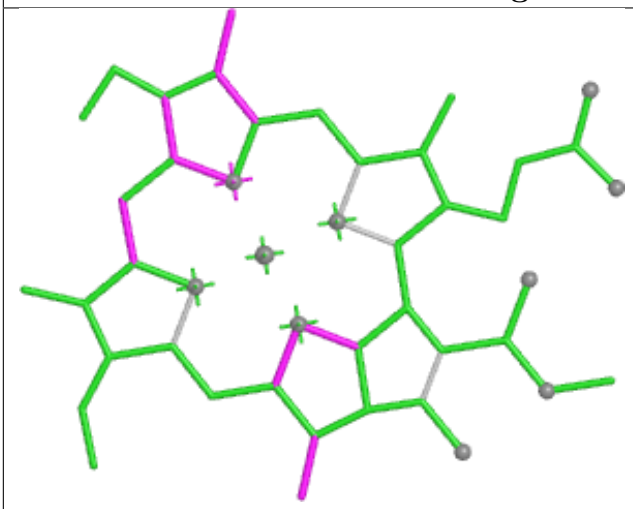


Torsions

Rings

Ligand CLA AB 603



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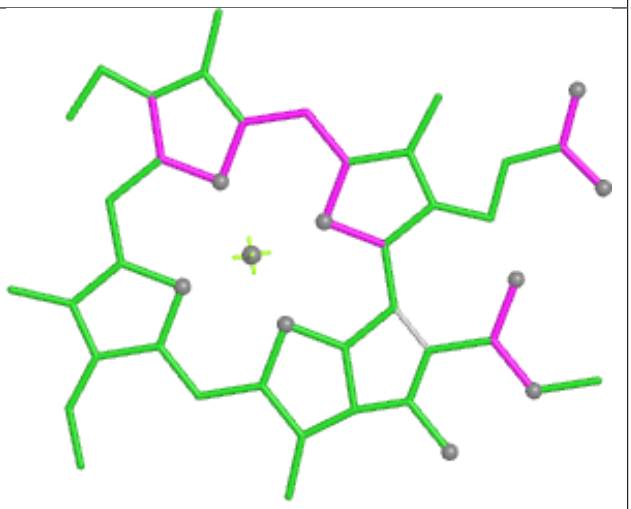

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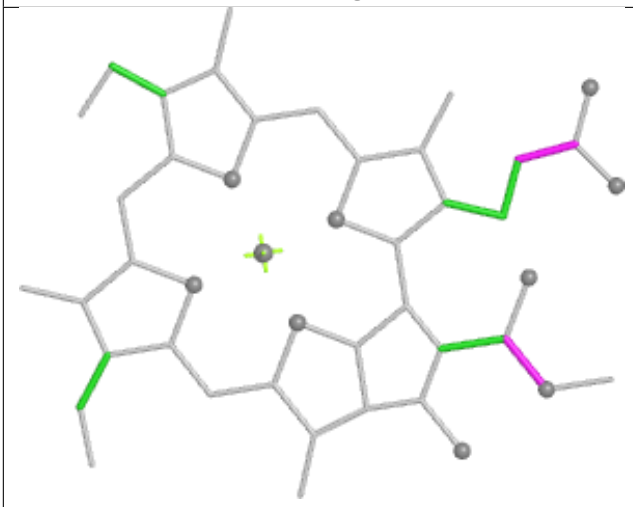
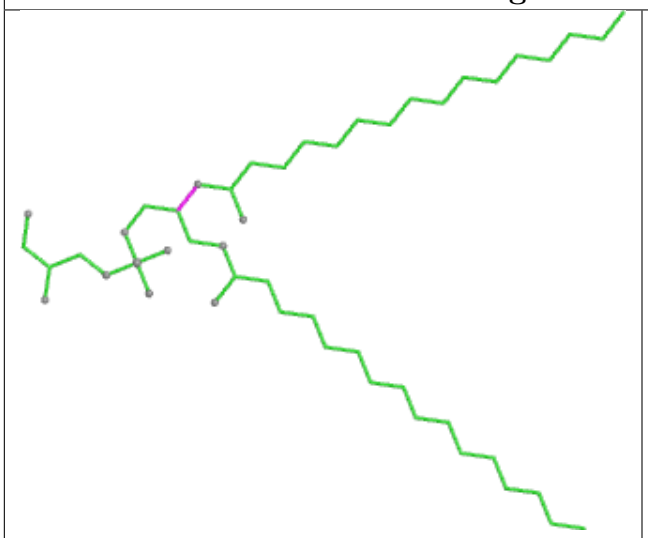


Torsions

Rings

Ligand LHG AK 624



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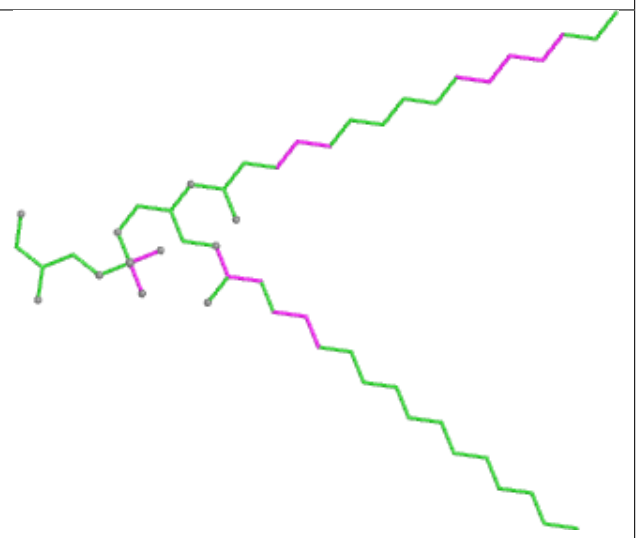

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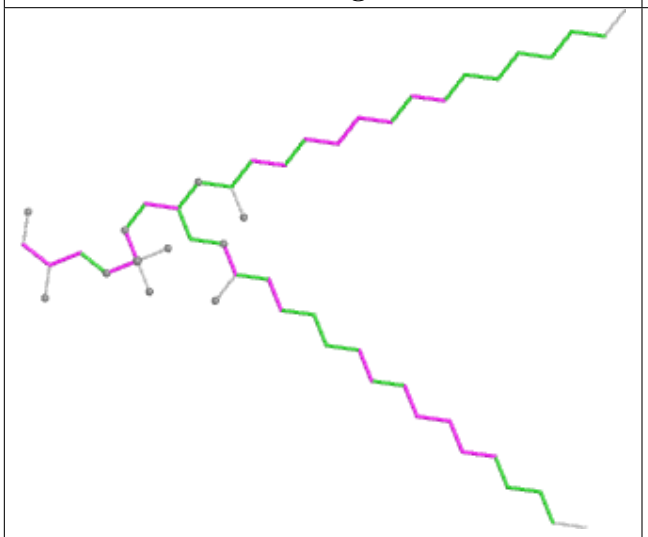

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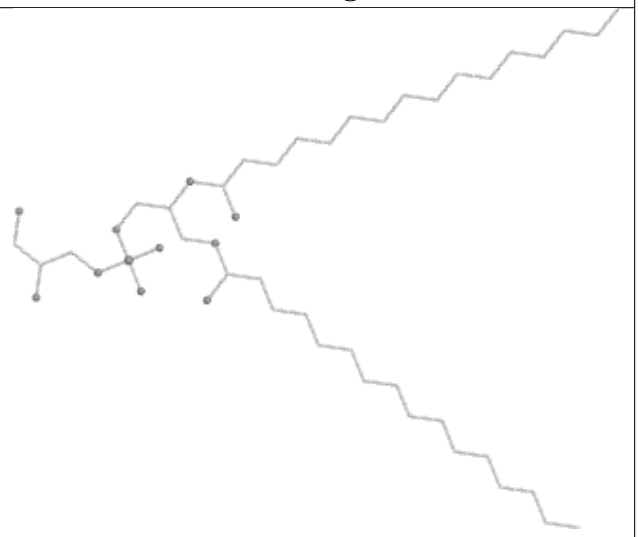
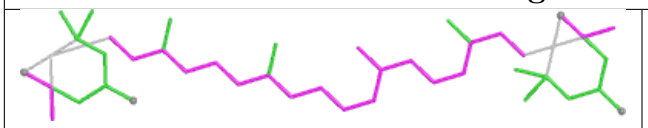


Rings

Ligand XAT q 617



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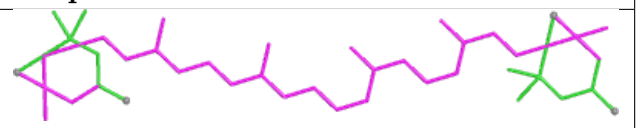

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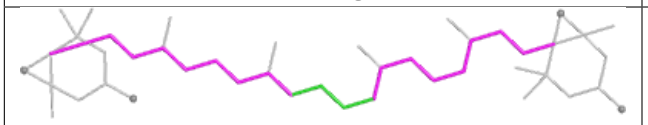

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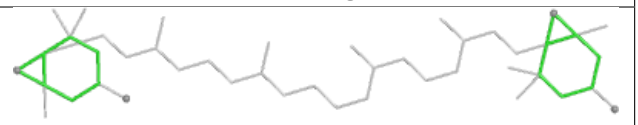
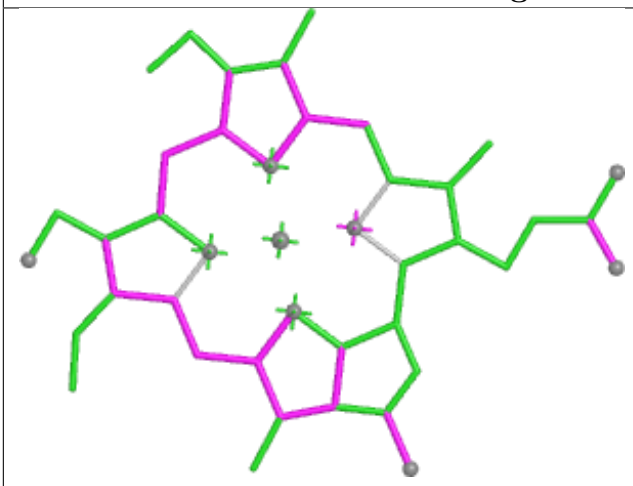


Rings

Ligand CHL AB 608



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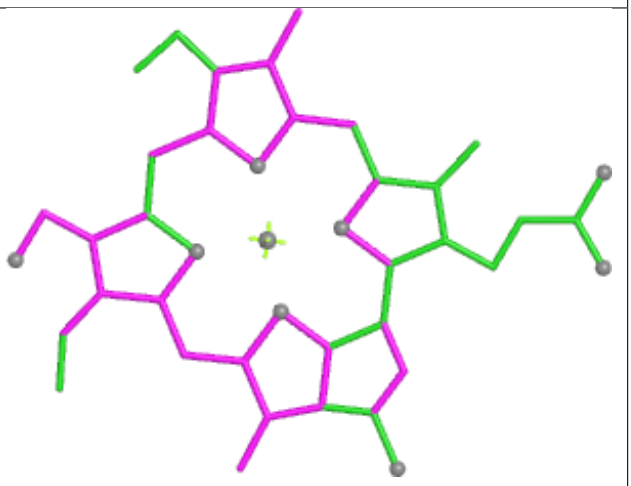
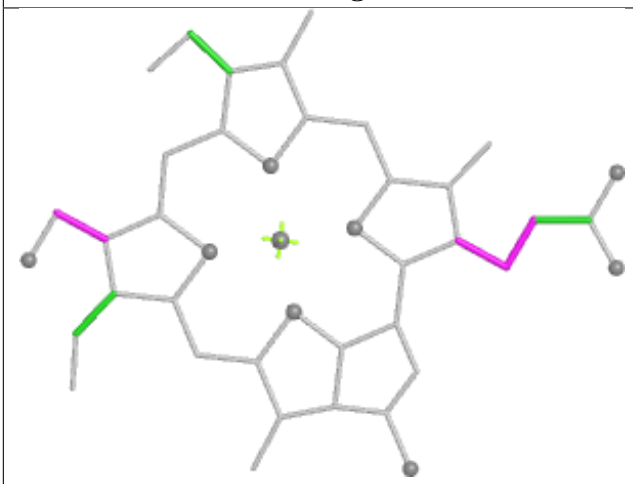


Bond angles



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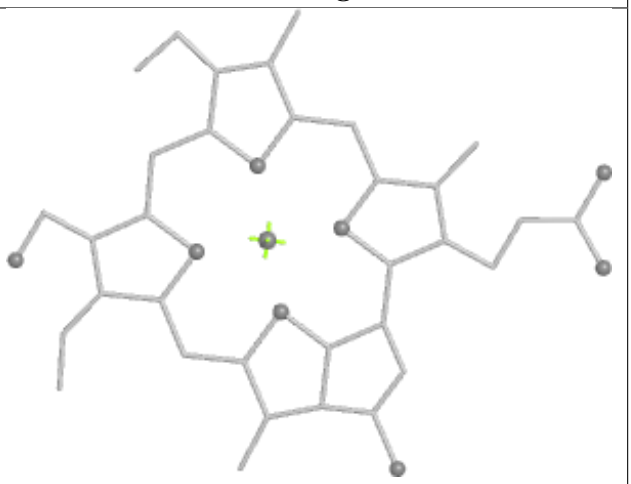
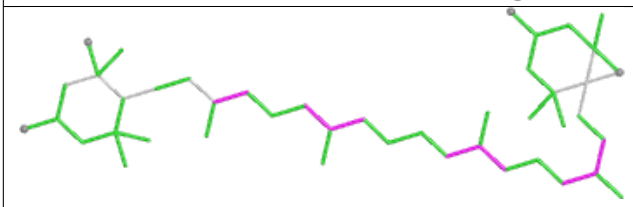


Rings

Ligand NEX AC 616



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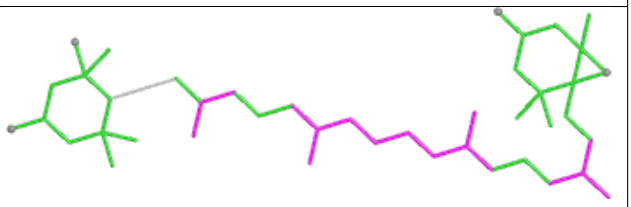

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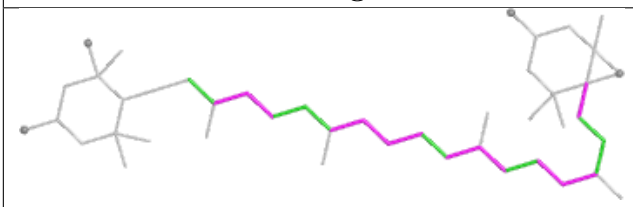

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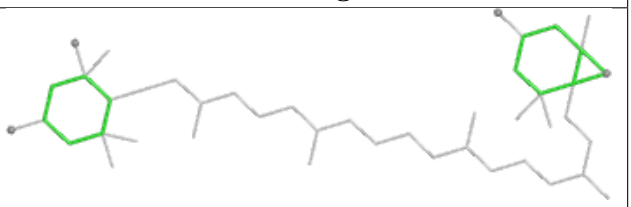
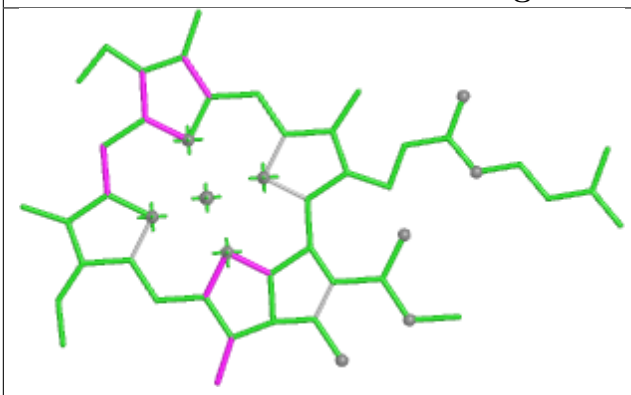
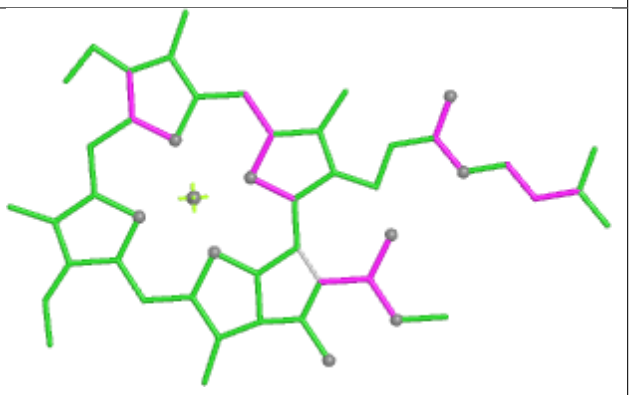
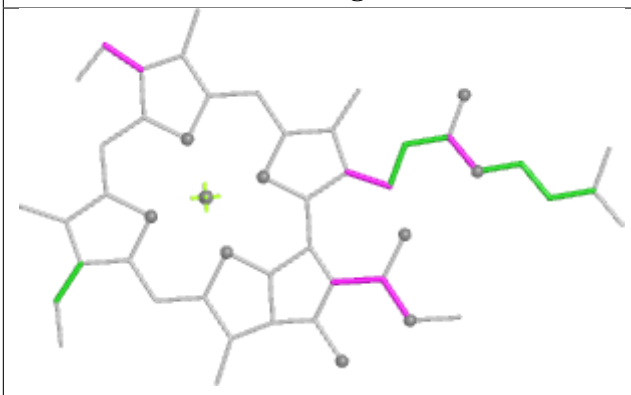
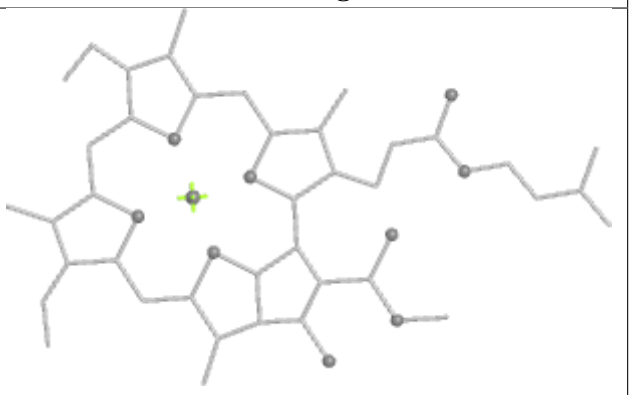
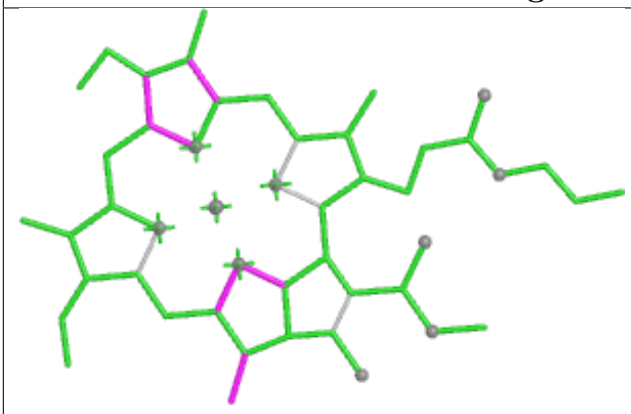
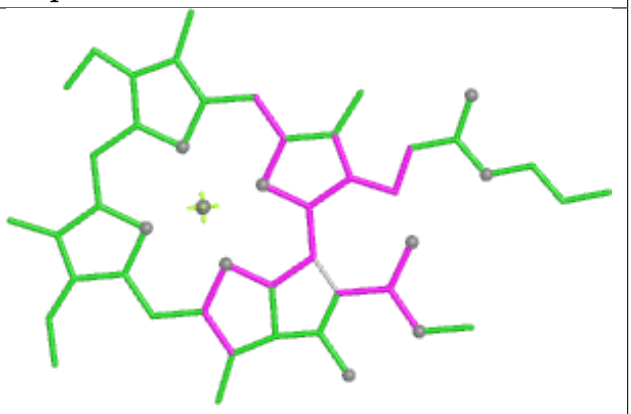
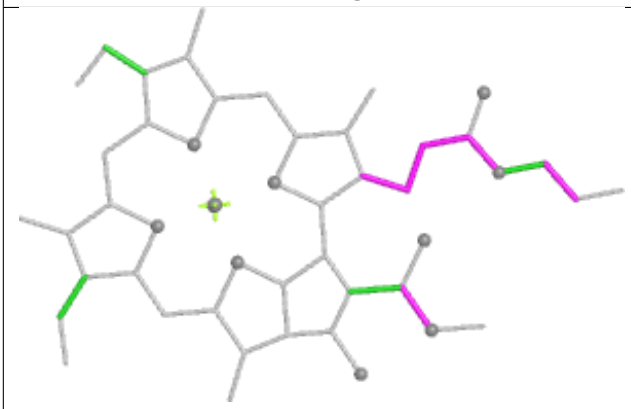
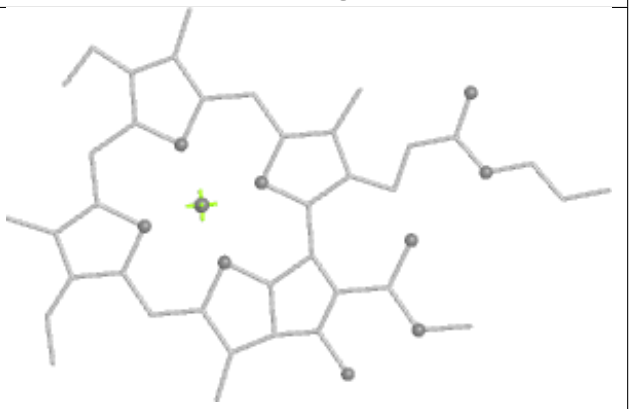
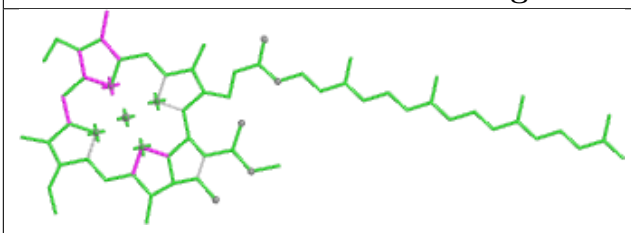
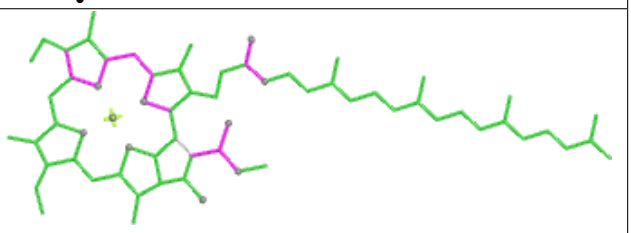
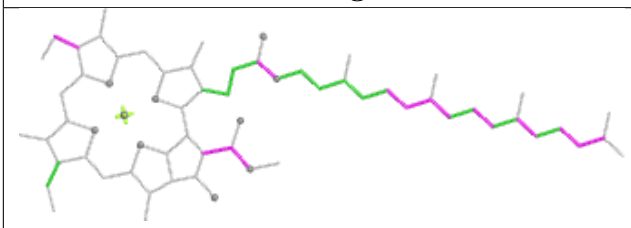
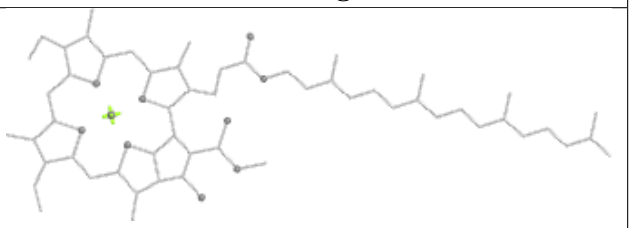


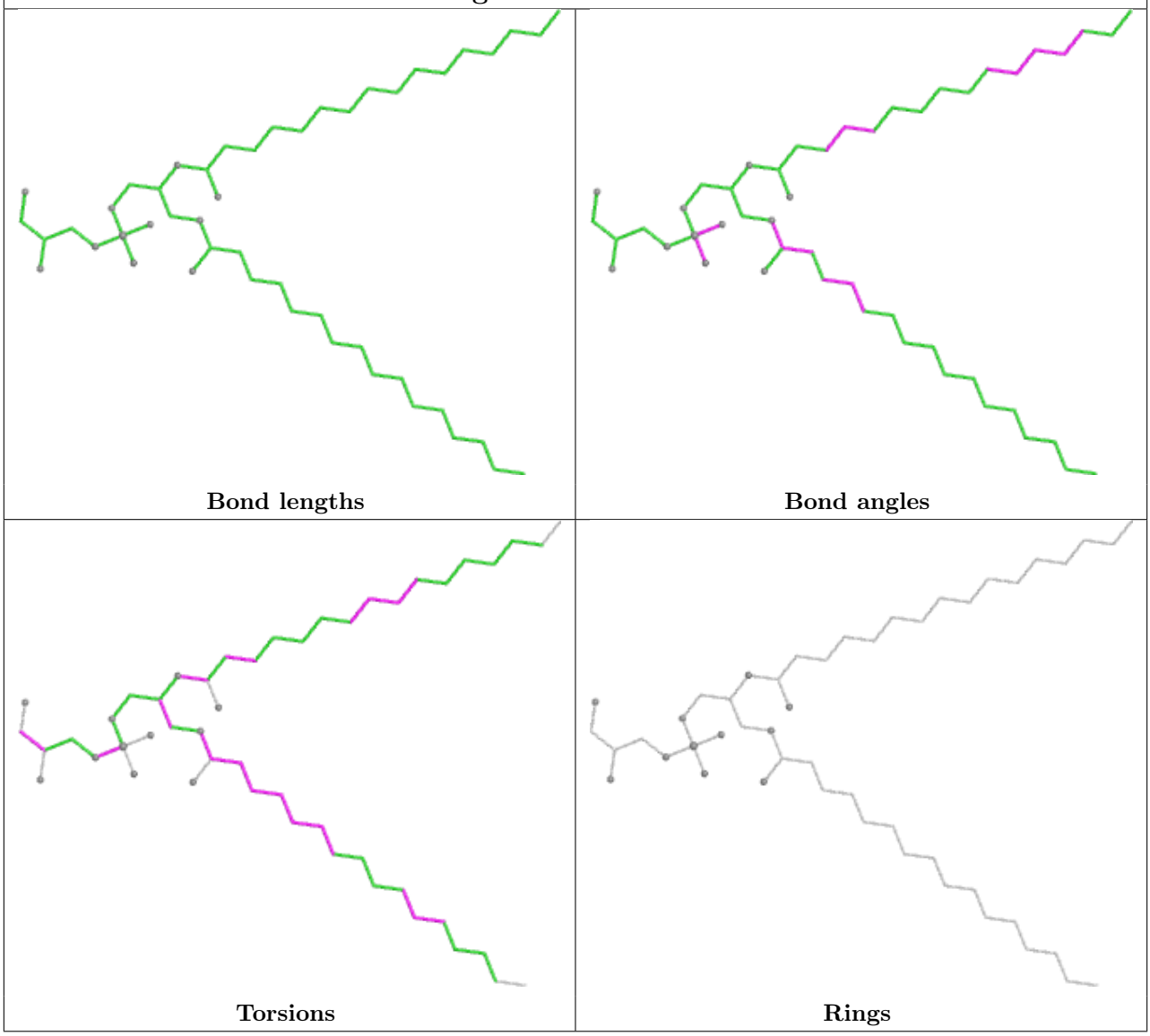
Rings

Ligand CLA AS 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

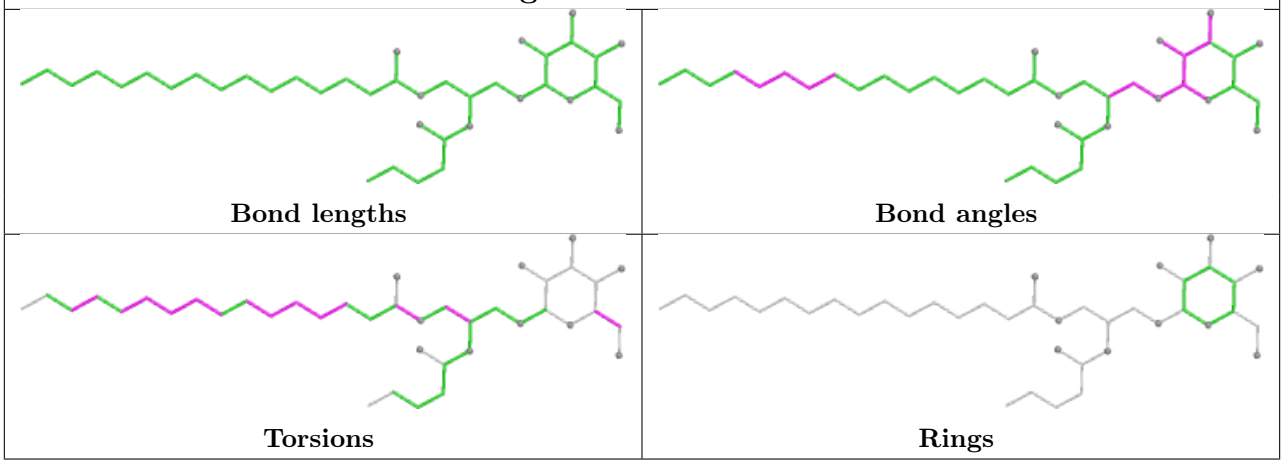
Ligand CLA p 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AQ 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

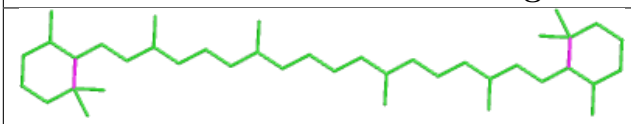
Ligand LHG v 301



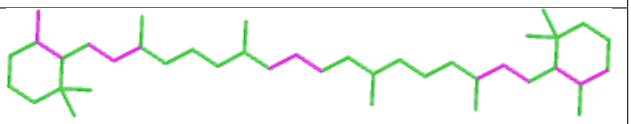
Ligand LMG O 624



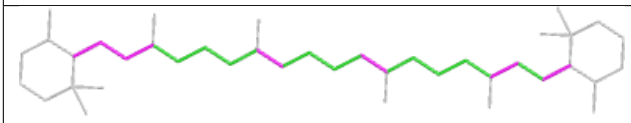
Ligand BCR F 101



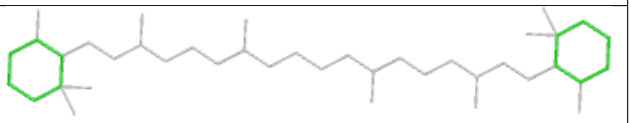
Bond lengths



Bond angles

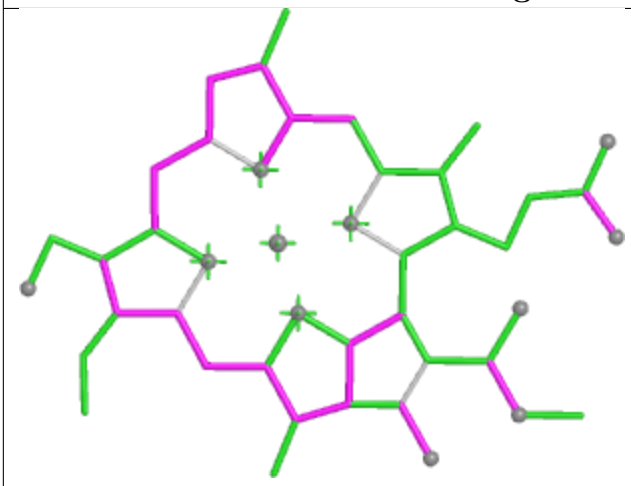


Torsions



Rings

Ligand CHL AS 302



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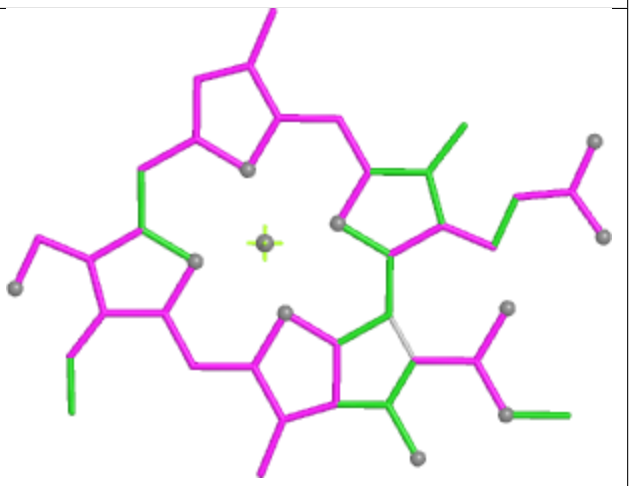
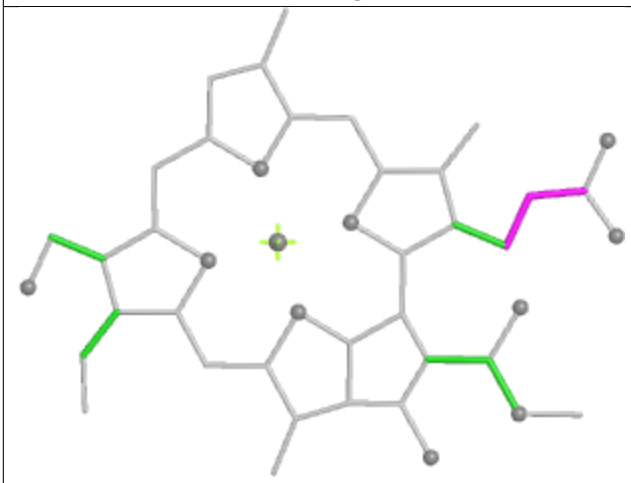


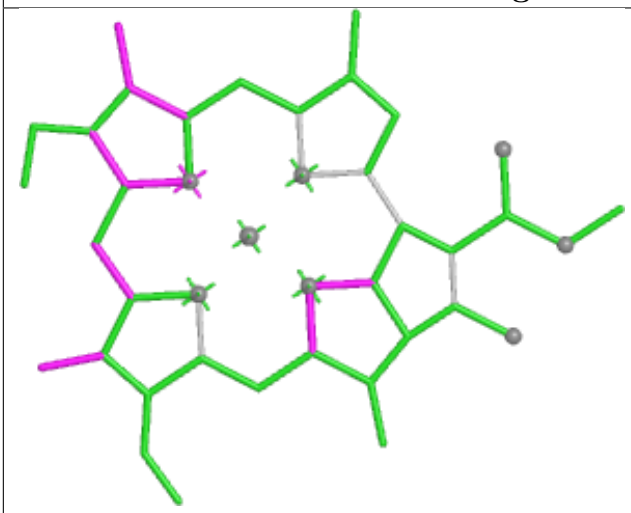
Bond angles



Torsions

Rings

Ligand CLA AF 609



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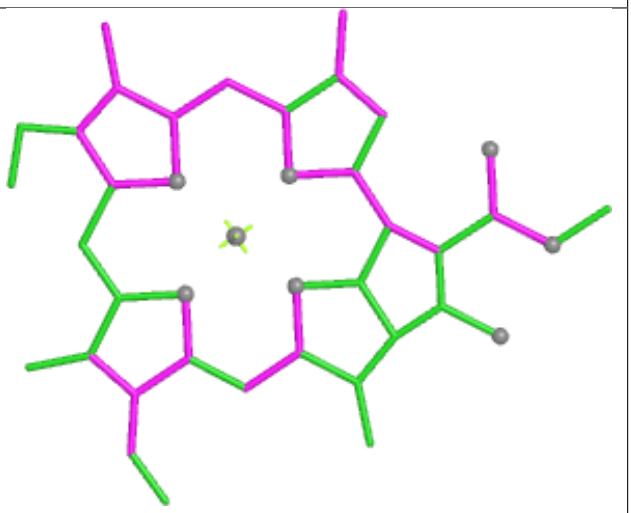
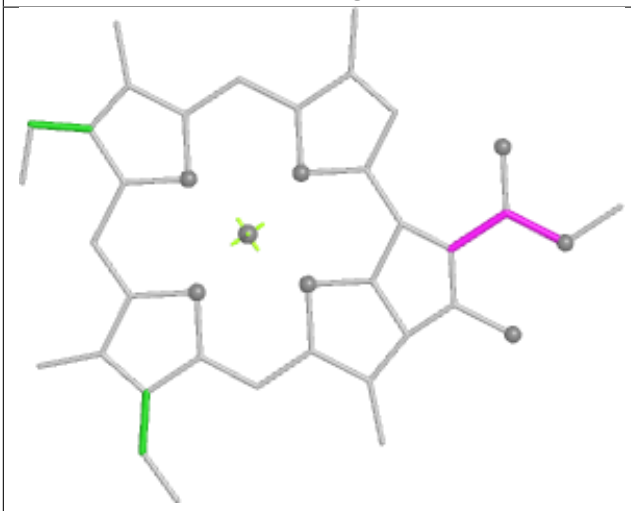


Bond angles



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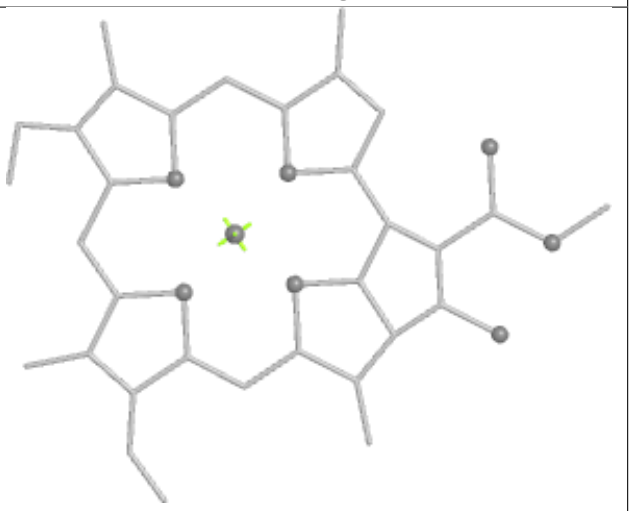
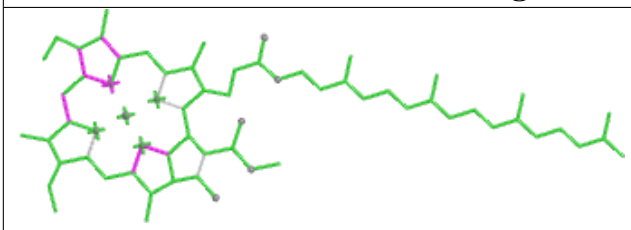
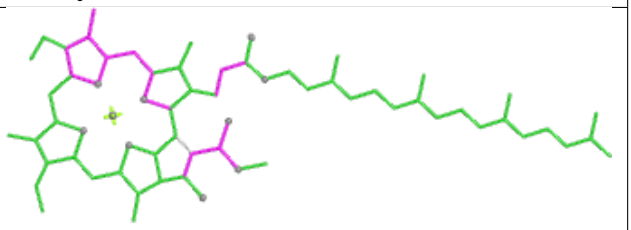


Rings

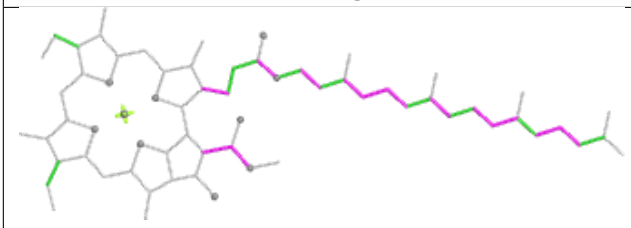
Ligand CLA AQ 610



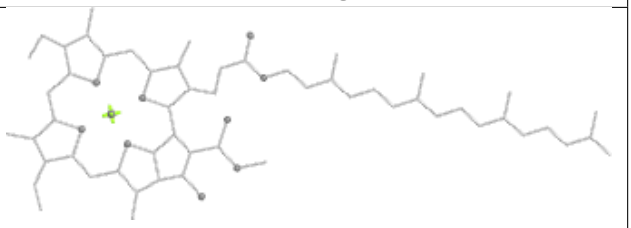
Bond lengths



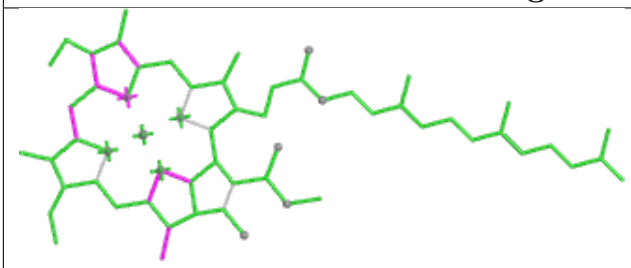
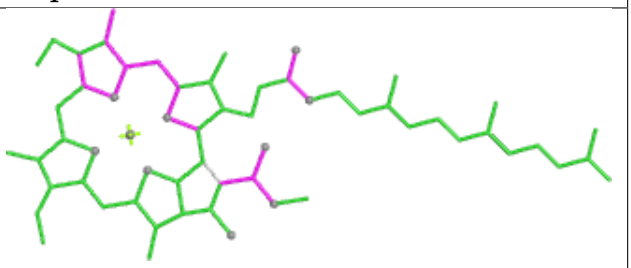
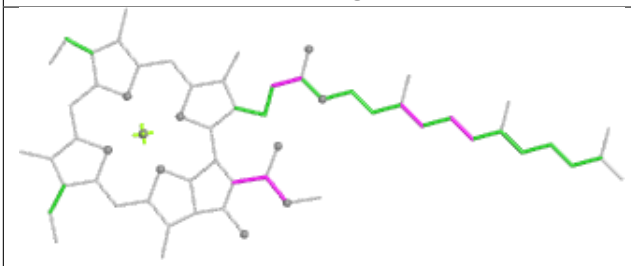
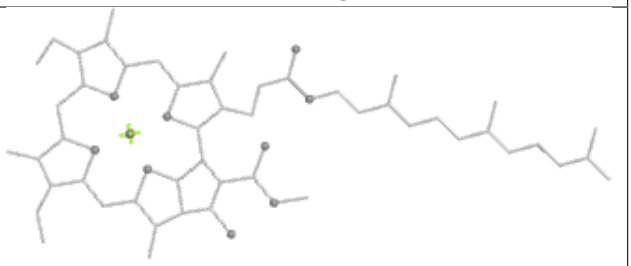
Bond angles



Torsions



Rings

Ligand CLA p 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

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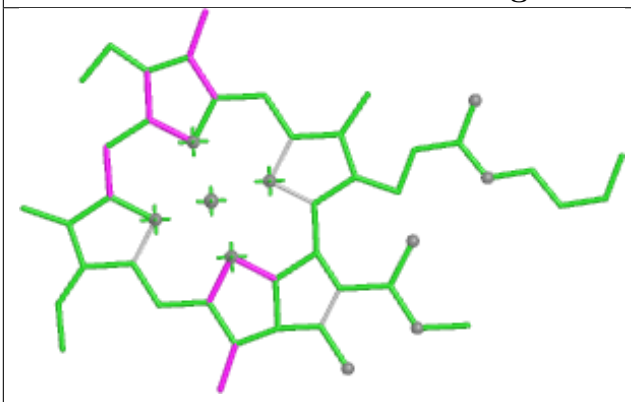
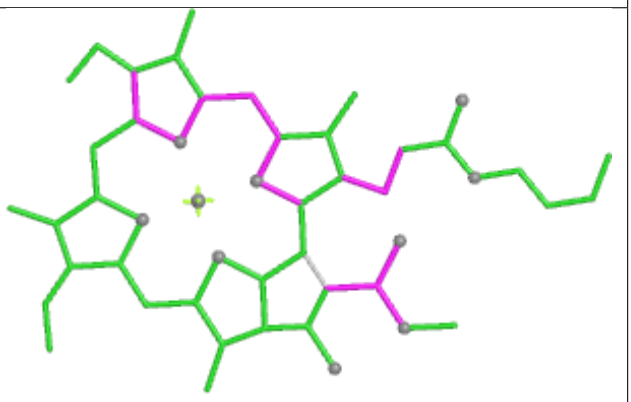
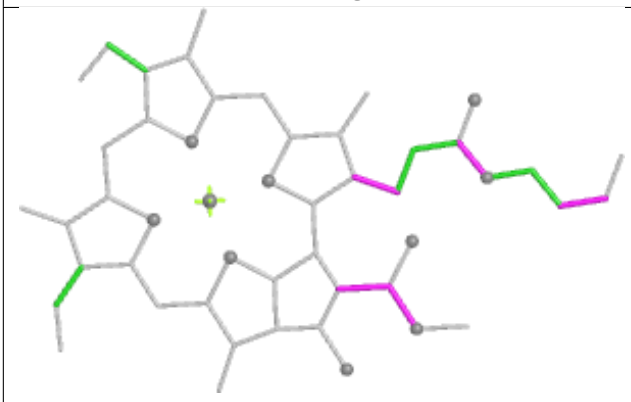
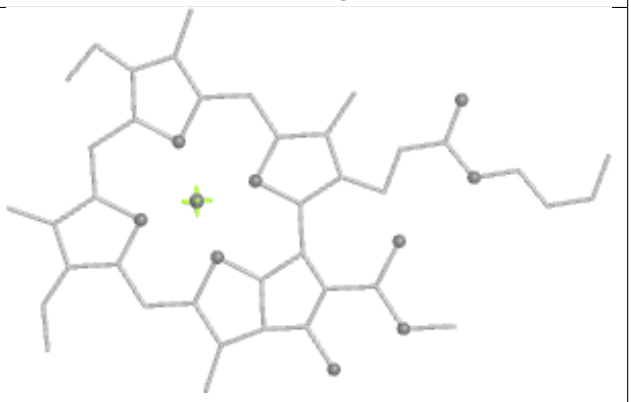
 Bond lengths	 Bond angles
 Torsions	 Rings

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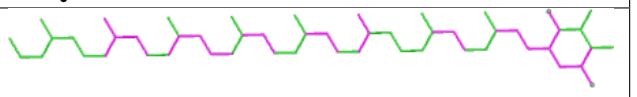
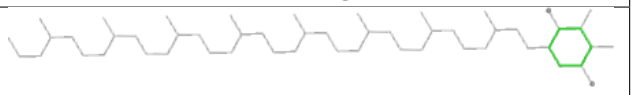
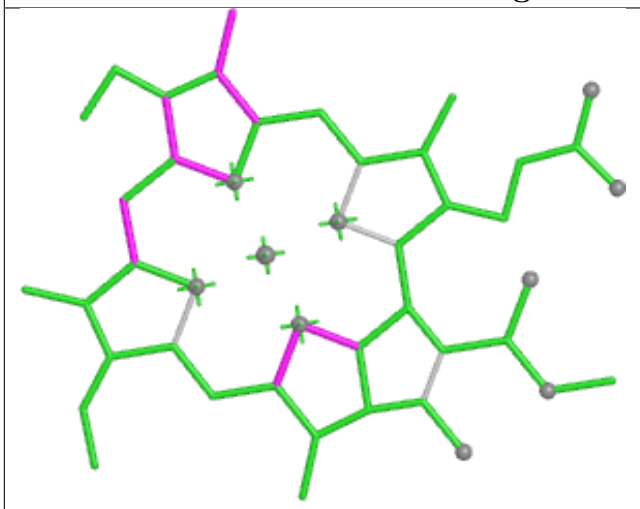
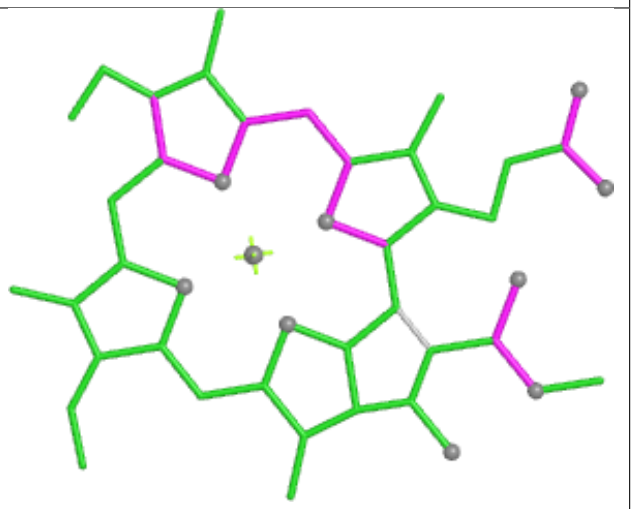
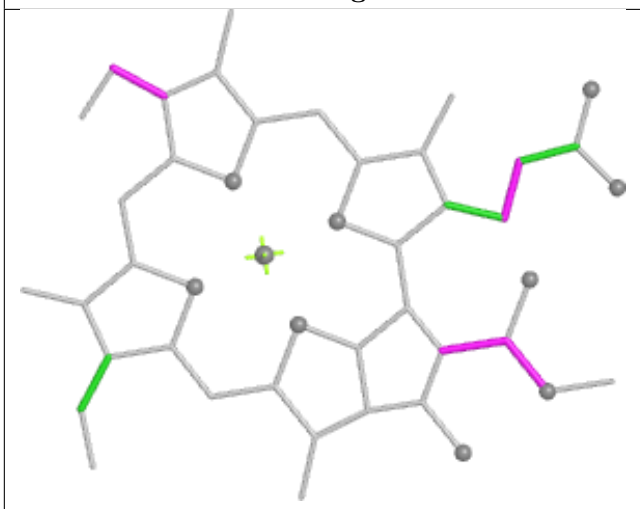
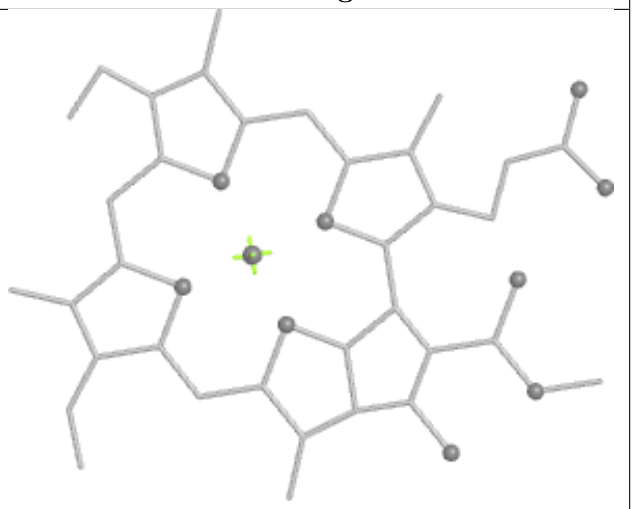
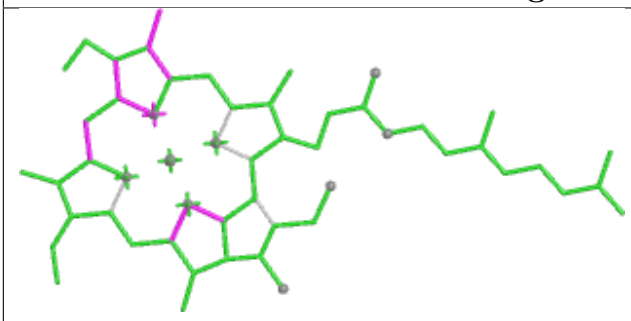
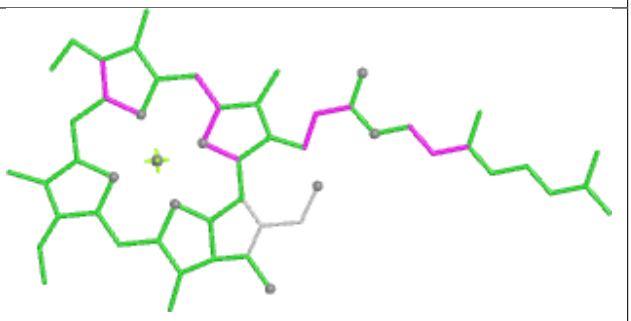
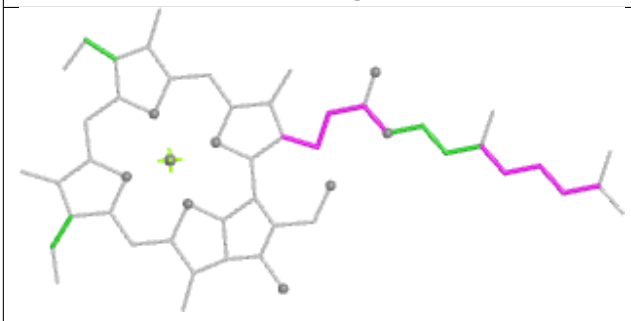
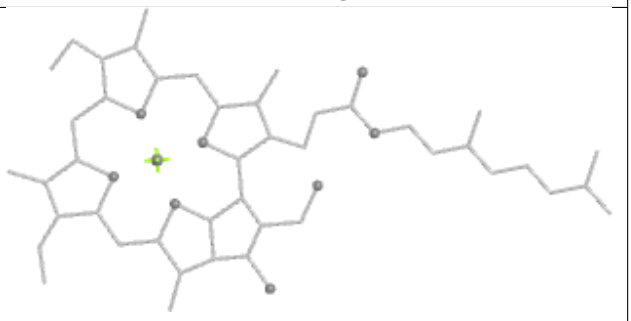
Bond lengths	 Bond angles
Torsions	 Rings

Ligand CLA AE 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA v 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

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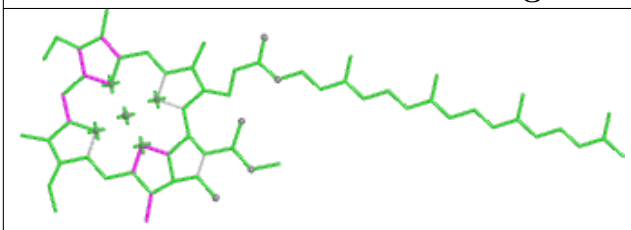
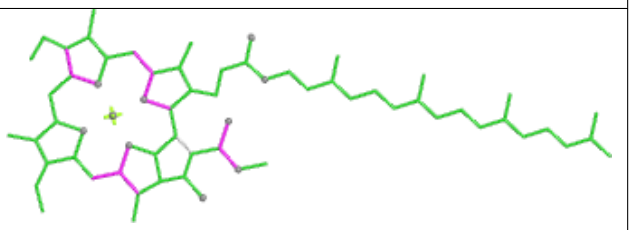
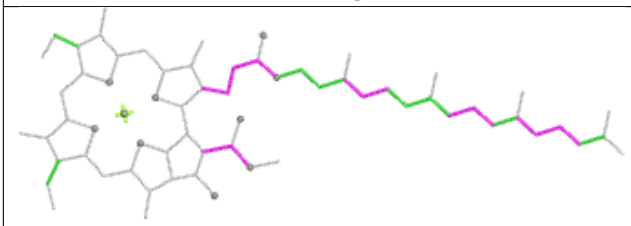
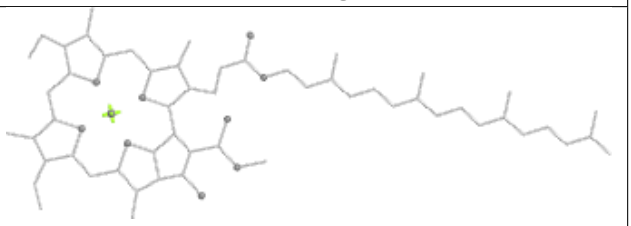
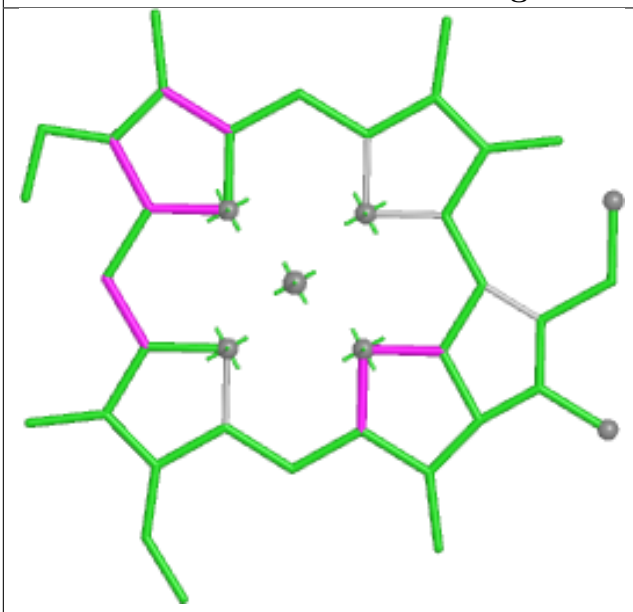
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AR 608



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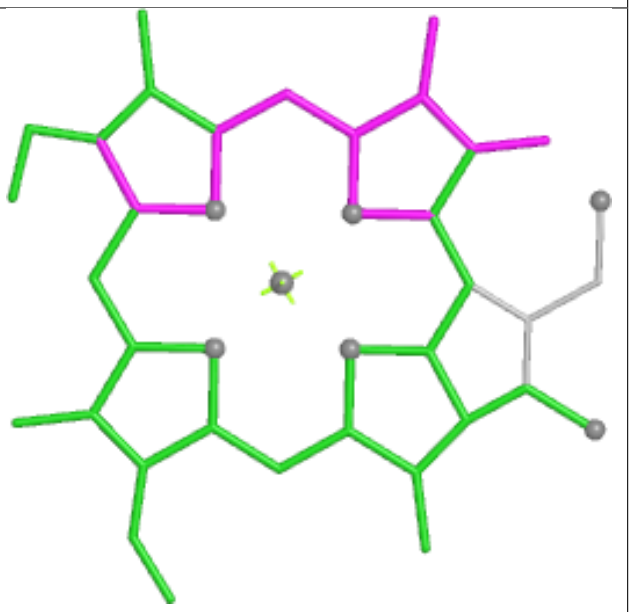

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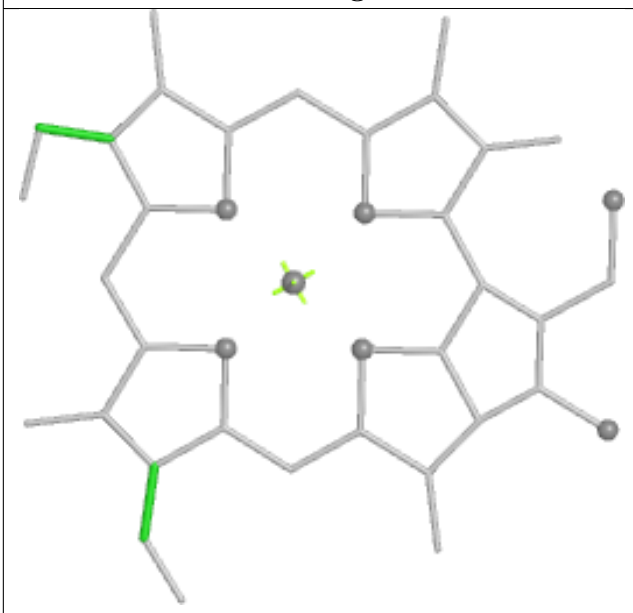

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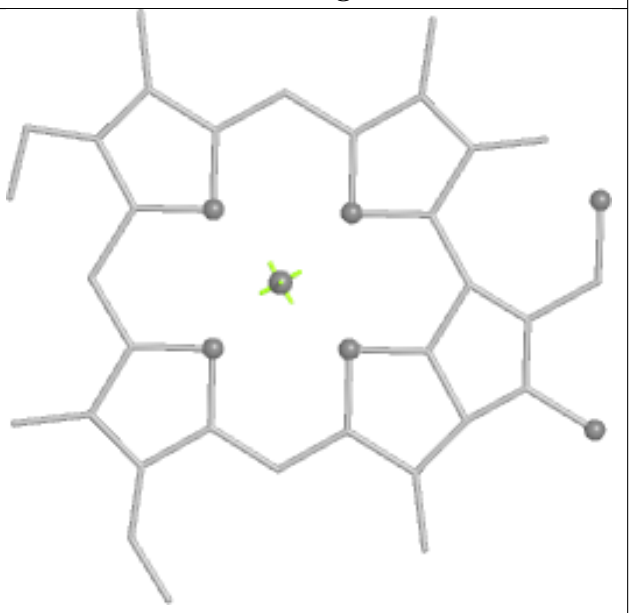
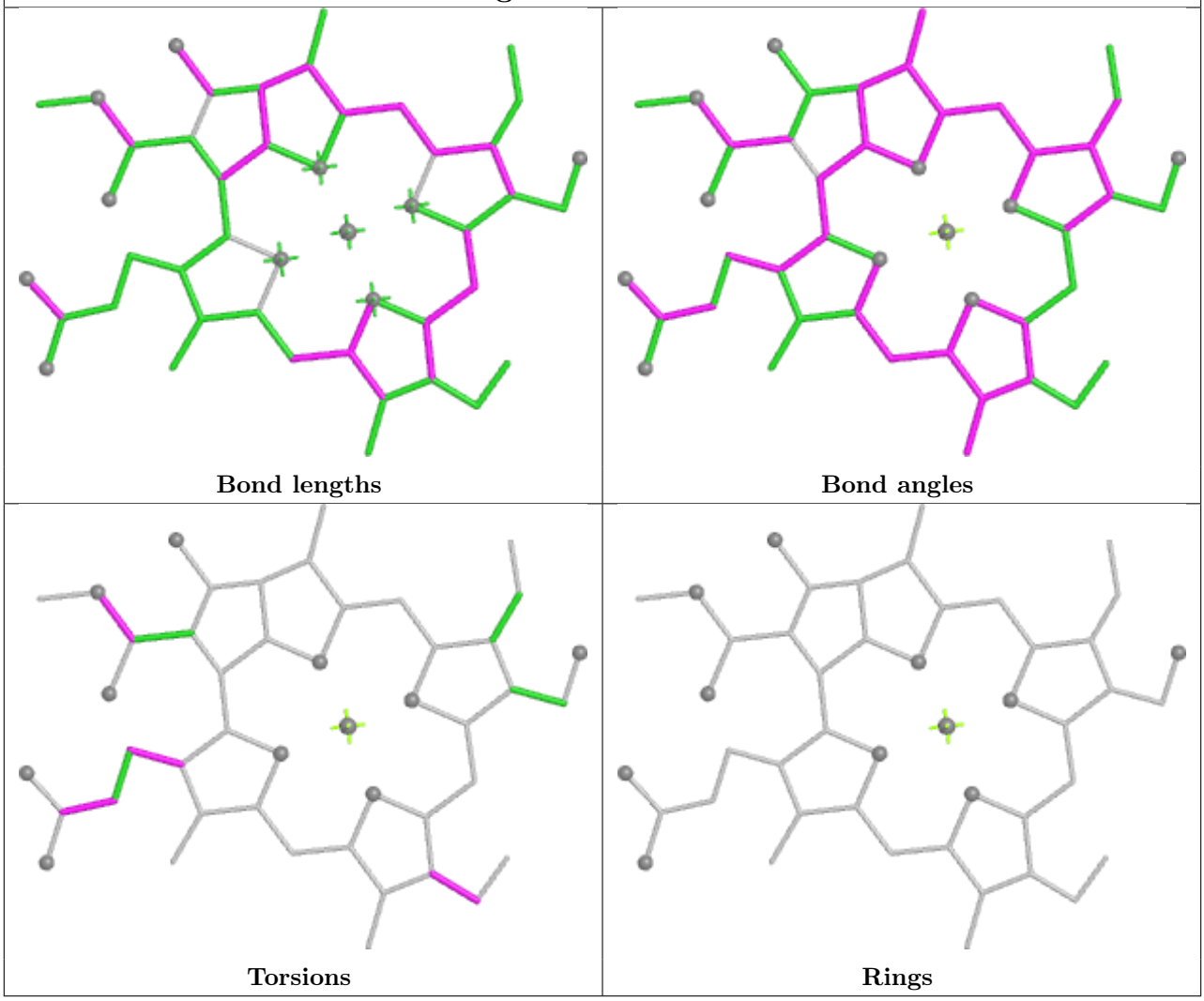
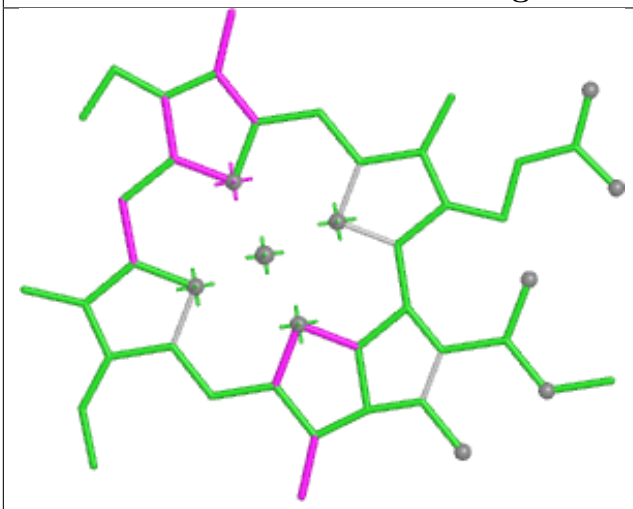


Rings

Ligand CHL 9 605



Ligand CLA AE 604



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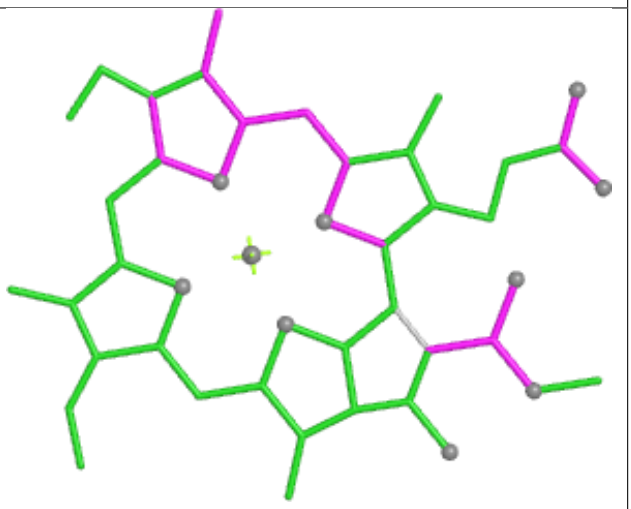

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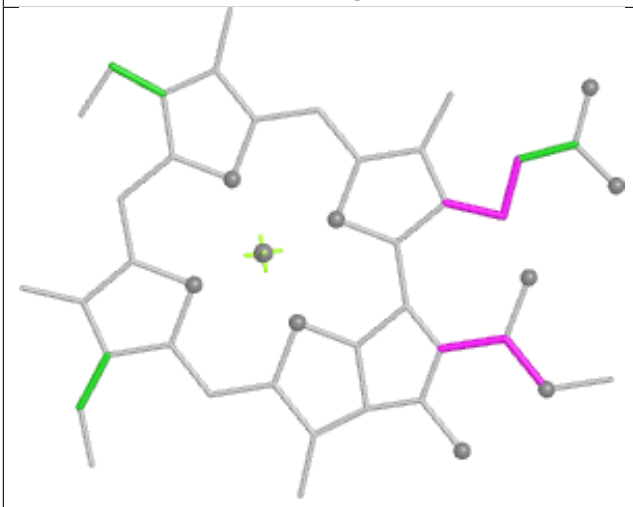
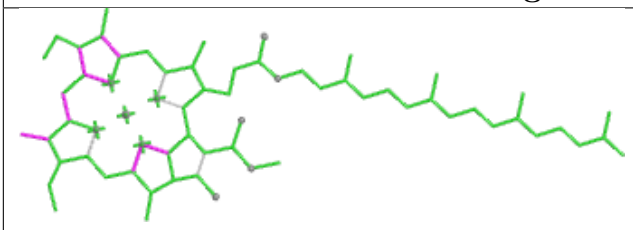


Torsions

Rings

Ligand CLA V 602



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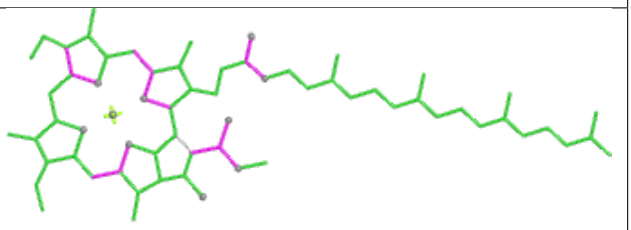
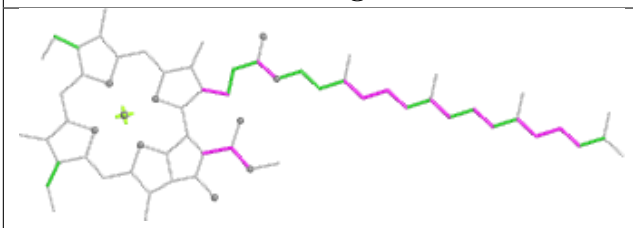


Bond angles



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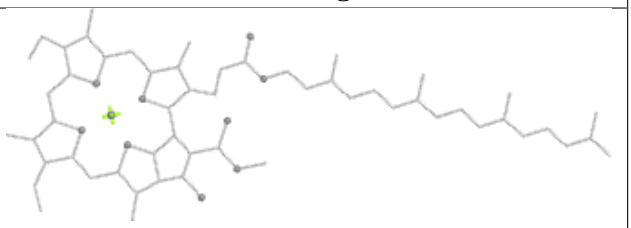
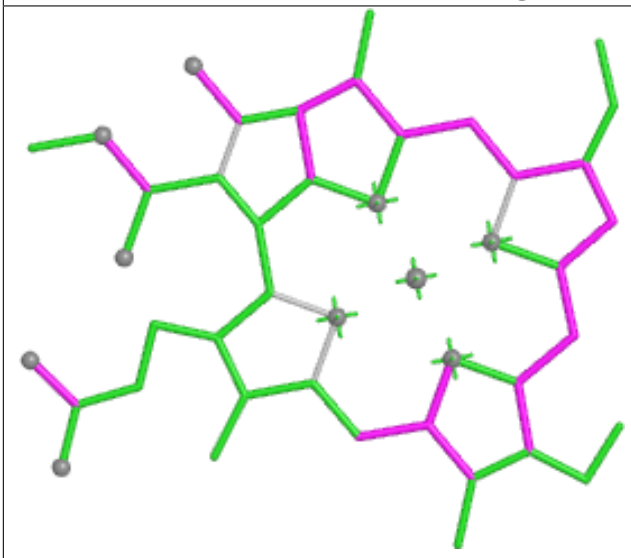


Rings

Ligand CHL AS 308



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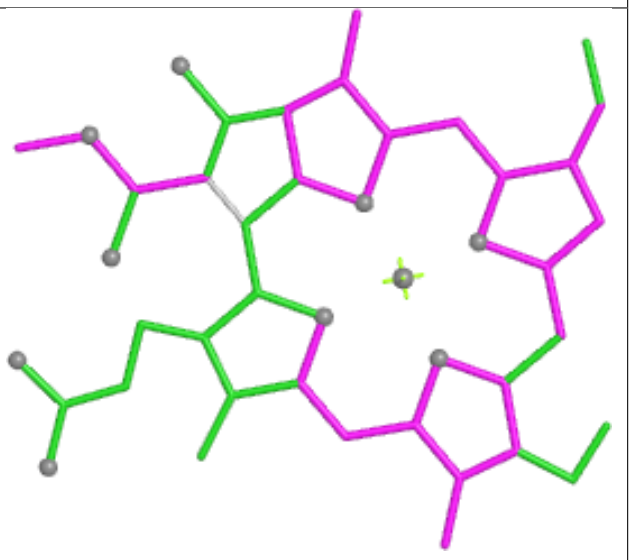

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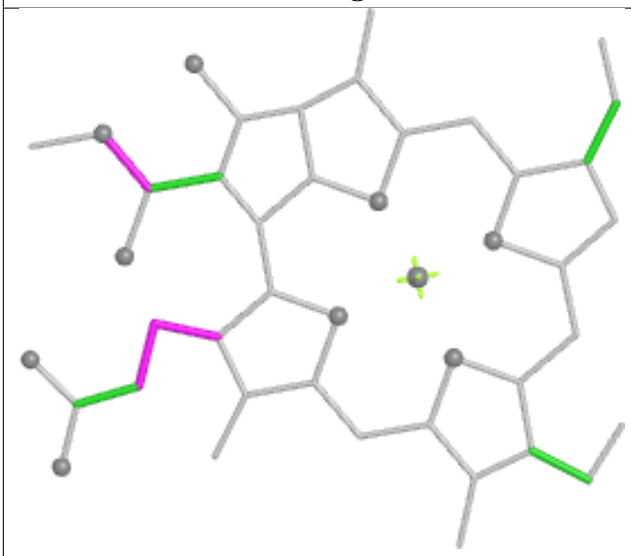
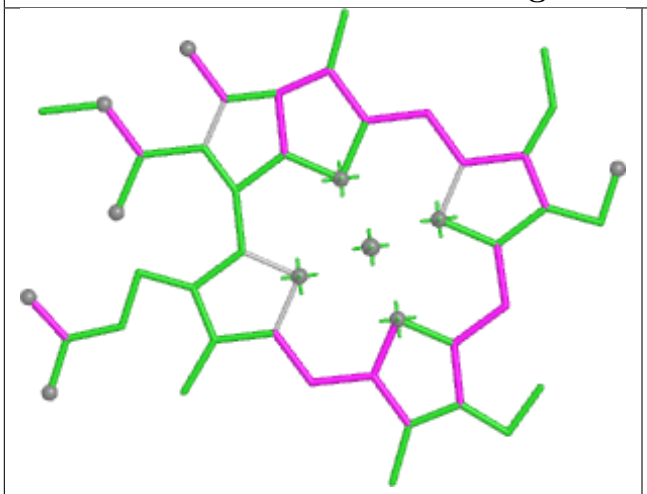


Torsions

Rings

Ligand CHL 0 605



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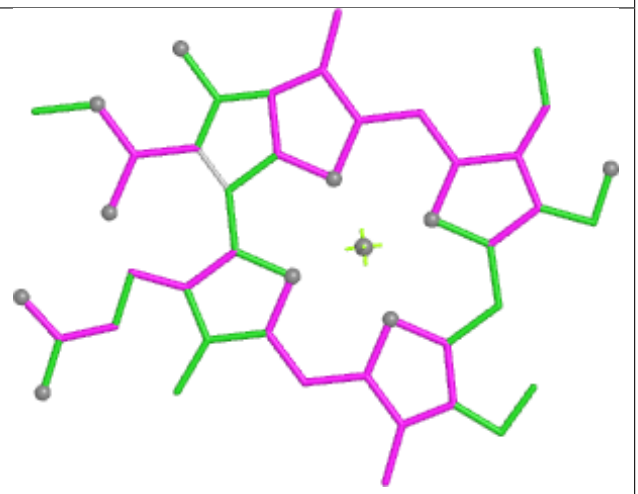

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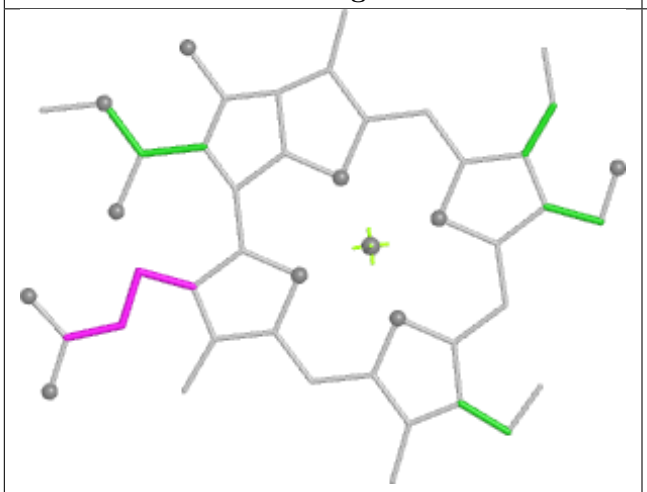

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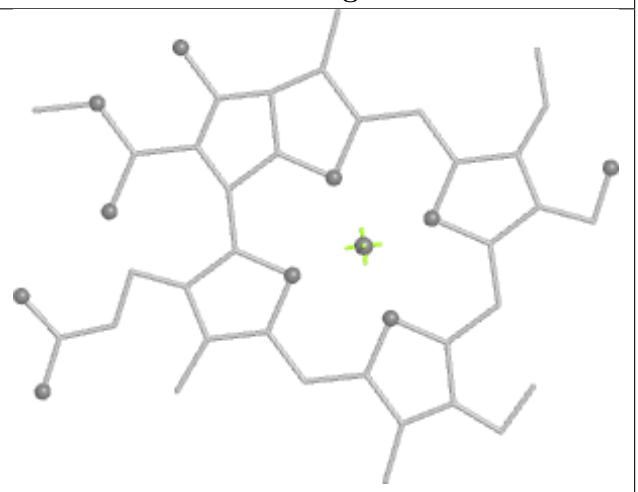
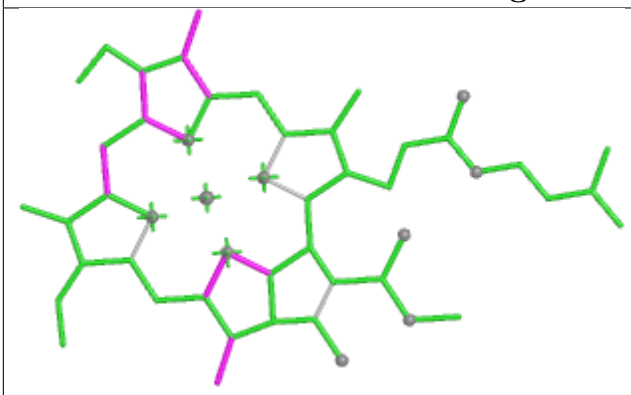
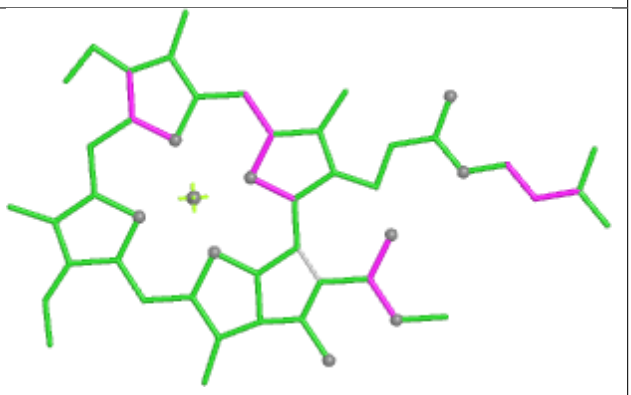
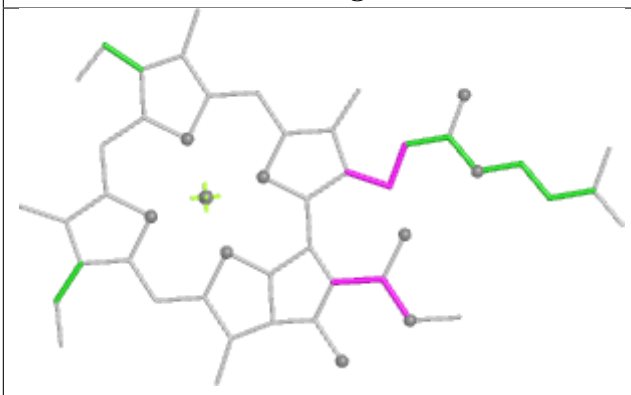
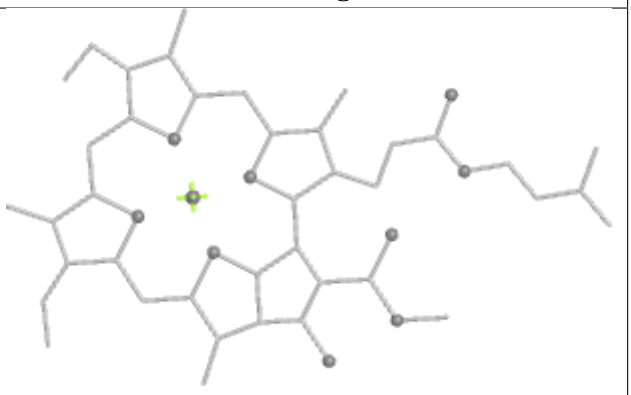
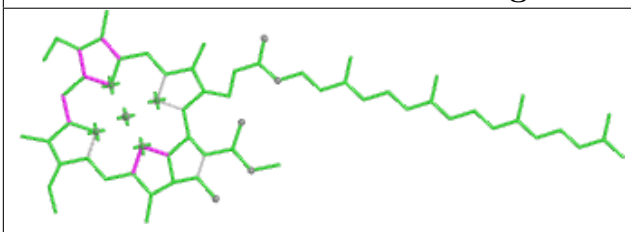
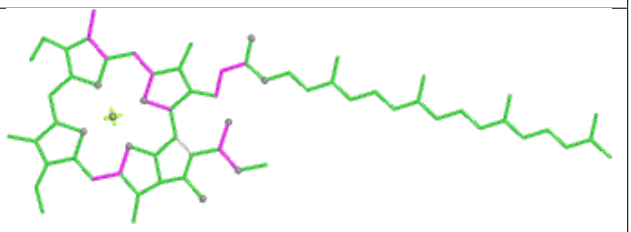
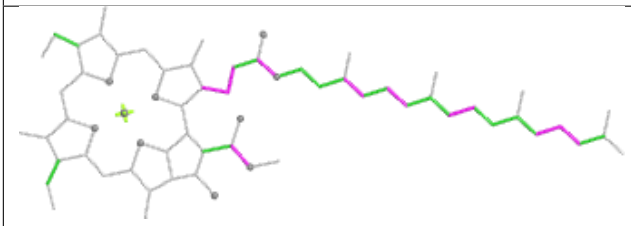
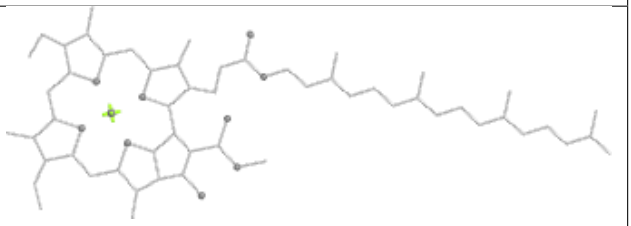
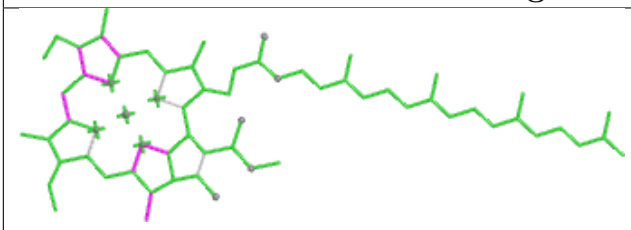


Rings

Ligand CLA AH 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AK 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 602



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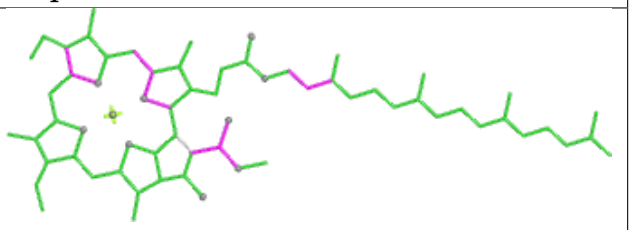
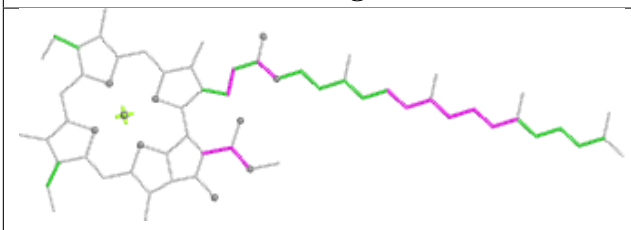


Bond angles



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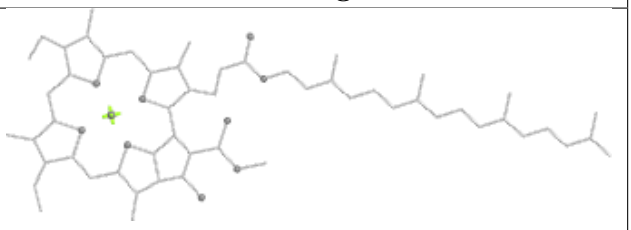
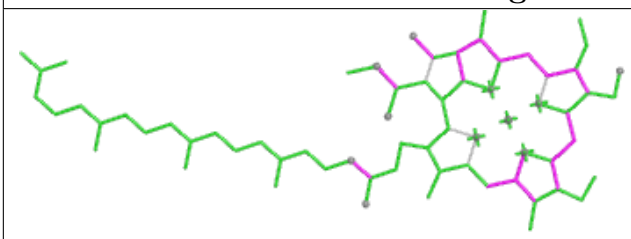
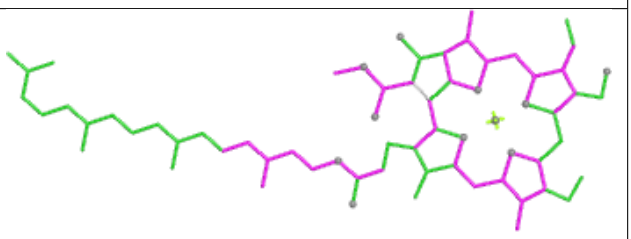


Rings

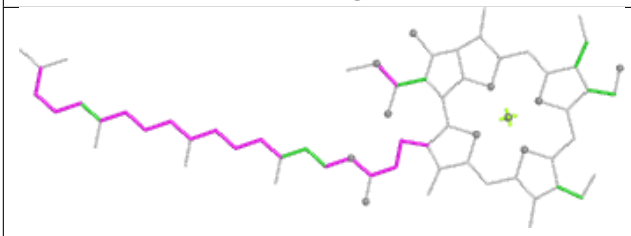
Ligand CHL AH 601



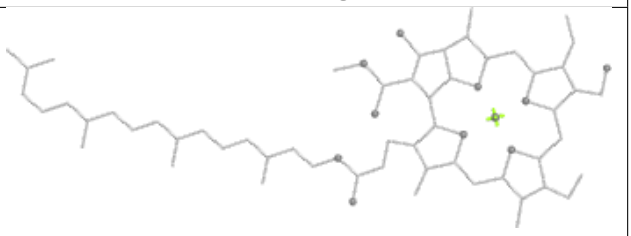
Bond lengths



Bond angles

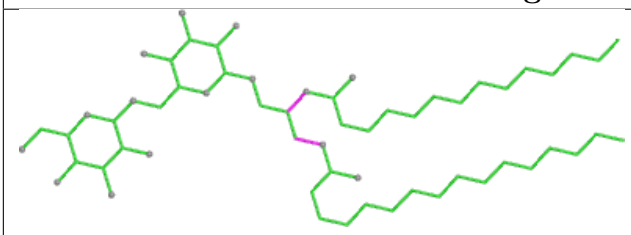


Torsions

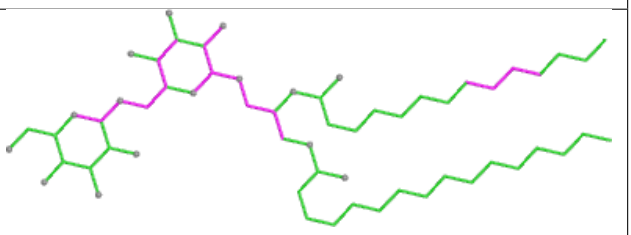


Rings

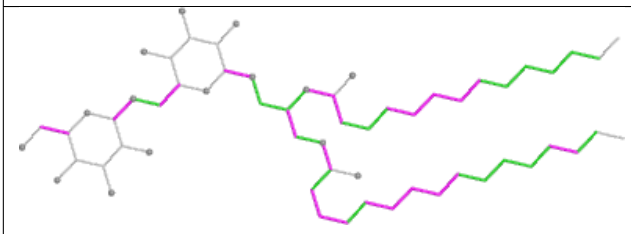
Ligand DGD J 411



Bond lengths



Bond angles



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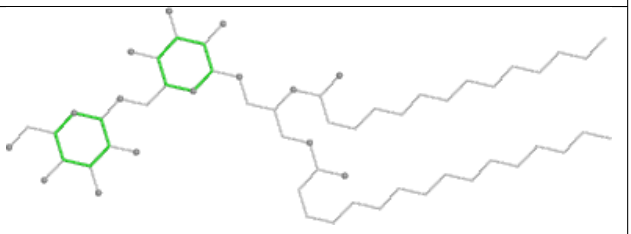
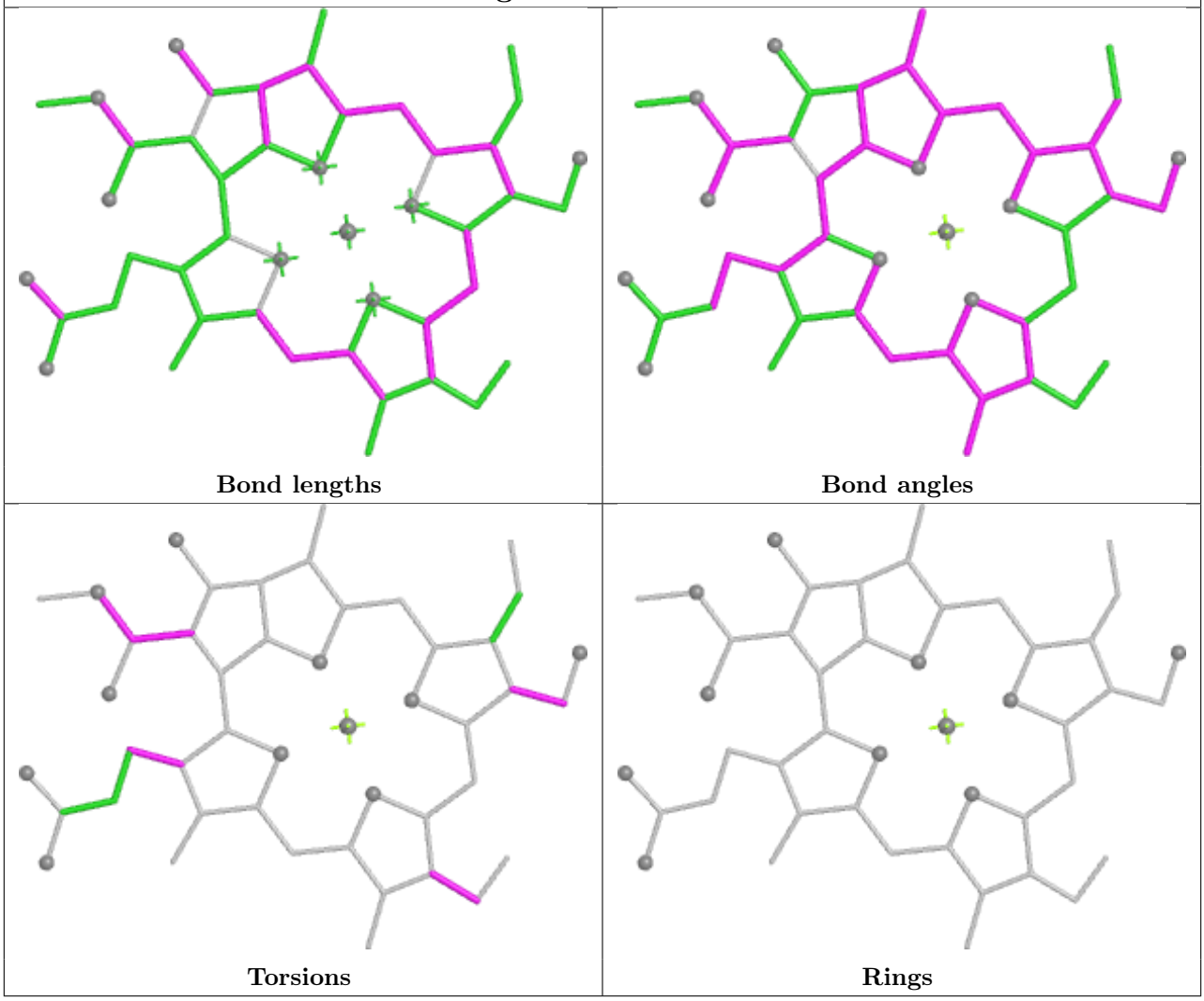
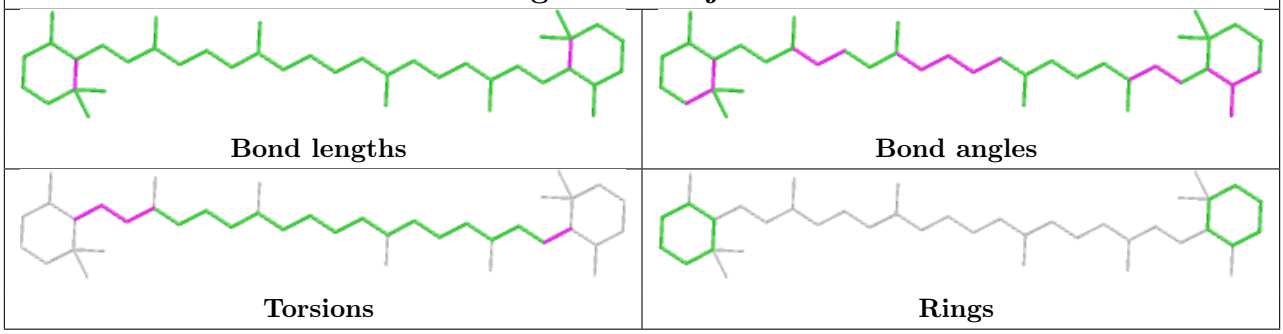


Rings

Ligand CHL 9 606



Ligand BCR j 101



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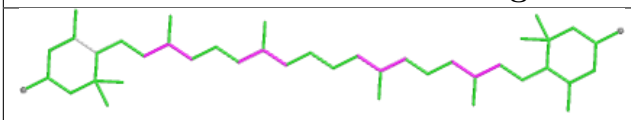
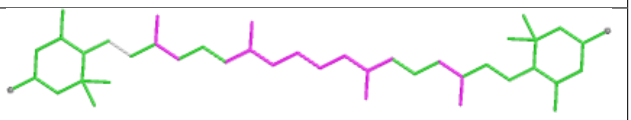
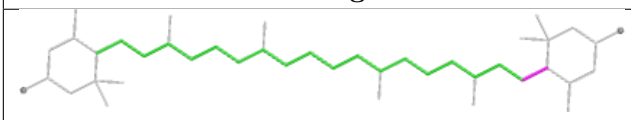
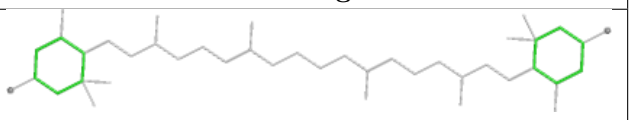
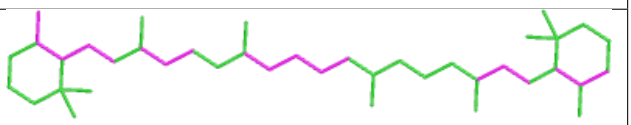
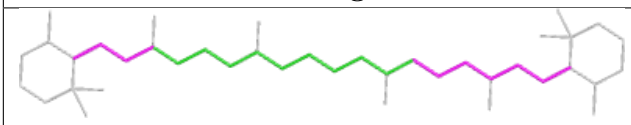
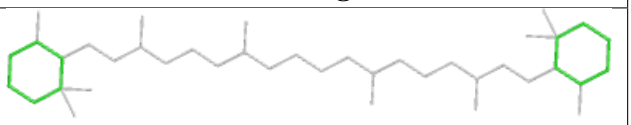
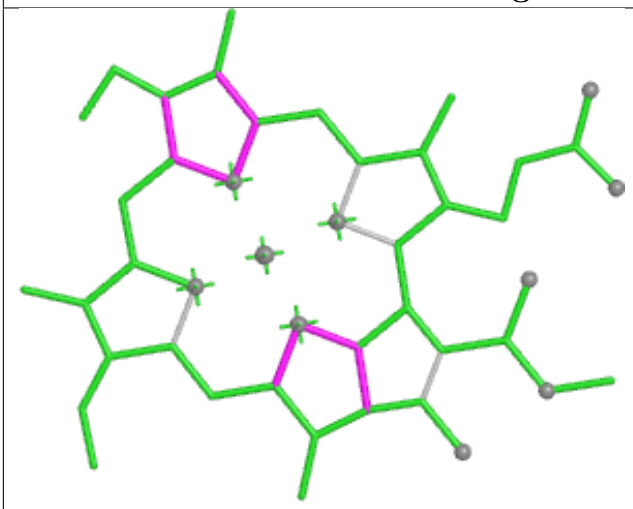
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR AB 612	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AF 610



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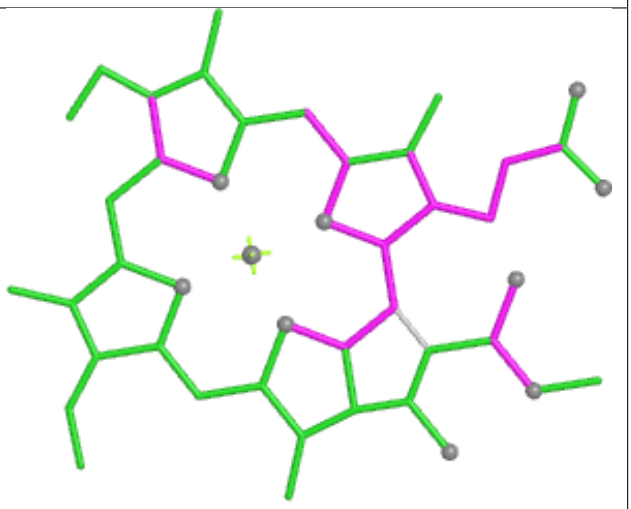
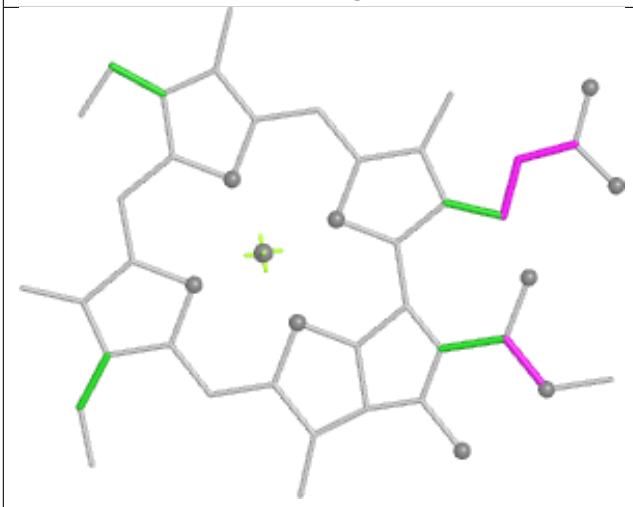


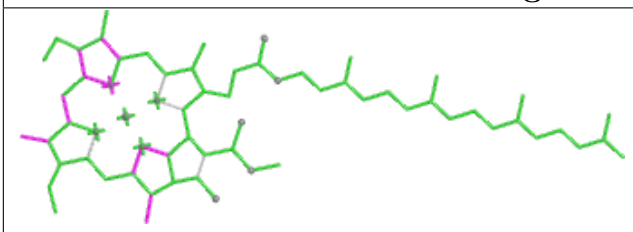
Bond angles



Torsions

Rings

Ligand CLA Q 403



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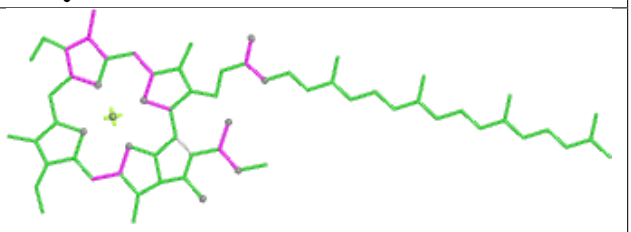
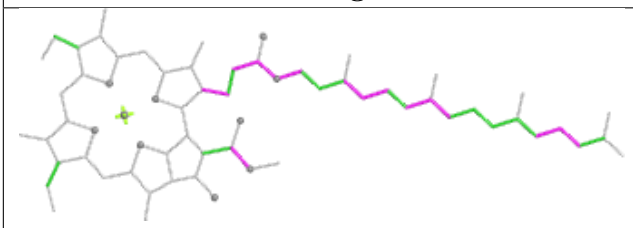


Bond angles



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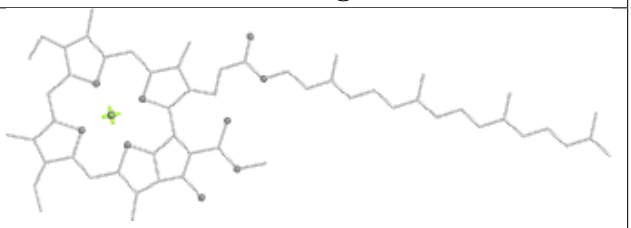
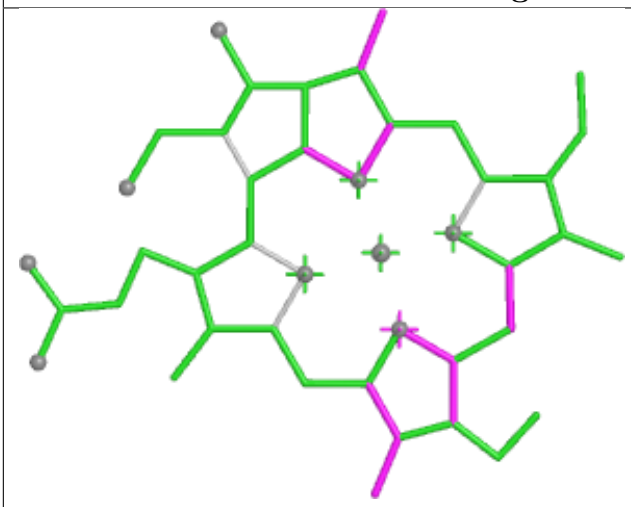
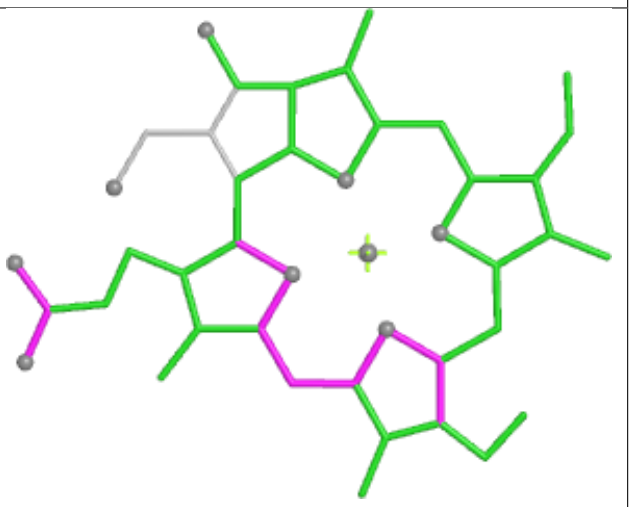
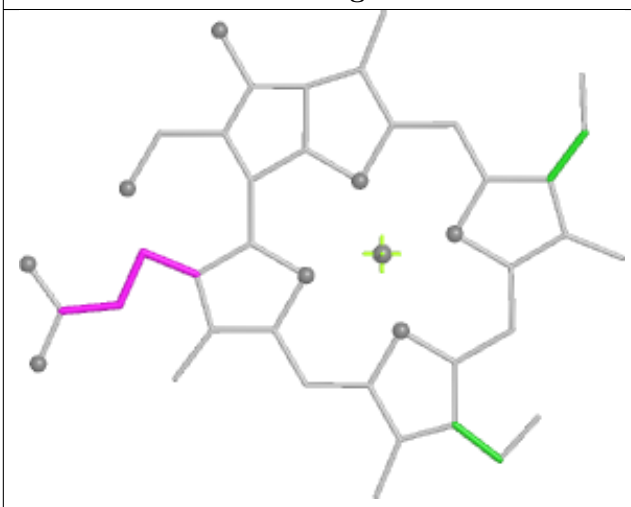
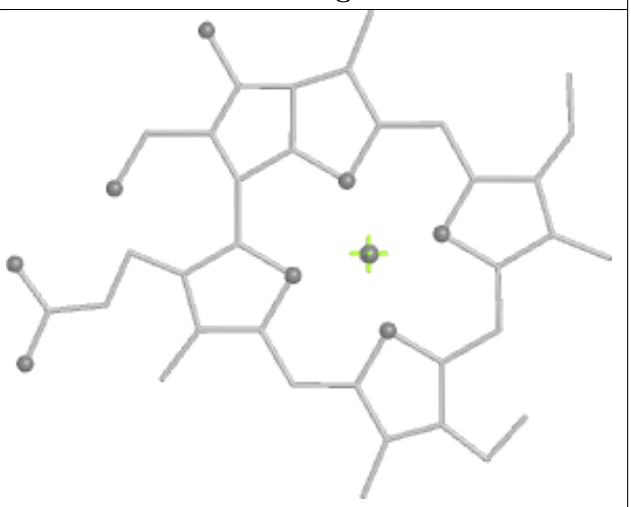


Rings

Ligand CLA AC 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

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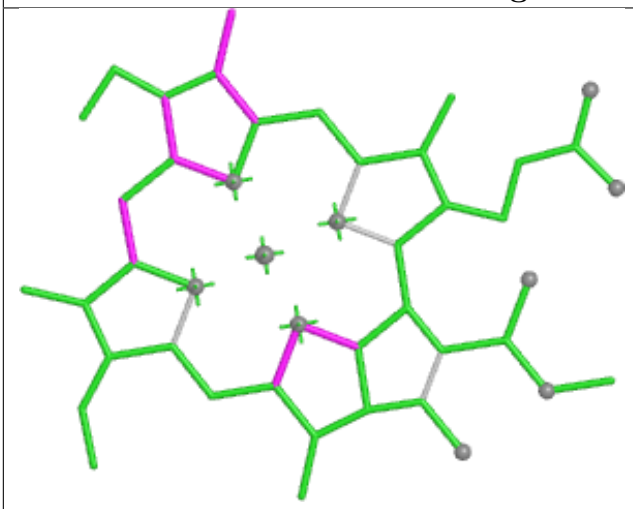

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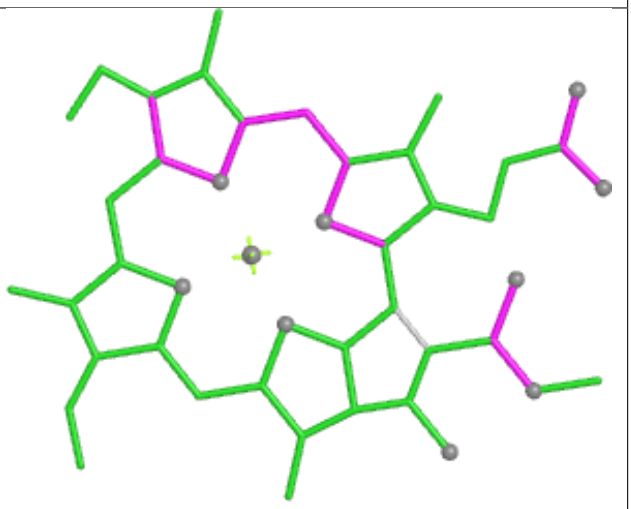
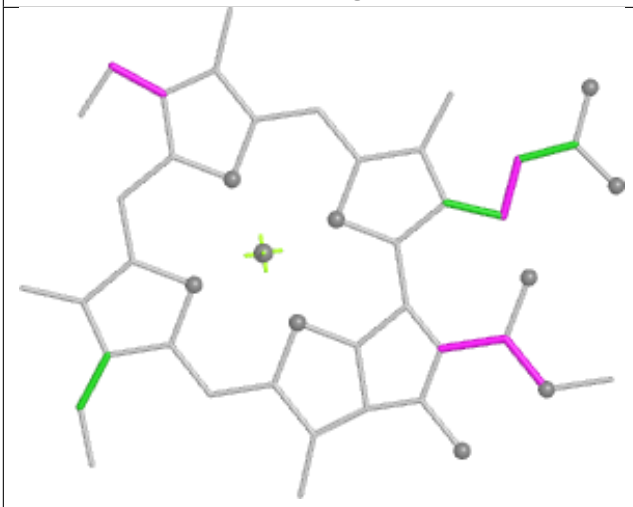


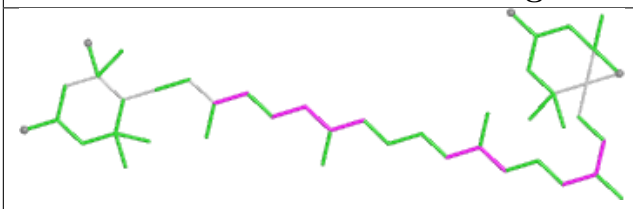
Bond angles



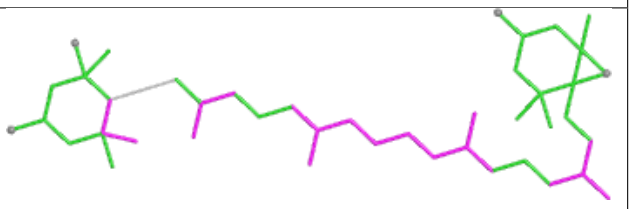
Torsions

Rings

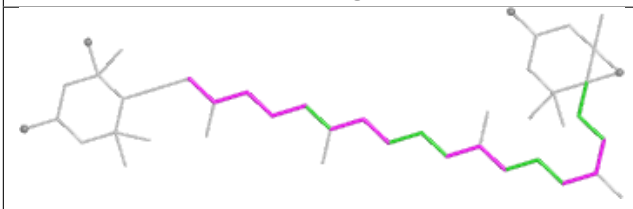
Ligand NEX v 317



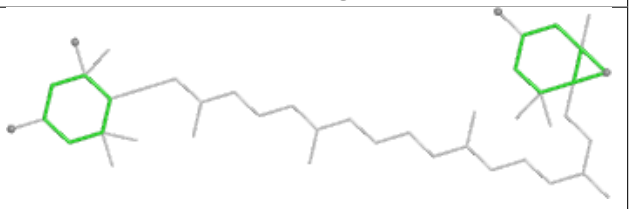
Bond lengths



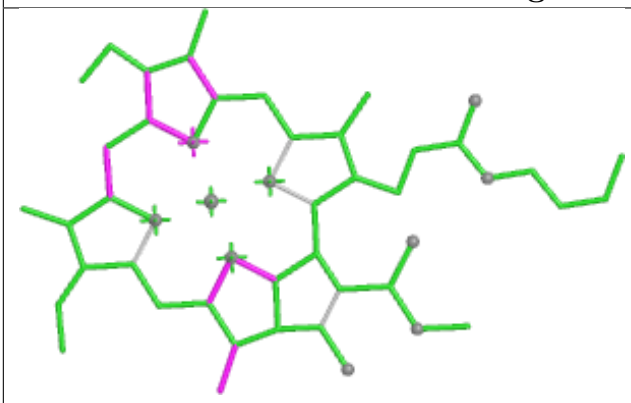
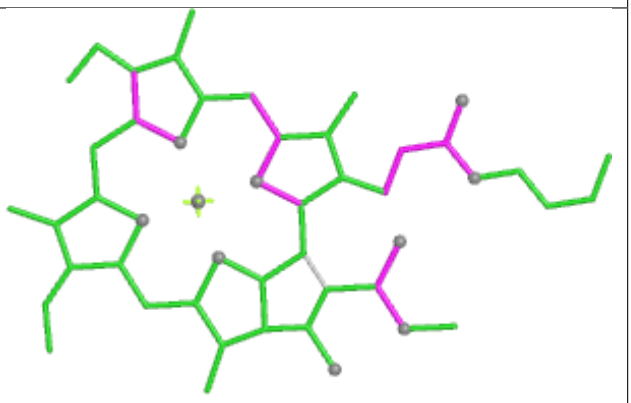
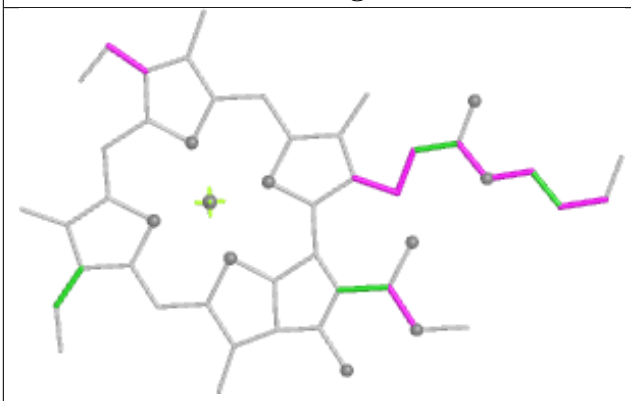
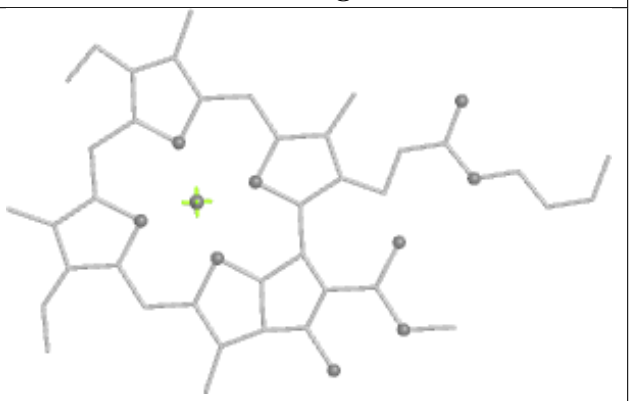
Bond angles

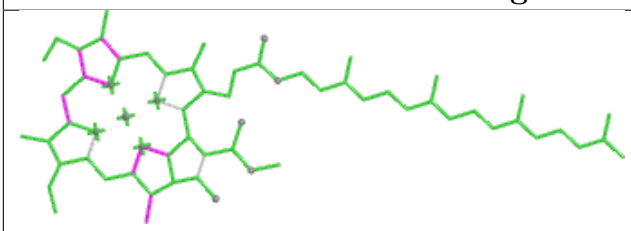
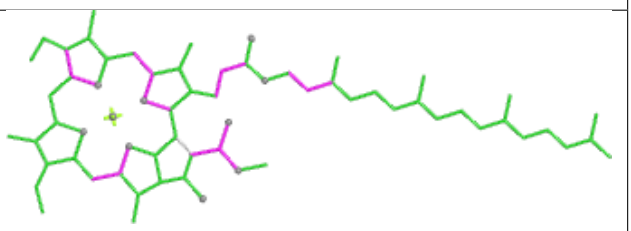
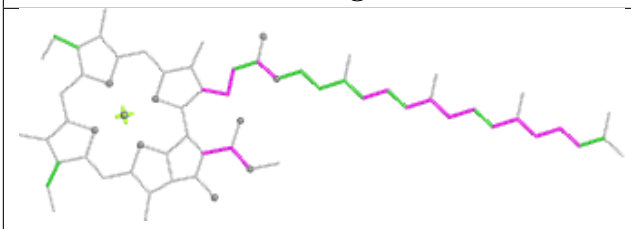
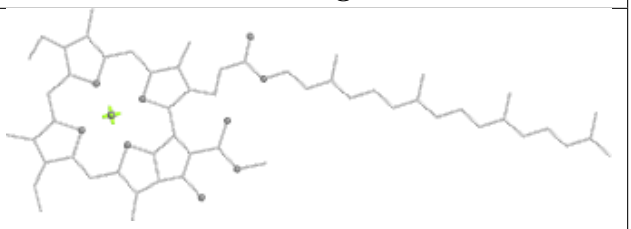


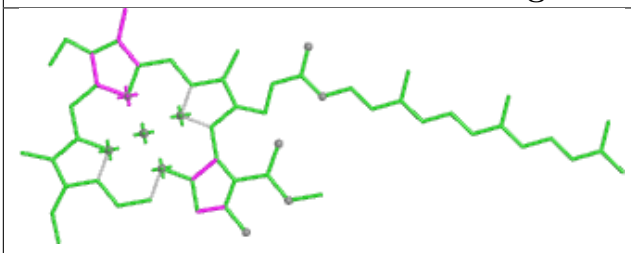
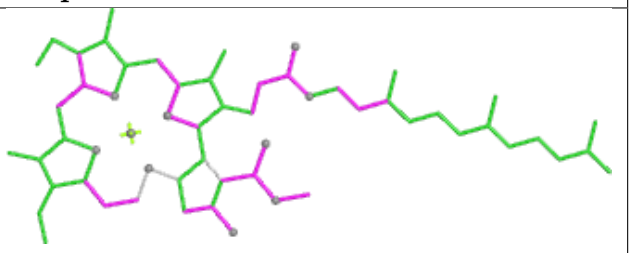
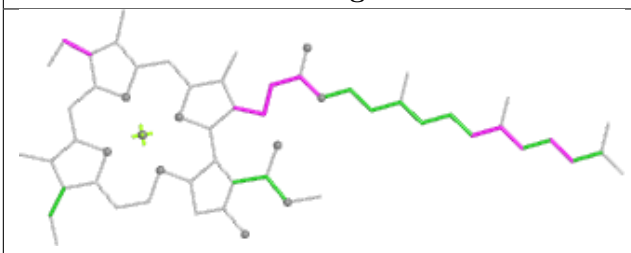
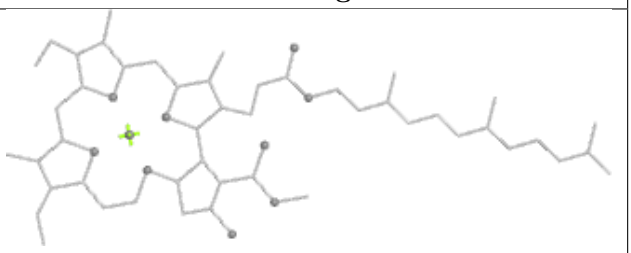
Torsions

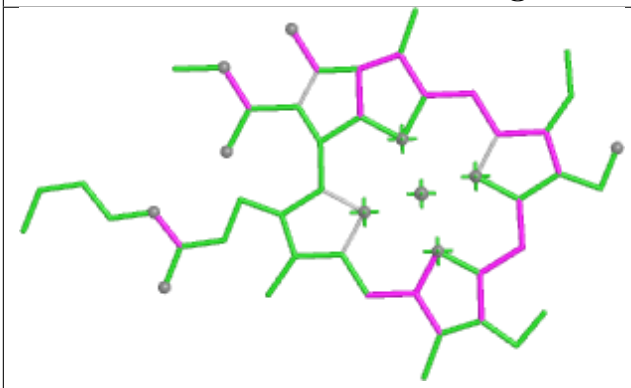
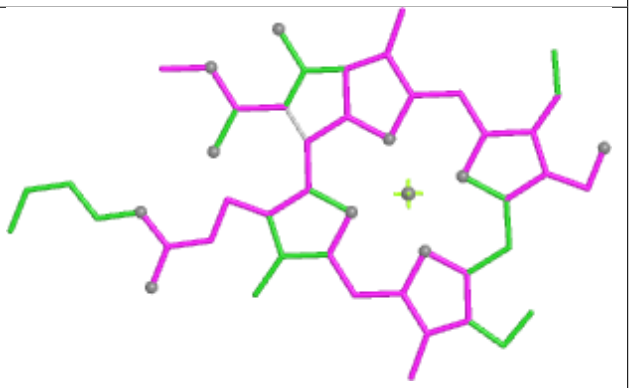
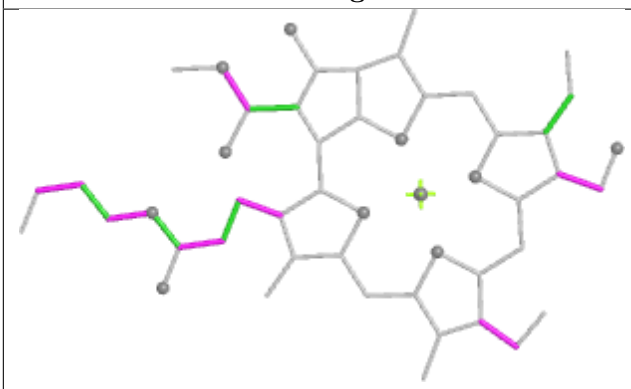
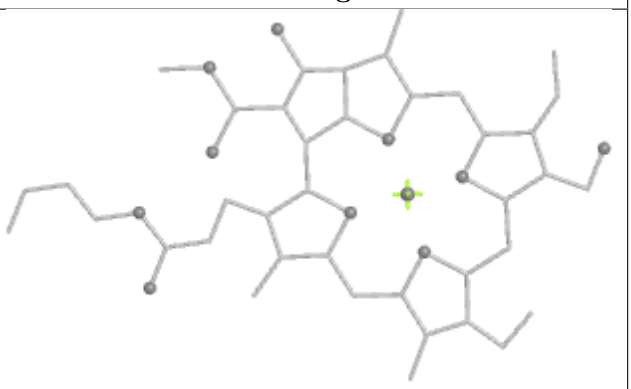


Rings

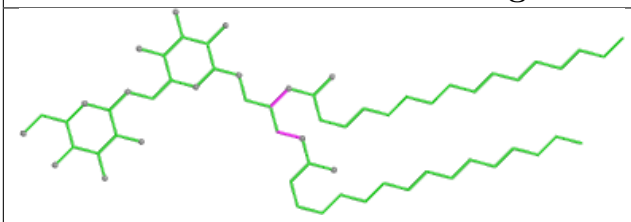
Ligand CLA v 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AU 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

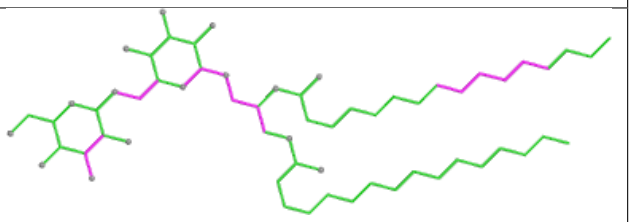
Ligand CLA q 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL AN 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

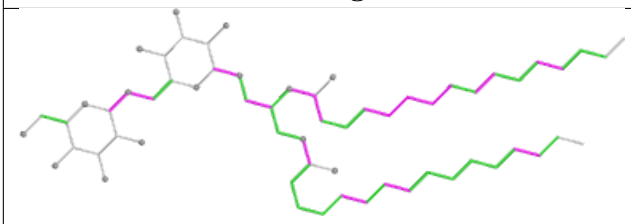
Ligand DGD AL 518



Bond lengths



Bond angles



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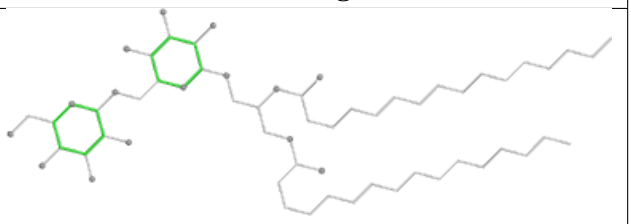
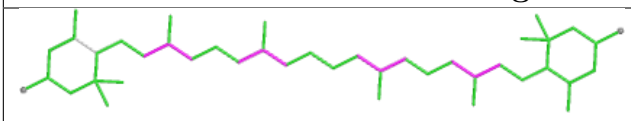
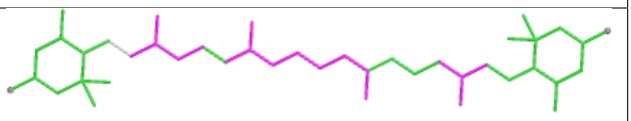


Rings

Ligand LUT AE 614

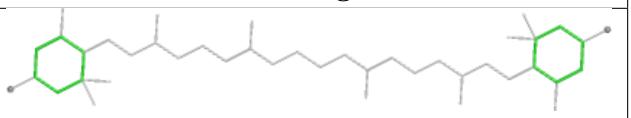


Bond lengths



Bond angles

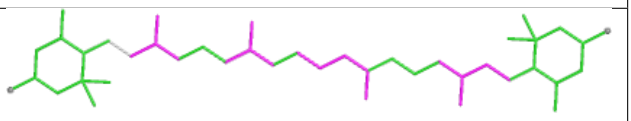
Torsions



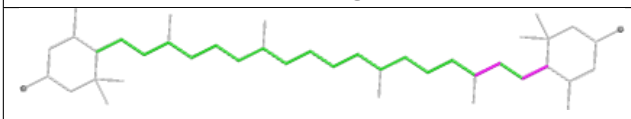
Rings

Ligand LUT AA 614

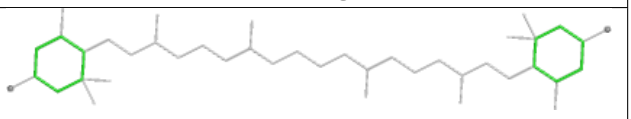
Bond lengths



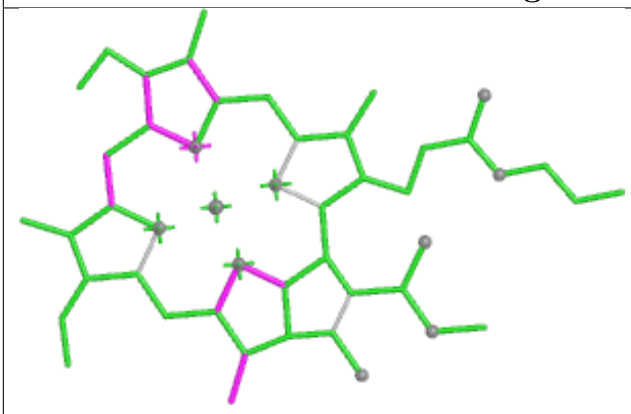
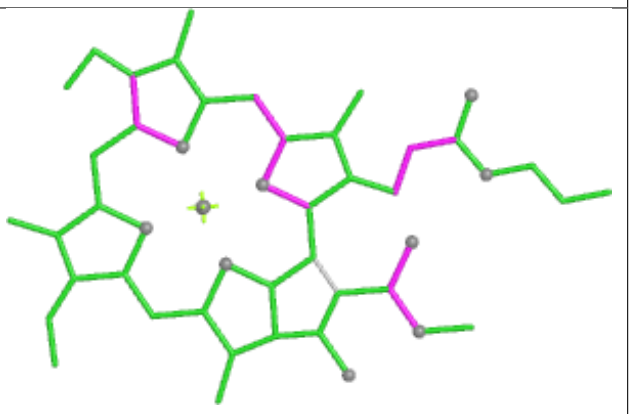
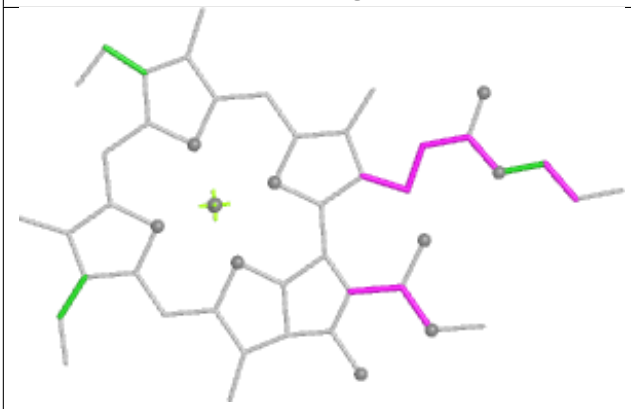
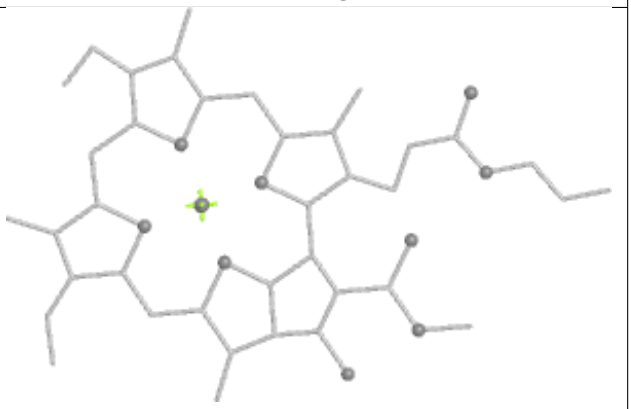
Bond angles

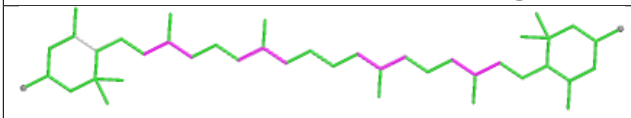
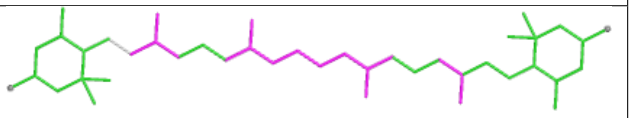
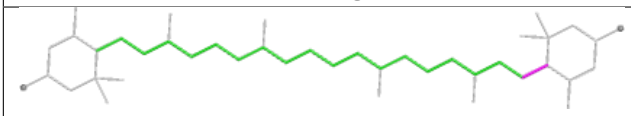
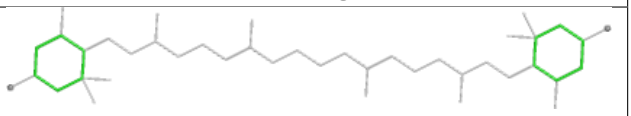


Torsions

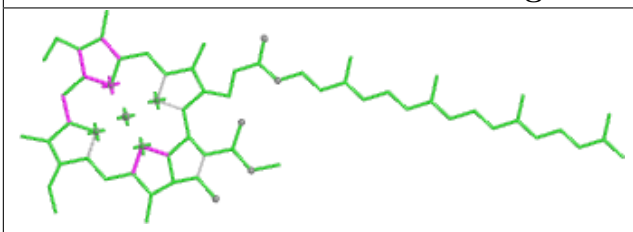


Rings

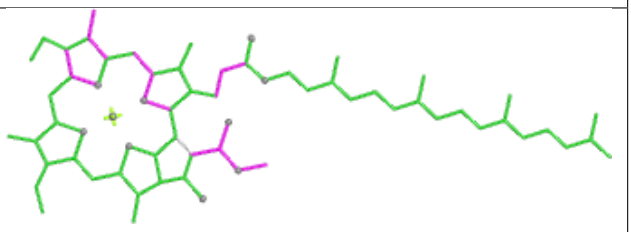
Ligand CLA V 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT AU 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

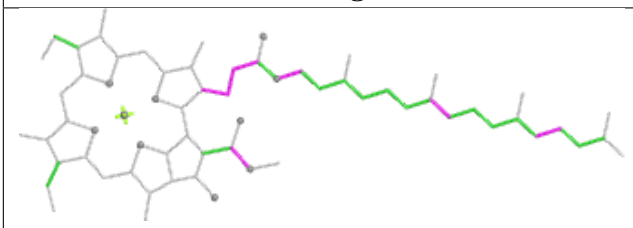
Ligand CLA P 504



Bond lengths



Bond angles



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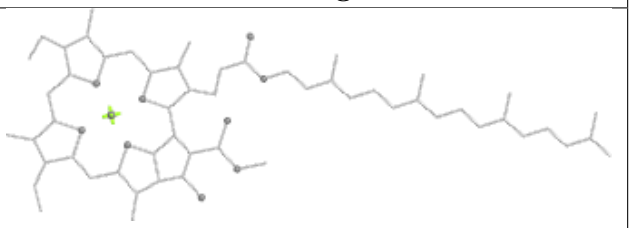
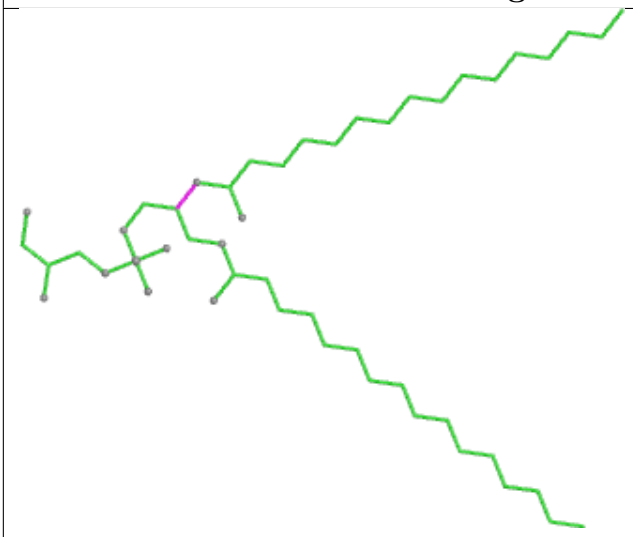


Rings

Ligand LHG AN 616



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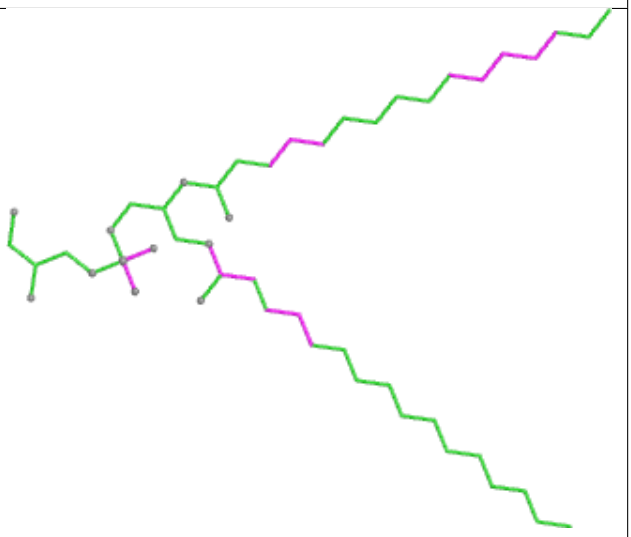
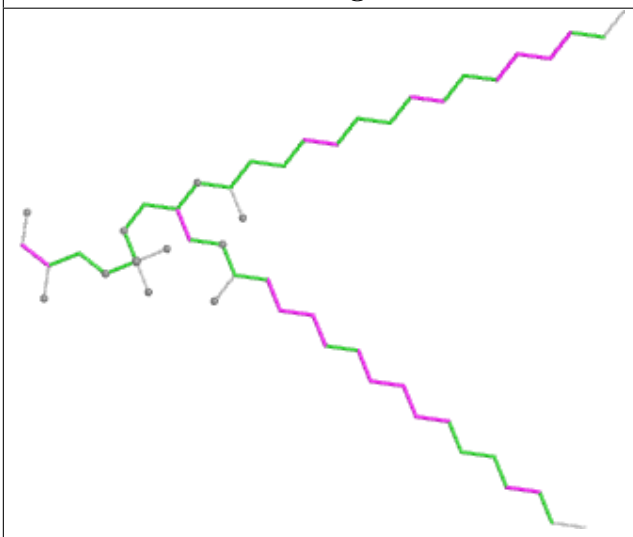


Bond angles



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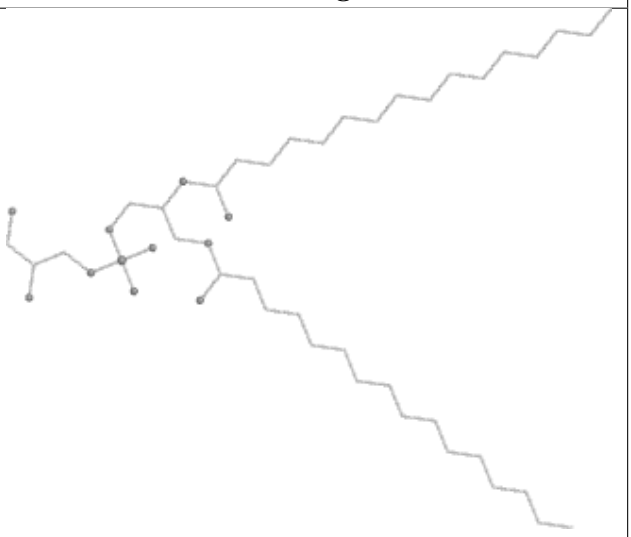
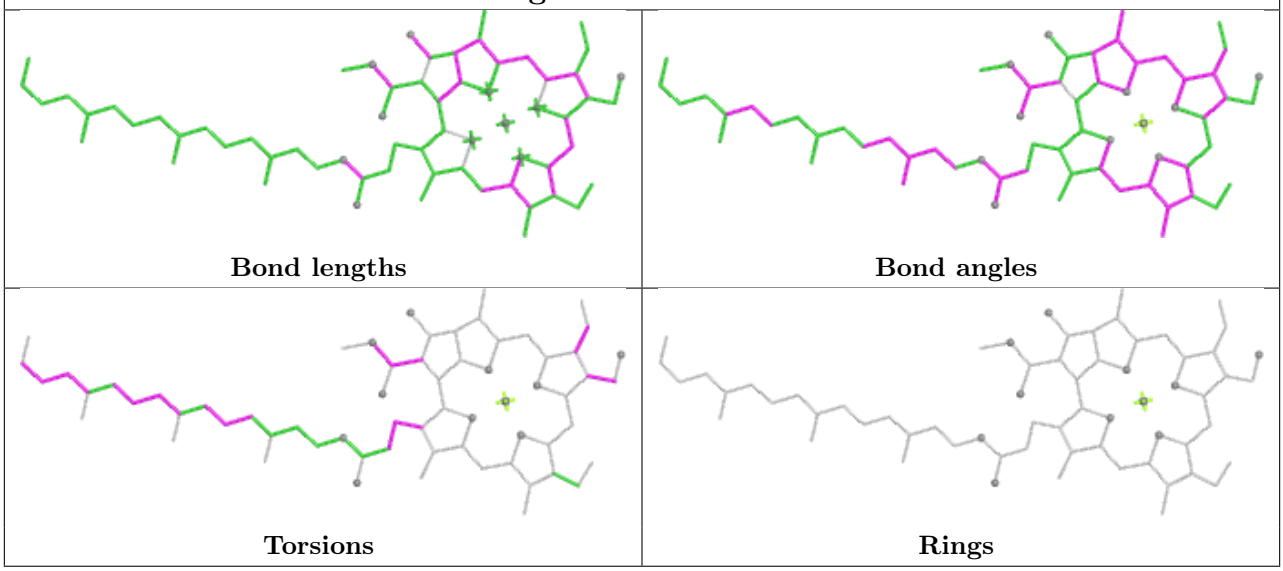
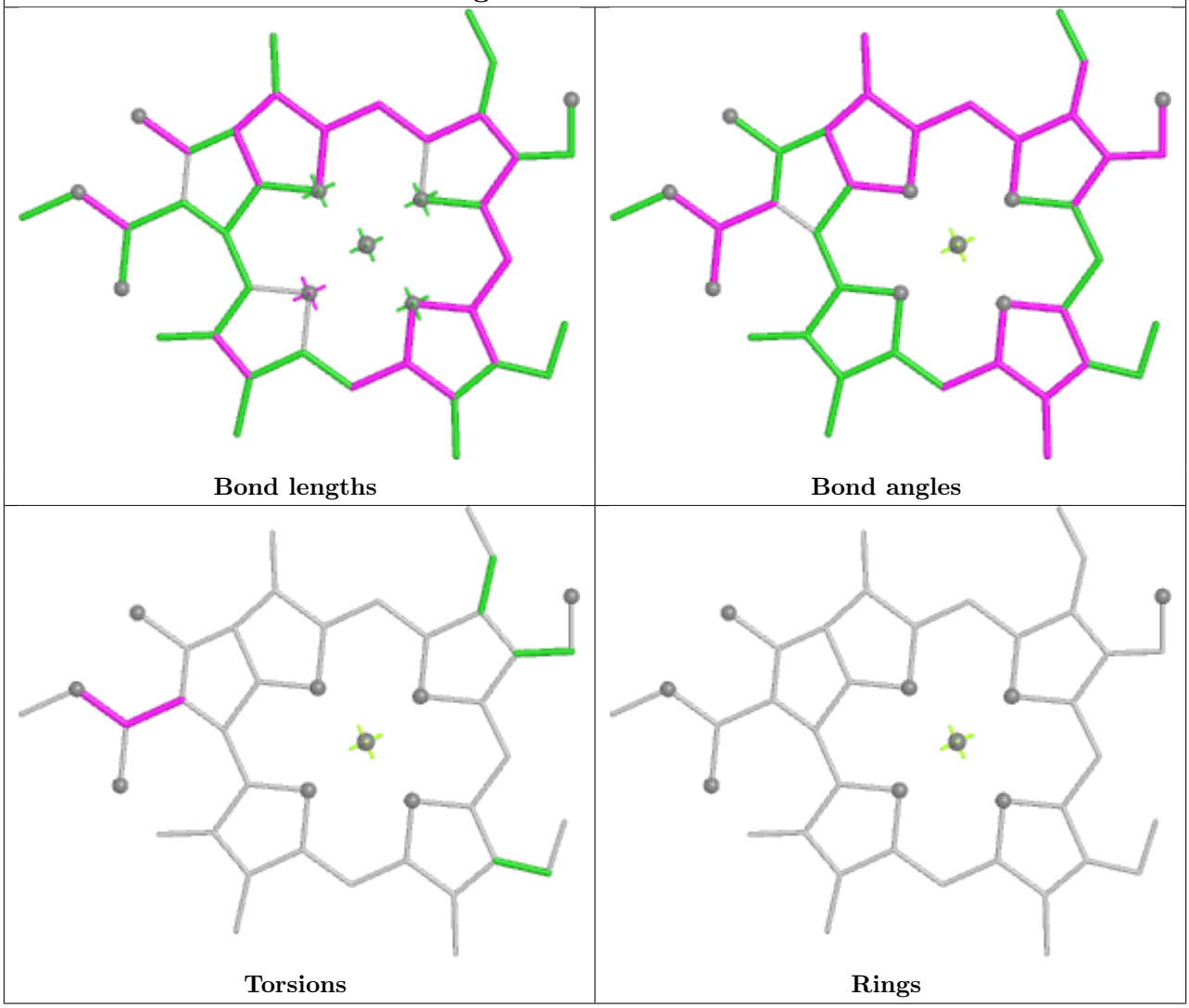


Rings

Ligand CHL 0 601



Ligand CHL AR 613



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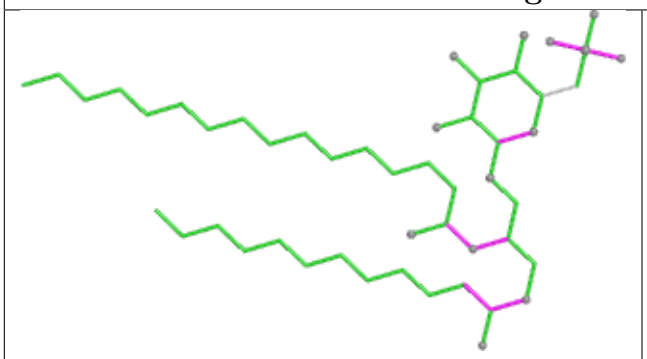

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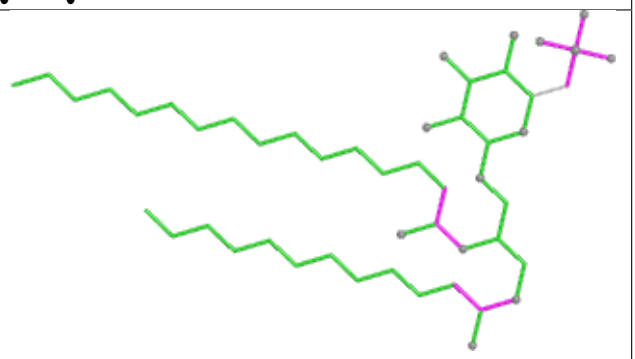

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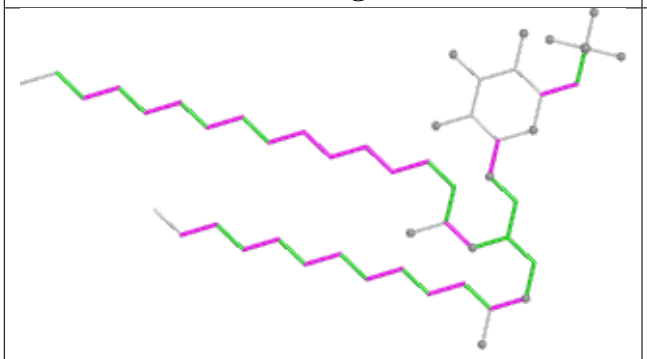

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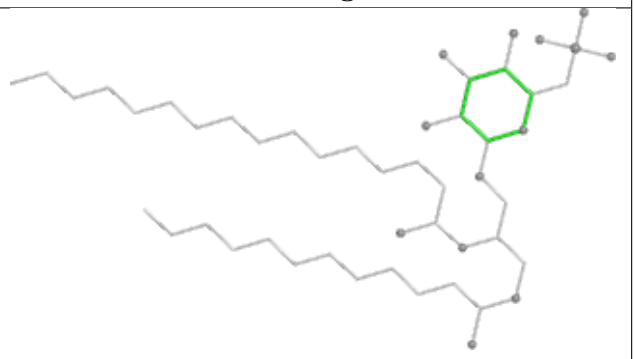
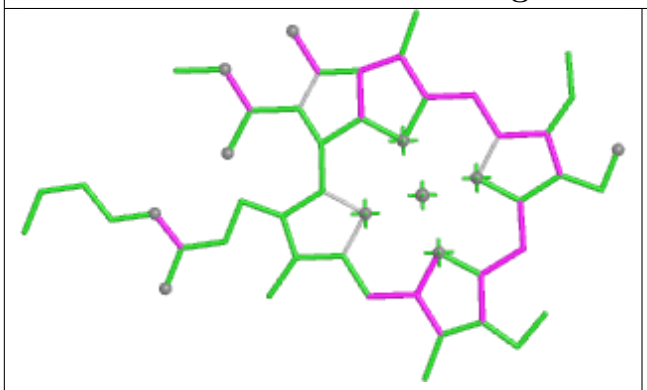


Rings

Ligand CHL AQ 606



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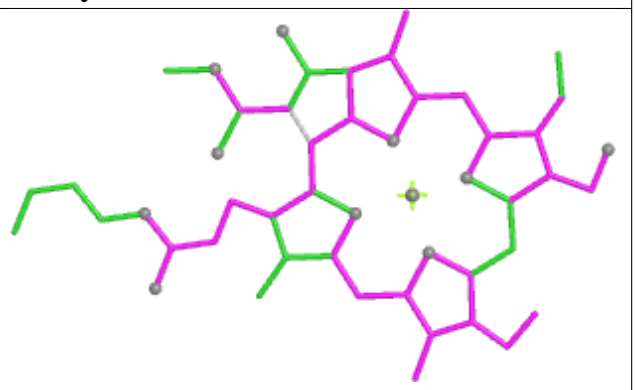

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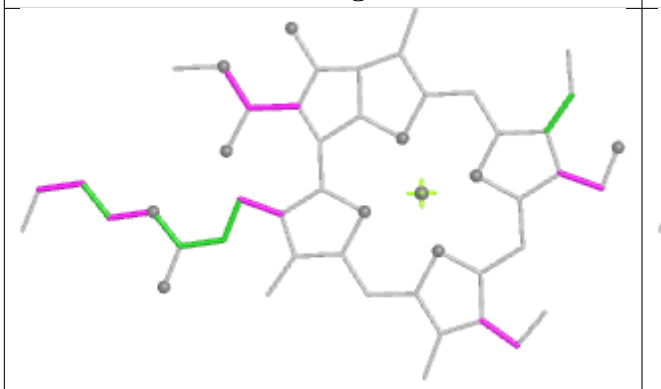
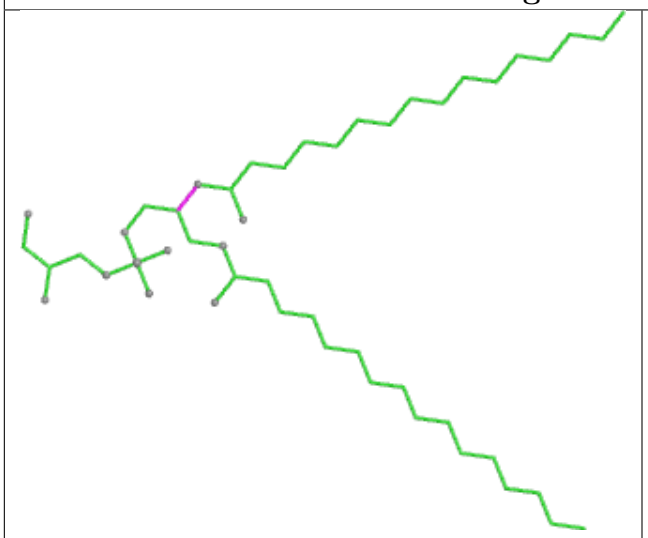


Torsions

Rings

Ligand LHG V 615



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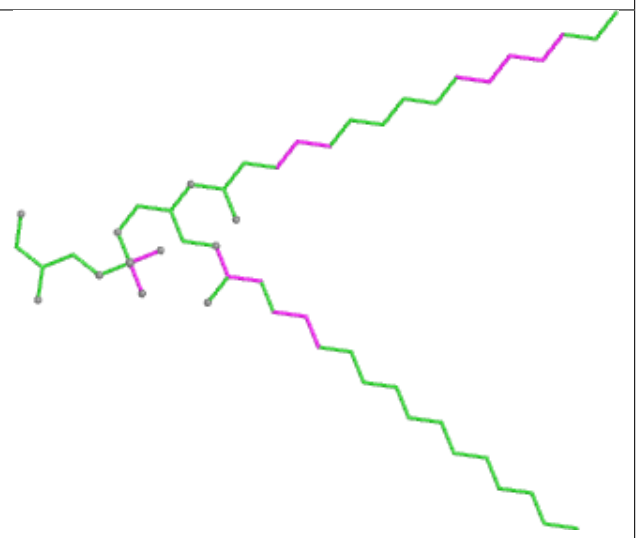

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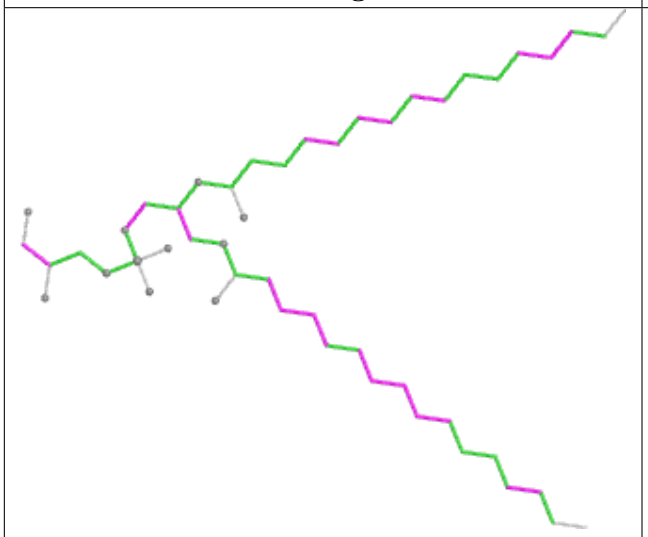

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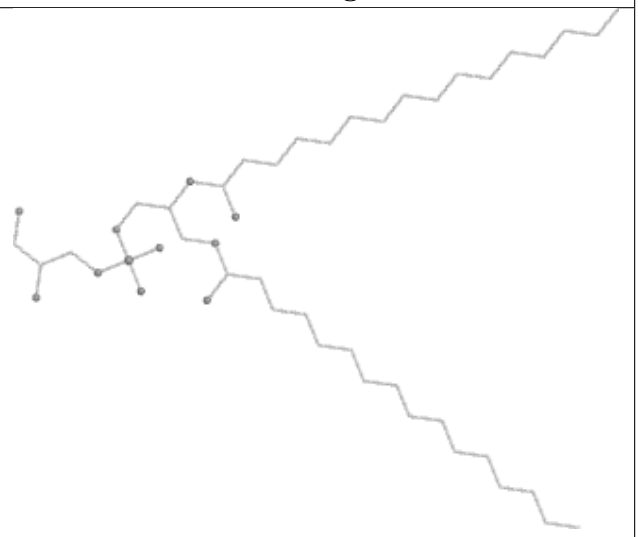
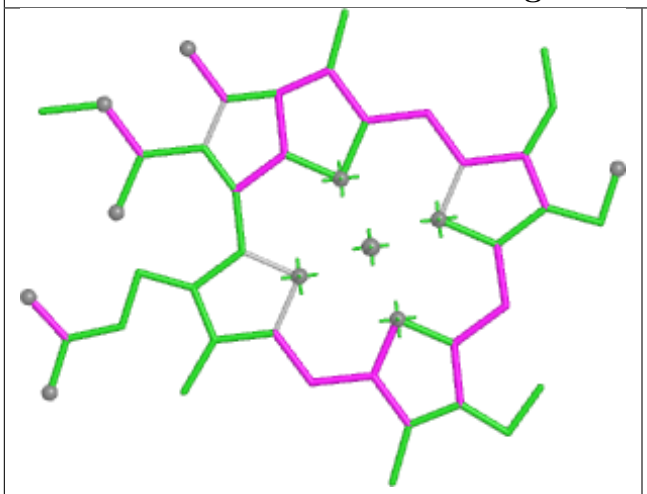


Rings

Ligand CHL V 616



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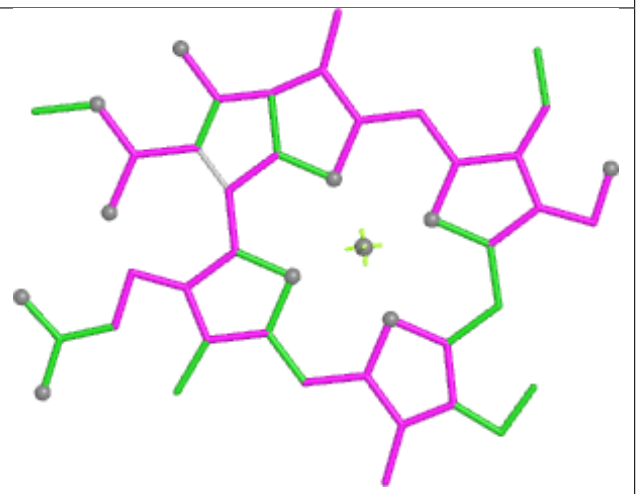
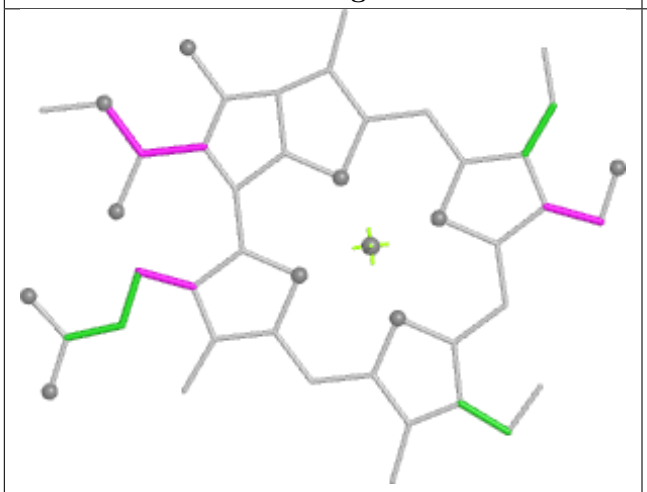


Bond angles



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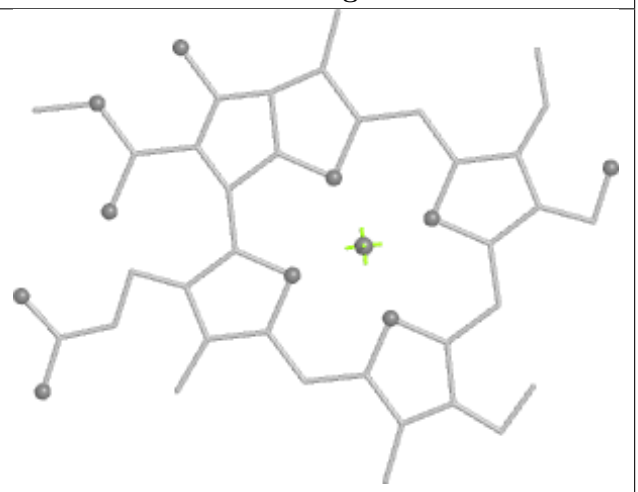
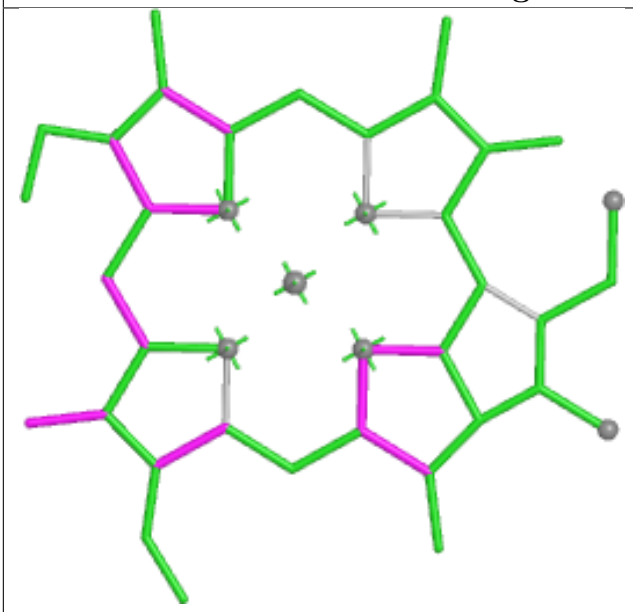


Rings

Ligand CLA AF 602



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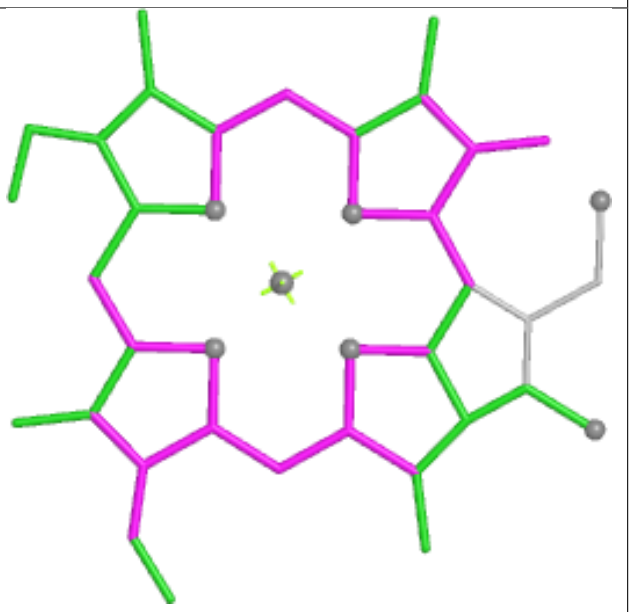
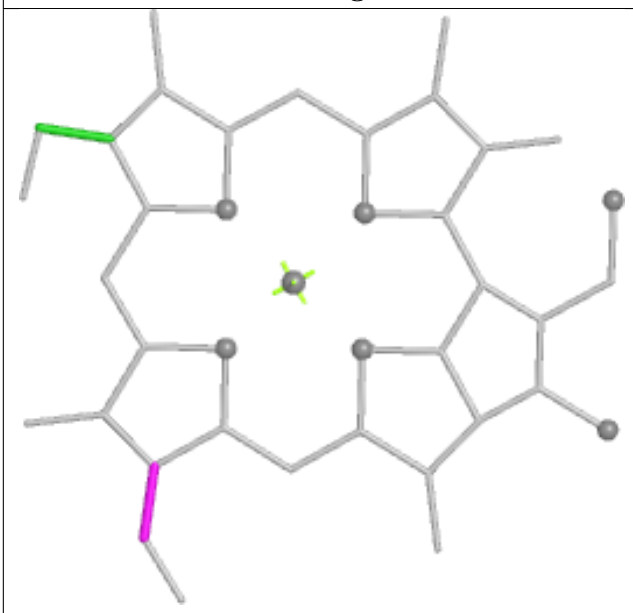


Bond angles



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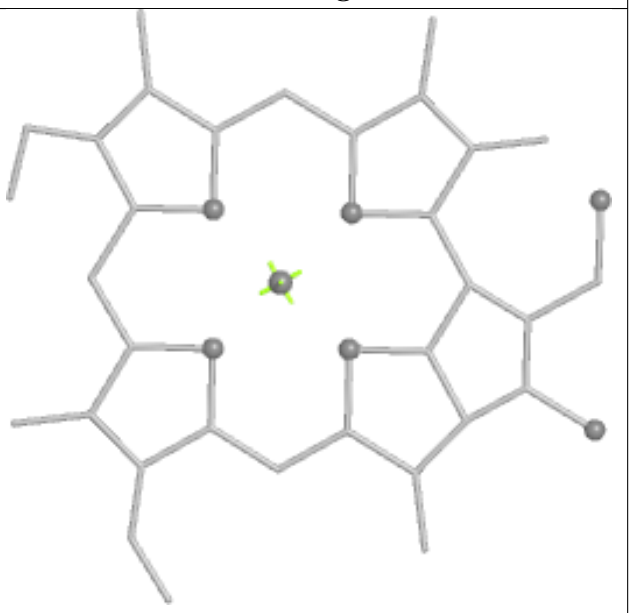
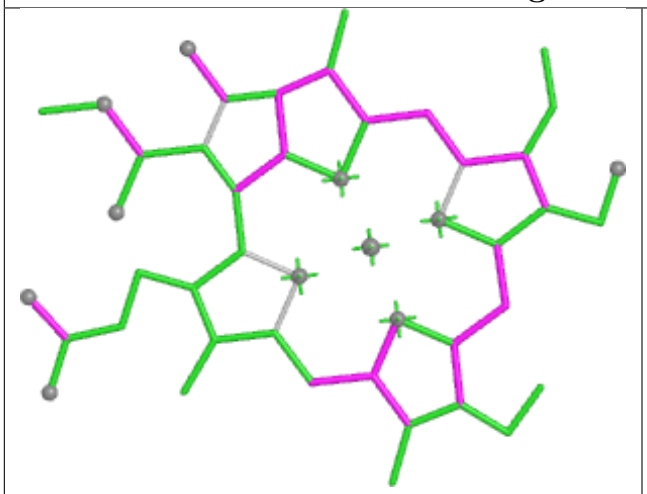


Rings

Ligand CHL v 307



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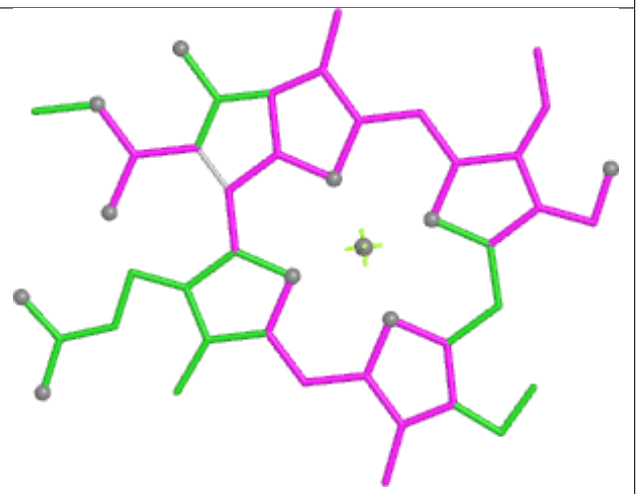
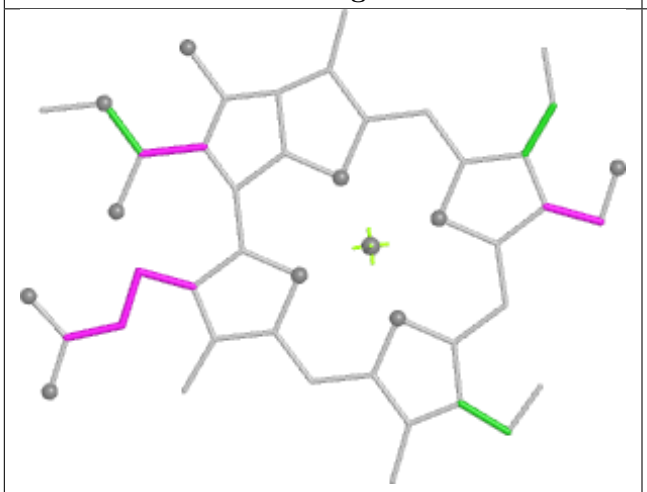


Bond angles



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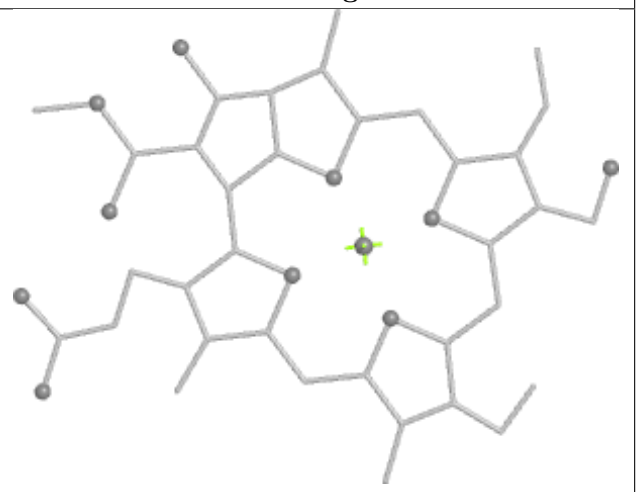
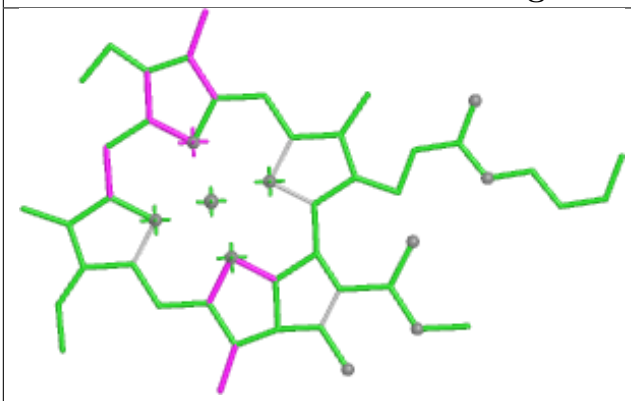
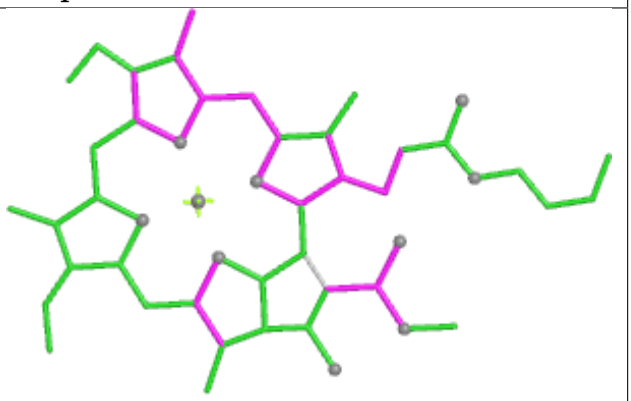
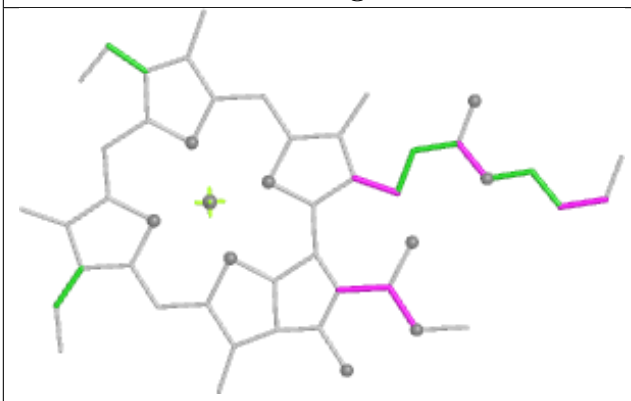
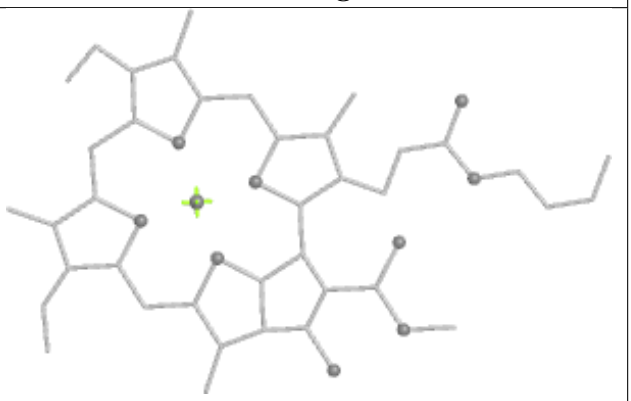
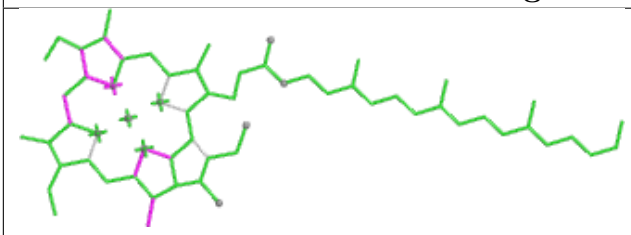
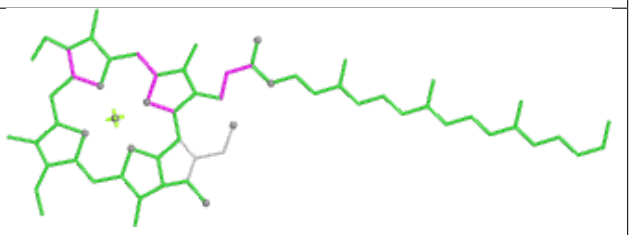
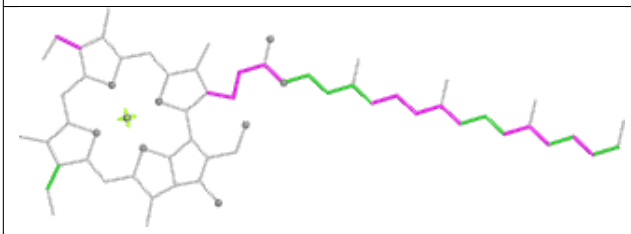
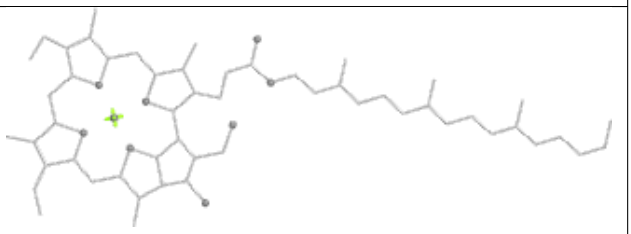


Rings

Ligand CLA q 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA V 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

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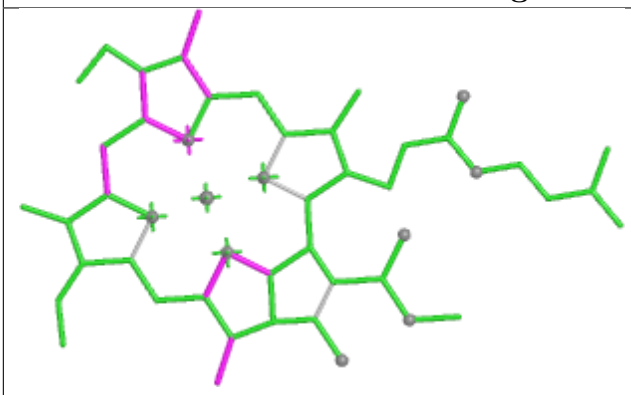
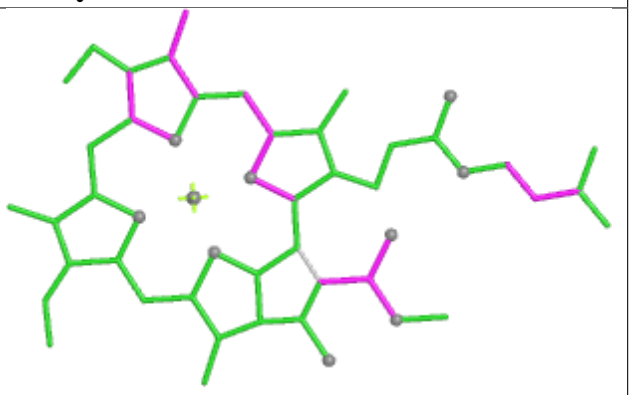
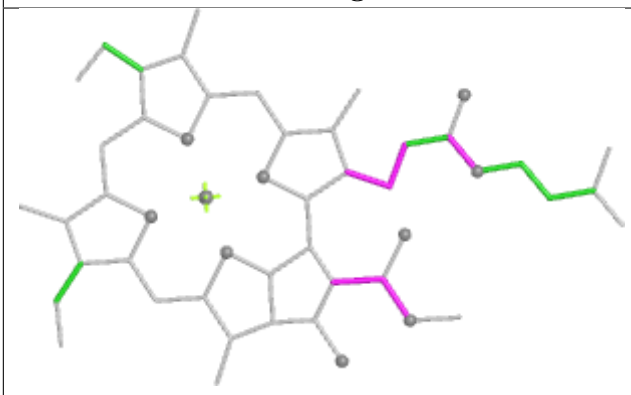
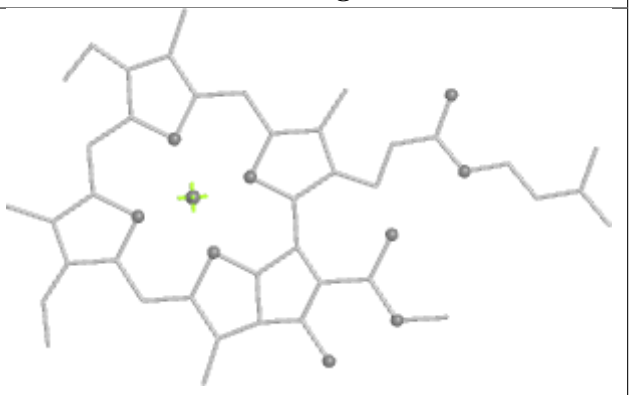
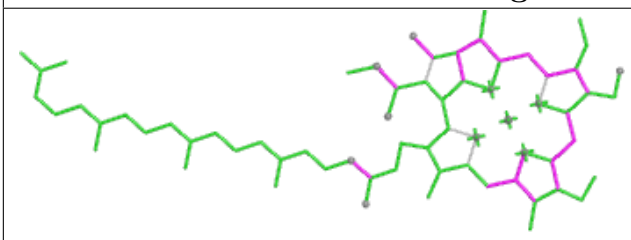
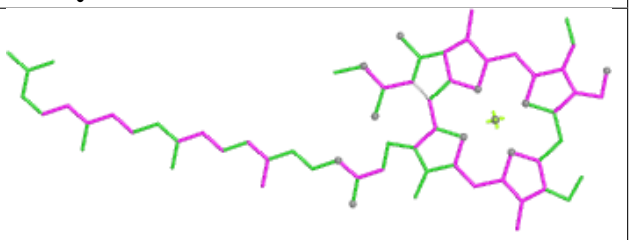
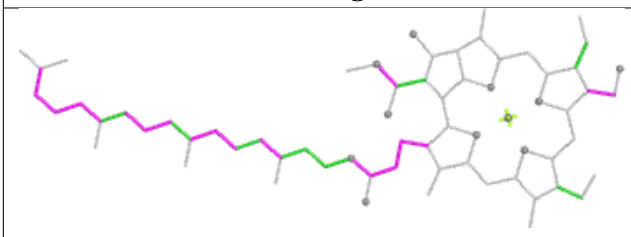
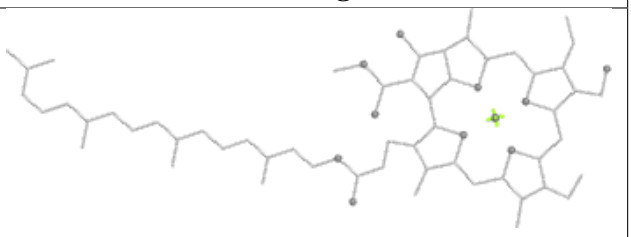
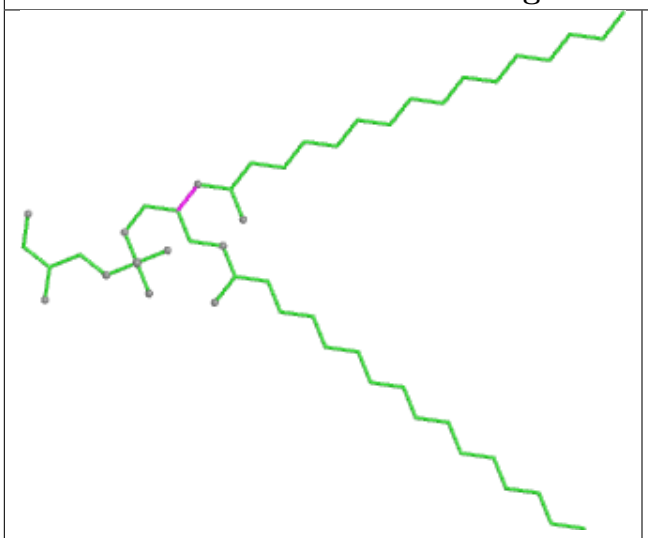
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL AQ 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG Q 406



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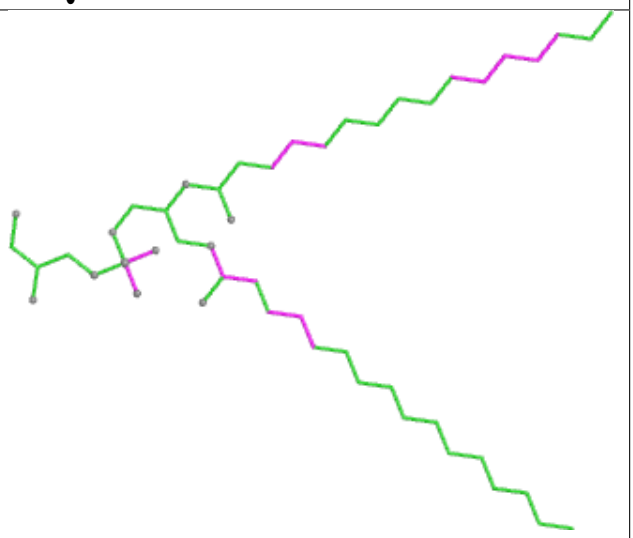
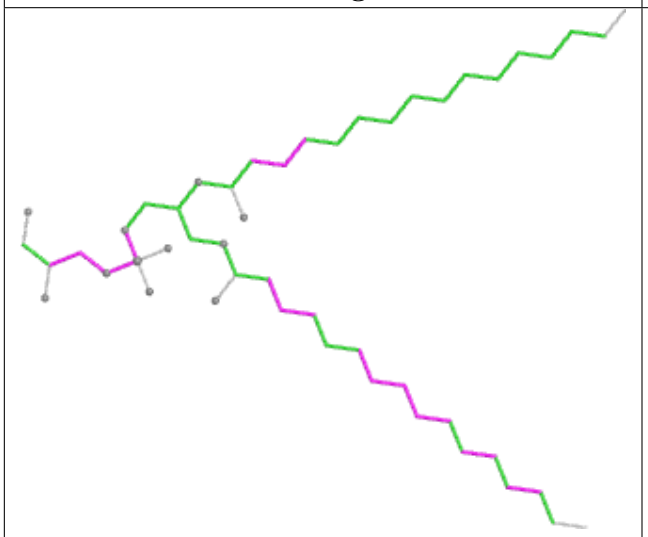
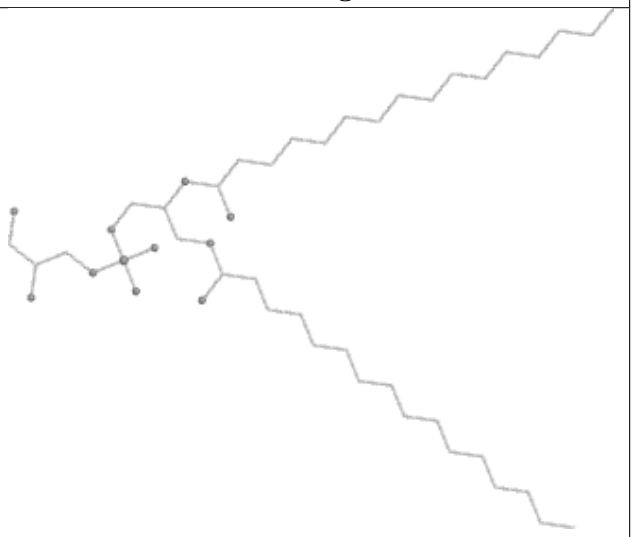


Bond angles

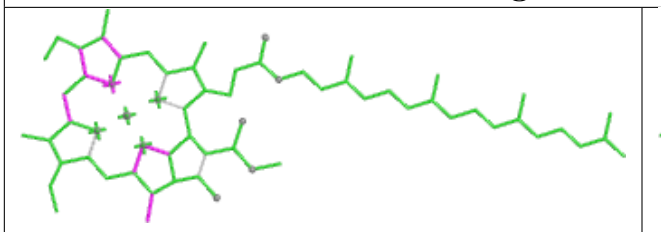


Torsions



Rings

Ligand CLA AK 609



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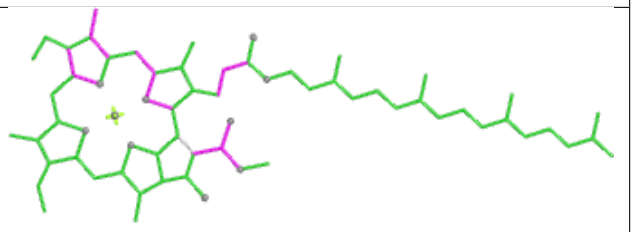
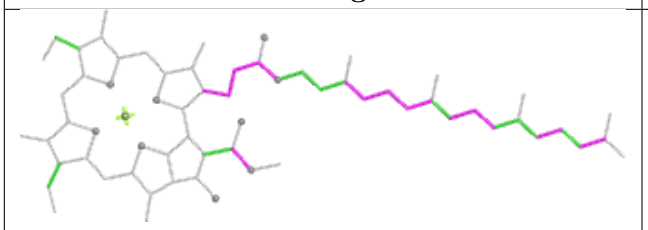


Bond angles



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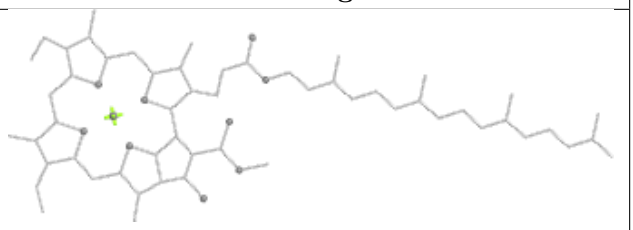
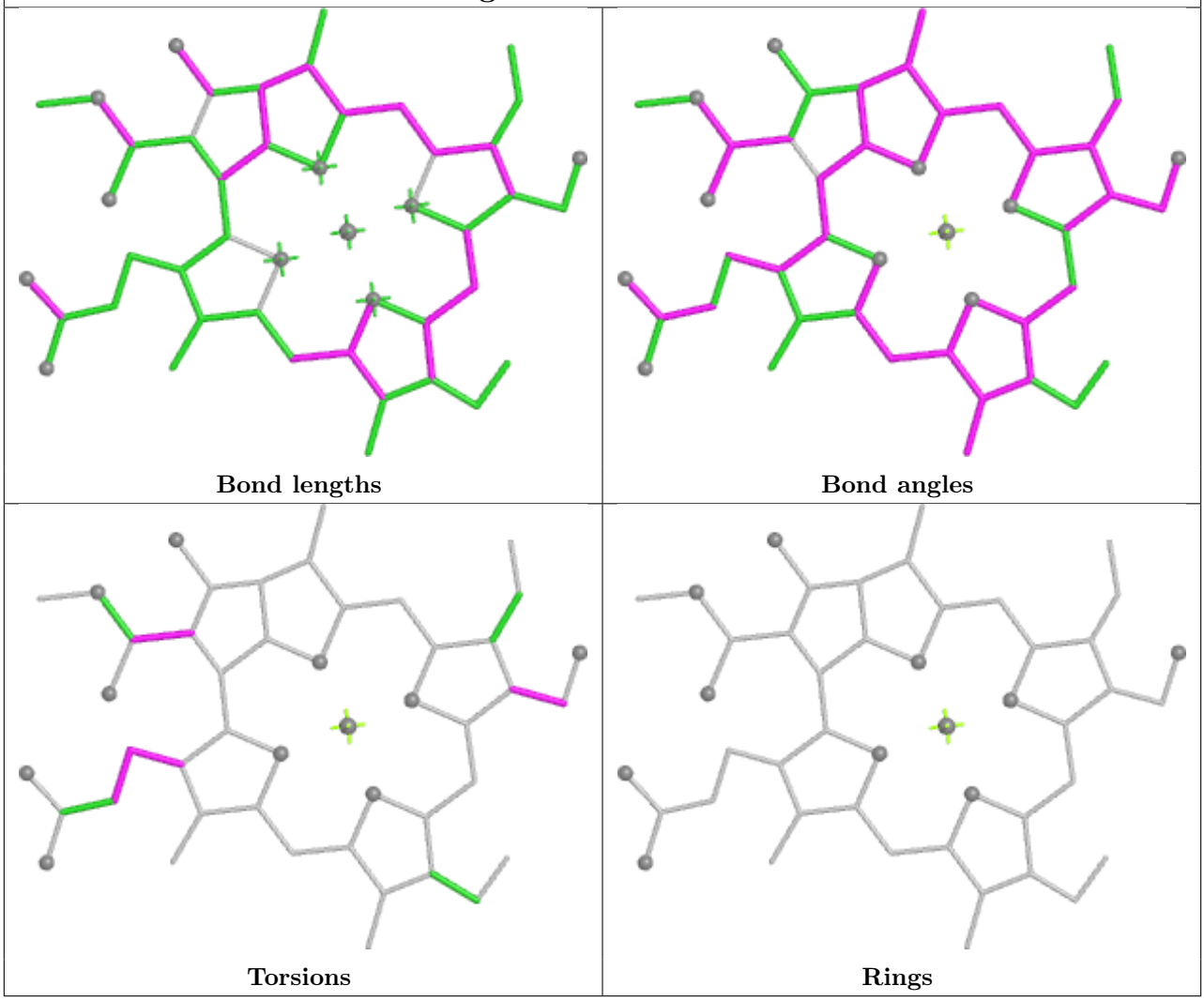
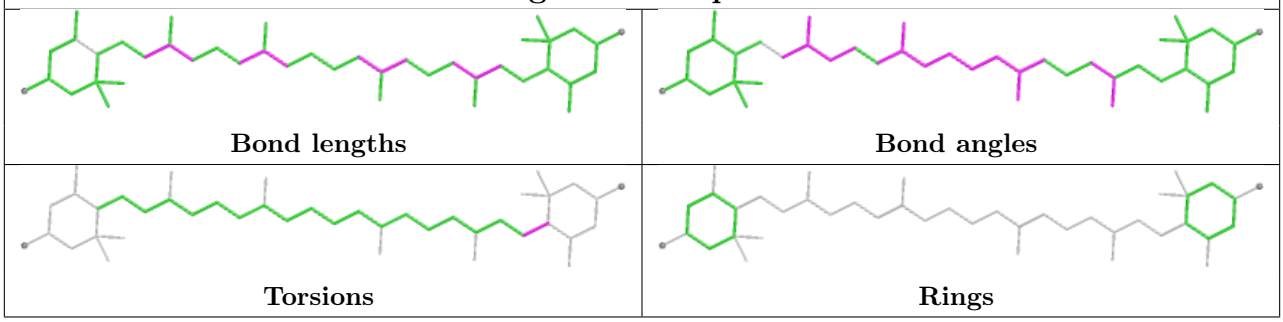


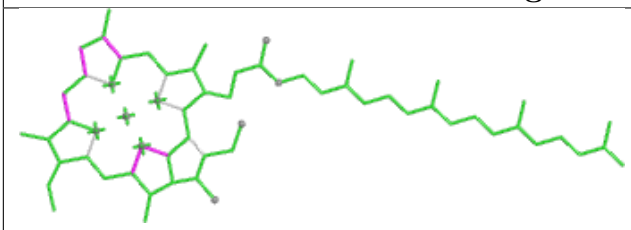
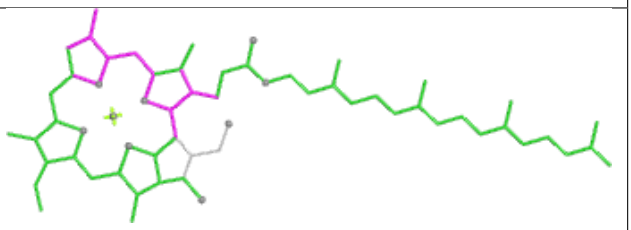
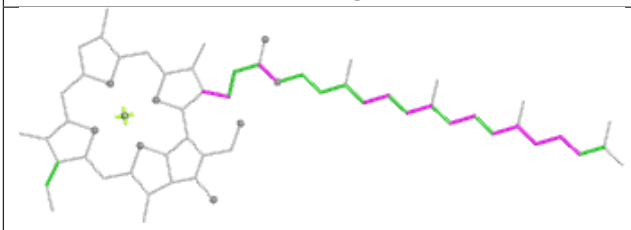
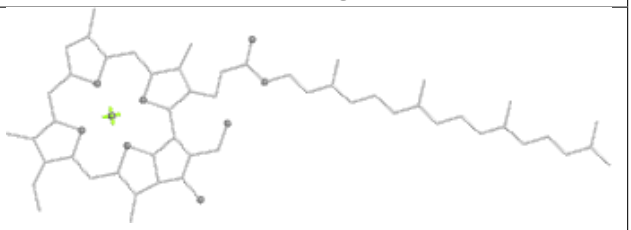
Rings

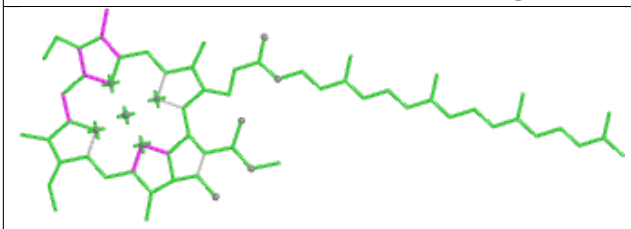
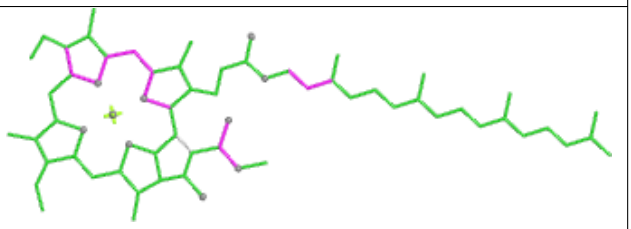
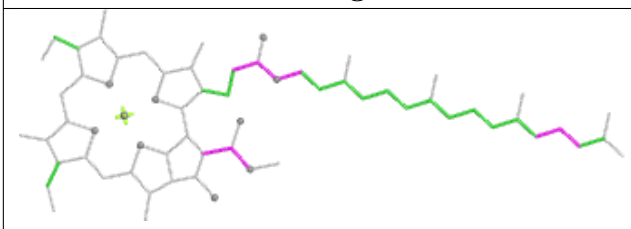
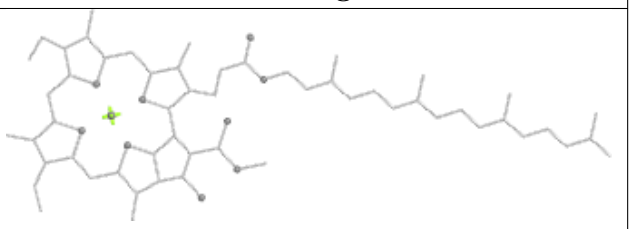
Ligand CHL AA 601



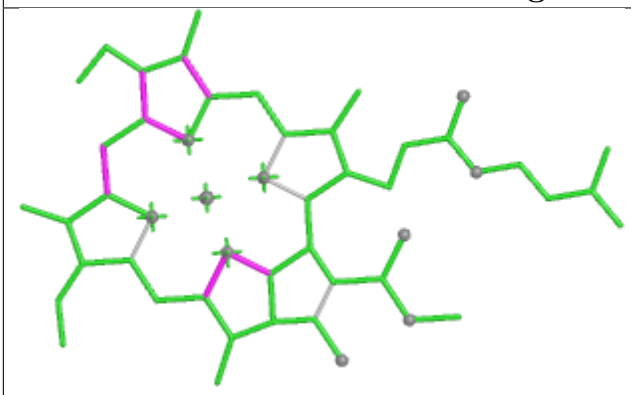
Ligand LUT q 614



Ligand CLA P 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AK 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA v 305



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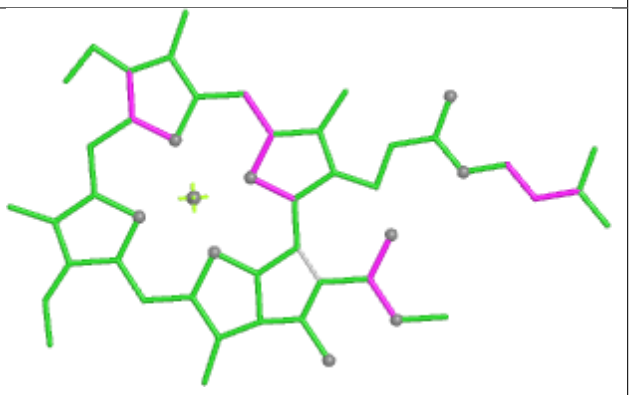

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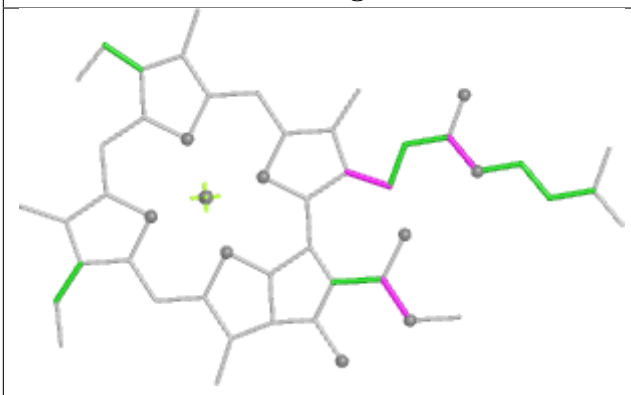

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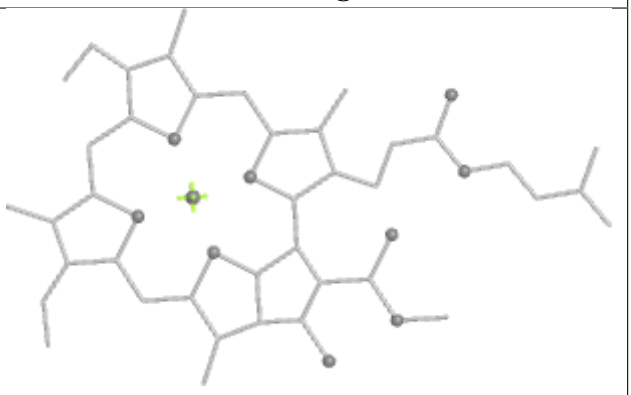
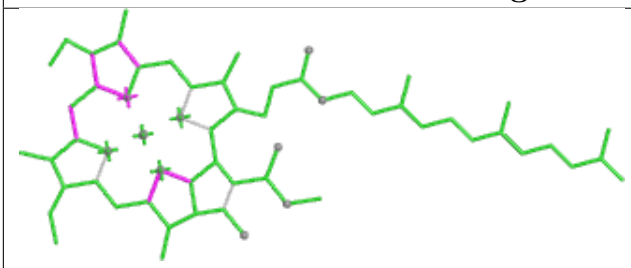


Rings

Ligand CLA AU 609



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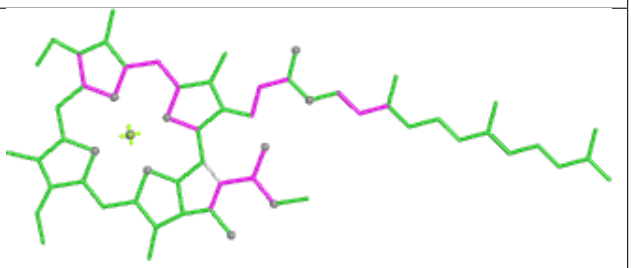

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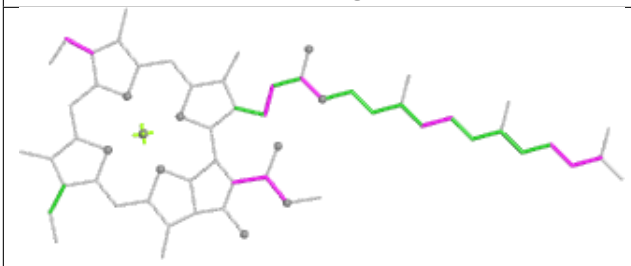

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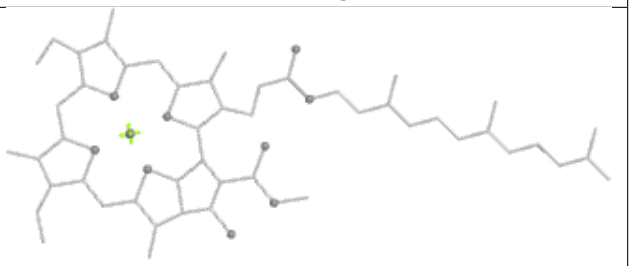
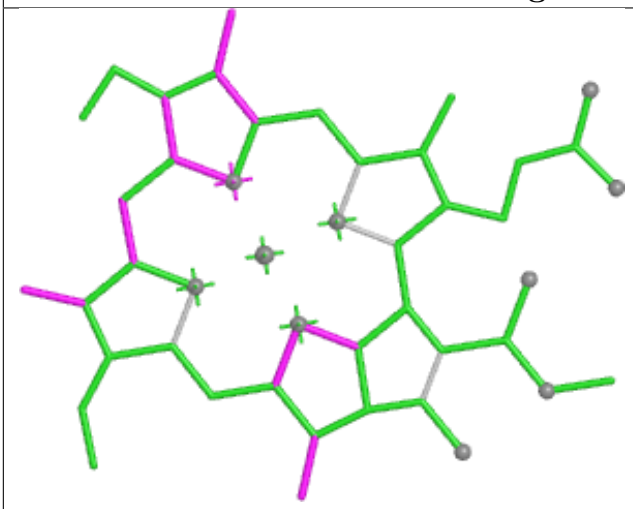


Rings

Ligand CLA 0 611



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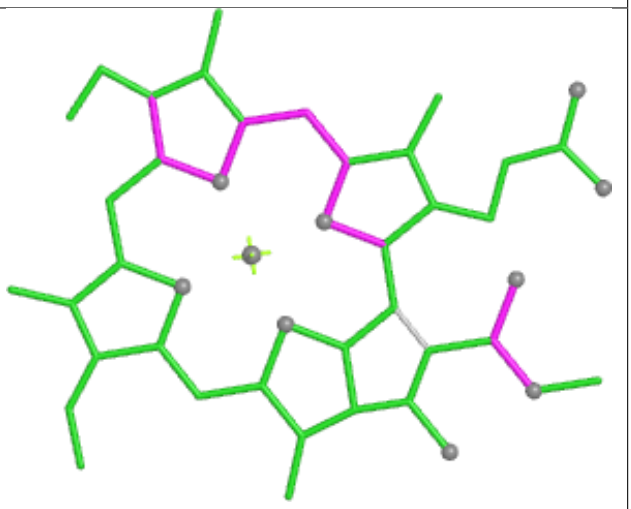
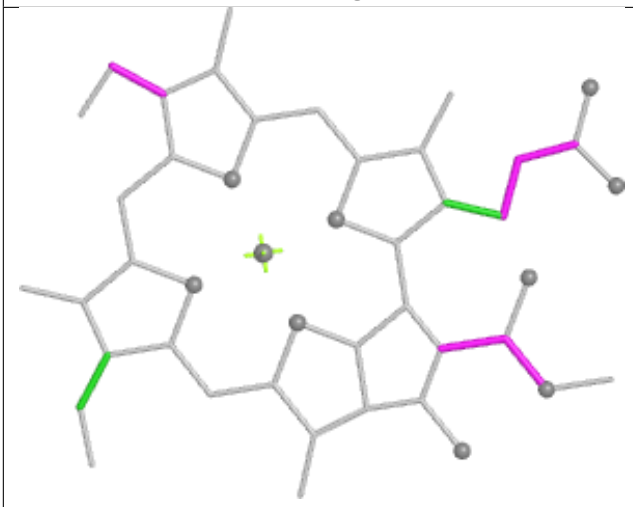
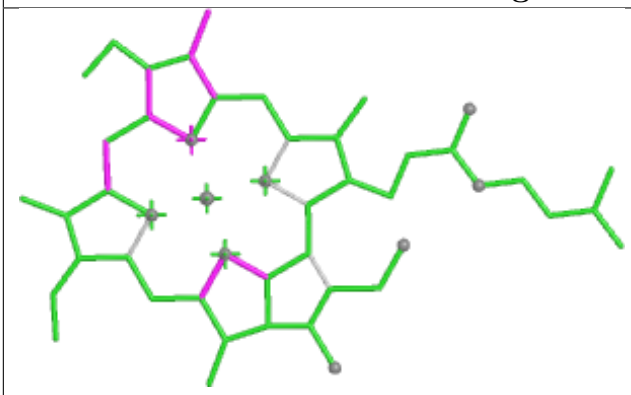
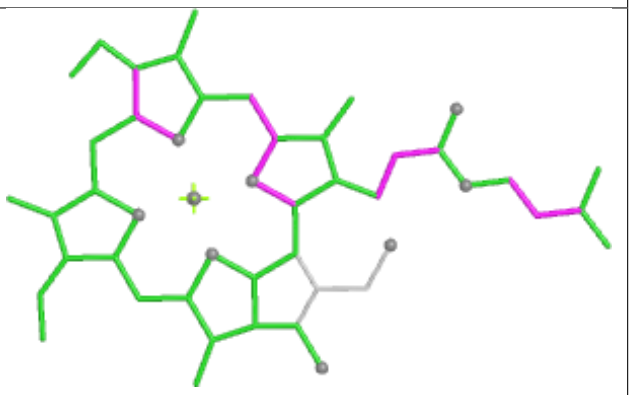


Bond angles



Torsions

Rings

Ligand CLA AE 608	
	
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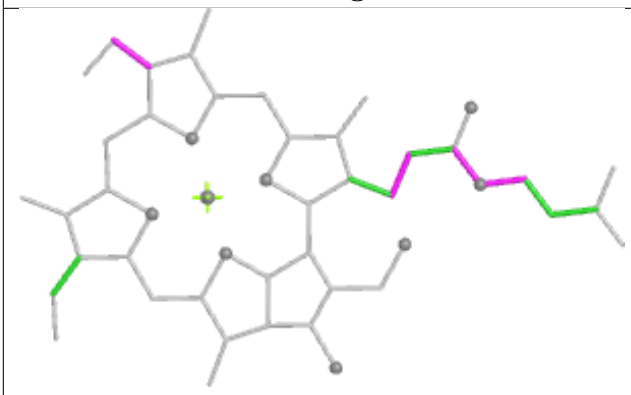
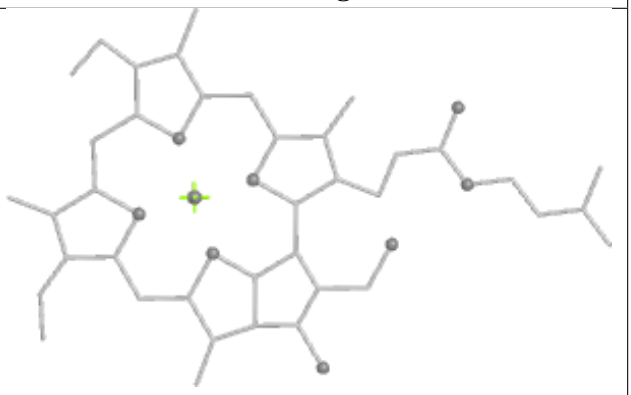
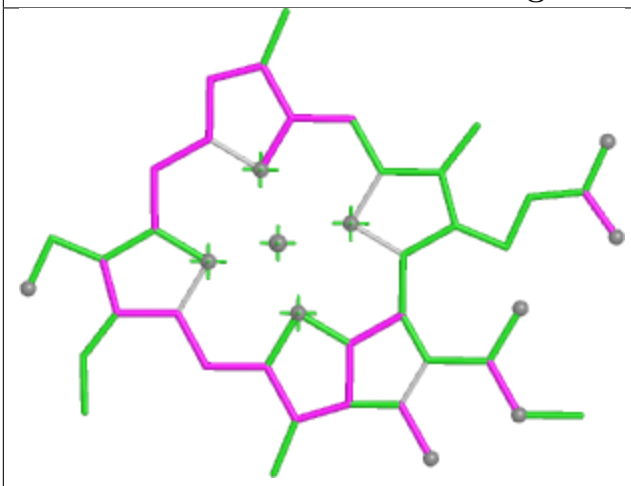
	
Torsions	**Rings**

Ligand CHL v 302



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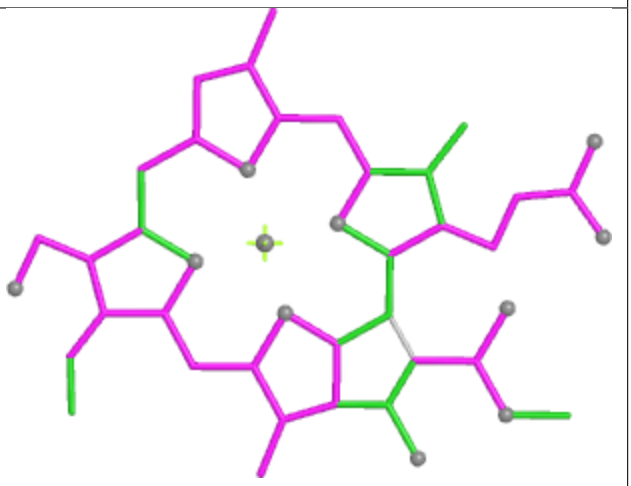
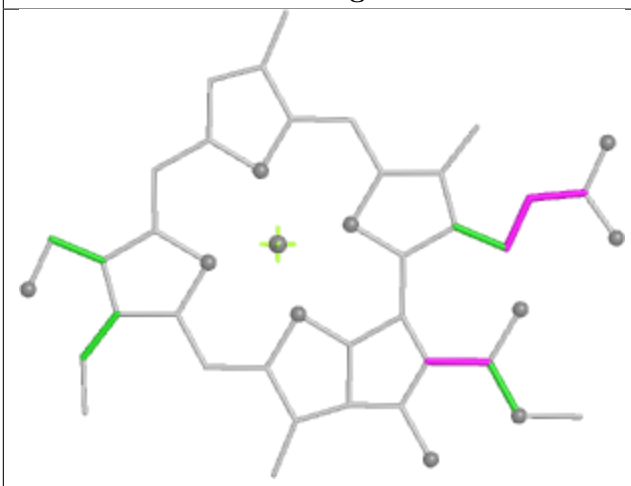


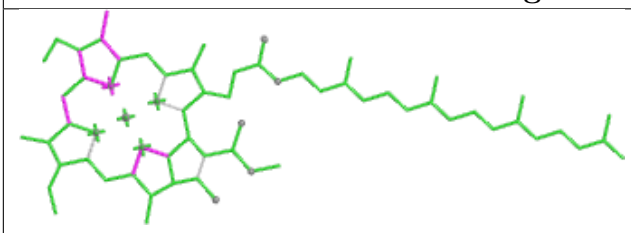
Bond angles



Torsions

Rings

Ligand CLA V 603



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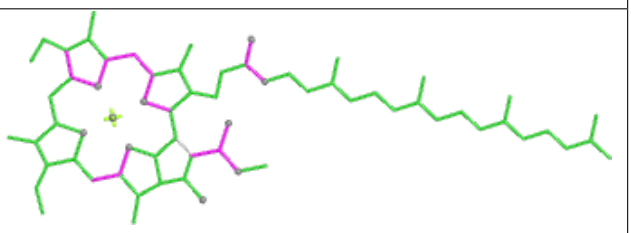
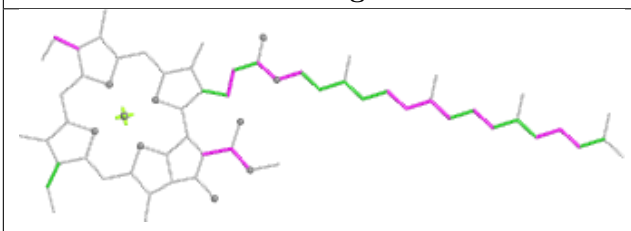
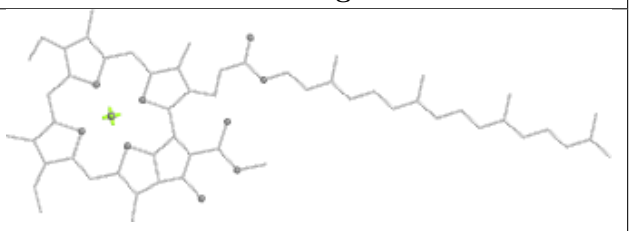


Bond angles

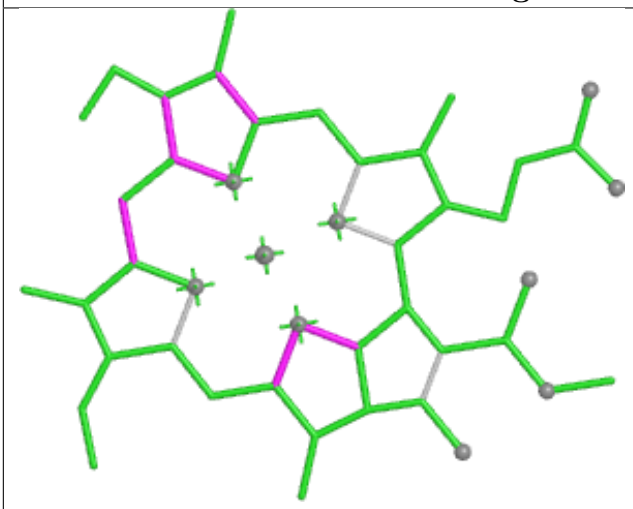


Torsions



Rings

Ligand CLA AF 604



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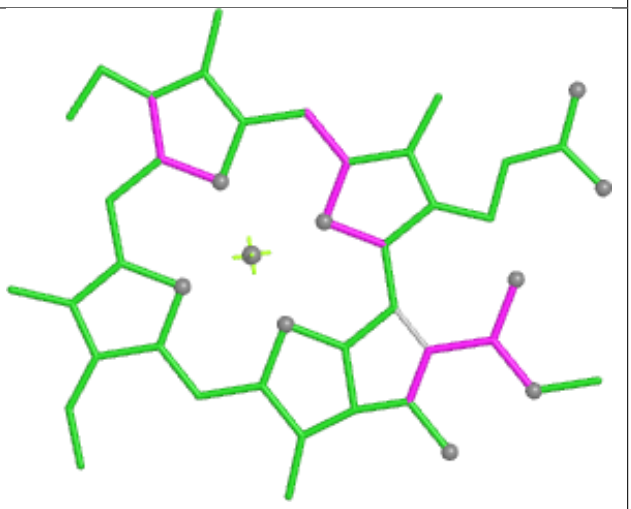

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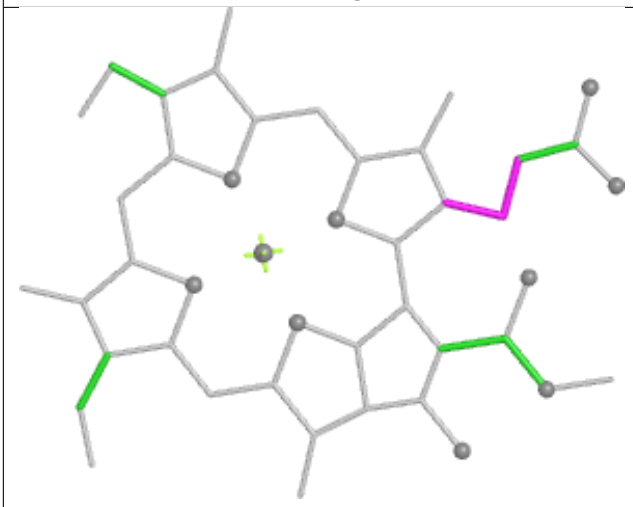
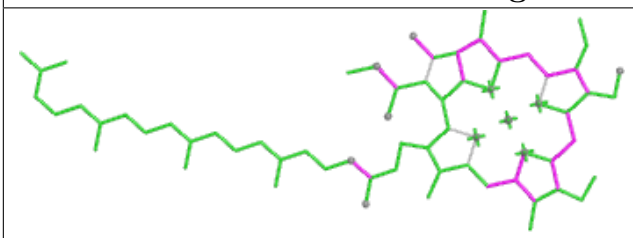


Torsions

Rings

Ligand CHL AN 606



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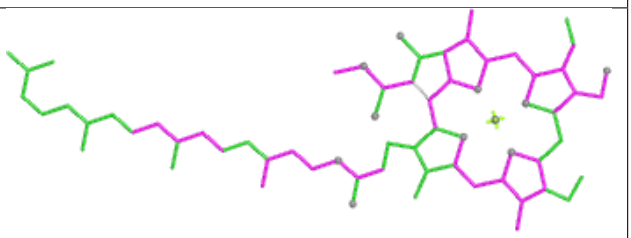
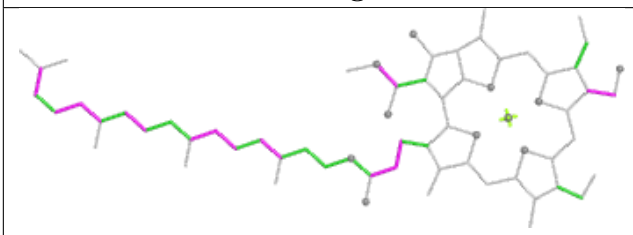
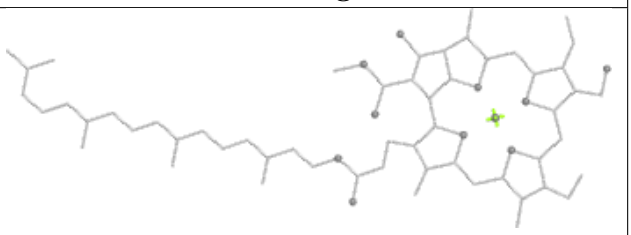


Bond angles

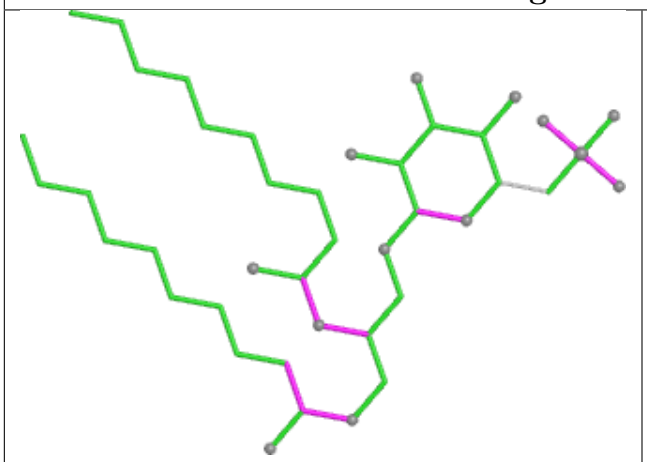


Torsions



Rings

Ligand SQD o 101



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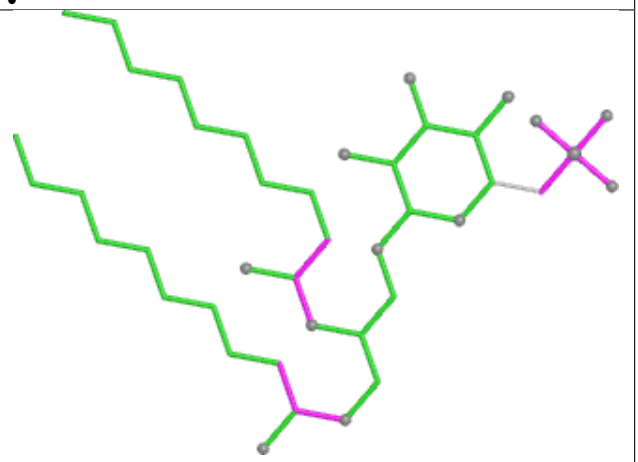
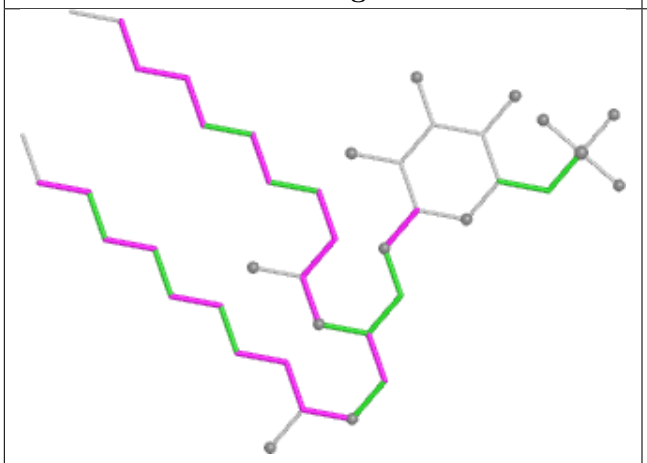


Bond angles



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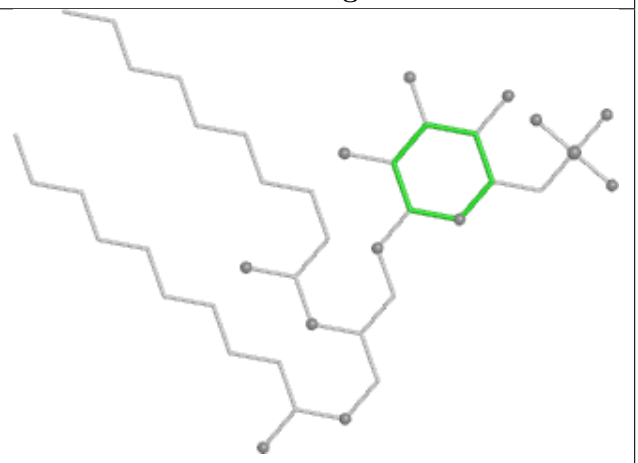
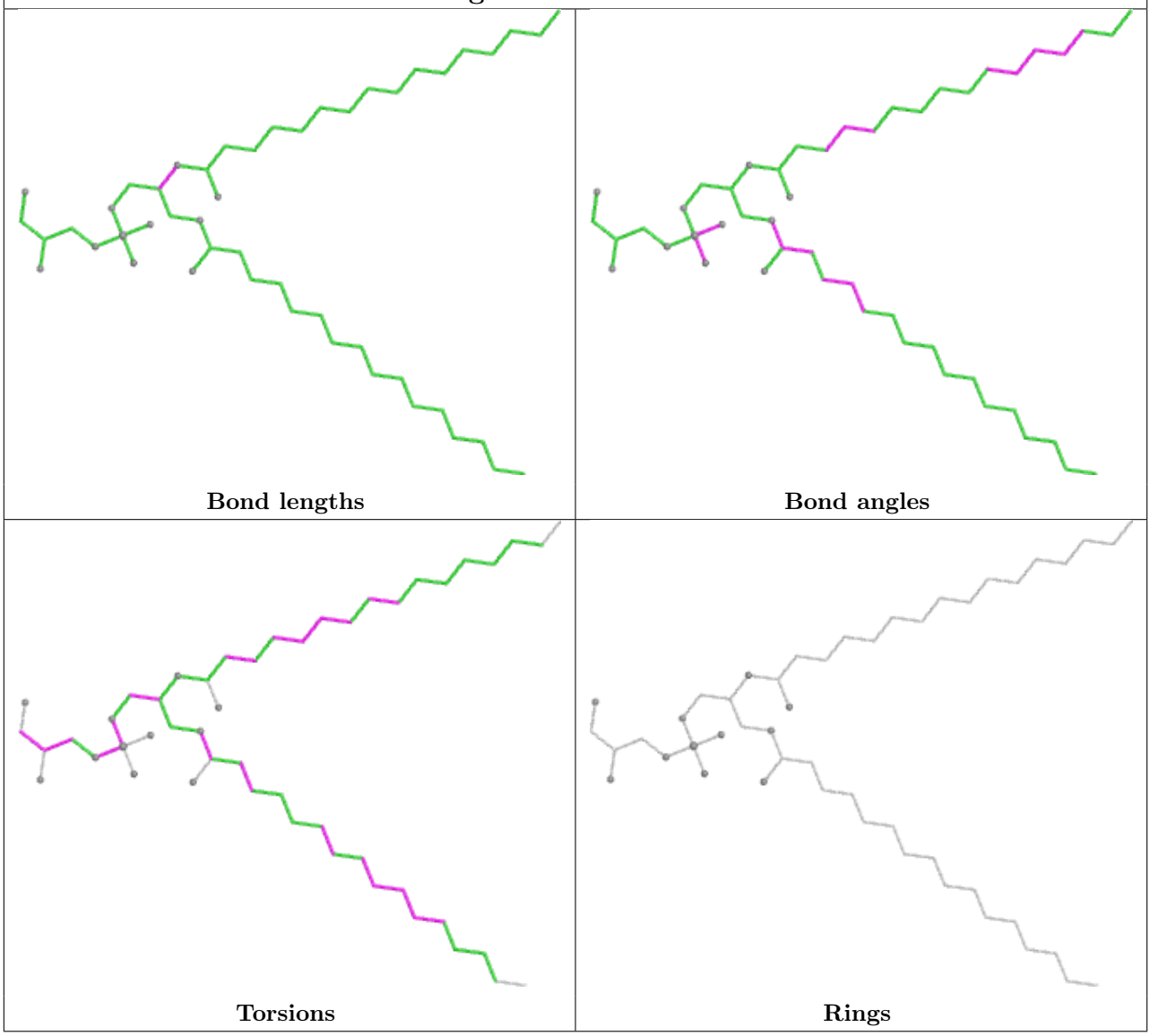
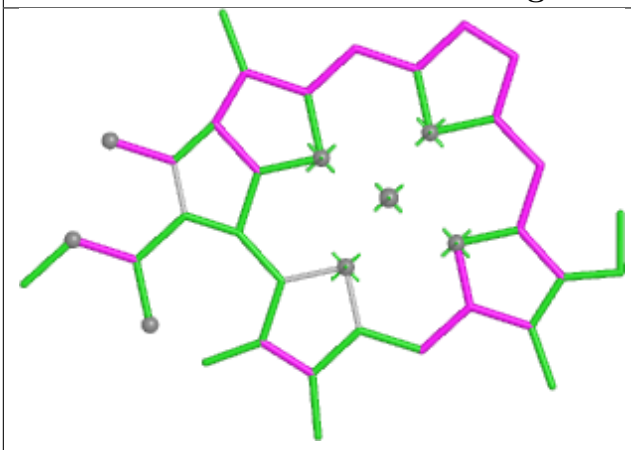


Rings

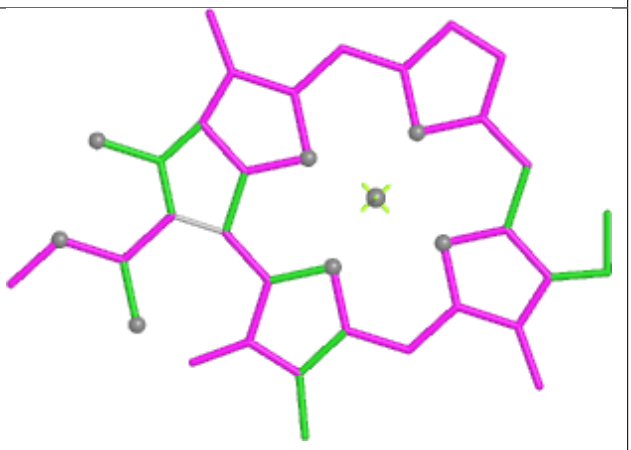
Ligand LHG O 623



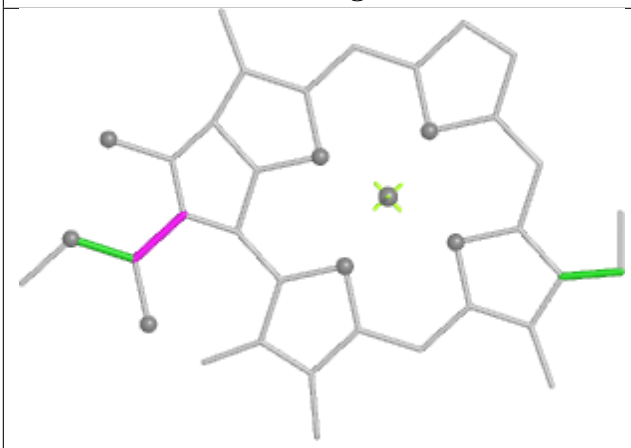
Ligand CHL v 308



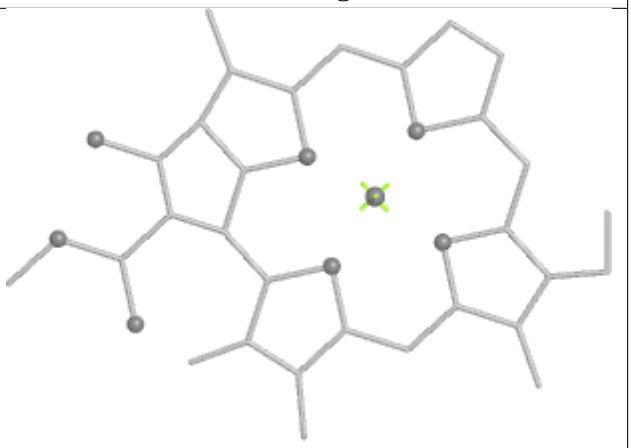
Bond lengths



Bond angles

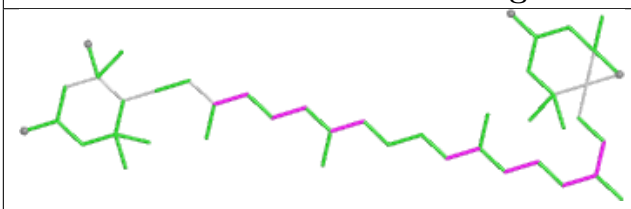


Torsions

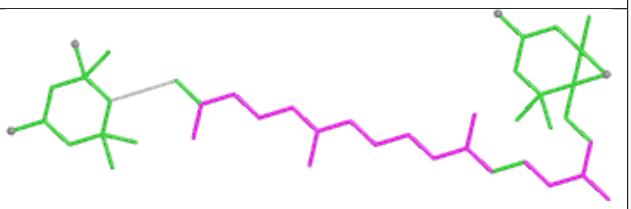


Rings

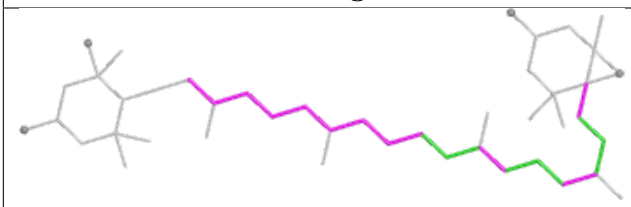
Ligand NEX AE 615



Bond lengths



Bond angles



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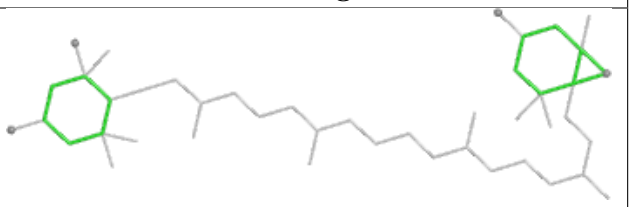
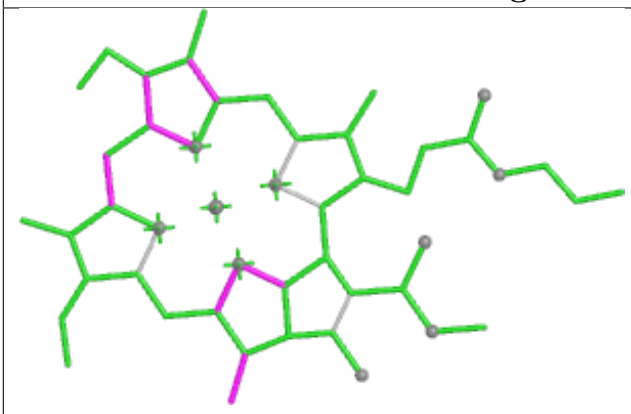


Rings

Ligand CLA AD 313



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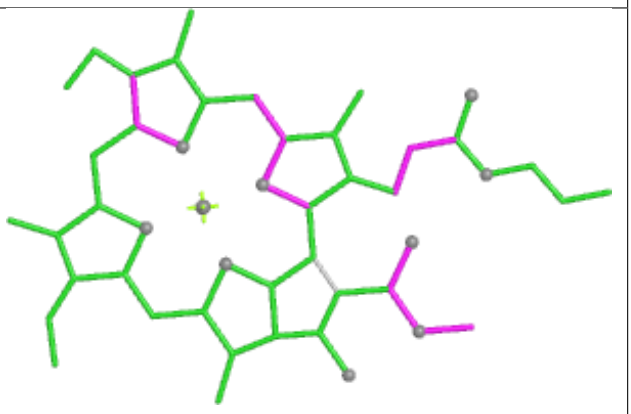

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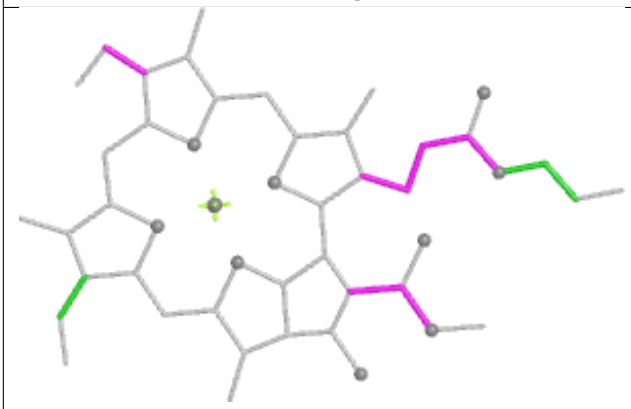

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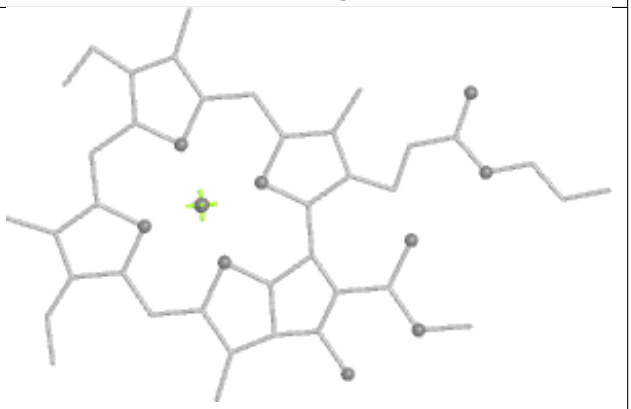
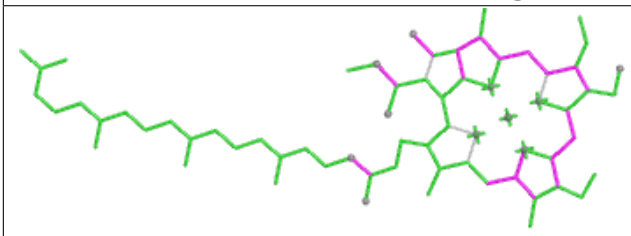


Rings

Ligand CHL AN 601



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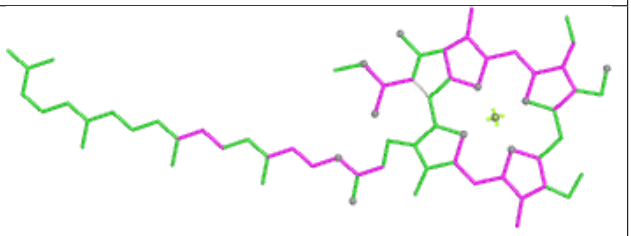
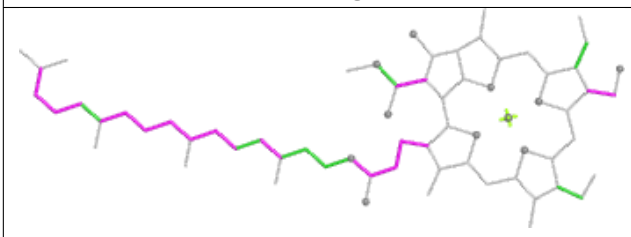


Bond angles



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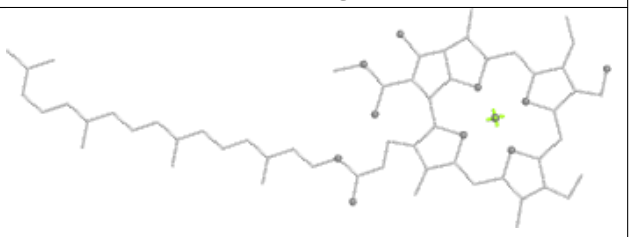
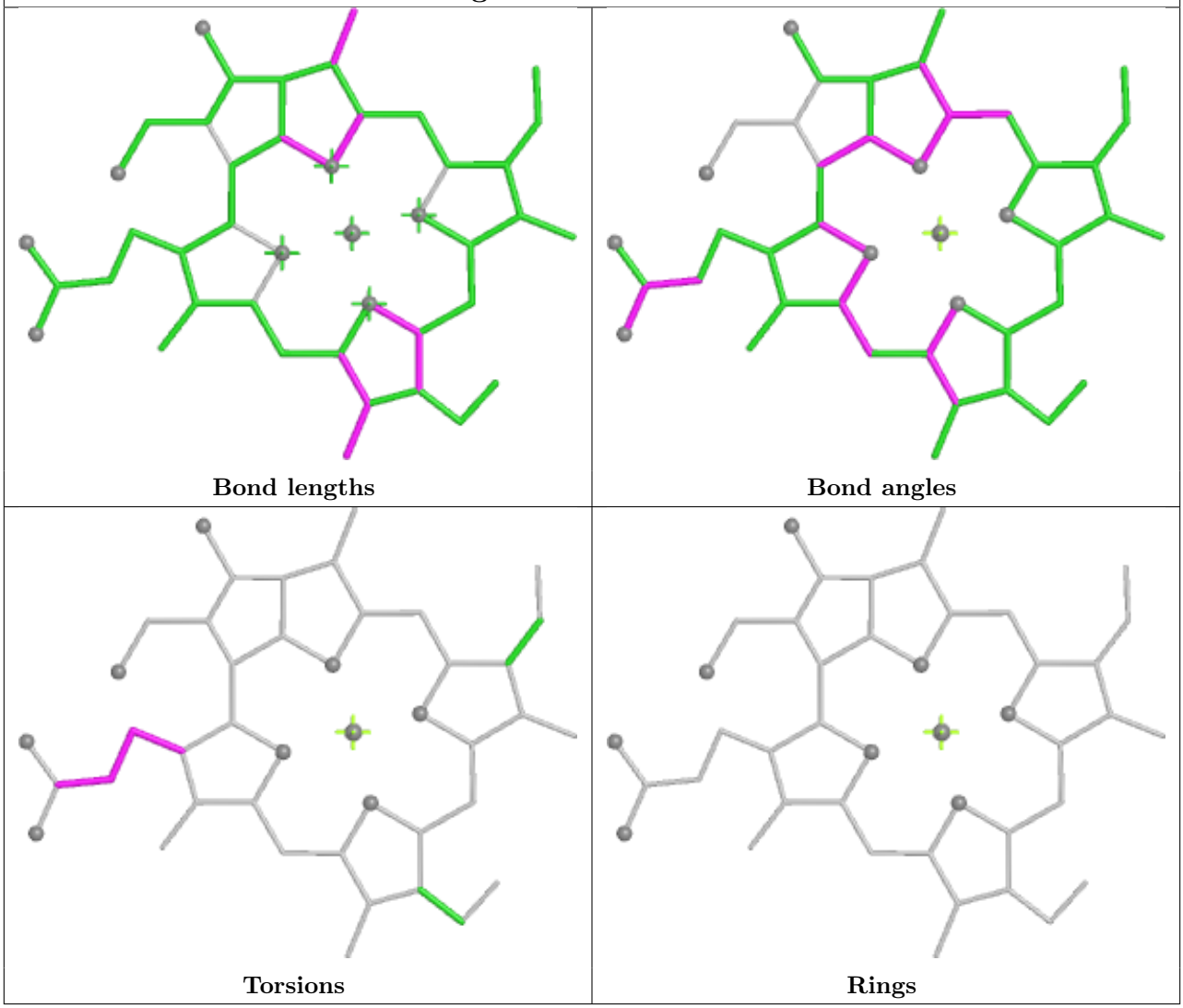
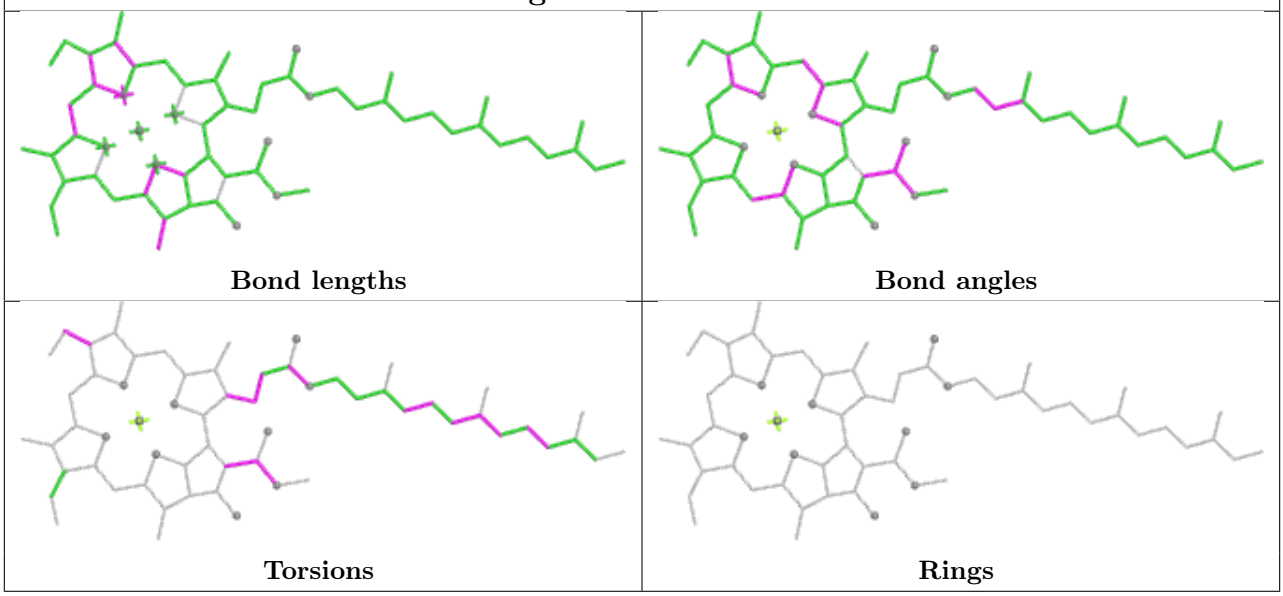


Rings

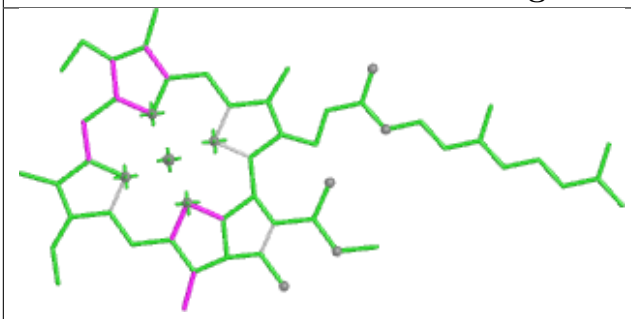
Ligand CLA AR 617



Ligand CLA v 303



Ligand CLA 9 613



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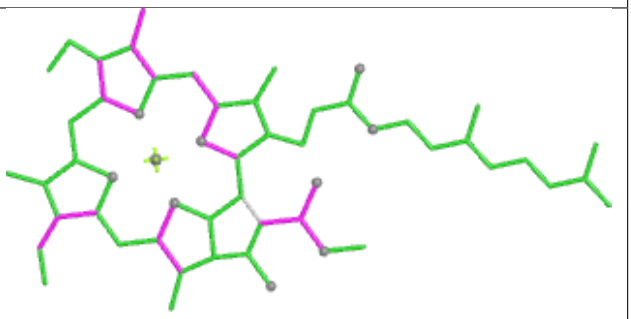
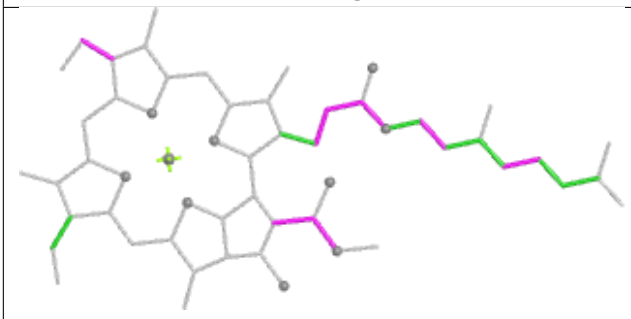


Bond angles



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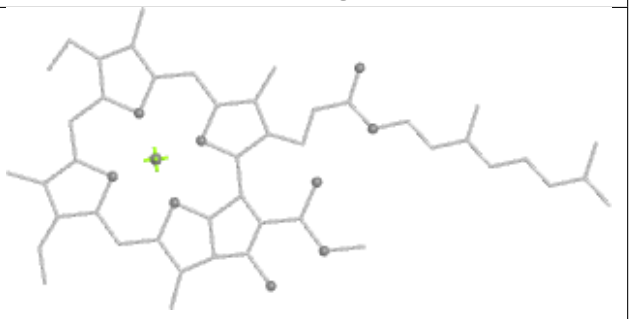
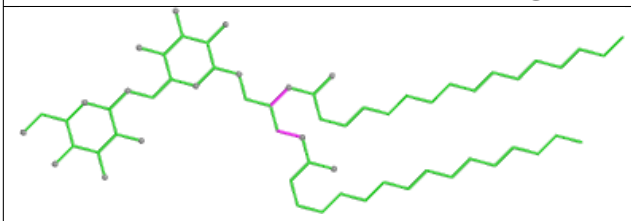


Rings

Ligand DGD j 102



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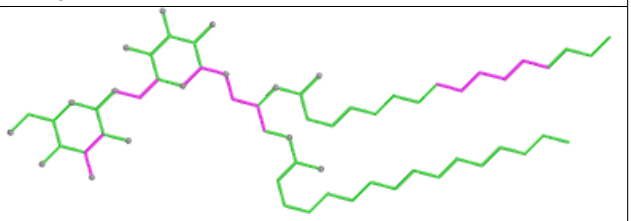
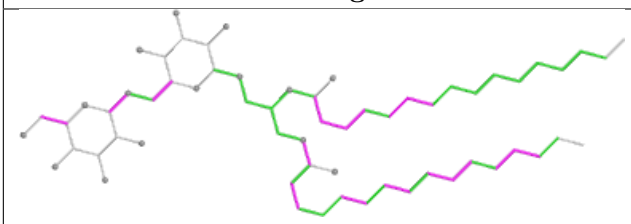


Bond angles



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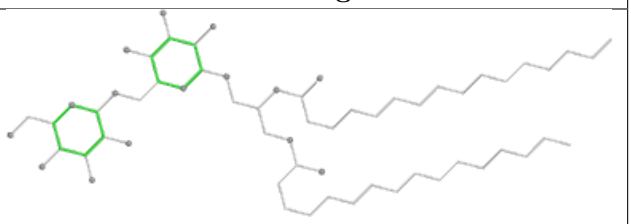
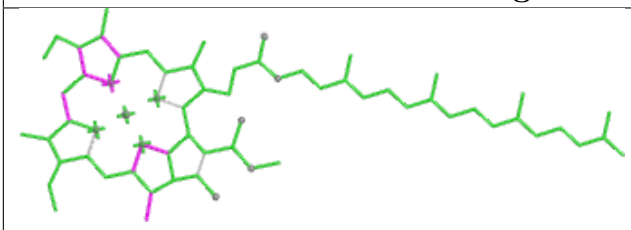


Rings

Ligand CLA AL 513



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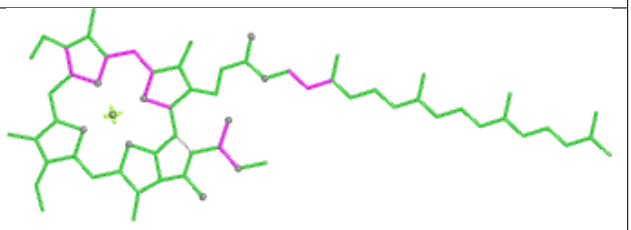
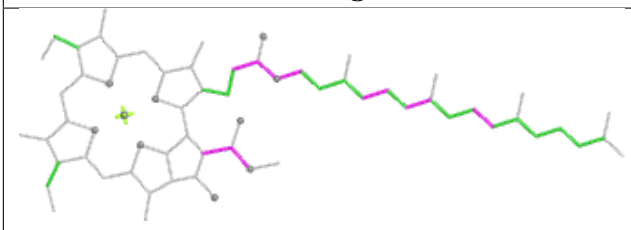


Bond angles



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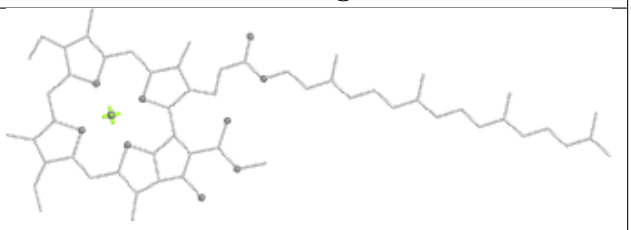
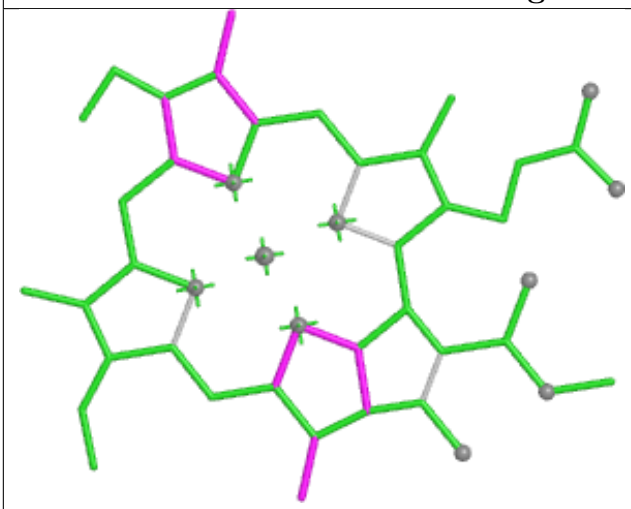
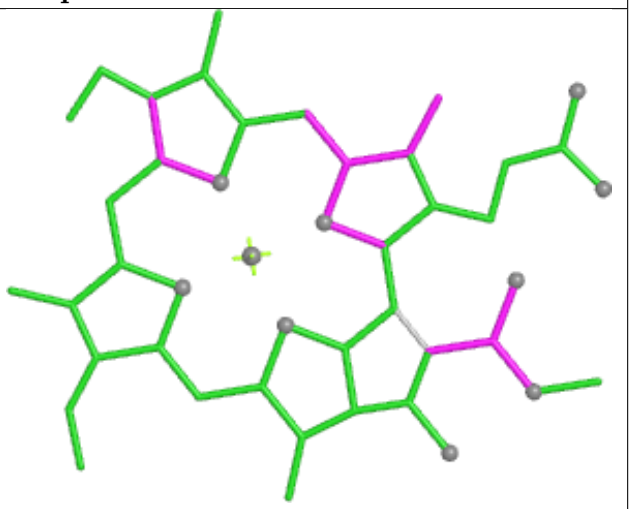


Rings

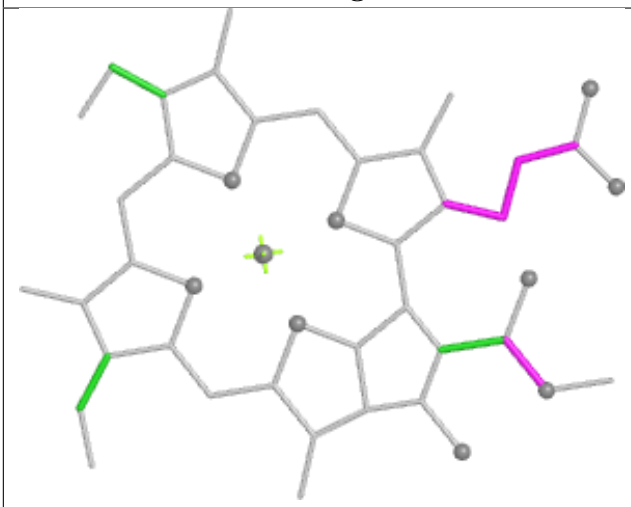
Ligand CLA q 618



Bond lengths



Bond angles



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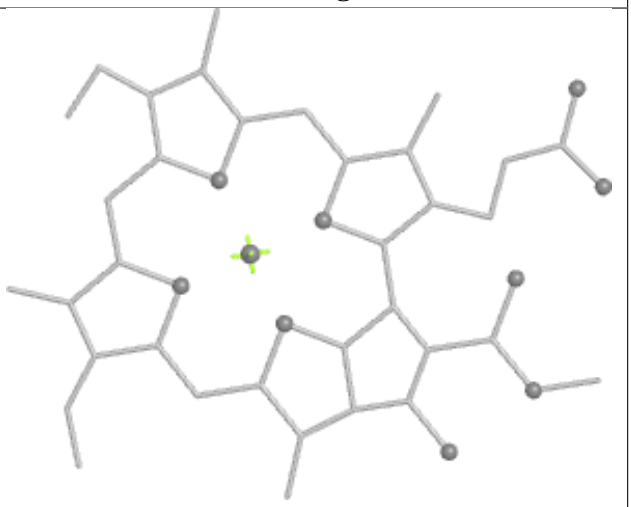
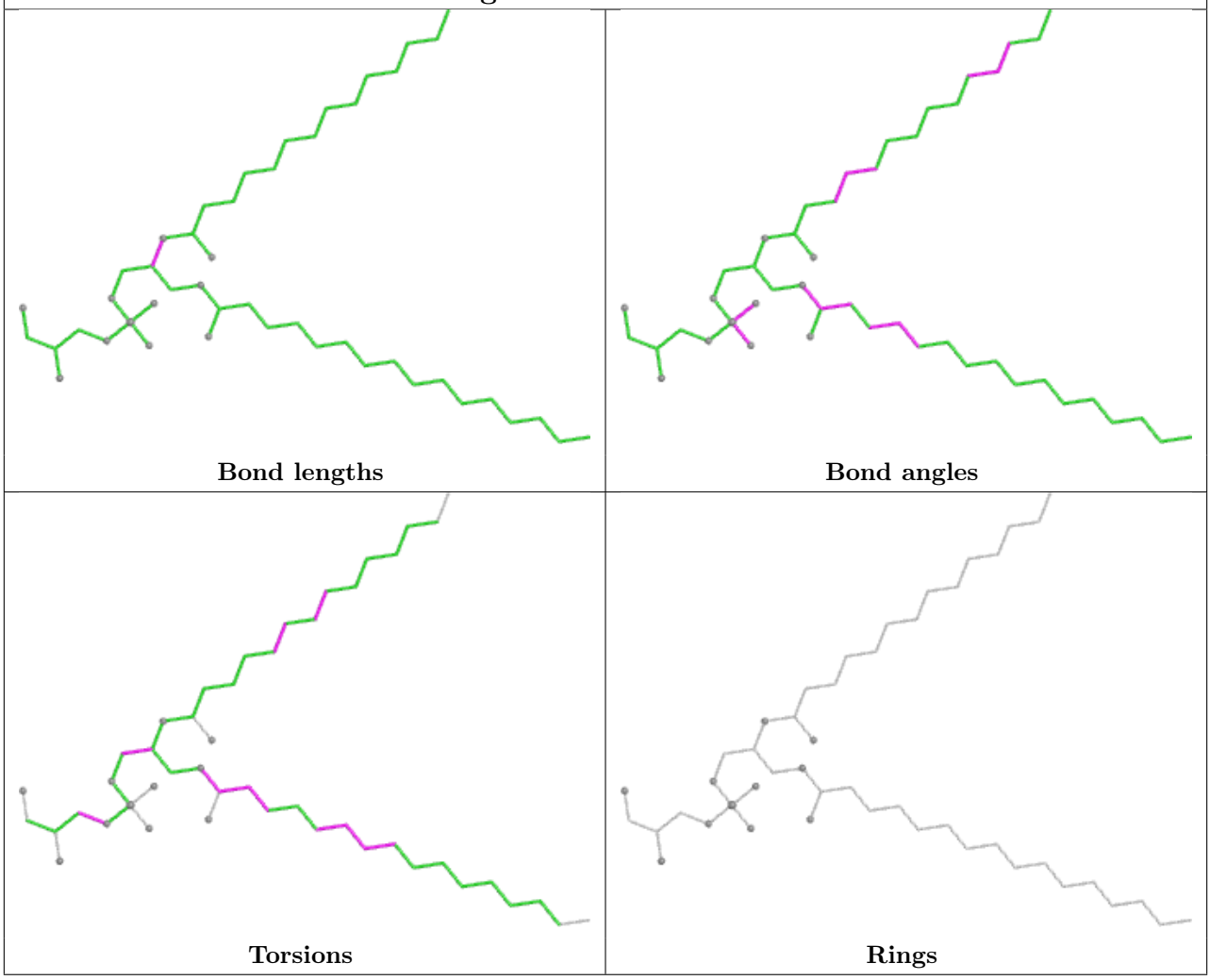
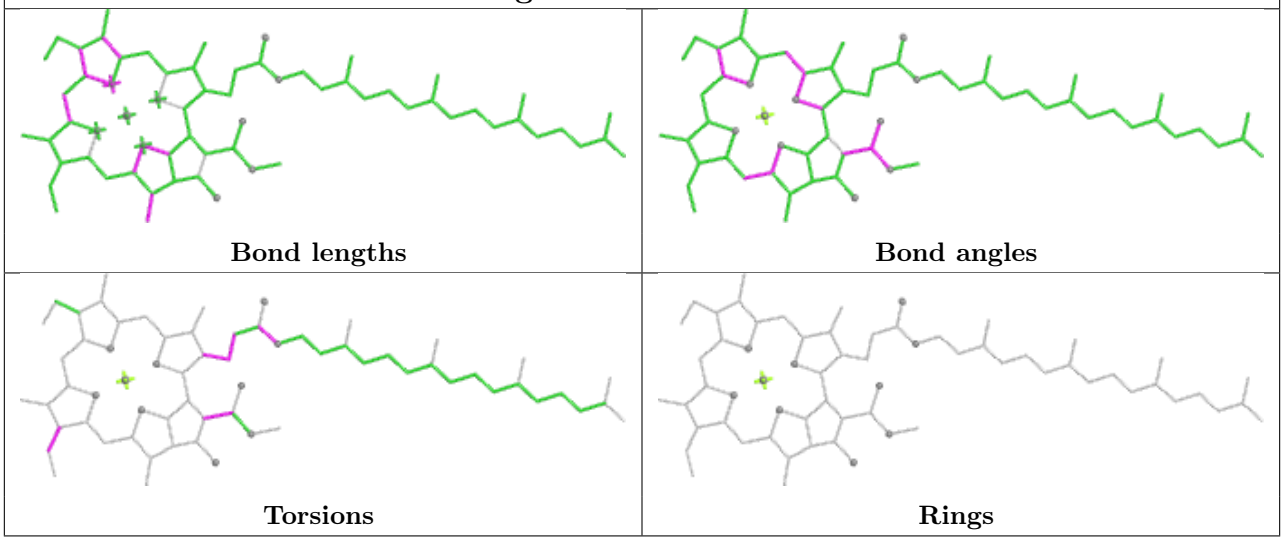


Rings

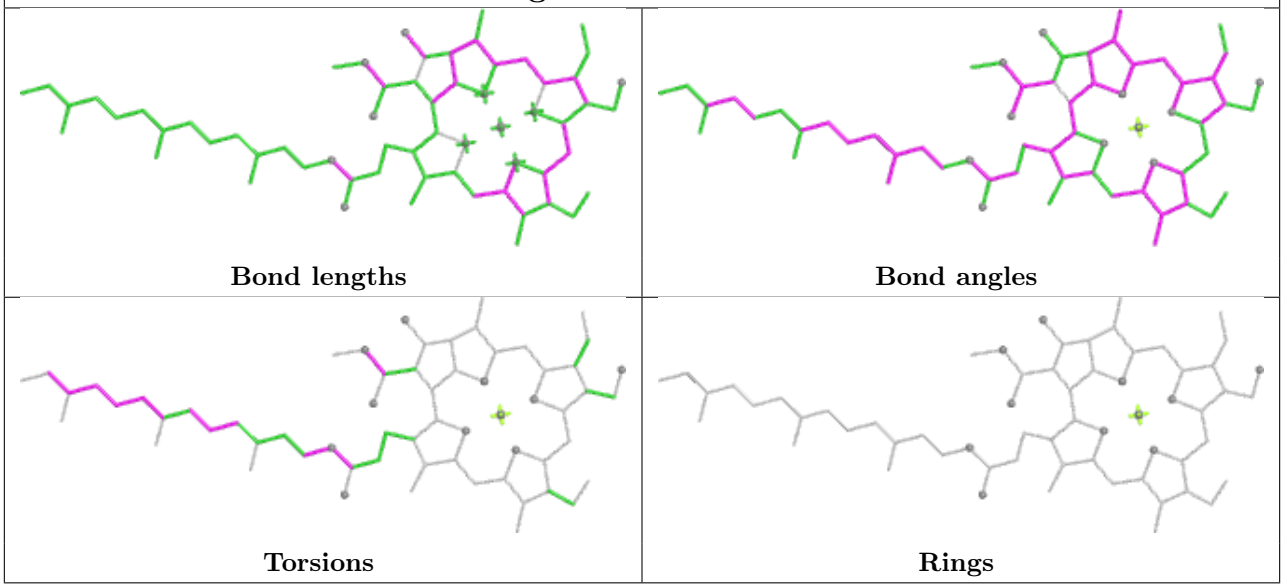
Ligand LHG AD 316



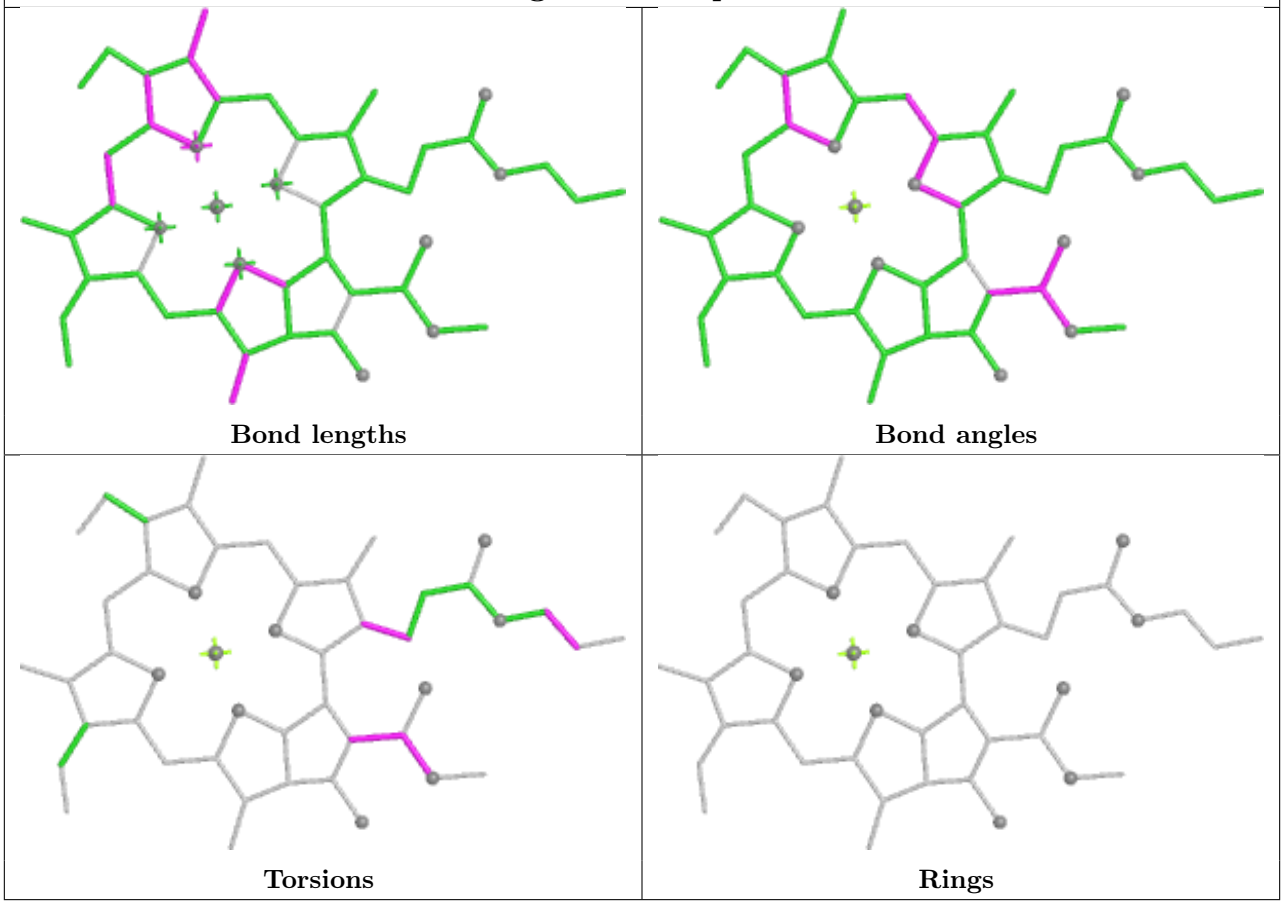
Ligand CLA AJ 405



Ligand CHL 9 609



Ligand CLA q 604



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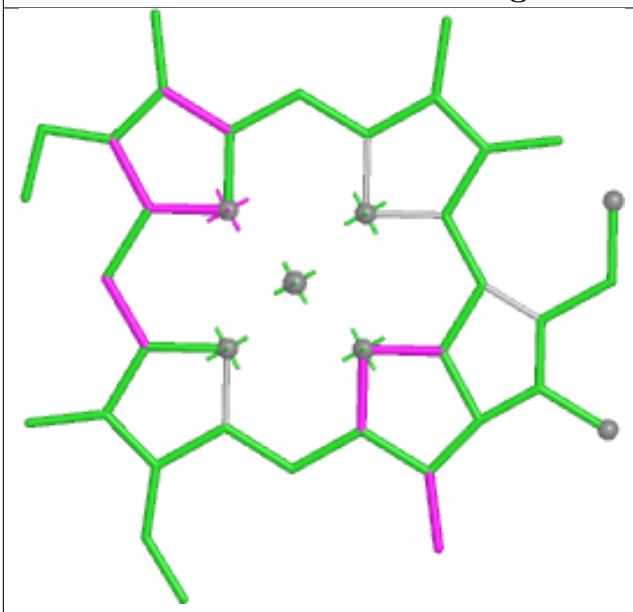
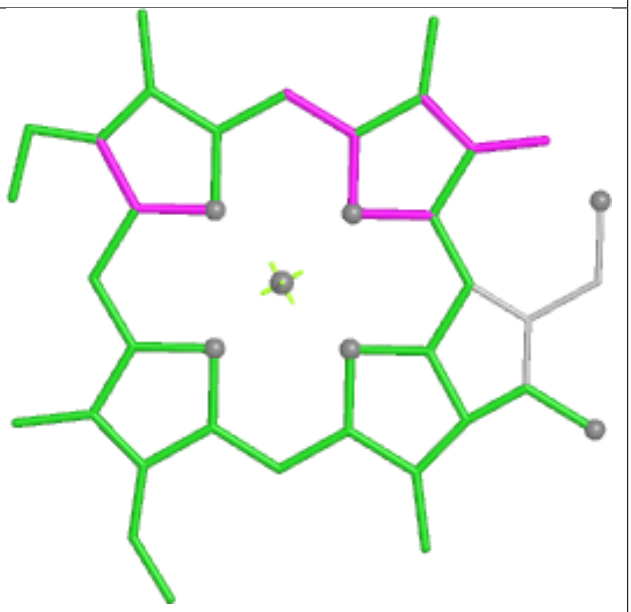
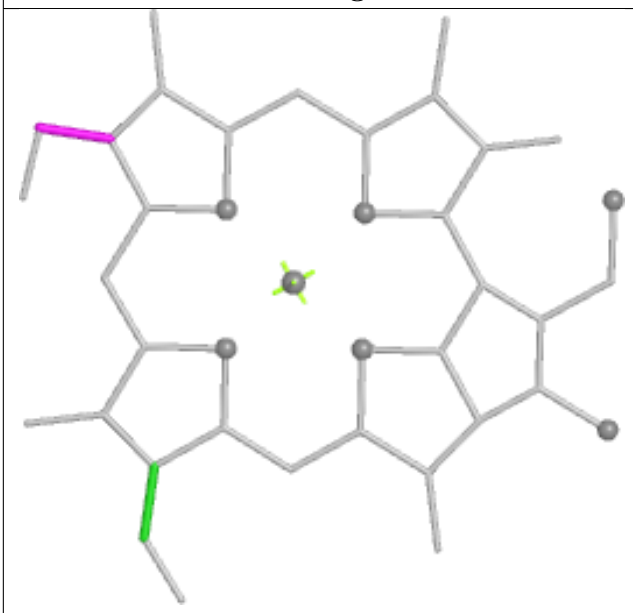


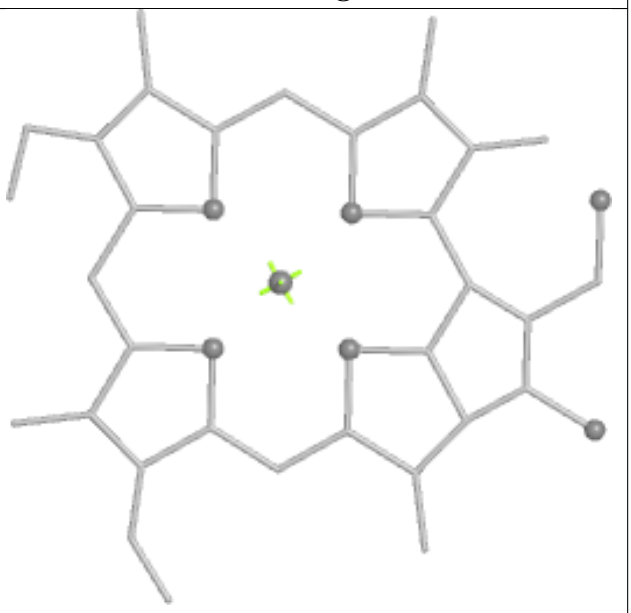
Bond lengths



Bond angles

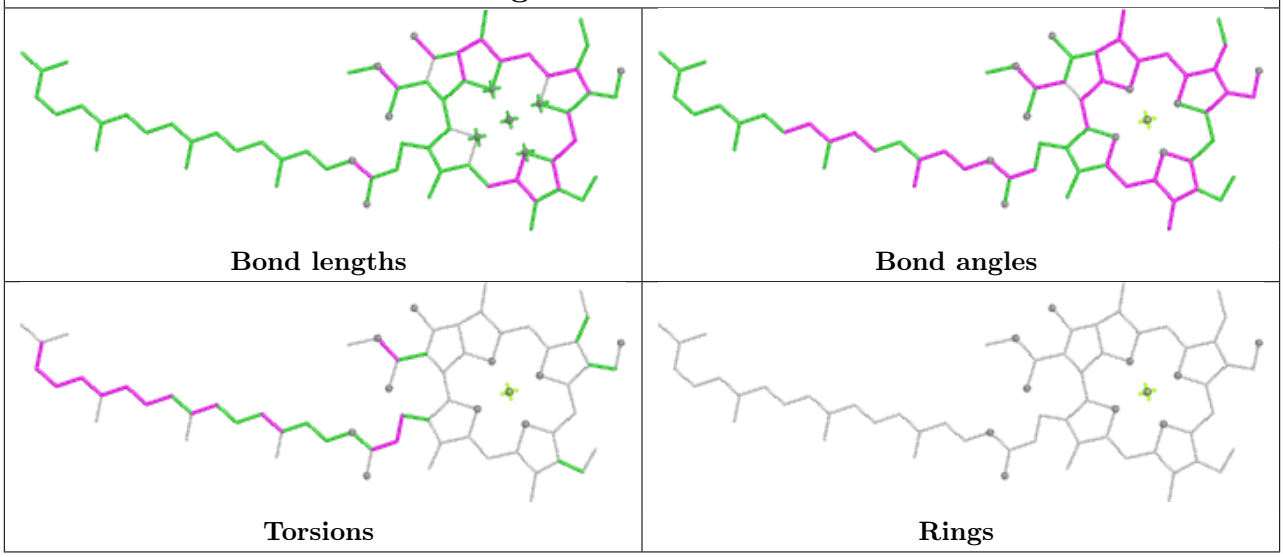


Torsions

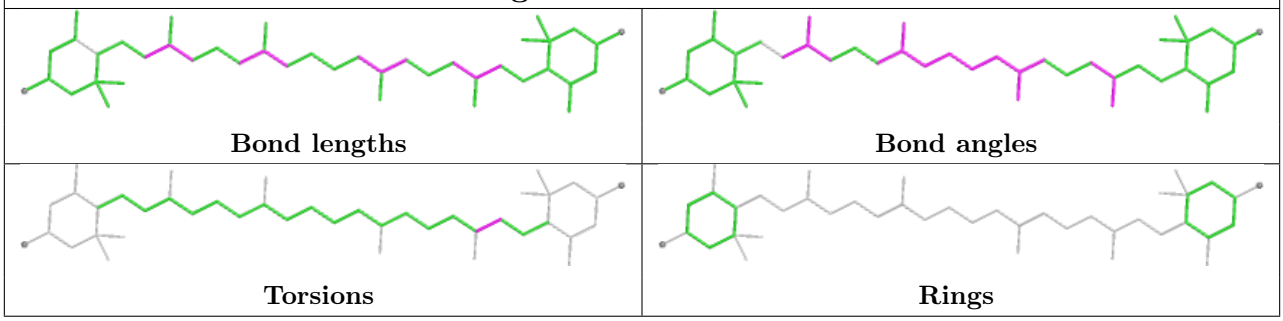


Rings

Ligand CHL AU 607



Ligand LUT AH 614



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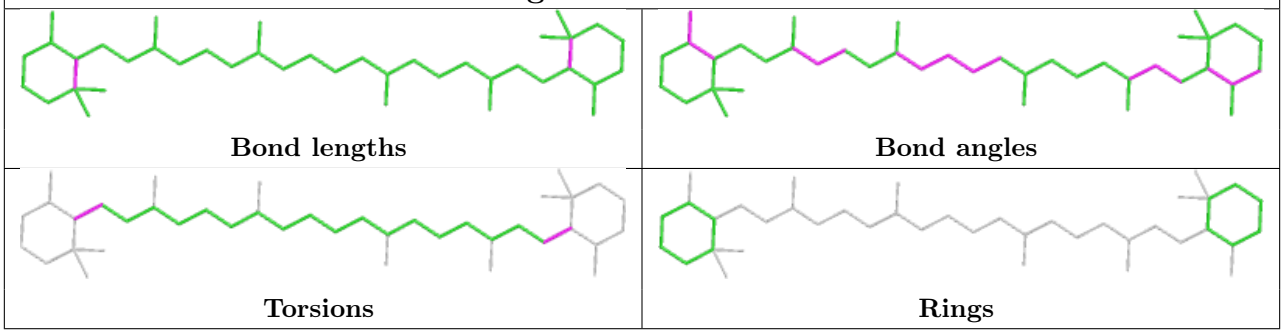

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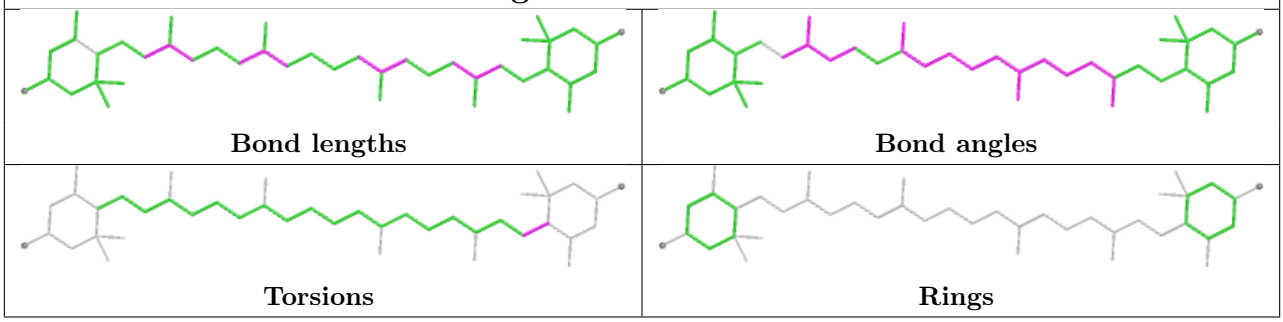
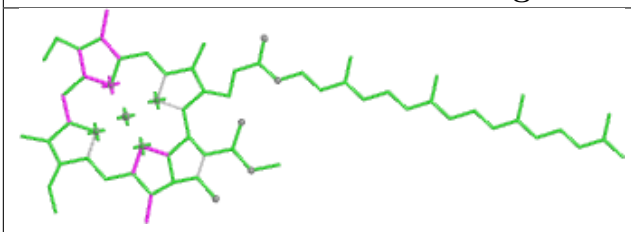
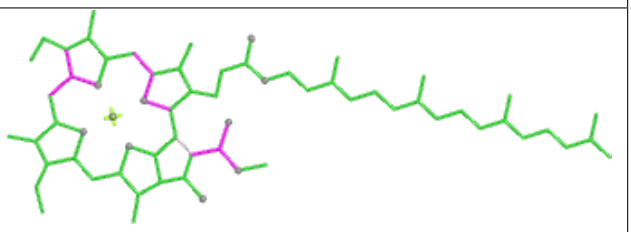
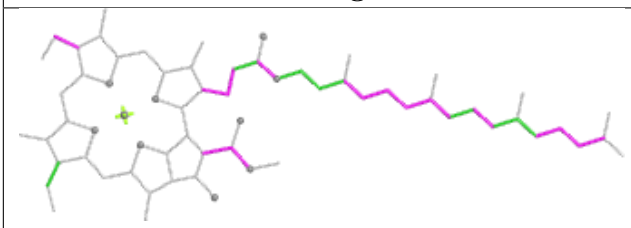
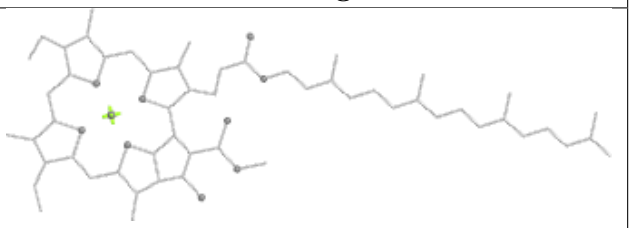
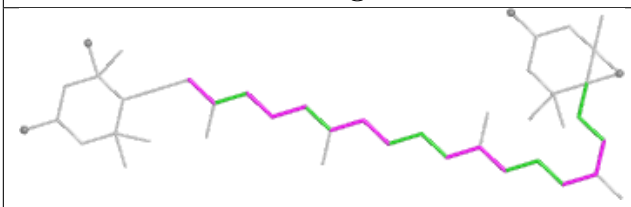
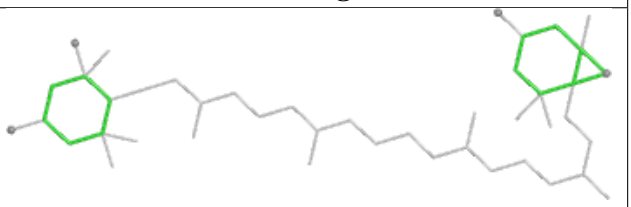
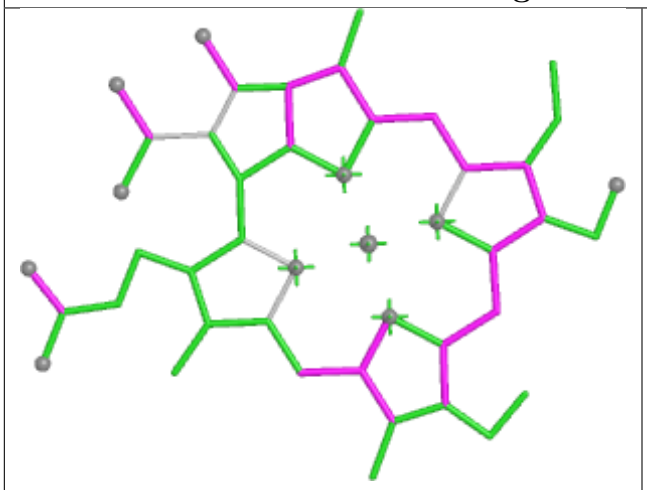


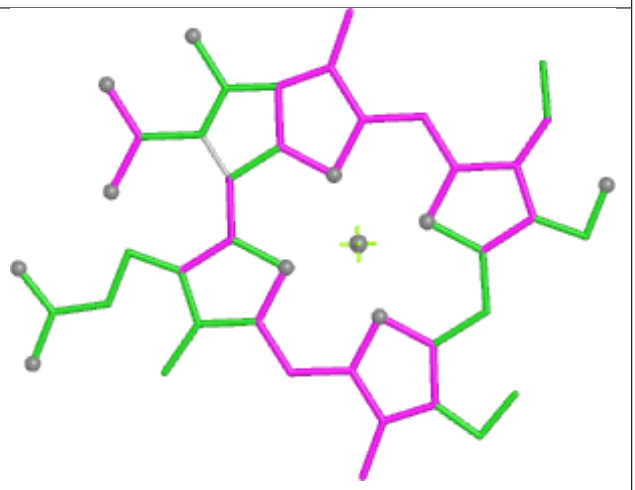
Ligand CLA AL 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NEX AS 317	
Bond lengths	Bond angles
 Torsions	 Rings

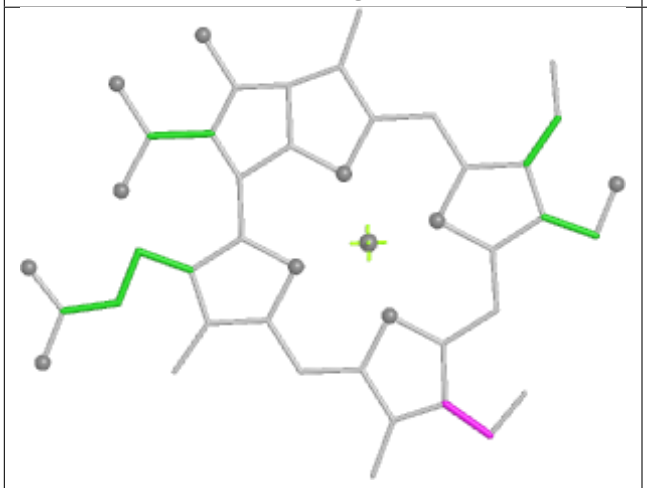
Ligand CHL AF 601



Bond lengths



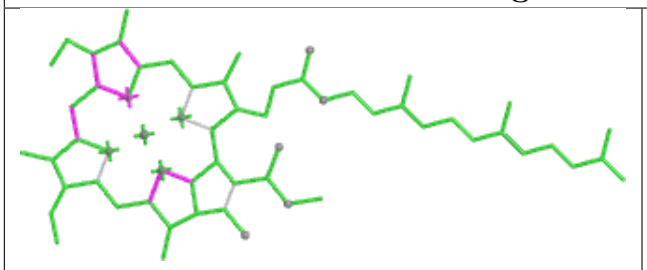
Bond angles



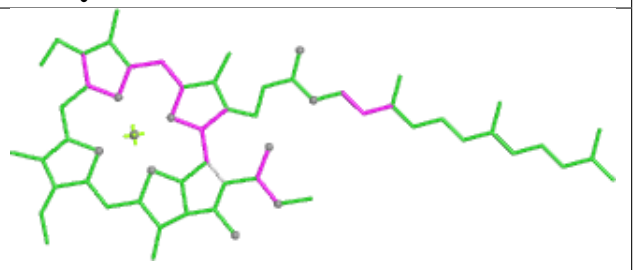
Torsions

Rings

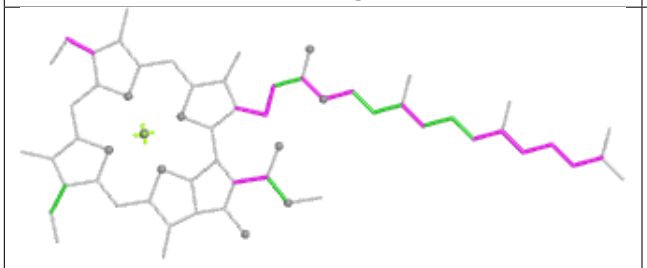
Ligand CLA AQ 611



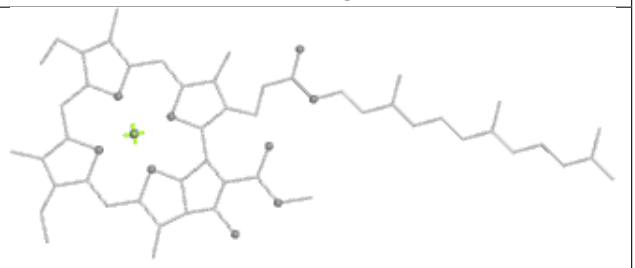
Bond lengths



Bond angles

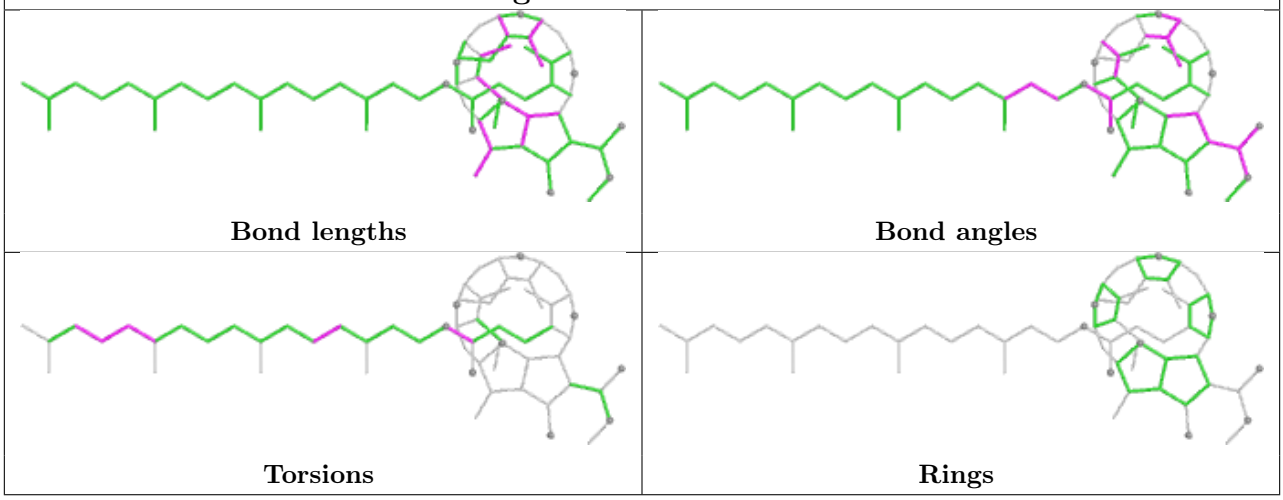


Torsions

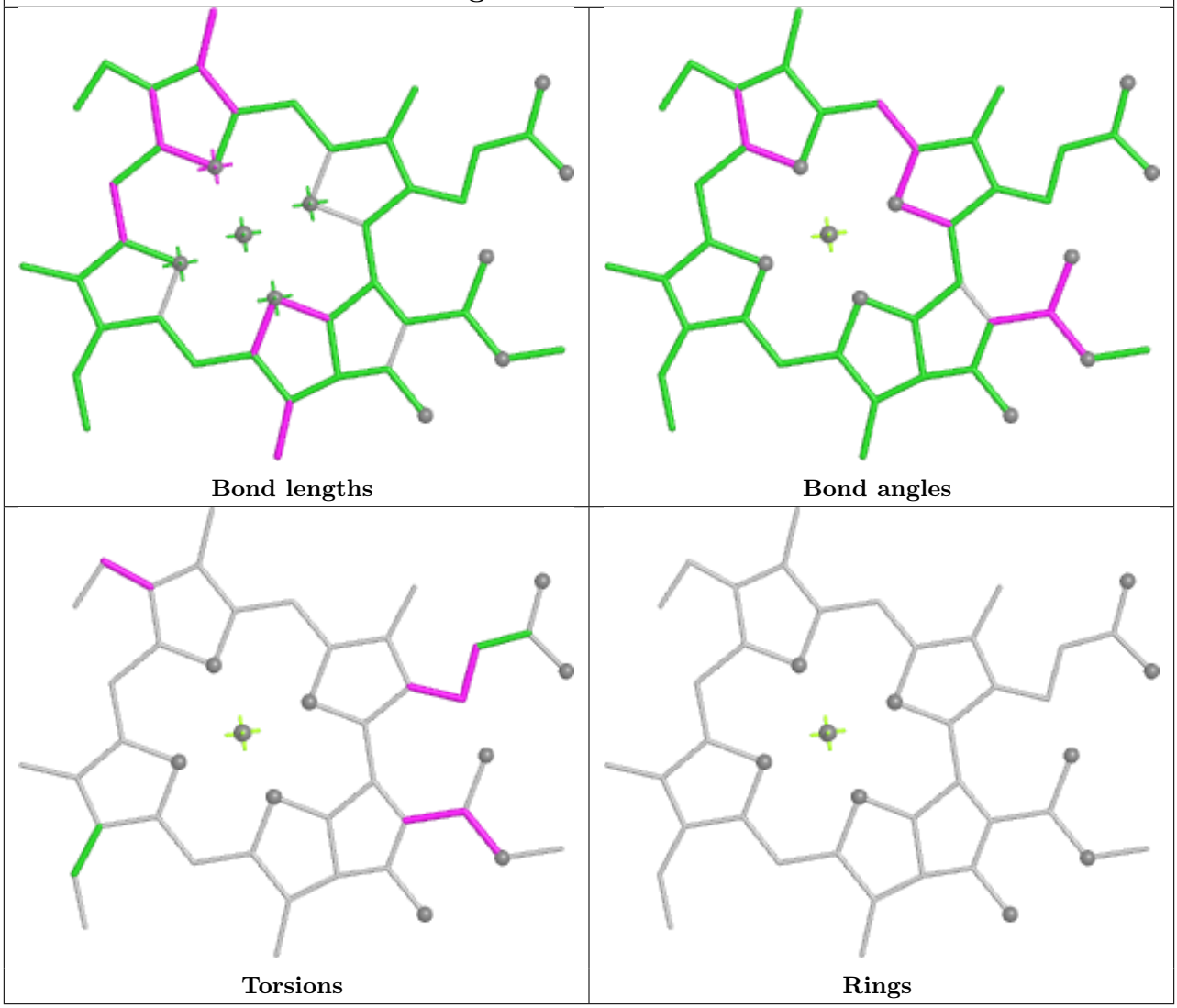


Rings

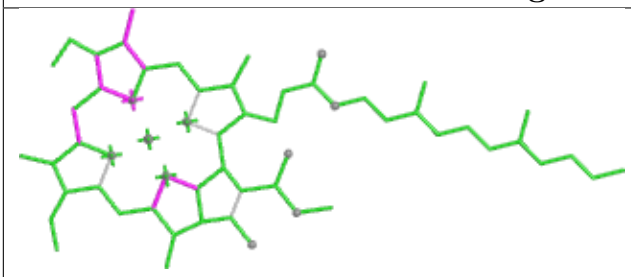
Ligand PHO AJ 407



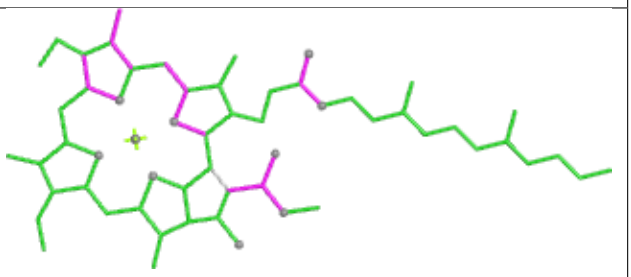
Ligand CLA AD 305



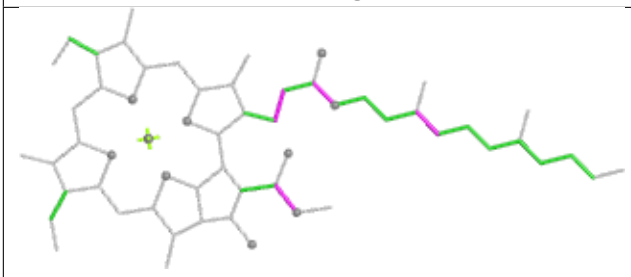
Ligand CLA 0 612



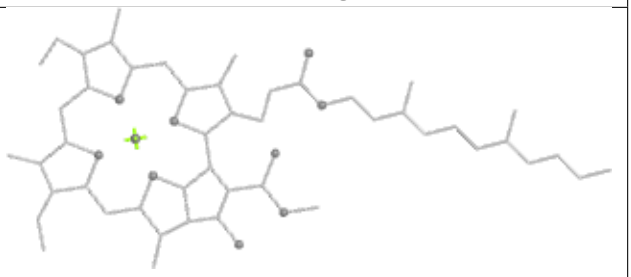
Bond lengths



Bond angles

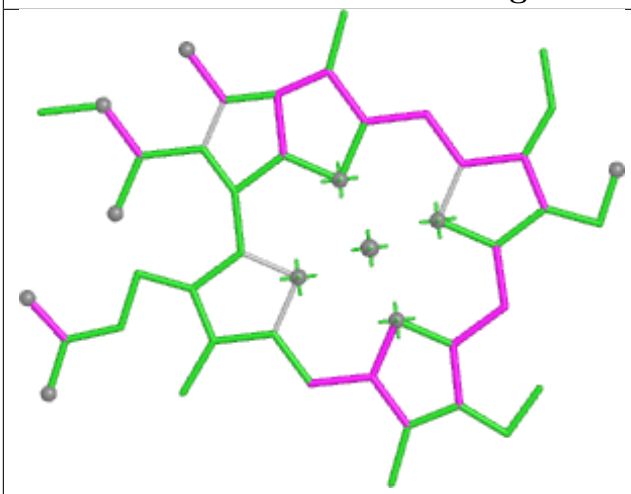


Torsions



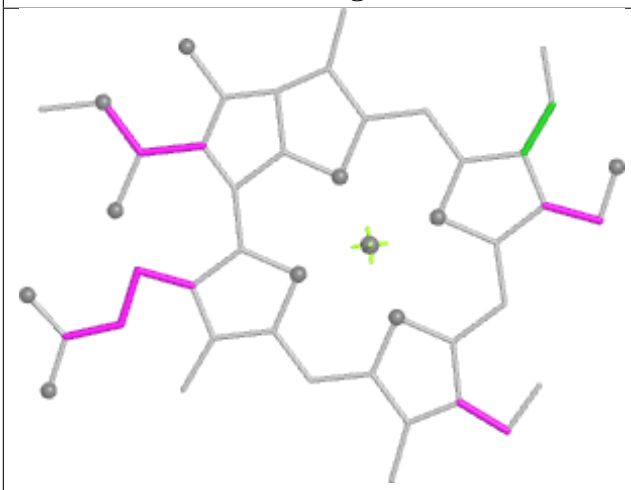
Rings

Ligand CHL AA 607



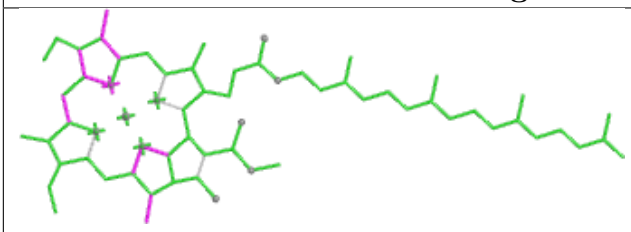
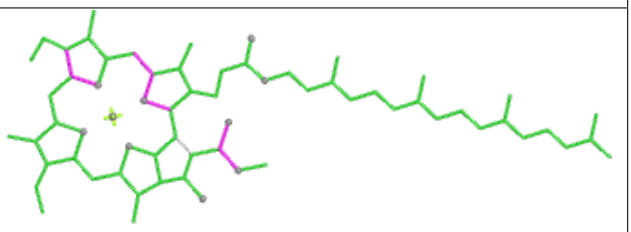
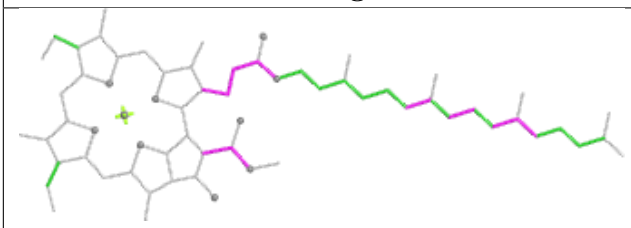
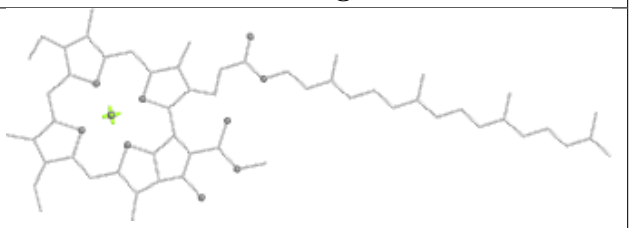
Bond lengths

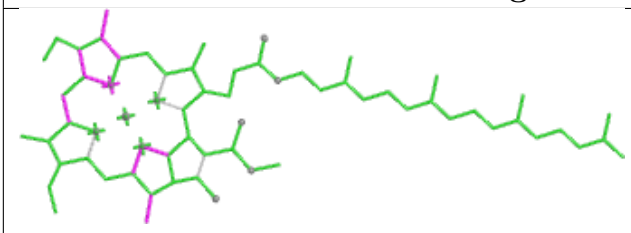
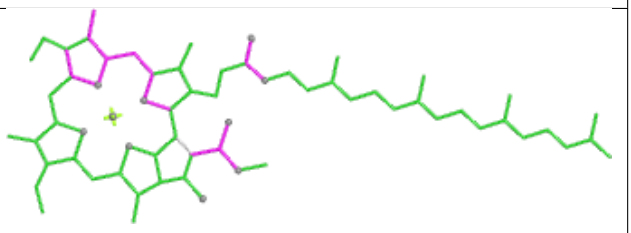
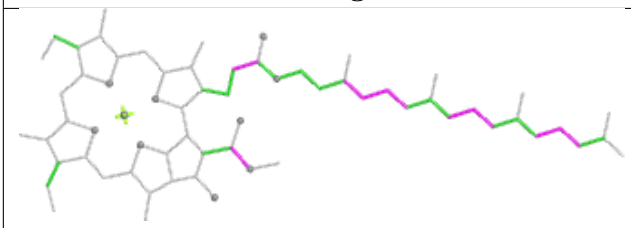
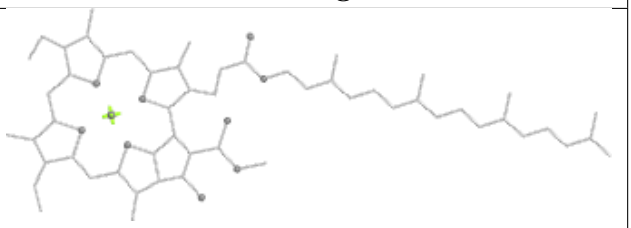
Bond angles



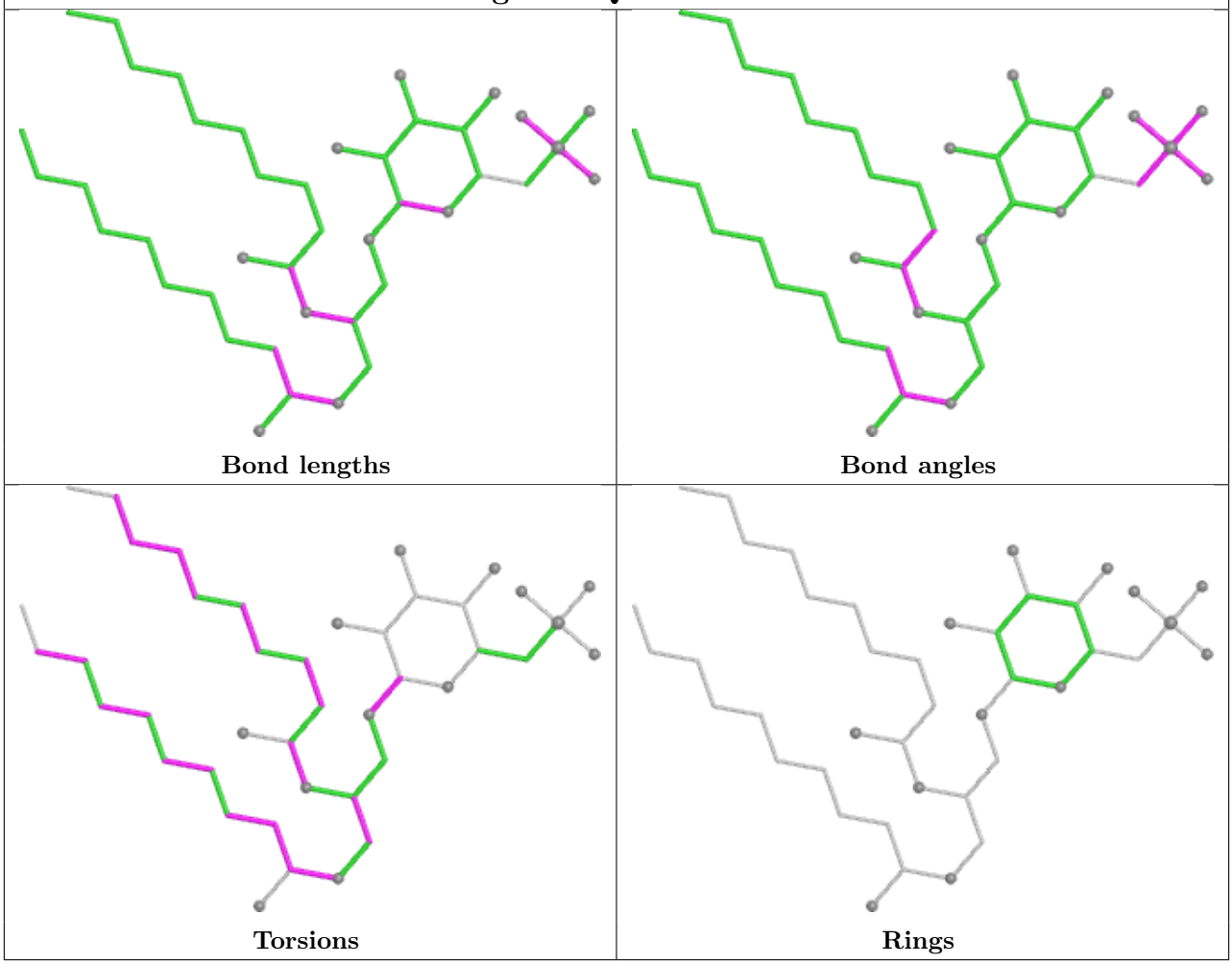
Torsions

Rings

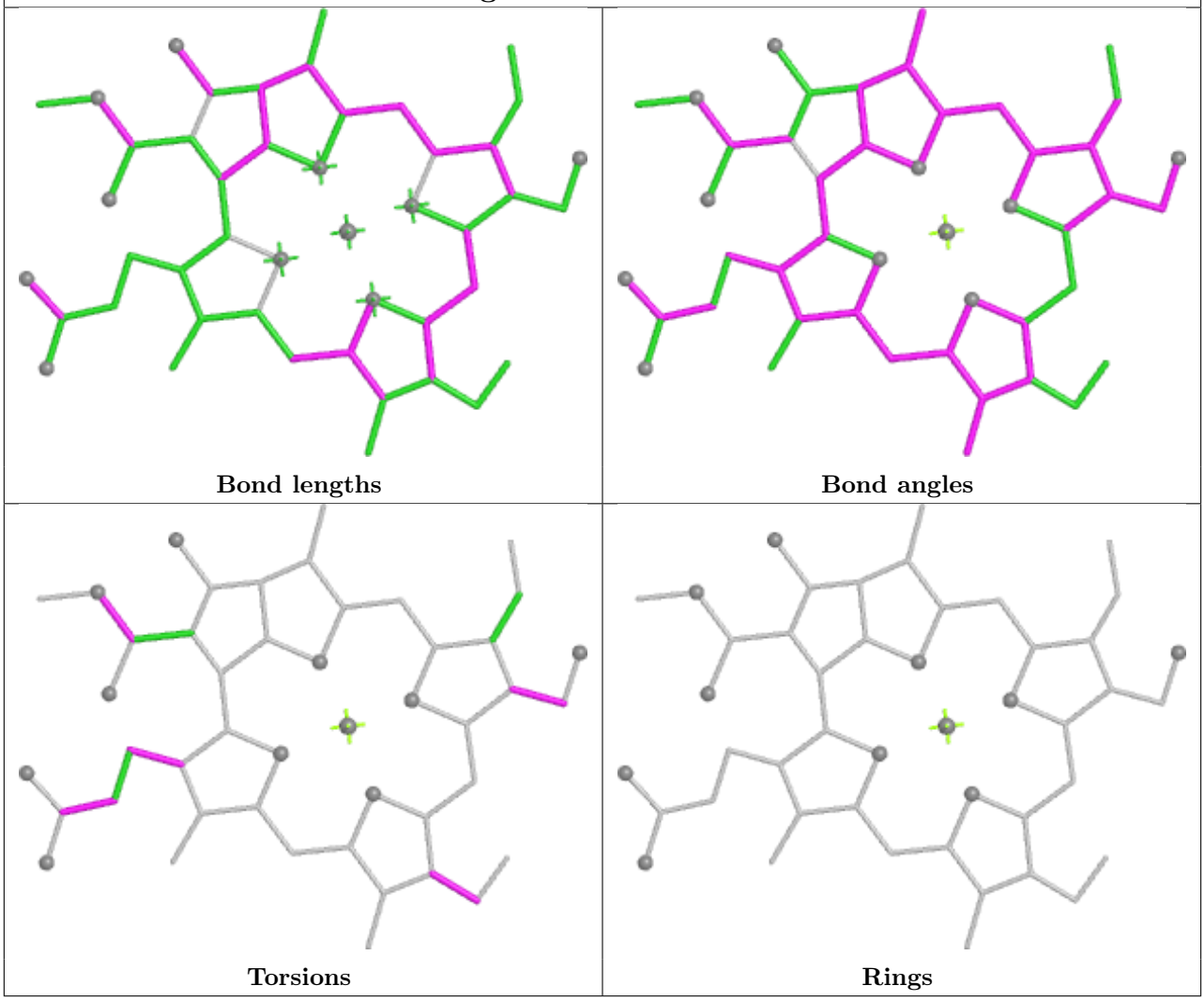
Ligand CLA AU 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AK 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

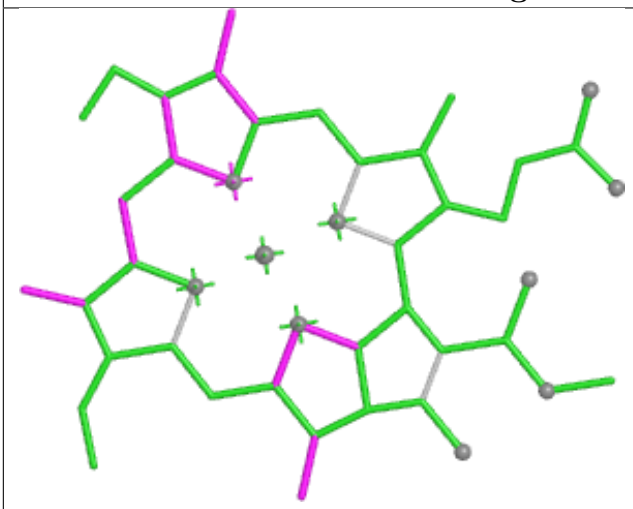
Ligand SQD AP 101



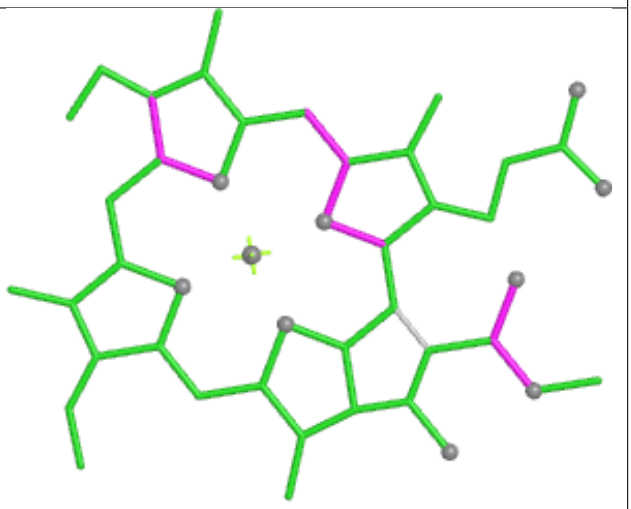
Ligand CHL AC 605



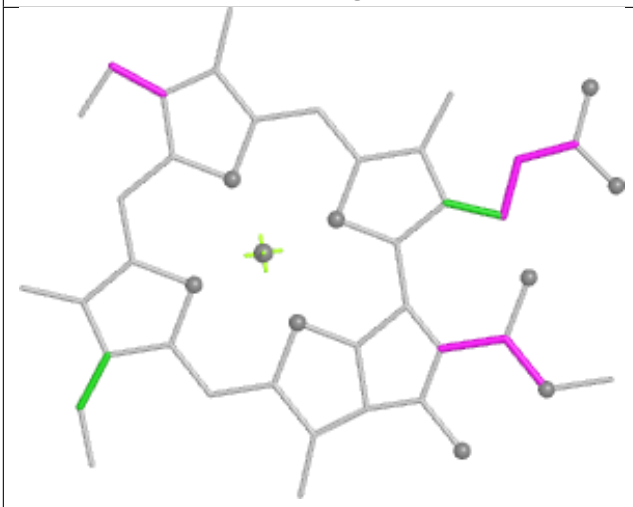
Ligand CLA AD 311



Bond lengths



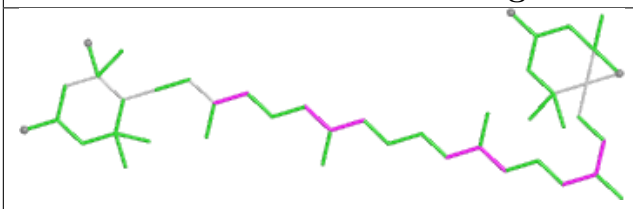
Bond angles



Torsions

Rings

Ligand NEX AU 616



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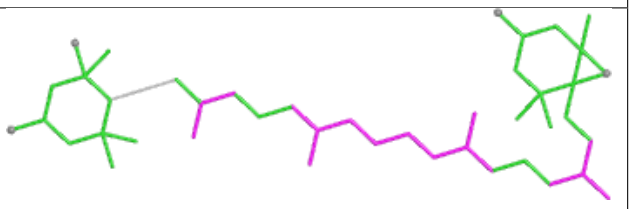
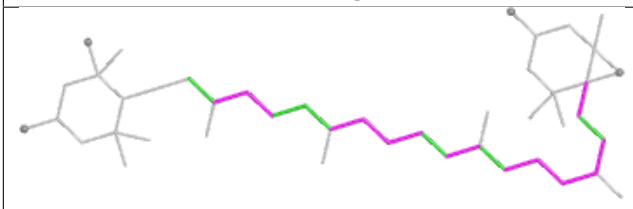
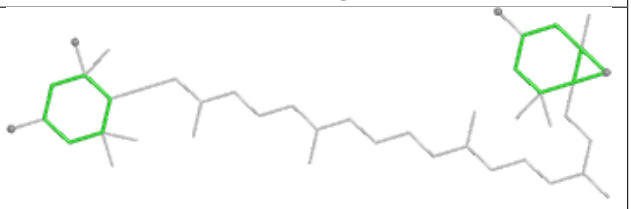


Bond angles

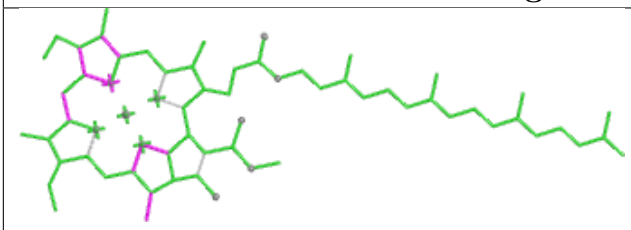


Torsions



Rings

Ligand CLA P 509



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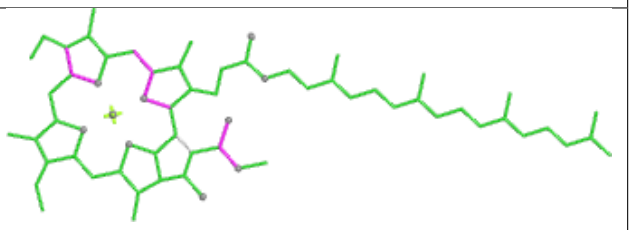
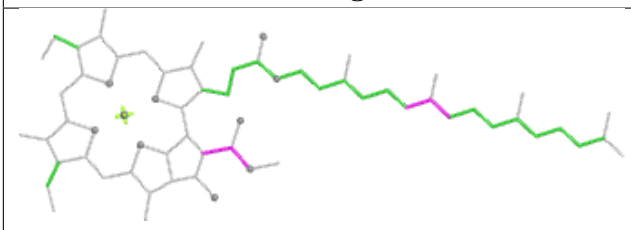


Bond angles



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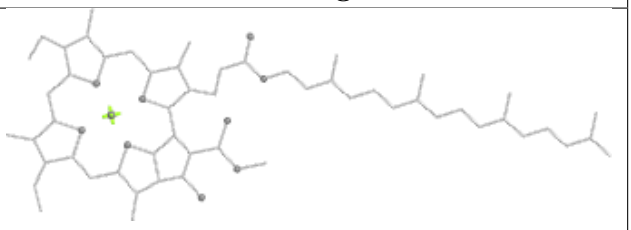
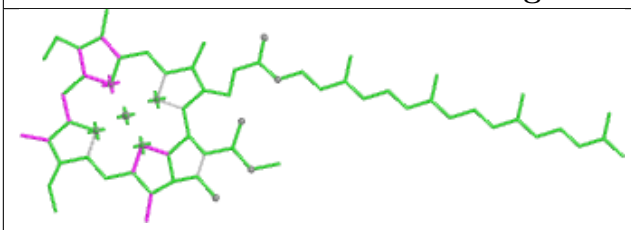


Rings

Ligand CLA O 616



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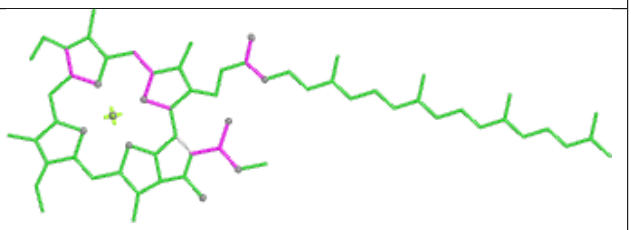
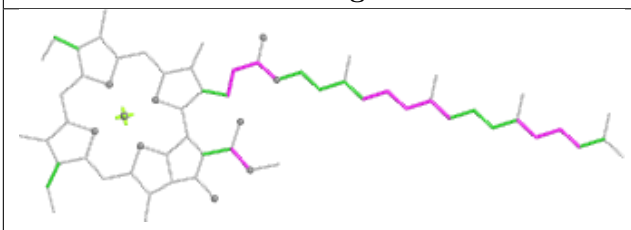


Bond angles



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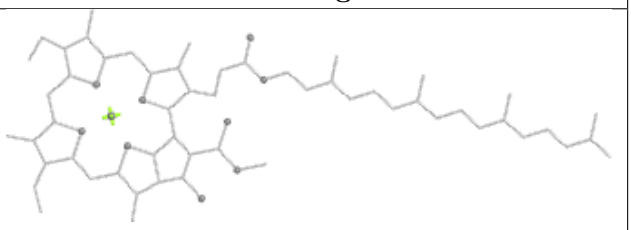
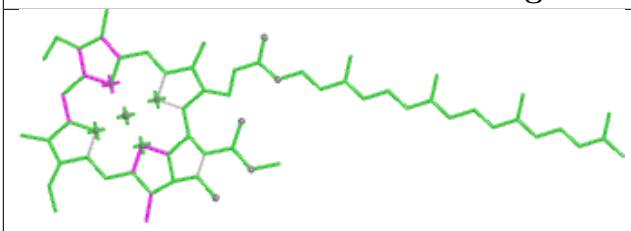


Rings

Ligand CLA P 511



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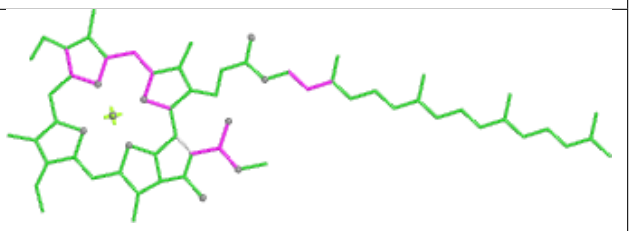
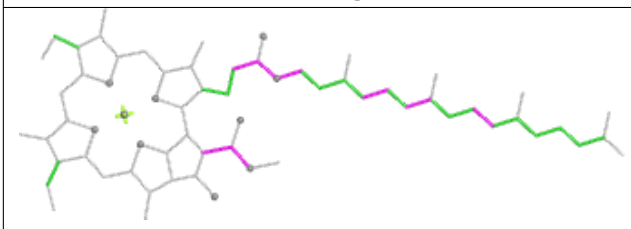
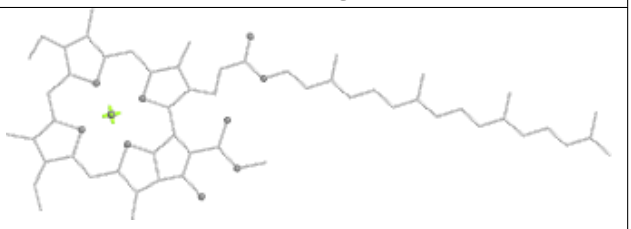


Bond angles

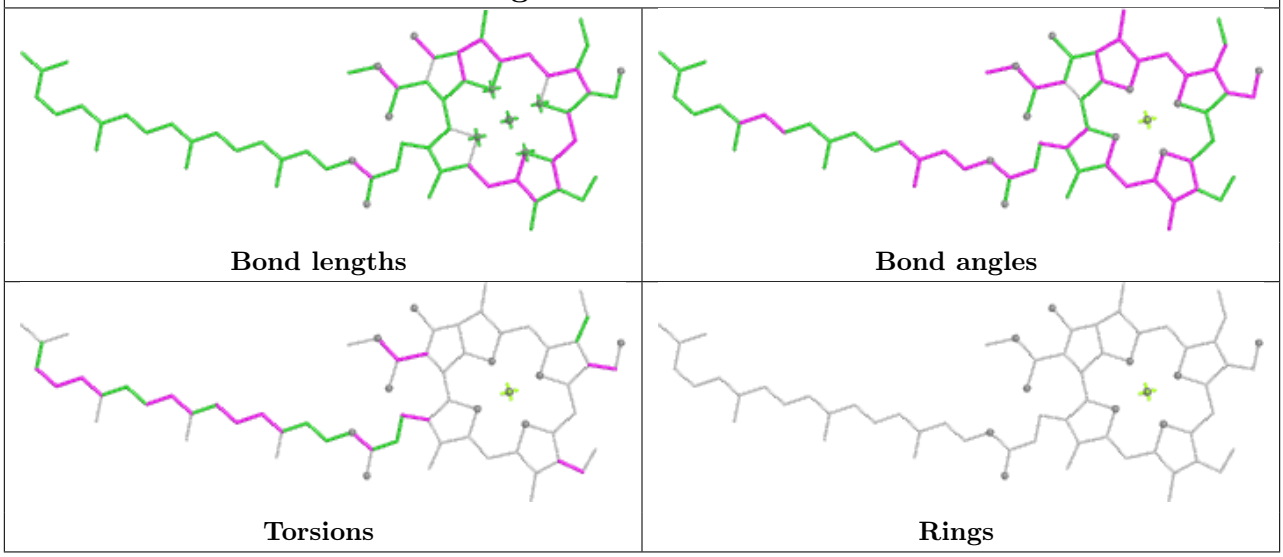


Torsions

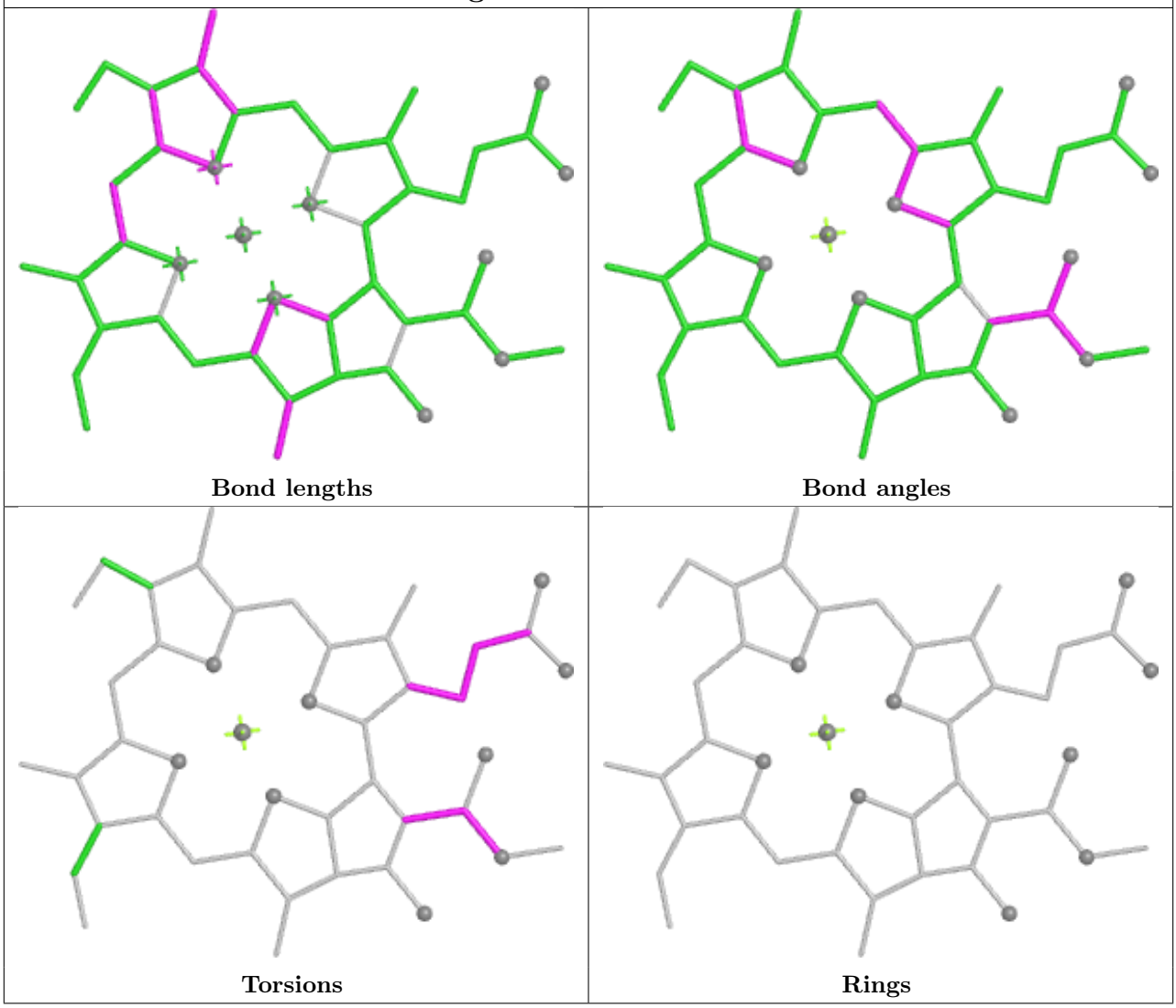


Rings

Ligand CHL AU 608



Ligand CLA AA 604



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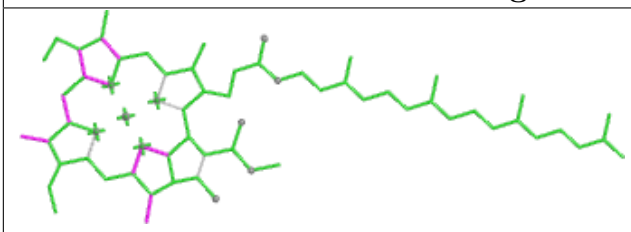
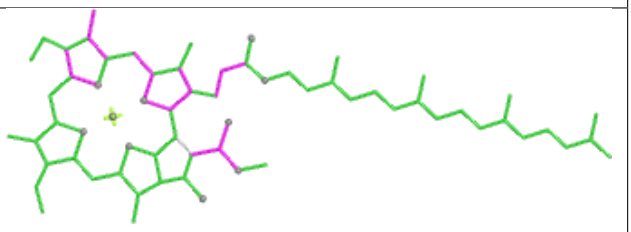
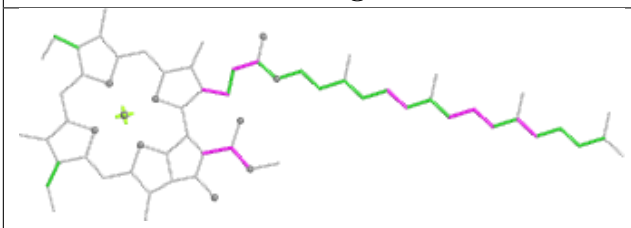


Bond lengths



Bond angles



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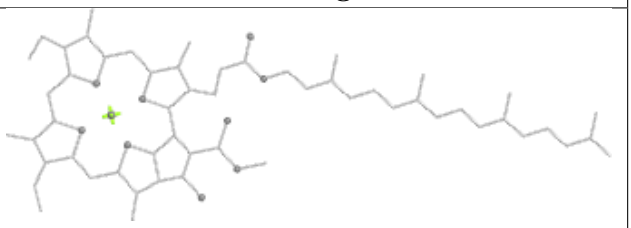
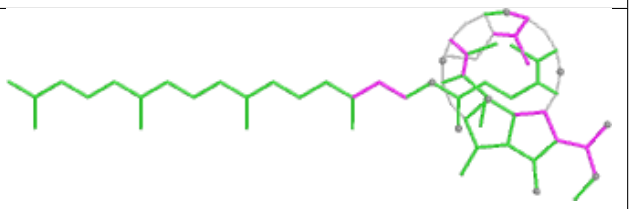


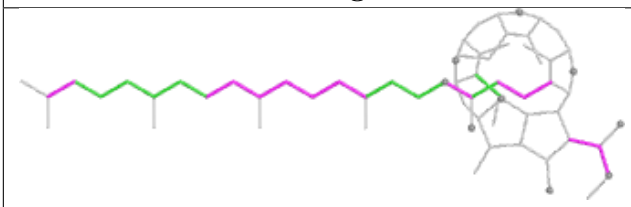
Rings

Ligand PHO AJ 408

Bond lengths



Bond angles



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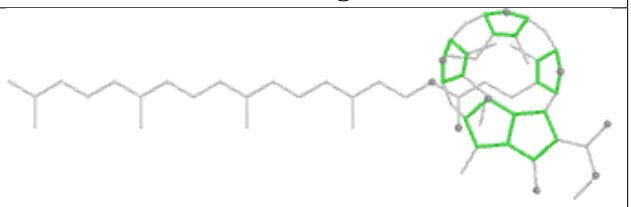
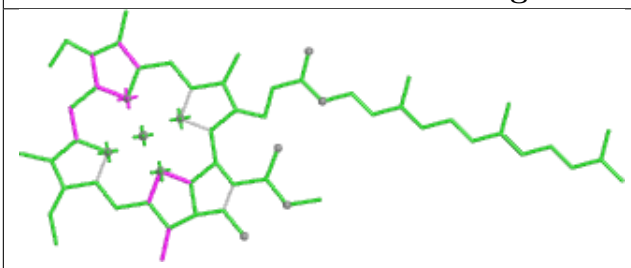
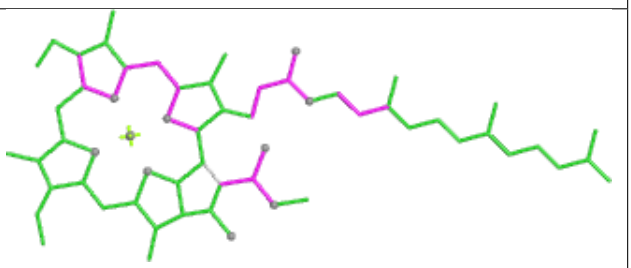


Rings

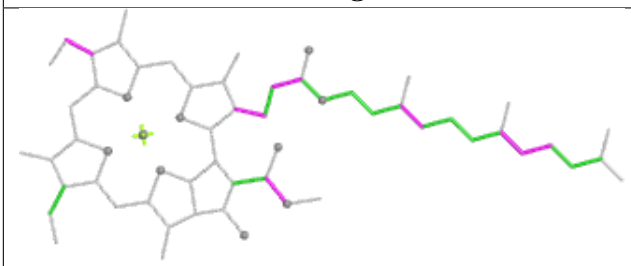
Ligand CLA AU 610



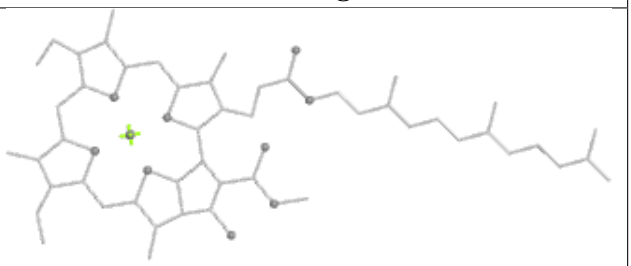
Bond lengths



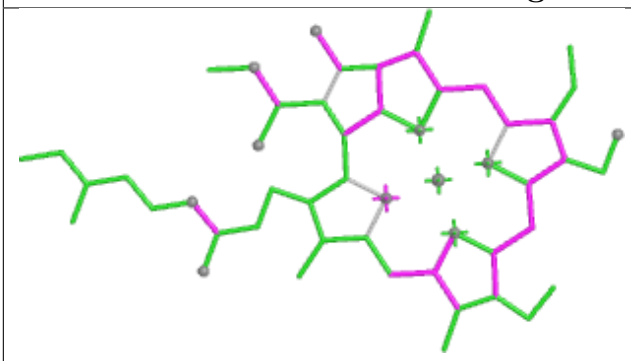
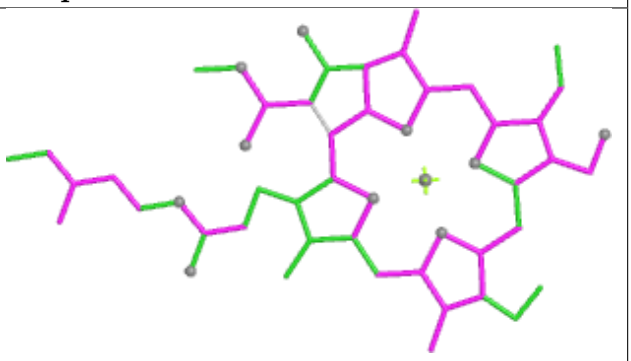
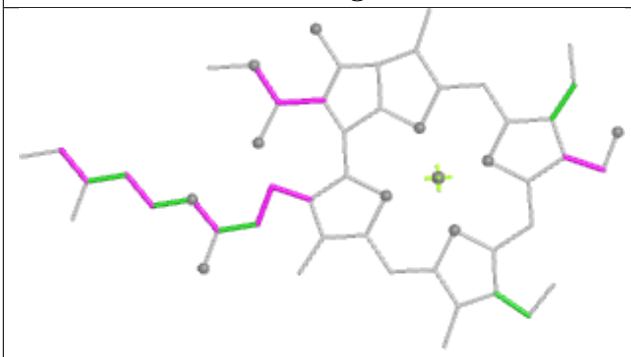
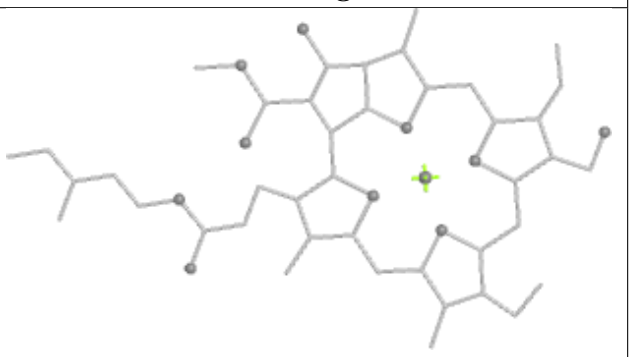
Bond angles

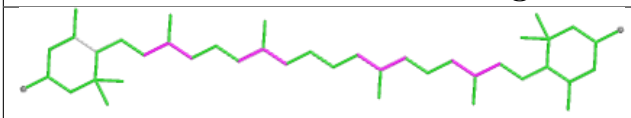
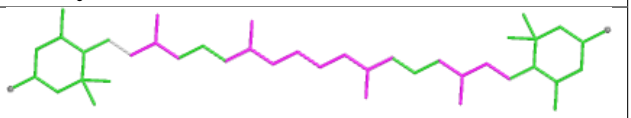
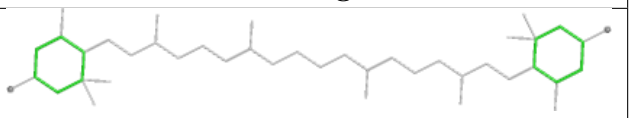


Torsions

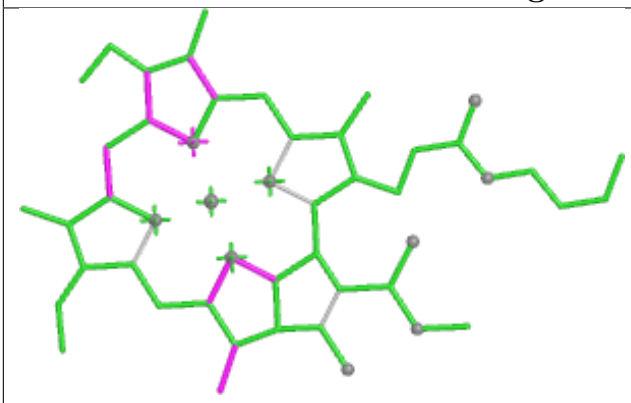


Rings

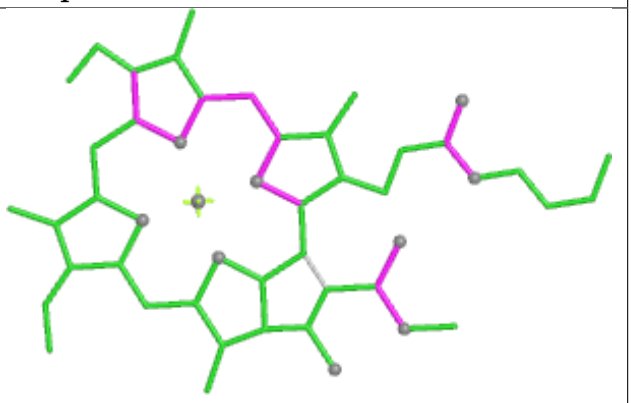
Ligand CHL q 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT AQ 616	
 Bond lengths	 Bond angles
Torsions	 Rings

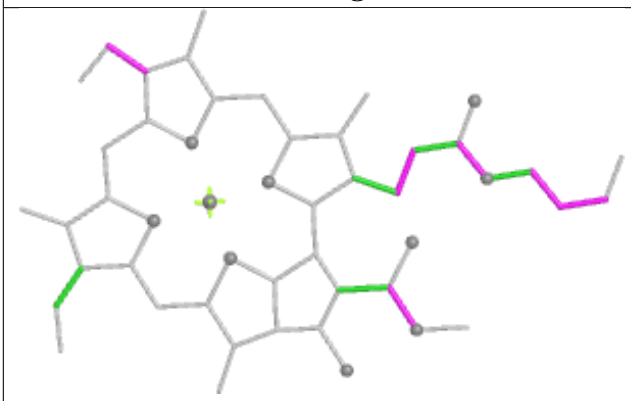
Ligand CLA q 611



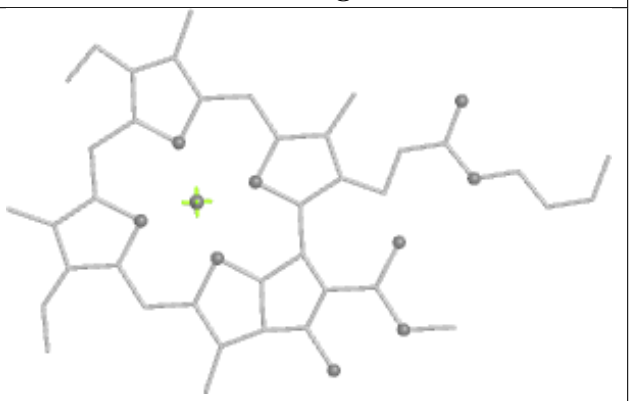
Bond lengths



Bond angles

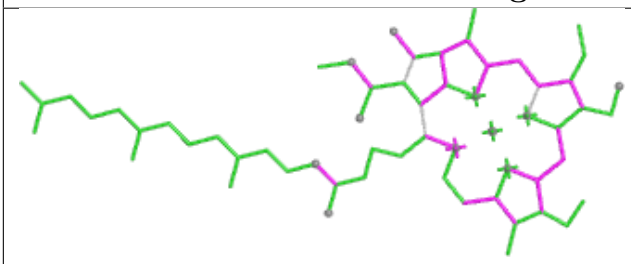


Torsions

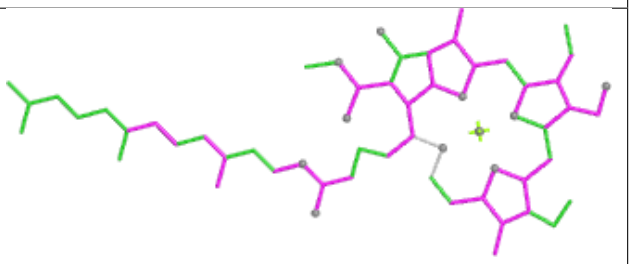


Rings

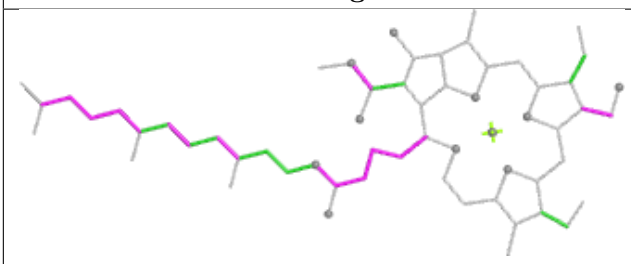
Ligand CHL AA 608



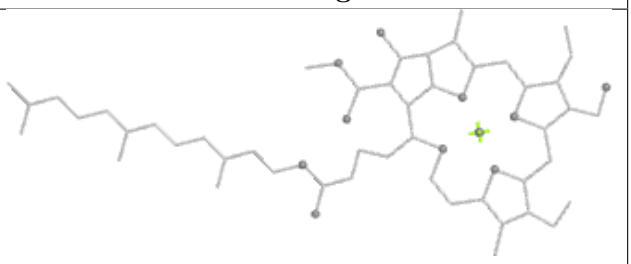
Bond lengths



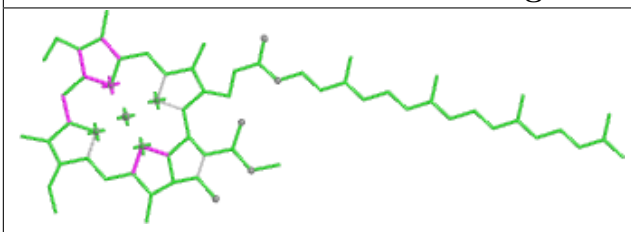
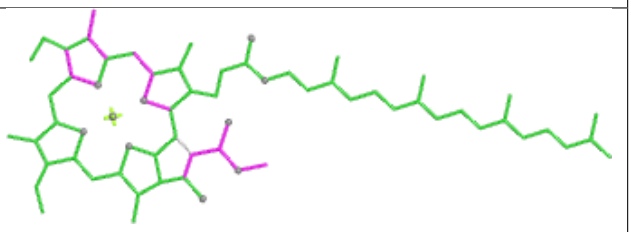
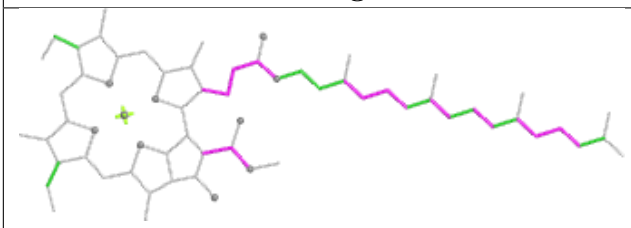
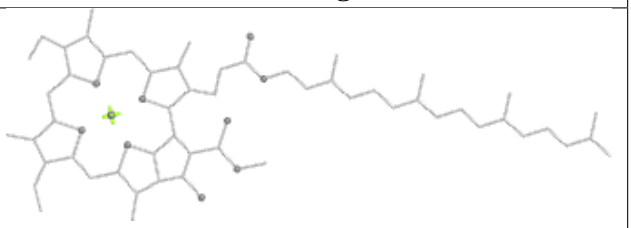
Bond angles



Torsions



Rings

Ligand CLA P 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

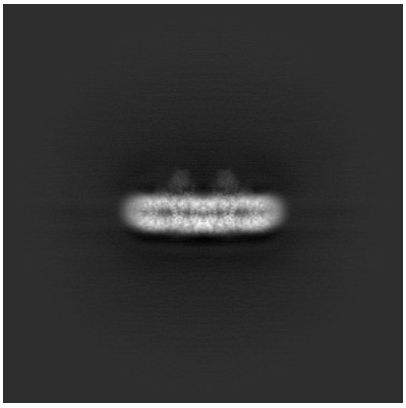
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-63018. These allow visual inspection of the internal detail of the map and identification of artifacts.

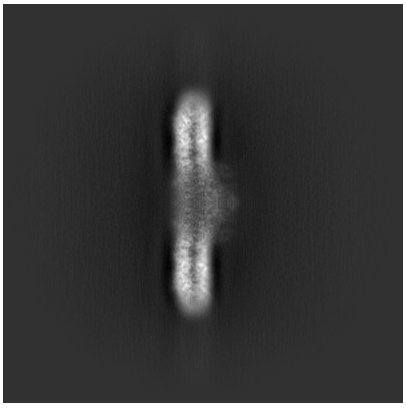
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

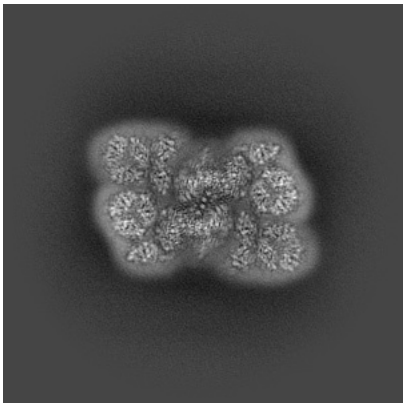
6.1.1 Primary map



X



Y

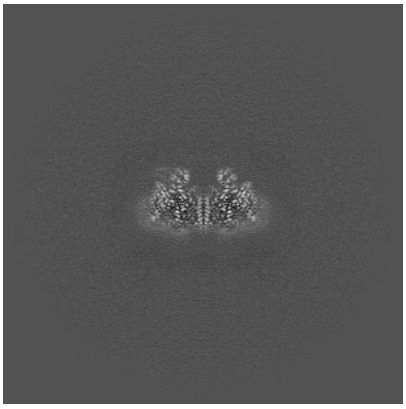


Z

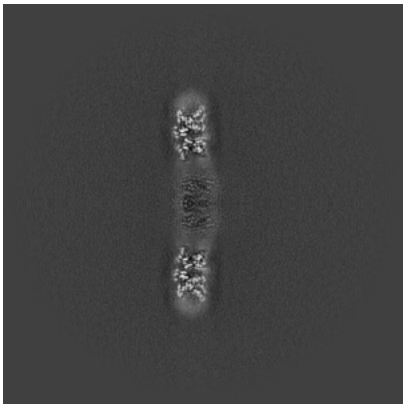
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

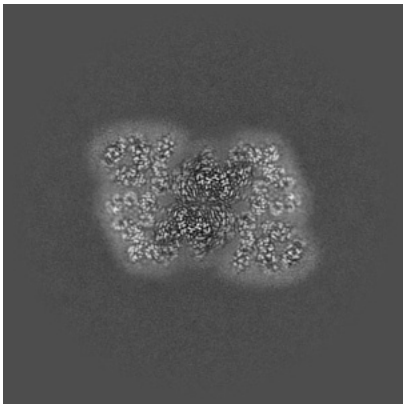
6.2.1 Primary map



X Index: 216



Y Index: 216

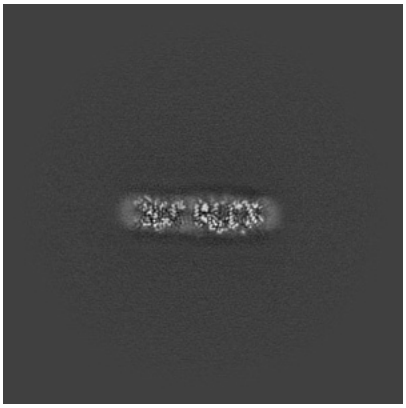


Z Index: 216

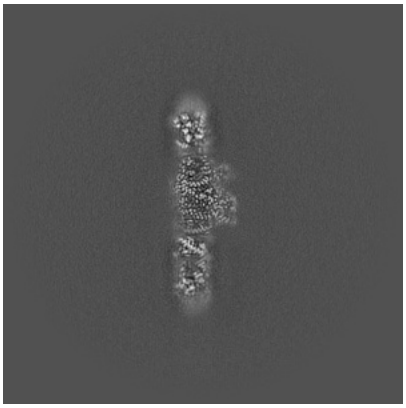
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

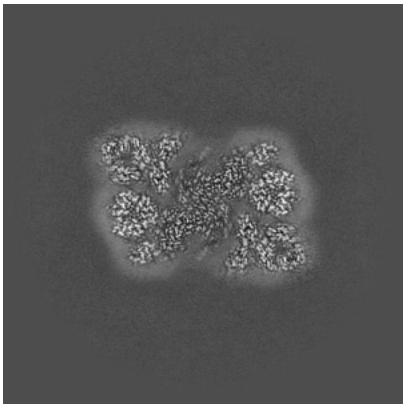
6.3.1 Primary map



X Index: 283



Y Index: 241

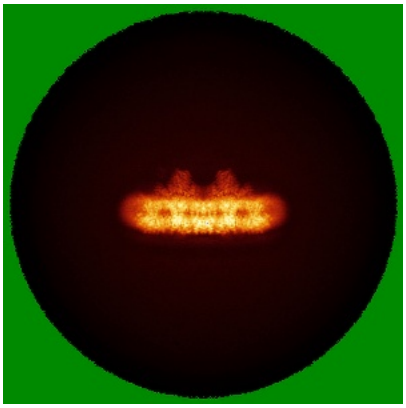


Z Index: 198

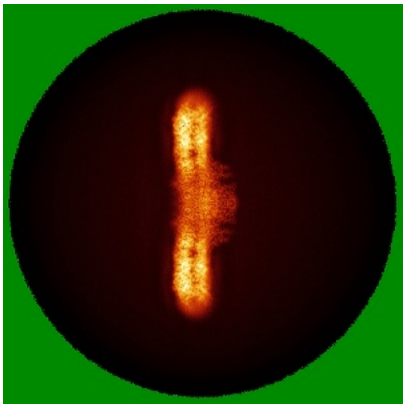
The images above show the largest variance slices of the map in three orthogonal directions.

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

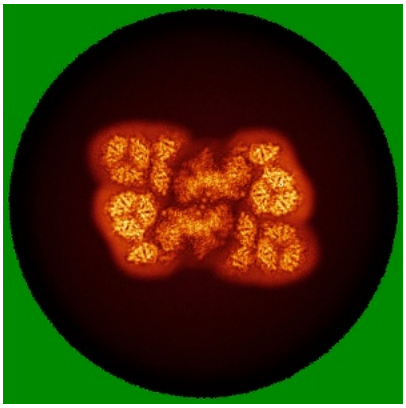
6.4.1 Primary map



X



Y

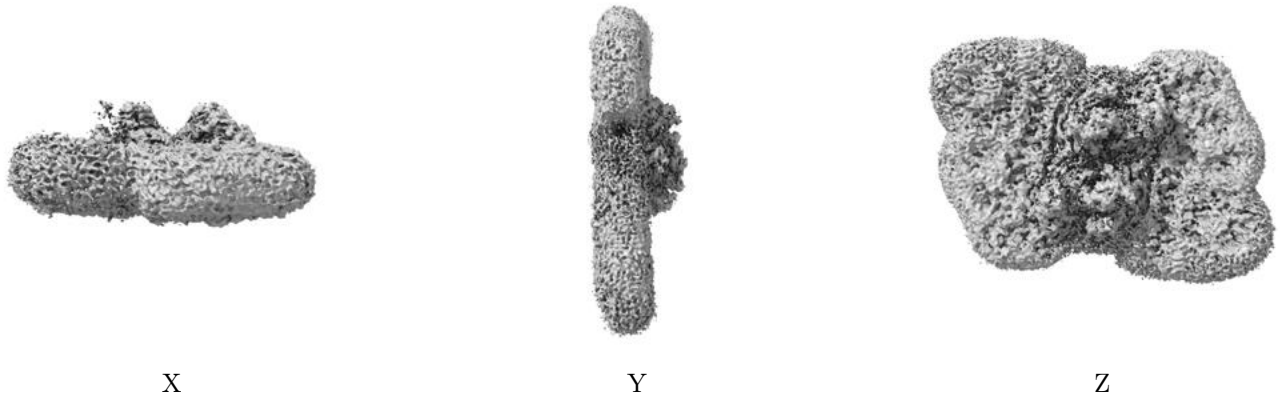


Z

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



The images above show the 3D surface view of the map at the recommended contour level 4.62. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

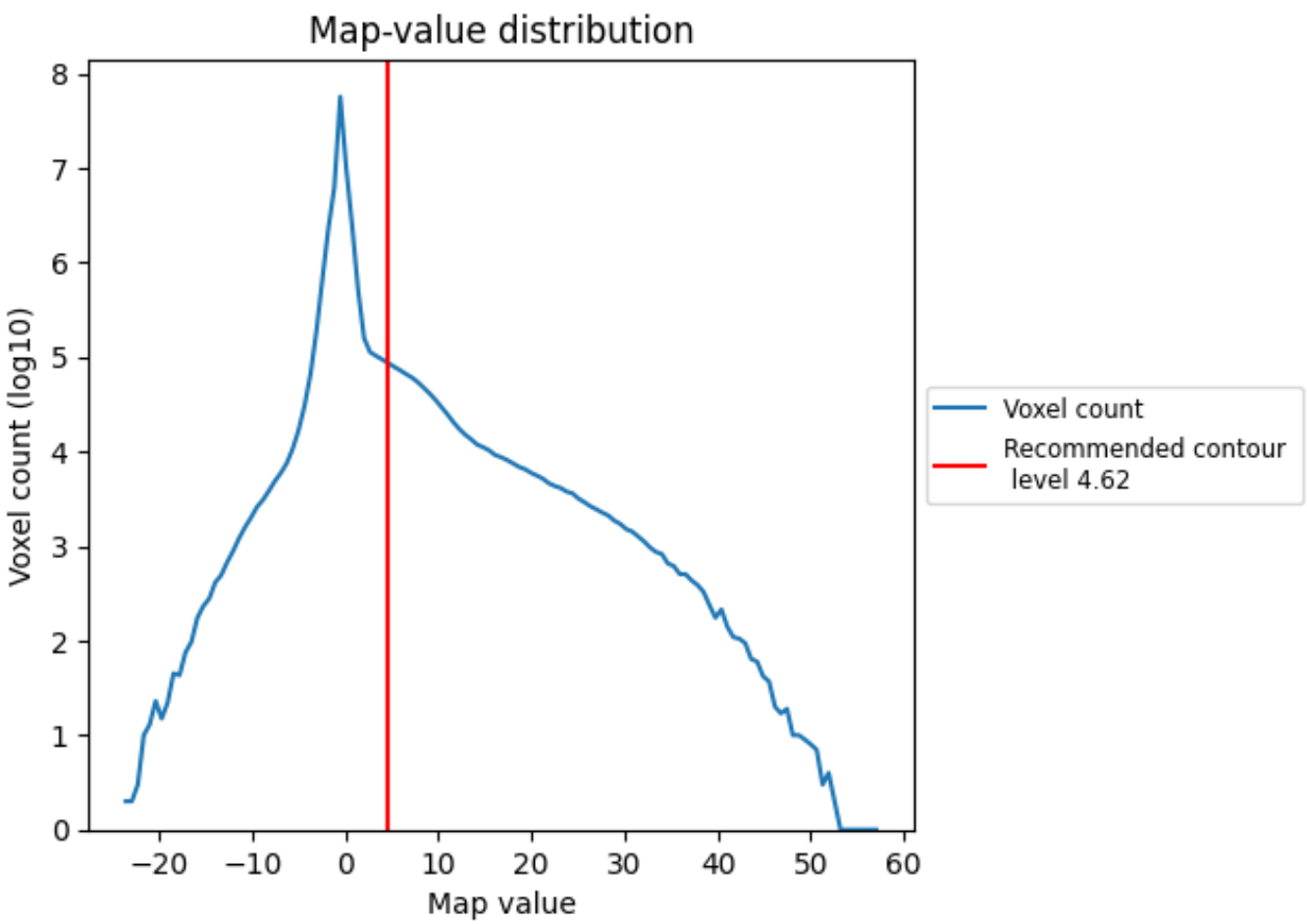
6.6 Mask visualisation (i)

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

7 Map analysis (i)

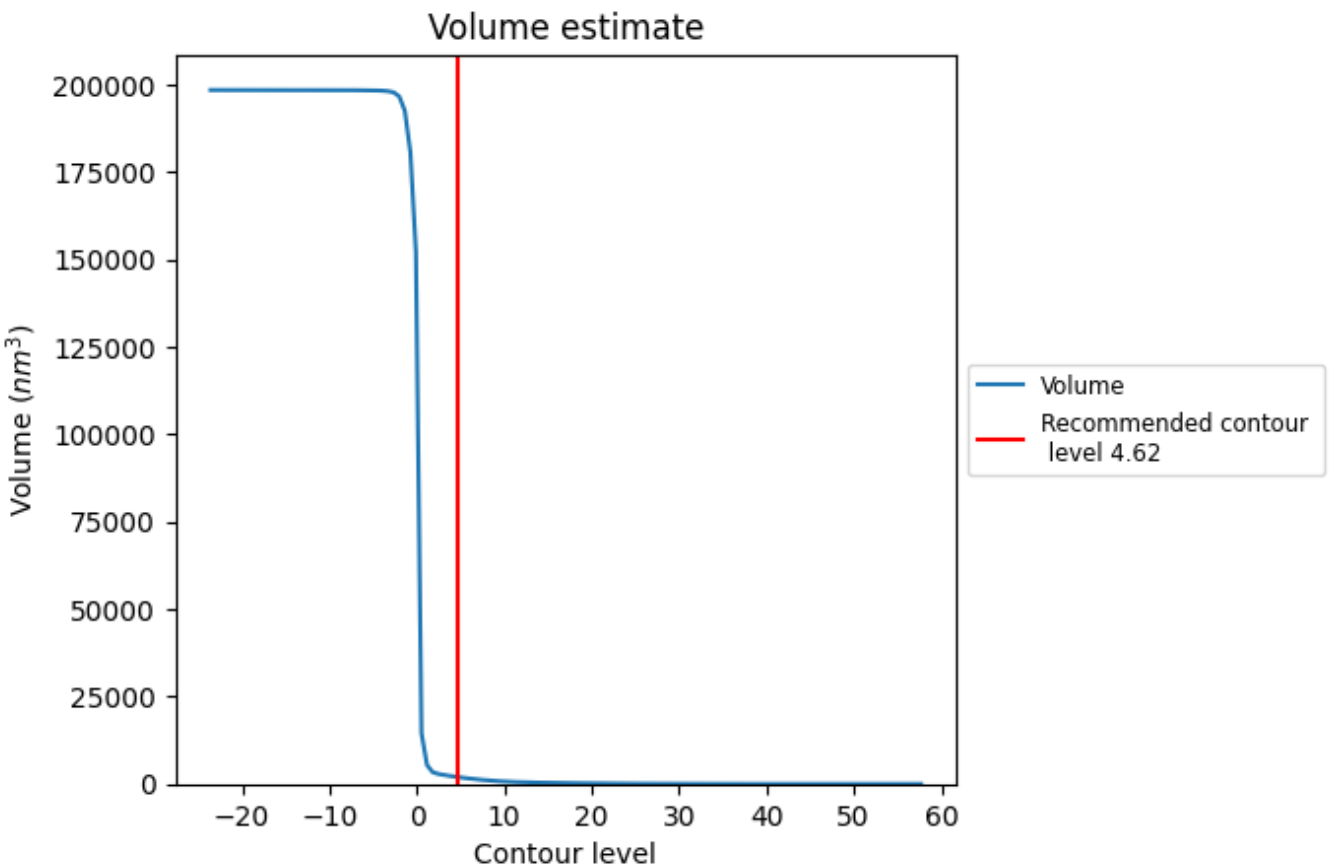
This section contains the results of statistical analysis of the map.

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.

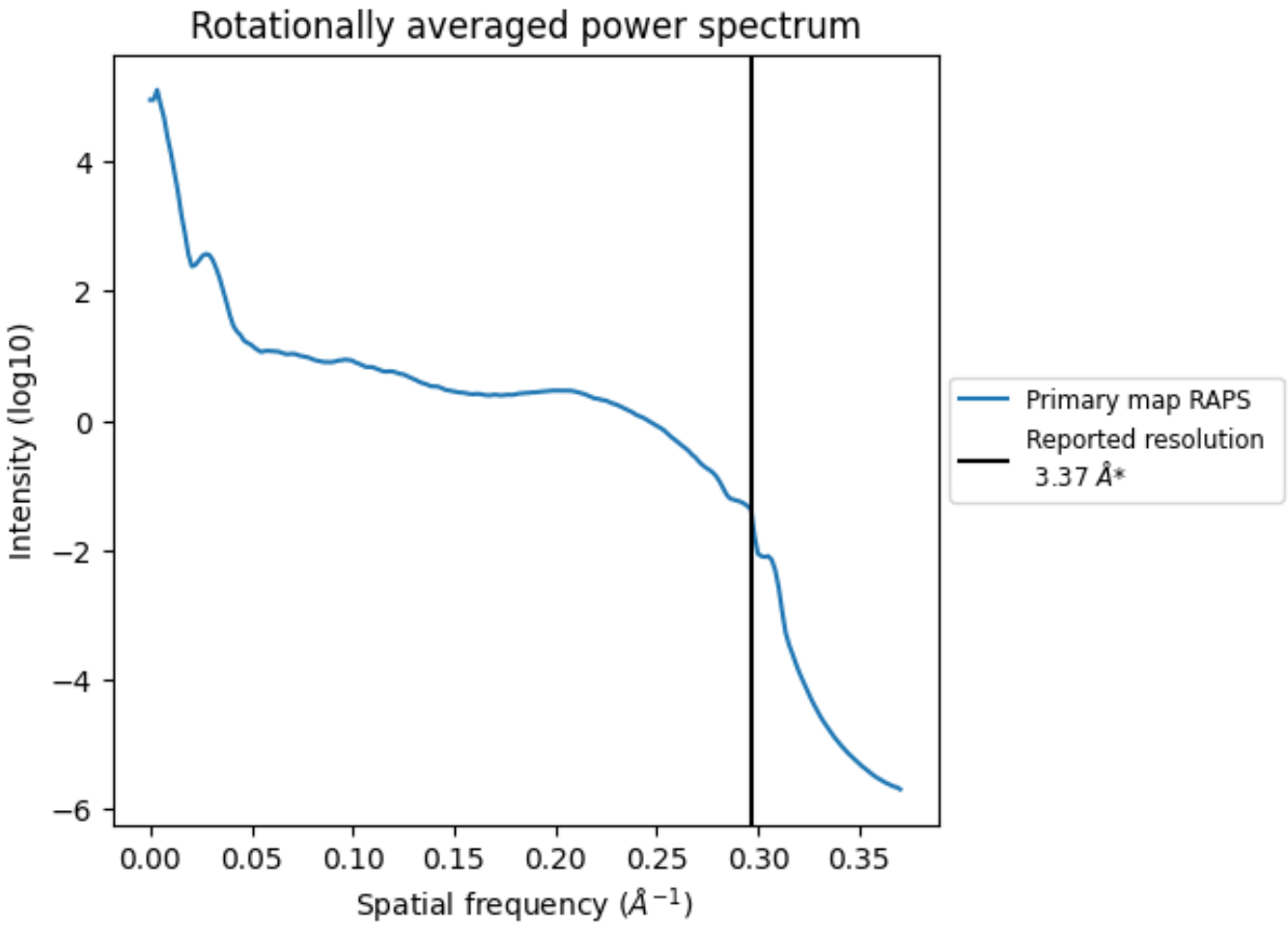
7.2 Volume estimate (i)



The volume at the recommended contour level is 1986 nm^3; this corresponds to an approximate mass of 1794 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 0.297 Å^{-1}

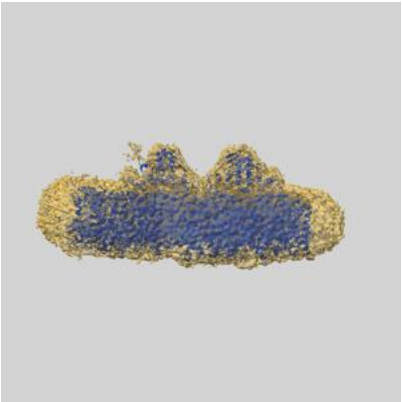
8 Fourier-Shell correlation (i)

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

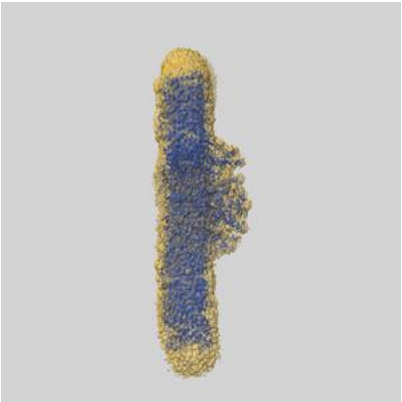
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-63018 and PDB model 9LE8. Per-residue inclusion information can be found in section 3 on page 39.

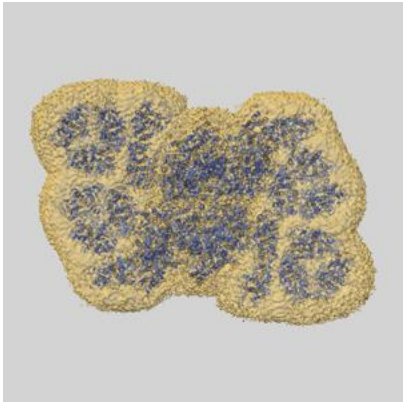
9.1 Map-model overlay (i)



X



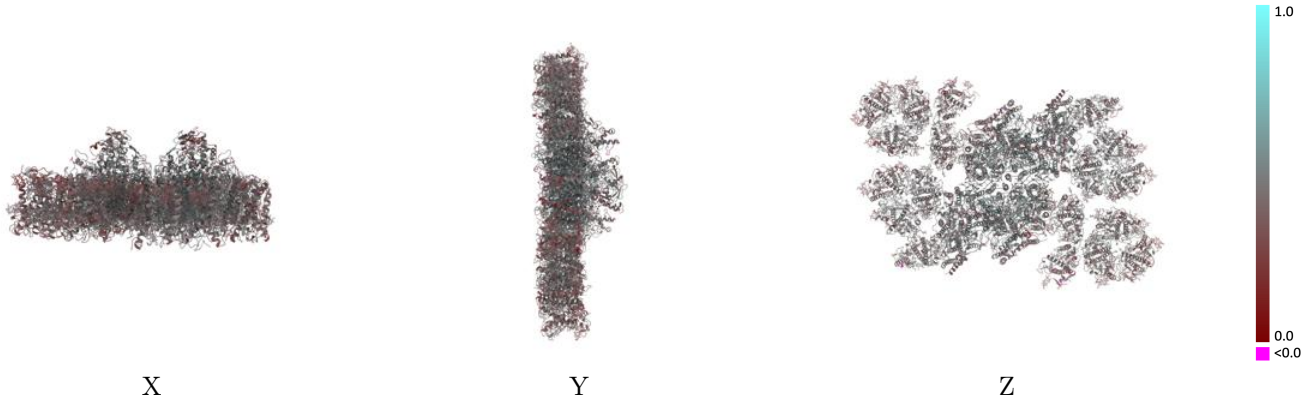
Y



Z

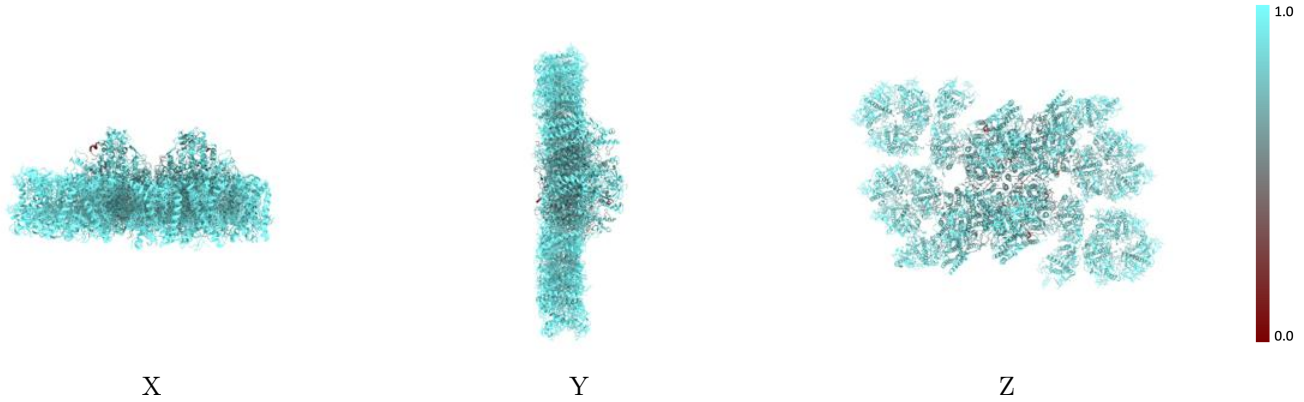
The images above show the 3D surface view of the map at the recommended contour level 4.62 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



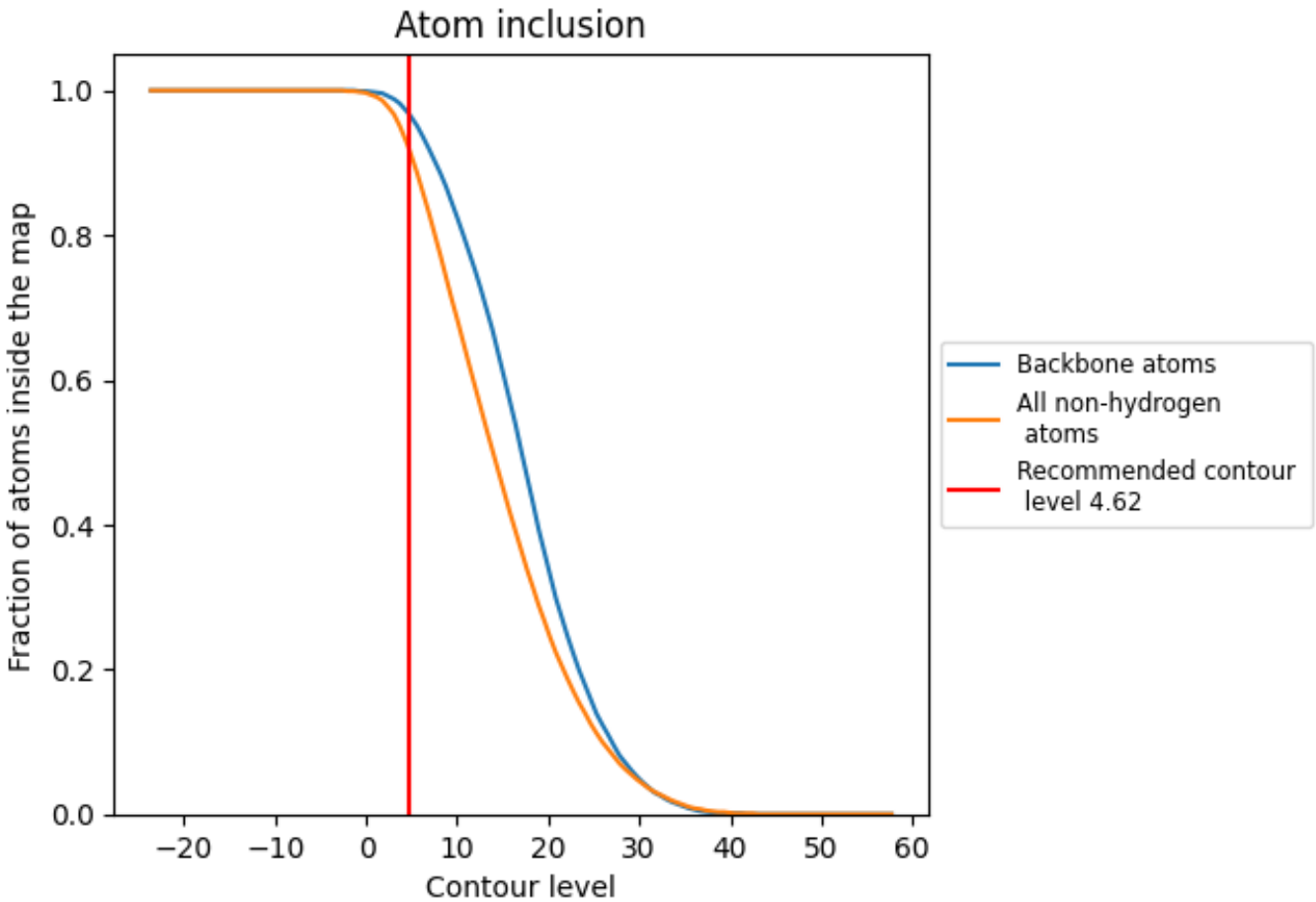
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.62).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (4.62) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9230	0.4360
0	0.9700	0.4170
9	0.9640	0.4100
AA	0.9680	0.3850
AB	0.9600	0.3670
AC	0.9650	0.4080
AD	0.9660	0.4130
AE	0.9710	0.3860
AF	0.9680	0.3800
AG	0.8560	0.4660
AH	0.9510	0.4410
AI	0.9500	0.3810
AJ	0.8850	0.4830
AK	0.8770	0.4650
AL	0.9060	0.4700
AM	0.9180	0.4930
AN	0.9700	0.4220
AO	0.8140	0.3990
AP	0.8640	0.4630
AQ	0.9680	0.4390
AR	0.9180	0.3920
AS	0.9780	0.4110
AT	0.8600	0.4620
AU	0.9490	0.4440
AV	0.9480	0.3860
E	0.9120	0.3980
F	0.8630	0.4070
I	0.9220	0.4780
J	0.8850	0.4830
K	0.9280	0.4550
M	0.7990	0.4550
O	0.8770	0.4620
P	0.9130	0.4710
Q	0.9160	0.4950
U	0.5710	0.3300

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Chain	Atom inclusion	Q-score
V	0.9700	0.4140
W	0.7290	0.3890
X	0.7340	0.2920
e	0.9190	0.3930
f	0.8500	0.3930
i	0.8970	0.4690
j	0.8200	0.3990
k	0.9260	0.4460
m	0.7790	0.4500
o	0.8760	0.4650
p	0.9720	0.4480
q	0.9130	0.3990
u	0.5400	0.3160
v	0.9760	0.4190
w	0.7180	0.4010
x	0.7100	0.3010