Full wwPDB EM Validation Report ⓘ

Sep 15, 2026 – 03:59 pm BST

PDB ID	:	5MDX / pdb_00005mdx
EMDB ID	:	EMD-3491
Title	:	Cryo-EM structure of the PSII supercomplex from Arabidopsis thaliana
Authors	:	van Bezouwen, L.S.; Caffarri, S.; Kale, R.S.; Kouril, R.; Thunnissen, A.M.W.H.; Oostergetel, G.T.; Boekema, E.J.
Deposited on	:	2016-11-13
Resolution	:	5.30 Å(reported)

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

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

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

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

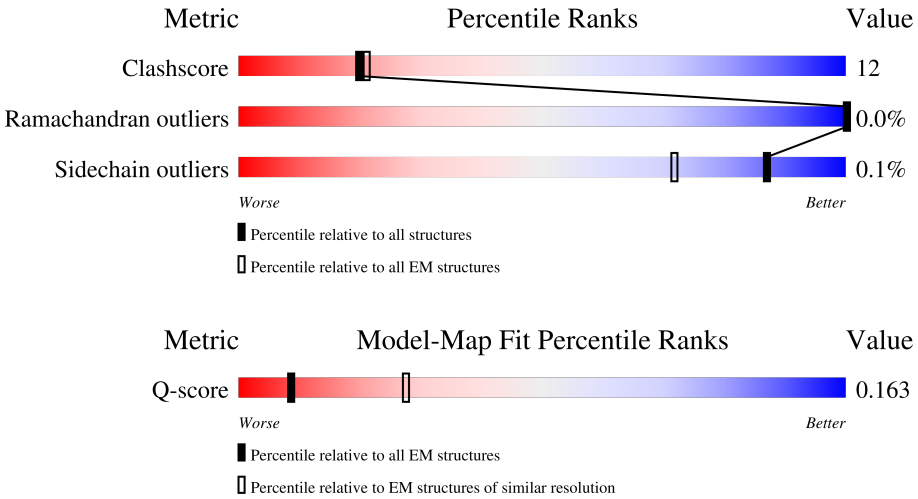
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 5.30 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.



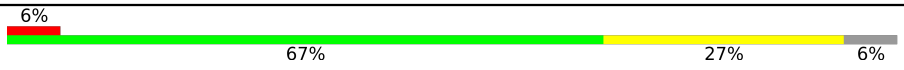
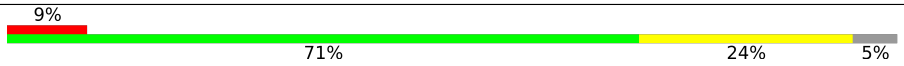
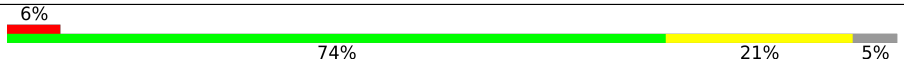
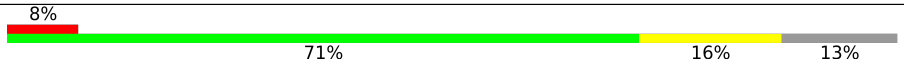
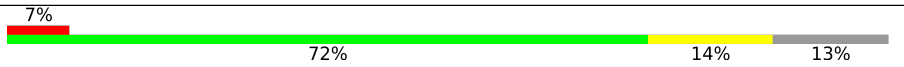
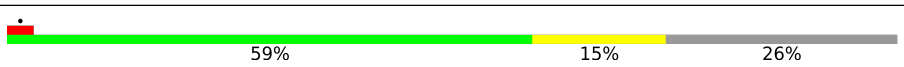
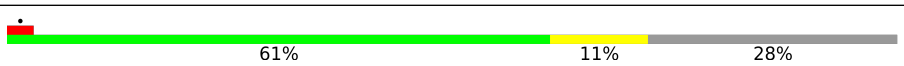
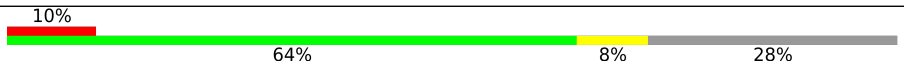
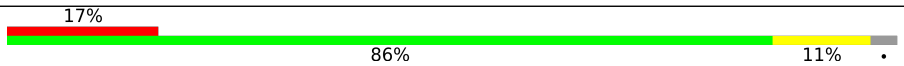
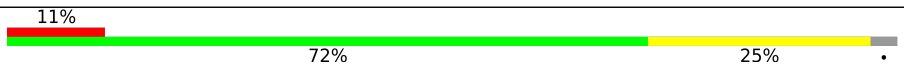
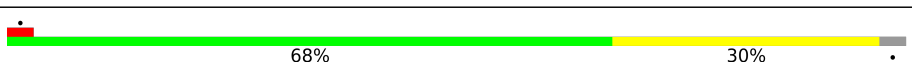
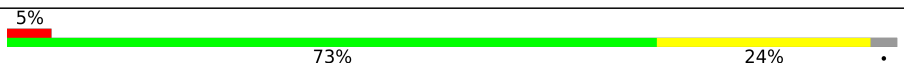
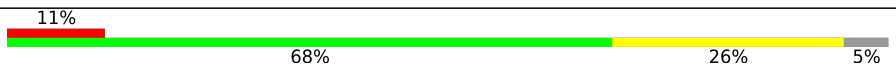
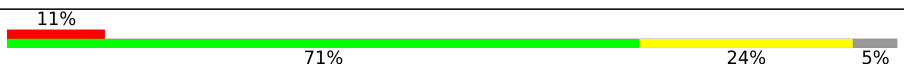
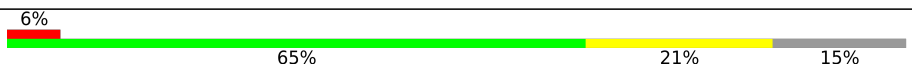
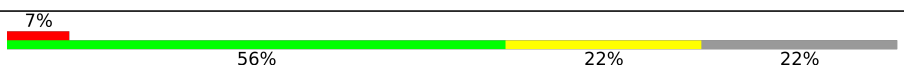
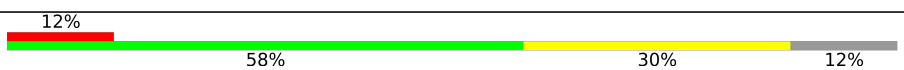
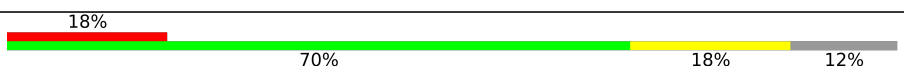
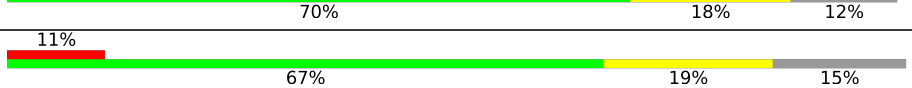
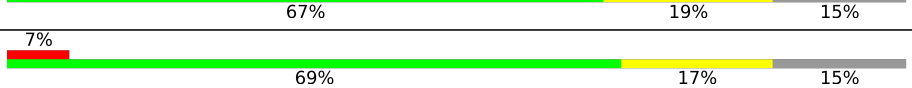
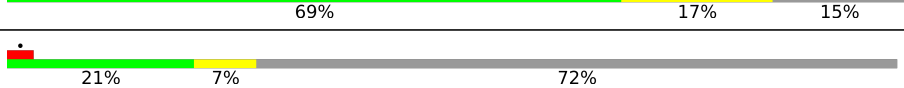
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	625 (4.80 - 5.80)

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

Mol	Chain	Length	Quality of chain
1	A	343	14% 70% 20% 10%
1	a	343	11% 75% 21% .
2	B	507	8% 67% 27% 6%
2	b	507	30% 69% 25% 6%

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Mol	Chain	Length	Quality of chain
3	C	459	
3	c	459	
4	D	352	
4	d	352	
5	E	83	
5	e	83	
6	F	39	
6	f	39	
7	H	72	
7	h	72	
8	I	36	
8	i	36	
9	K	37	
9	k	37	
10	L	38	
10	l	38	
11	M	34	
11	m	34	
12	O	247	
12	o	247	
13	T	33	
13	t	33	
14	W	54	
14	w	54	
15	X	116	

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Mol	Chain	Length	Quality of chain
15	x	116	8% 20% 8% 72%
16	Z	62	8% 68% 31%
16	z	62	6% 73% 26%
17	R	250	18% 52% 22% 25%
17	r	250	18% 52% 22% 25%
18	S	232	8% 66% 25% 8%
18	s	232	8% 66% 24% 8%
19	1	224	27% 82% 16%
19	2	224	31% 79% 18%
19	3	224	38% 81% 17%
19	5	224	27% 82% 16%
19	6	224	31% 78% 20%
19	7	224	38% 81% 17%
19	G	224	16% 78% 20%
19	N	224	77% 21%
19	Y	224	11% 76% 21%
19	g	224	16% 78% 20%
19	n	224	77% 21%
19	y	224	11% 77% 21%
20	4	210	41% 67% 30%
20	8	210	41% 67% 30%

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
22	CLA	4	301	-	-	X	-
22	CLA	8	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	R	302	-	-	X	-

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 78324 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	308	Total	C	N	O	S	0	0
			2388	1558	392	426	12		
1	a	330	Total	C	N	O	S	0	0
			2584	1688	426	457	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	478	Total	C	N	O	S	0	0
			3752	2459	635	646	12		
2	b	478	Total	C	N	O	S	0	0
			3752	2459	635	646	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		
3	c	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	336	Total	C	N	O	S	0	0
			2675	1770	438	455	12		
4	d	336	Total	C	N	O	S	0	0
			2675	1770	438	455	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	72	Total 586	C 386	N 93	O 107	0	0
5	e	72	Total 586	C 386	N 93	O 107	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit beta (PsbF).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	29	Total 224	C 147	N 40	O 36	S 1	0	0
6	f	29	Total 224	C 147	N 40	O 36	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	52	Total 389	C 257	N 61	O 69	S 2	0	0
7	h	52	Total 389	C 257	N 61	O 69	S 2	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	36	Total 290	C 205	N 40	O 44	S 1	0	0
9	k	36	Total 290	C 205	N 40	O 44	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	36	Total 302	C 200	N 47	O 55	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	36	Total 302	C 200	N 47	O 55	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	29	Total 226	C 158	N 32	O 36	0	0
11	m	29	Total 226	C 158	N 32	O 36	0	0

- Molecule 12 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	193	Total 1487	C 951	N 235	O 297	S 4	0	0
12	o	193	Total 1487	C 951	N 235	O 297	S 4	0	0

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

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

- Molecule 14 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	46	Total 372	C 247	N 53	O 71	S 1	0	0
14	w	46	Total 372	C 247	N 53	O 71	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	X	32	Total 226	C 149	N 35	O 42	0	0
15	x	32	Total 226	C 149	N 35	O 42	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		
16	z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		

- Molecule 17 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	188	Total	C	N	O	S	0	0
			1459	953	238	265	3		
17	r	188	Total	C	N	O	S	0	0
			1459	953	238	265	3		

- Molecule 18 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	214	Total	C	N	O	S	0	0
			1653	1082	270	297	4		
18	s	214	Total	C	N	O	S	0	0
			1653	1082	270	297	4		

- Molecule 19 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	N	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	Y	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	g	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	n	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	y	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	1	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	2	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	3	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	5	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	6	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	7	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		

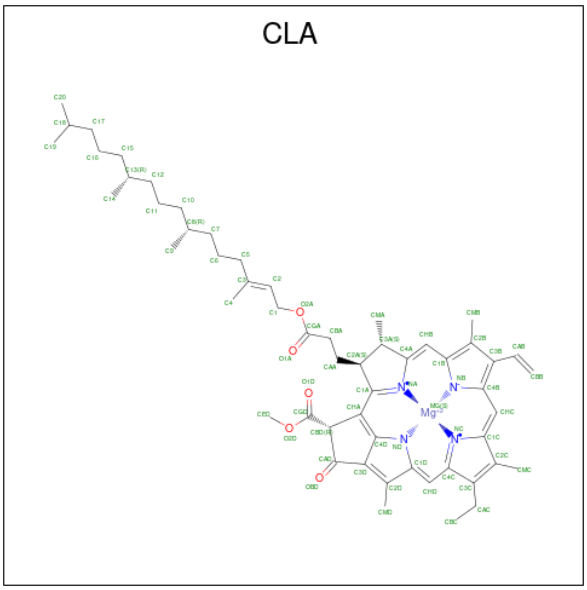
- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		
20	8	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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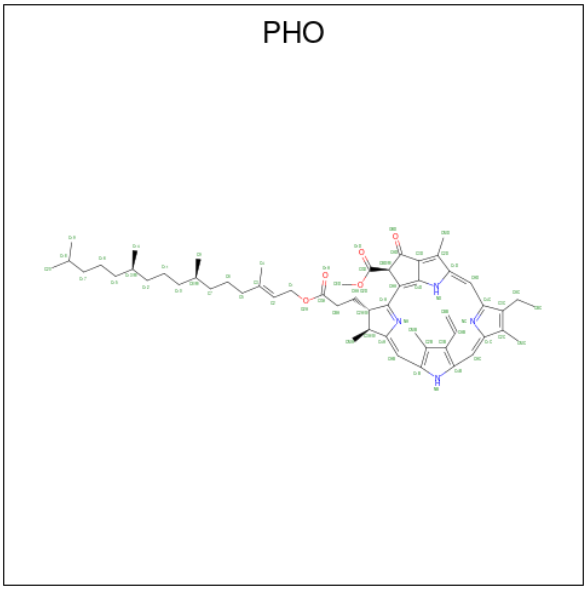
Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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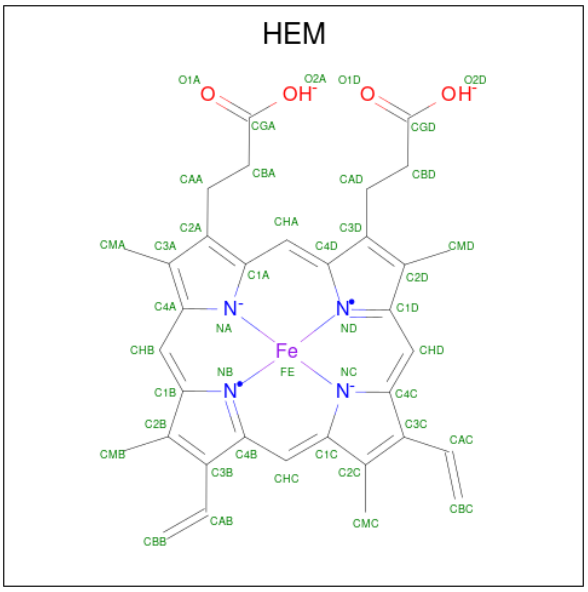
Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



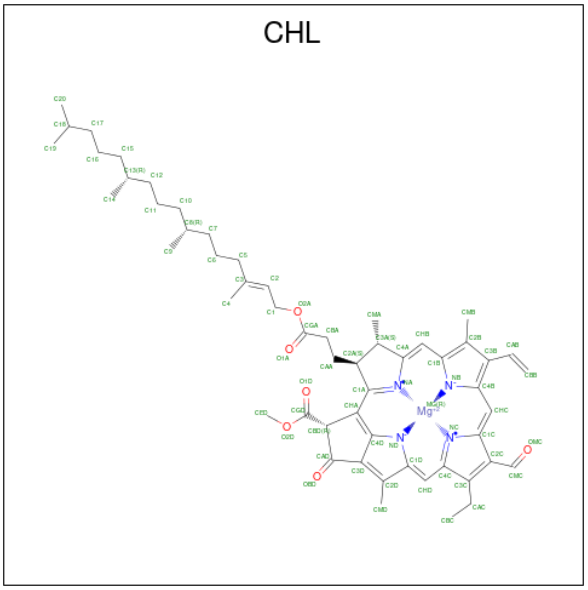
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	N	O	0
			44	35	4	5	
23	D	1	Total	C	N	O	0
			44	35	4	5	
23	a	1	Total	C	N	O	0
			44	35	4	5	
23	d	1	Total	C	N	O	0
			44	35	4	5	

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 25 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
25	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
25	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
25	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	r	1	Total	C	Mg	N	O	0
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25	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
25	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	7	1	Total	C	Mg	N	O	0
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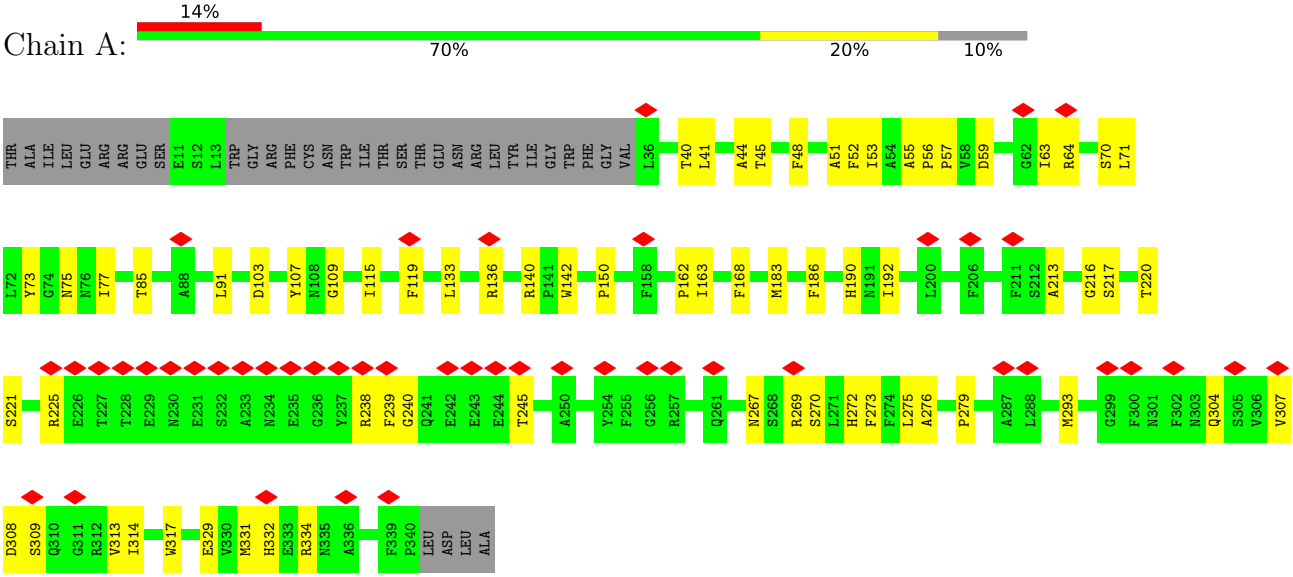
Mol	Chain	Residues	Atoms					AltConf
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			46	35	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

3 Residue-property plots (i)

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

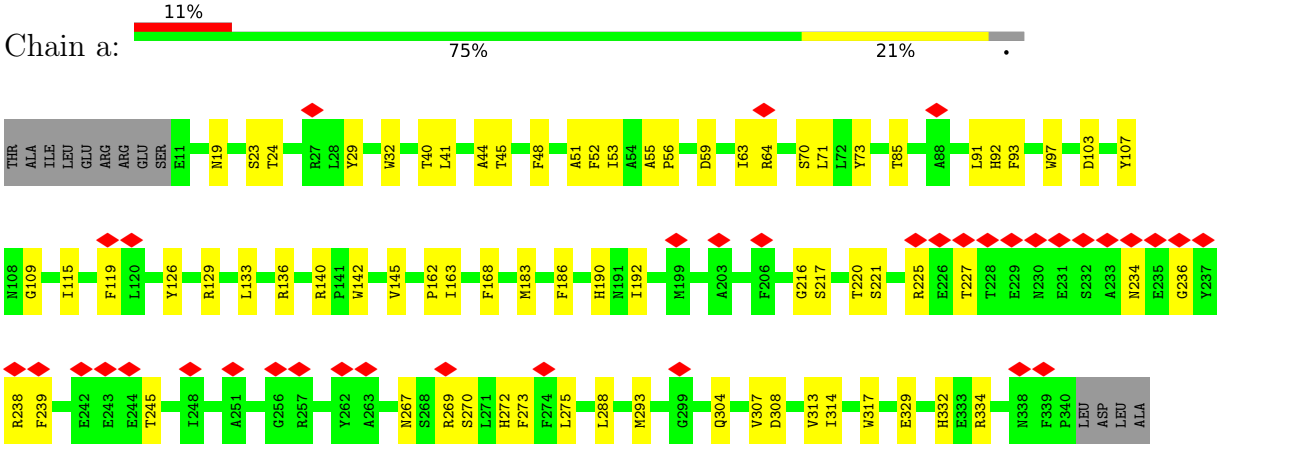
• Molecule 1: Photosystem II protein D1

Chain A:



• Molecule 1: Photosystem II protein D1

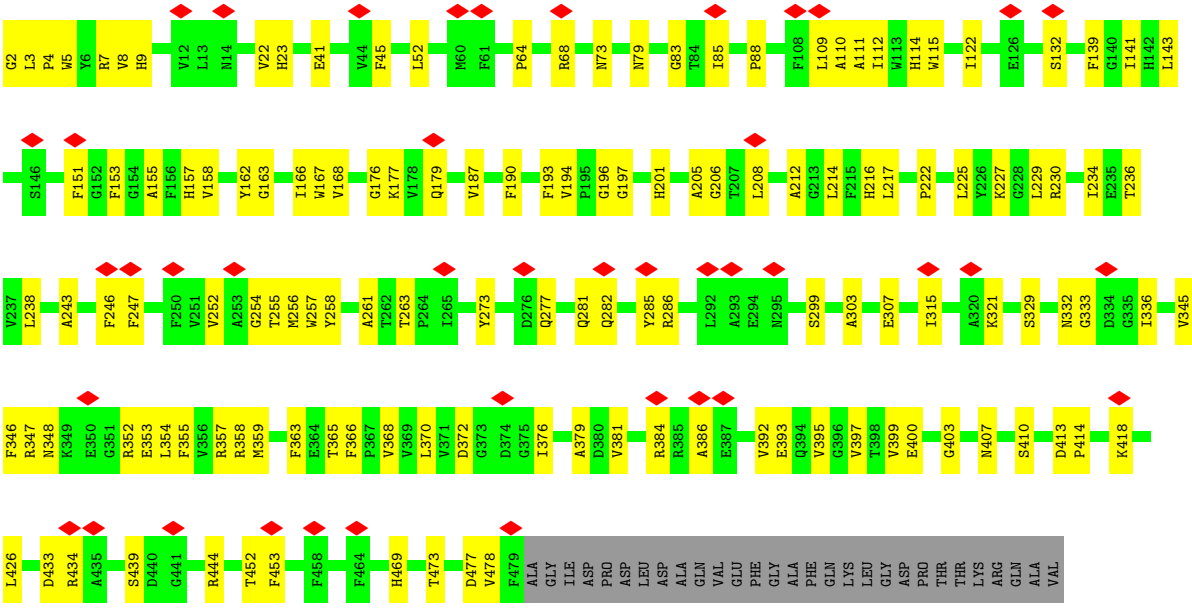
Chain a:



• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:

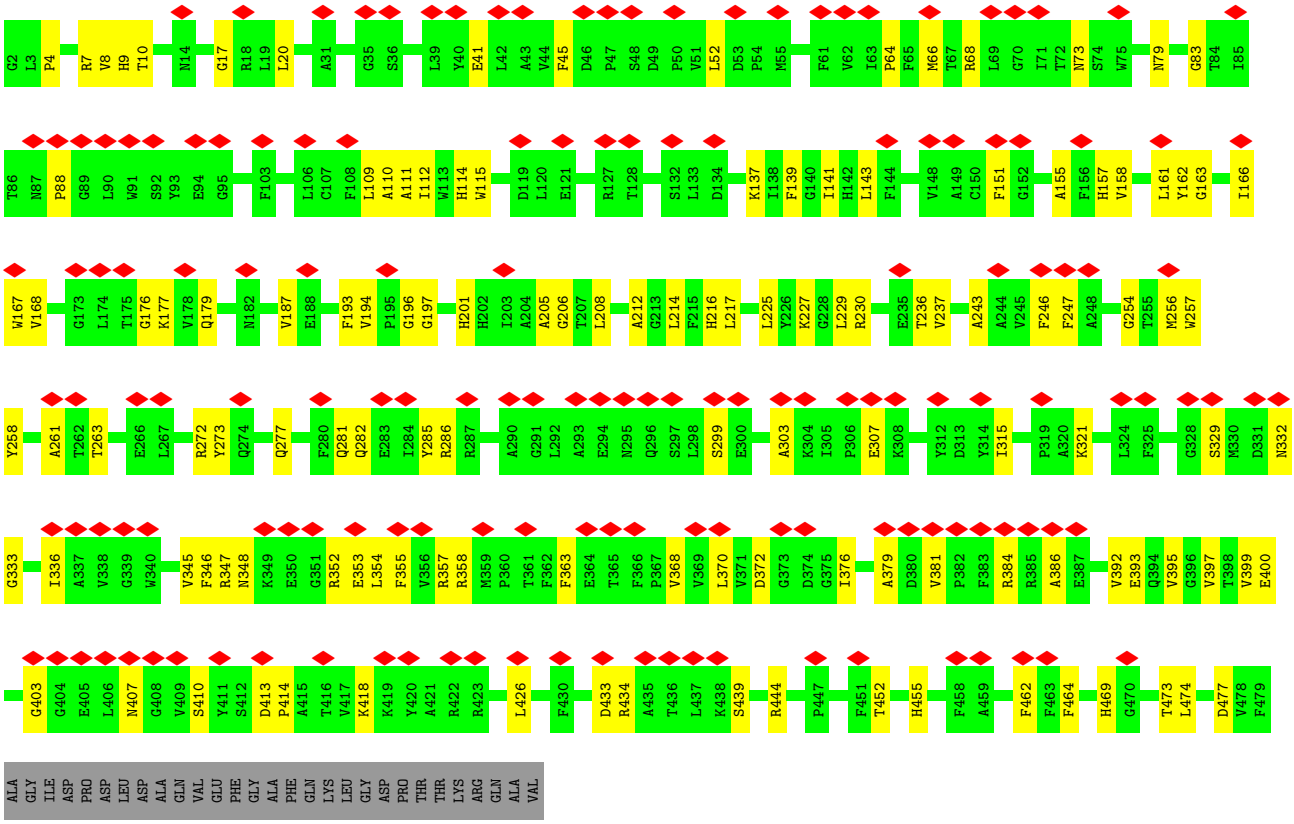




• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

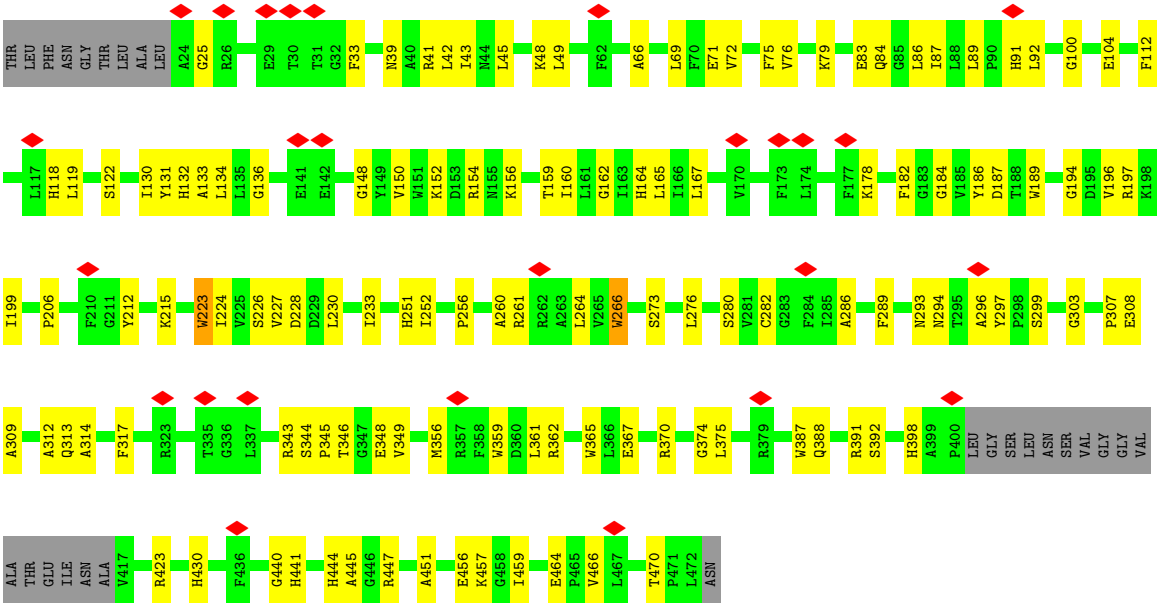




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

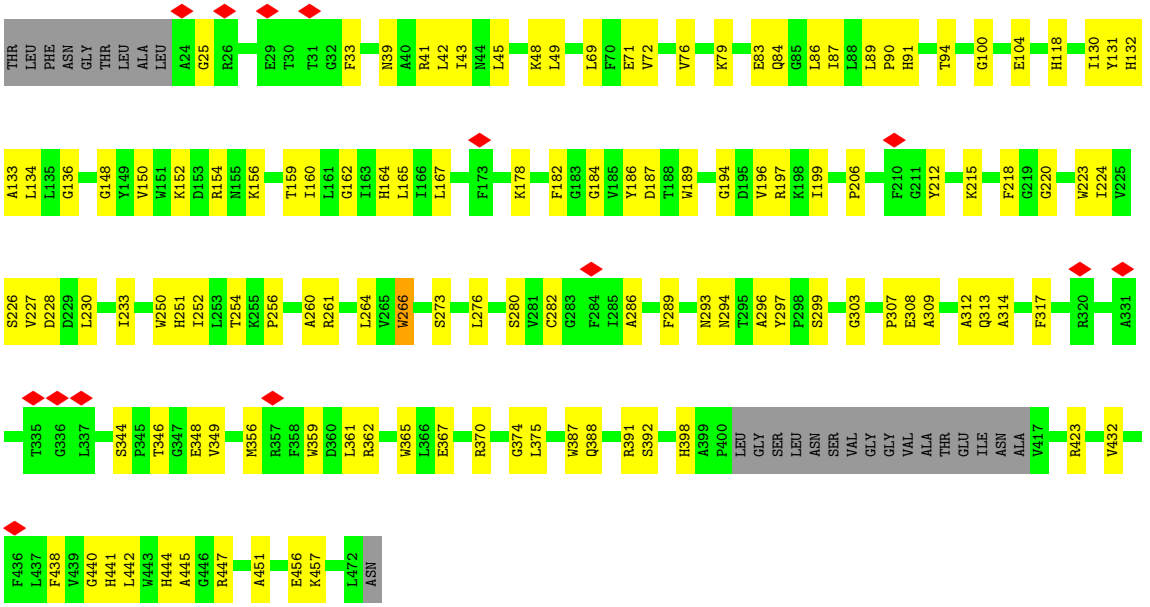




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

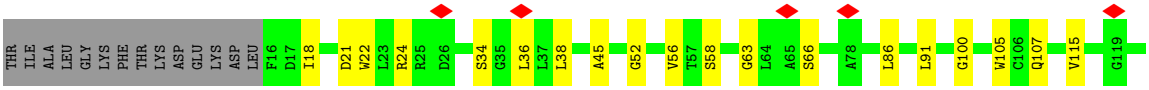


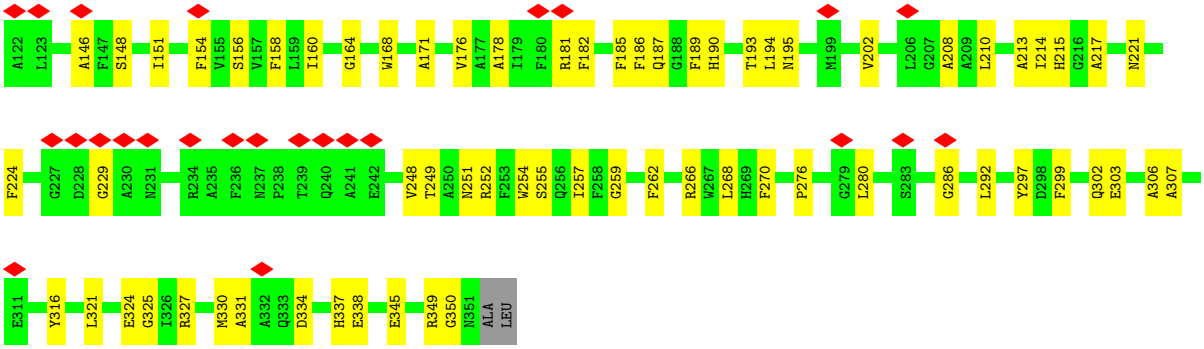


• Molecule 4: Photosystem II D2 protein

Chain D:

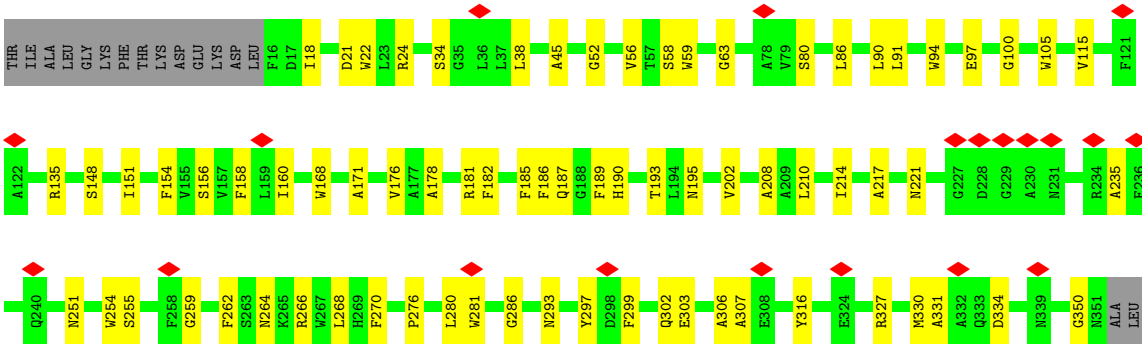






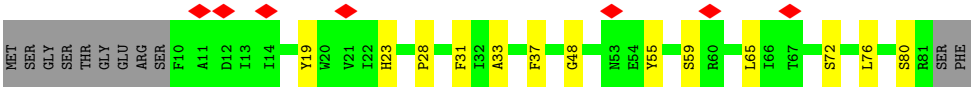
• Molecule 4: Photosystem II D2 protein





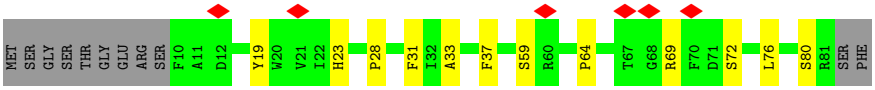
• Molecule 5: Cytochrome b559 subunit alpha





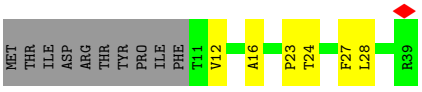
• Molecule 5: Cytochrome b559 subunit alpha





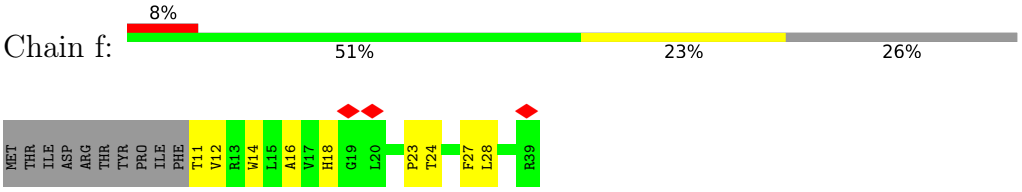
• Molecule 6: Cytochrome b559 subunit beta (PsbF)





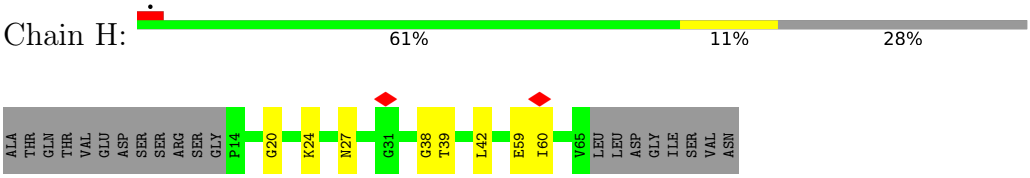
• Molecule 6: Cytochrome b559 subunit beta (PsbF)

Chain f:



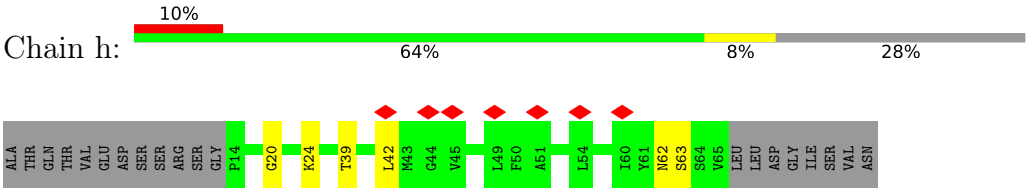
• Molecule 7: Photosystem II reaction center protein H

Chain H:



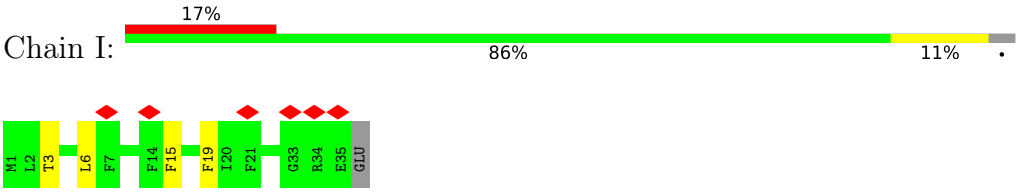
• Molecule 7: Photosystem II reaction center protein H

Chain h:



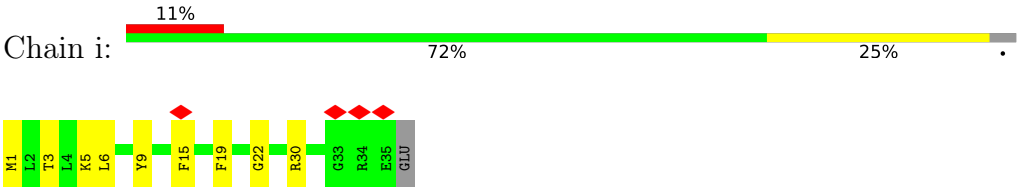
• Molecule 8: Photosystem II reaction center protein I

Chain I:



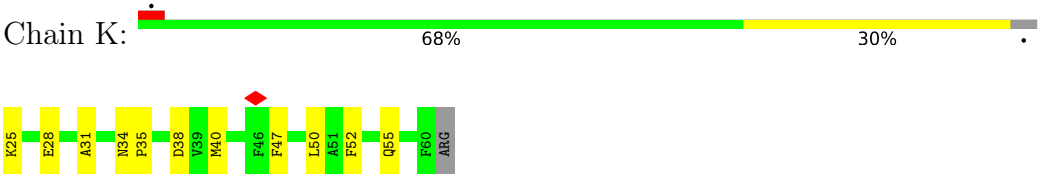
• Molecule 8: Photosystem II reaction center protein I

Chain i:



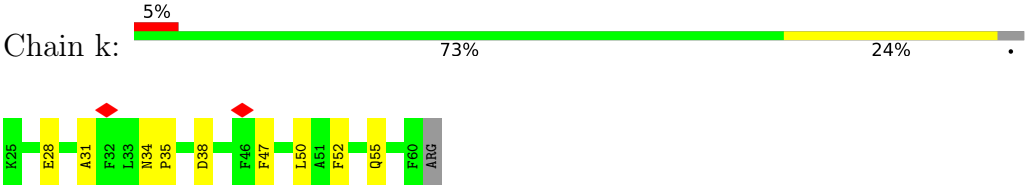
• Molecule 9: Photosystem II reaction center protein K

Chain K:



• Molecule 9: Photosystem II reaction center protein K

Chain k:



• Molecule 10: Photosystem II reaction center protein L

Chain L:

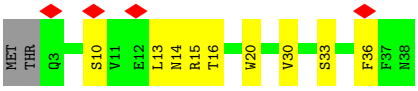




• Molecule 10: Photosystem II reaction center protein L

Chain l:

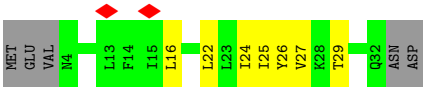




• Molecule 11: Photosystem II reaction center protein M

Chain M:

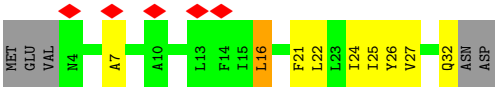




• Molecule 11: Photosystem II reaction center protein M

Chain m:

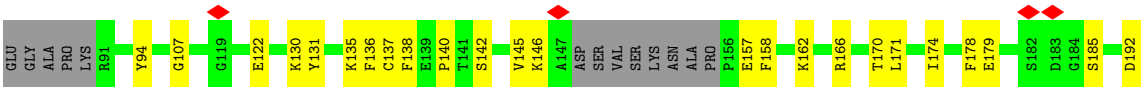


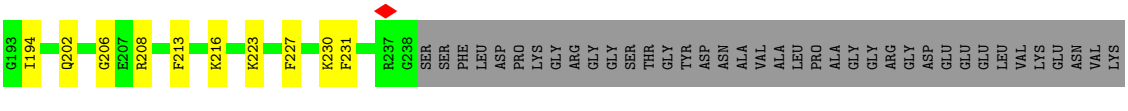


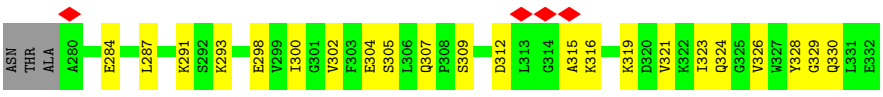
• Molecule 12: Oxygen-evolving enhancer protein 1-1, chloroplastic

Chain O:





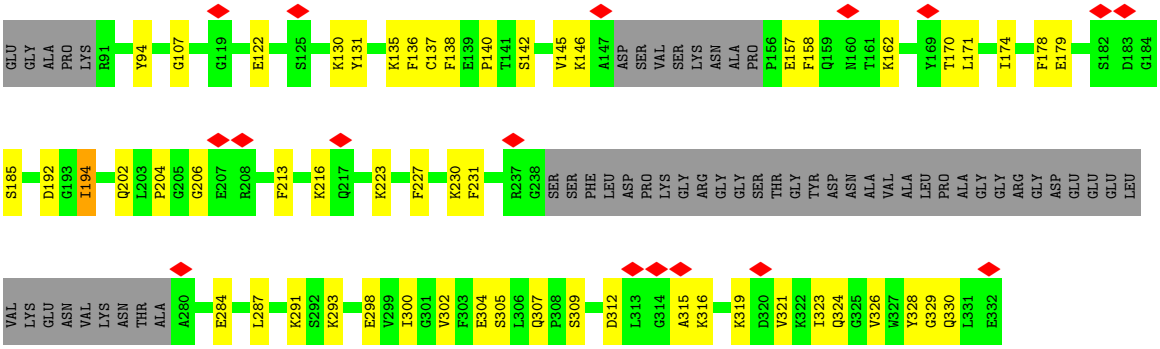




• Molecule 12: Oxygen-evolving enhancer protein 1-1, chloroplastic

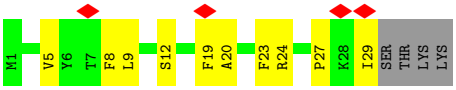
Chain o:





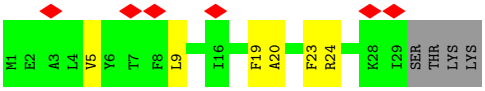
• Molecule 13: Photosystem II reaction center protein T





• Molecule 13: Photosystem II reaction center protein T





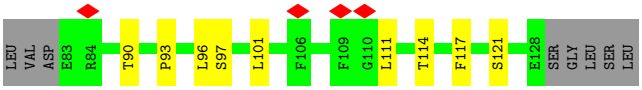
• Molecule 14: Photosystem II reaction center W protein, chloroplastic





• Molecule 14: Photosystem II reaction center W protein, chloroplastic

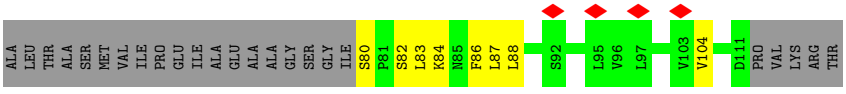




• Molecule 15: Photosystem II reaction center protein X

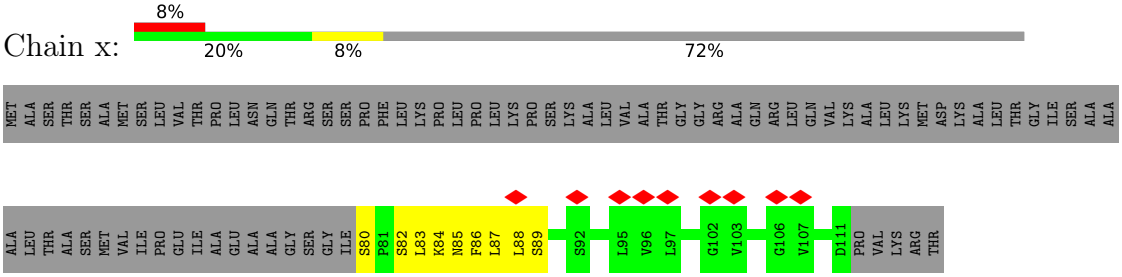






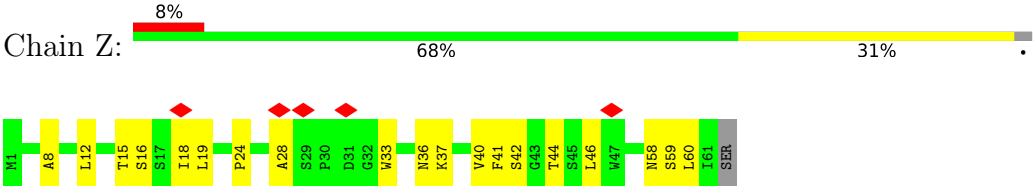
• Molecule 15: Photosystem II reaction center protein X

Chain x:



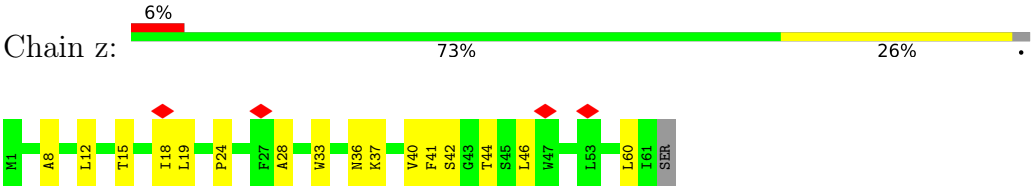
• Molecule 16: Photosystem II reaction center protein Z

Chain Z:



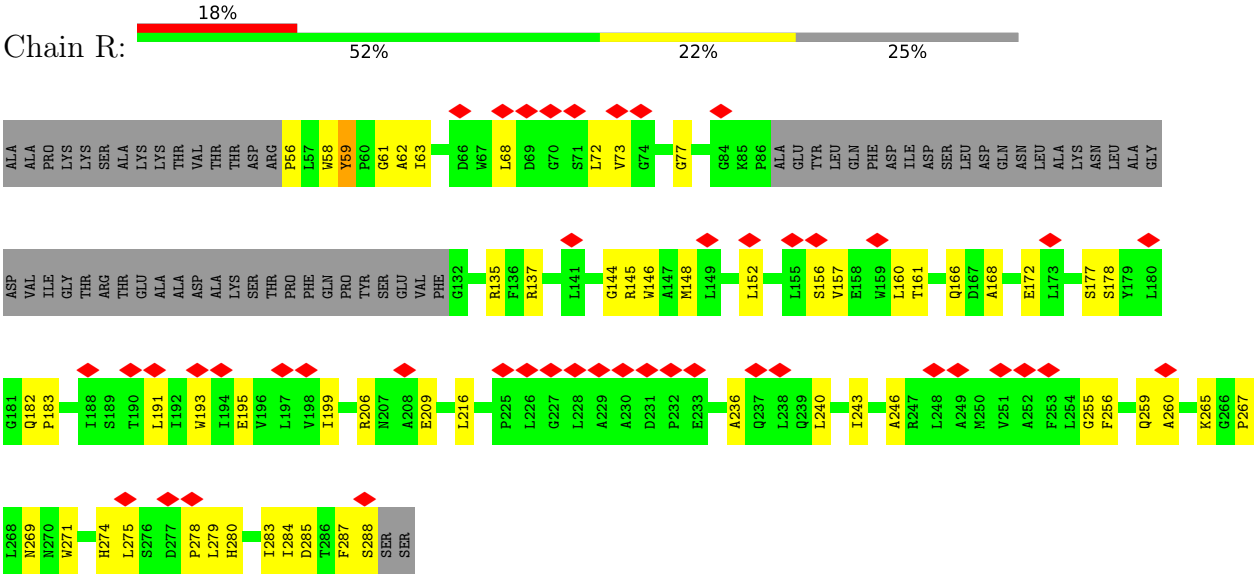
• Molecule 16: Photosystem II reaction center protein Z

Chain z:



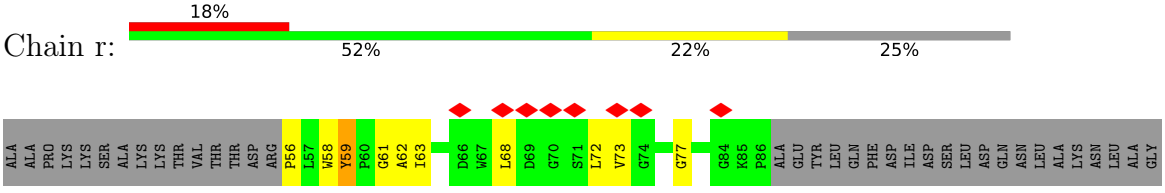
• Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic

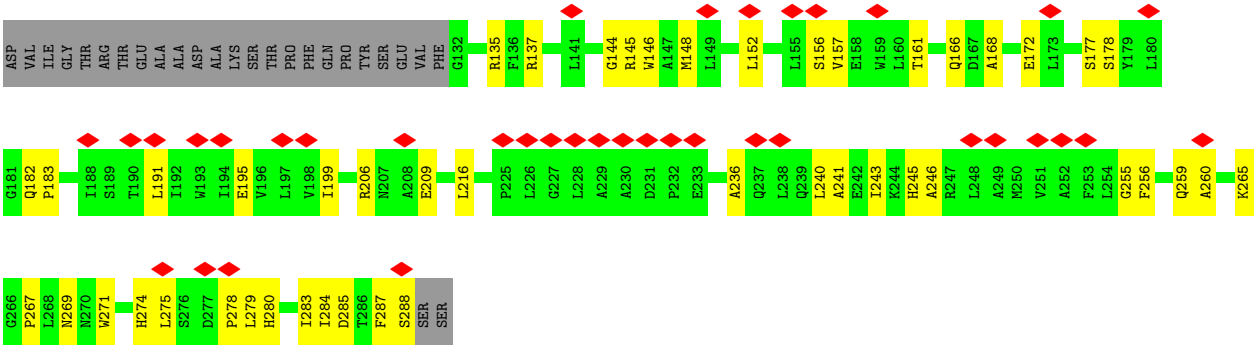
Chain R:



• Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic

Chain r:

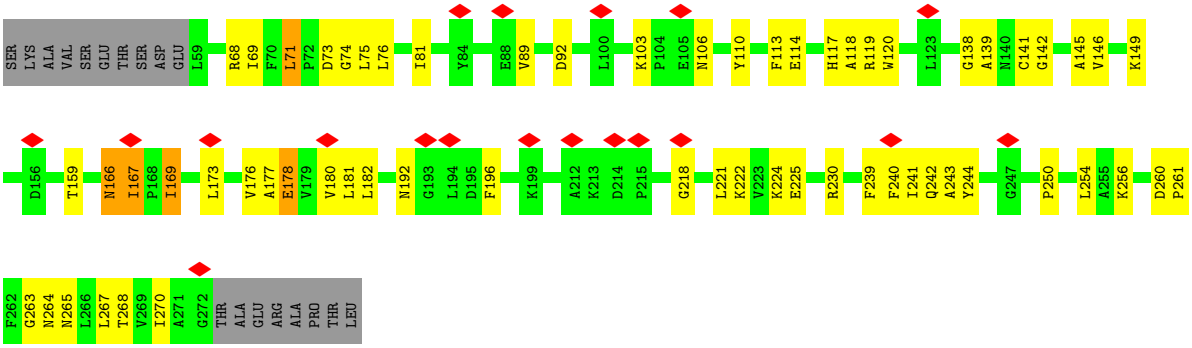




• Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic

Chain S:

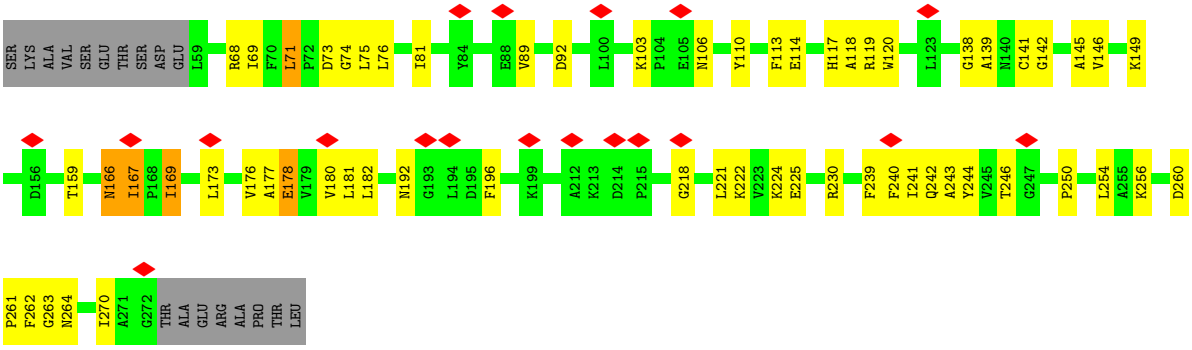




• Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic

Chain s:

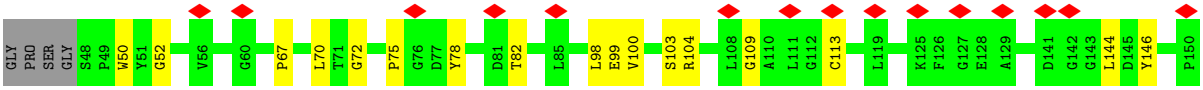


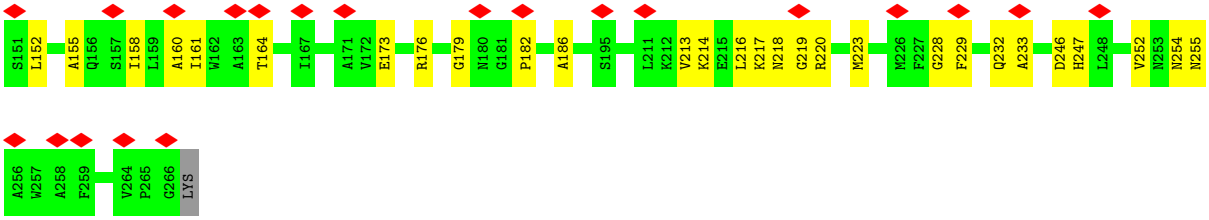


• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain G:



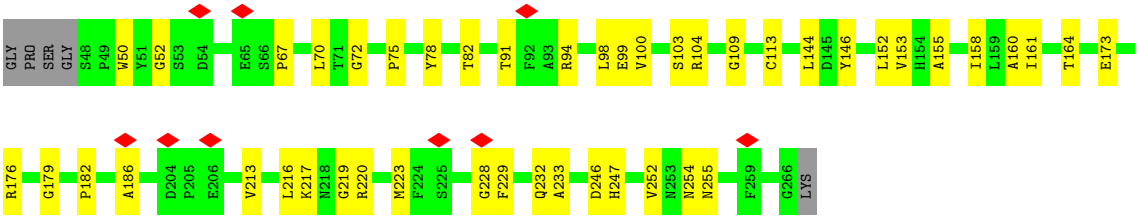




• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain N:

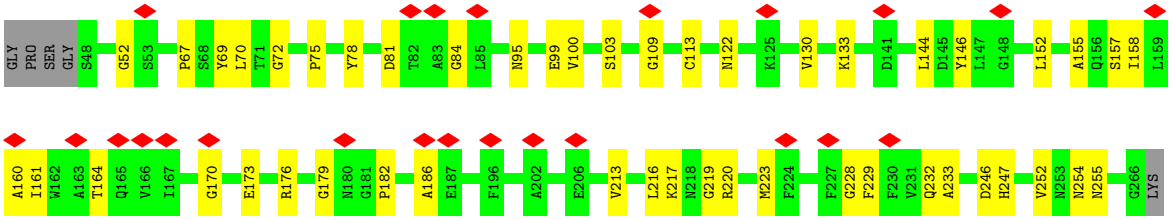




• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain Y:

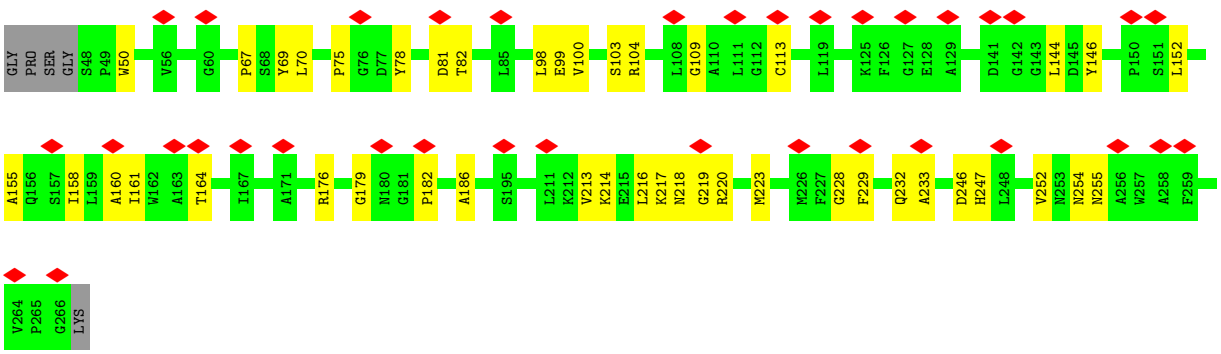




• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain g:

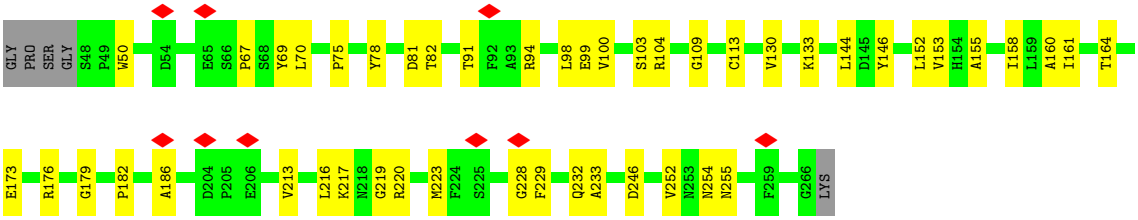




• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain n:

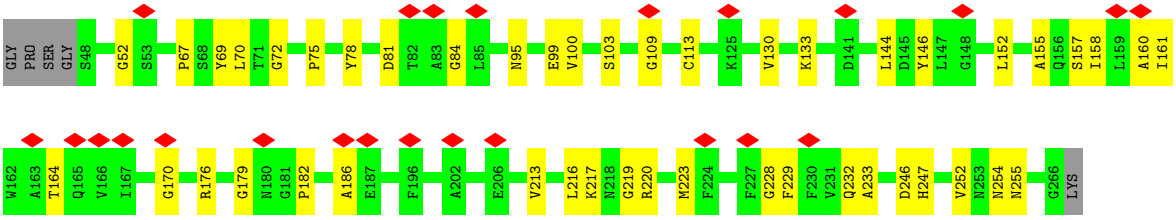




• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain y:

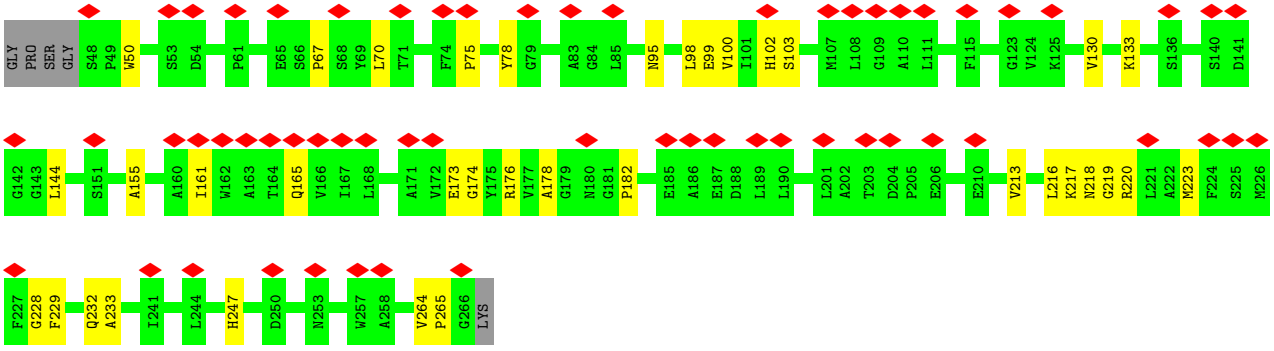




• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 1:

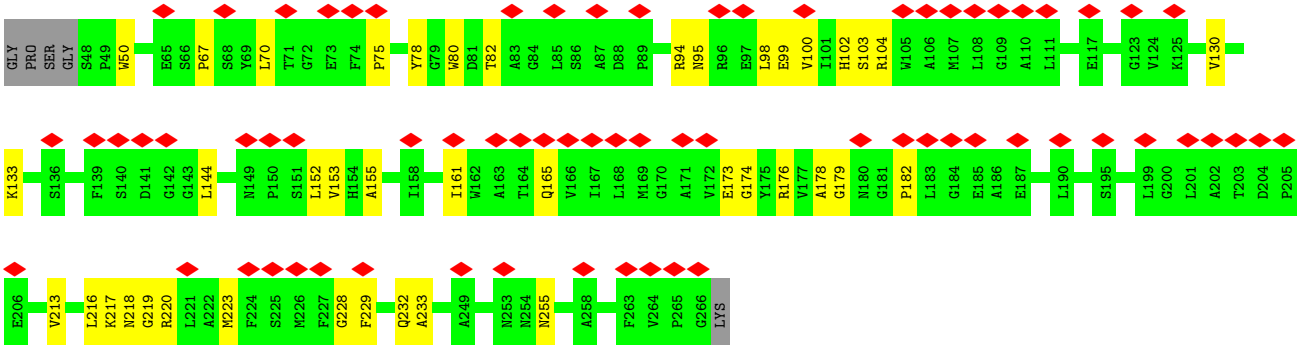




• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

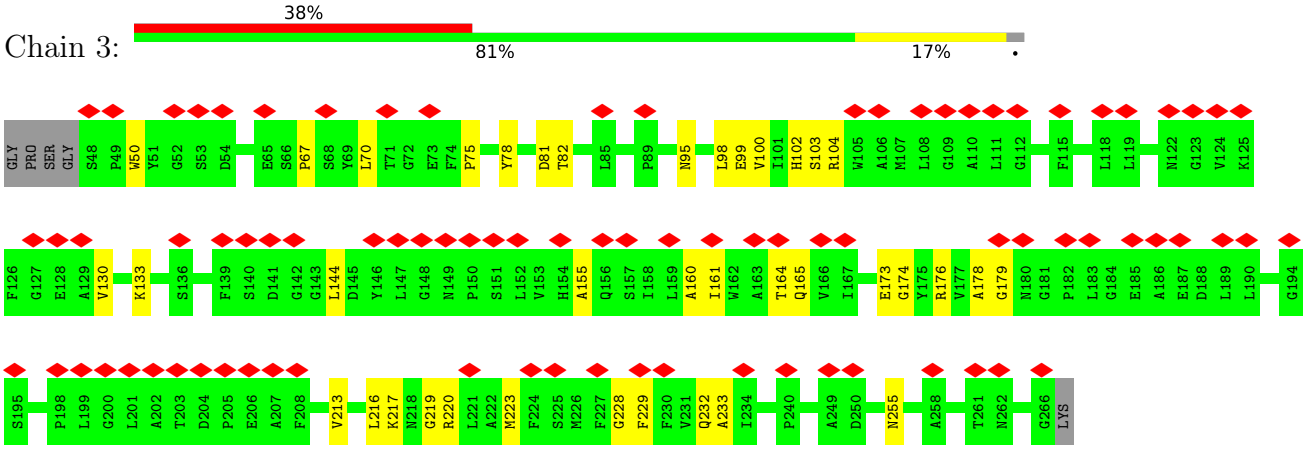
Chain 2:





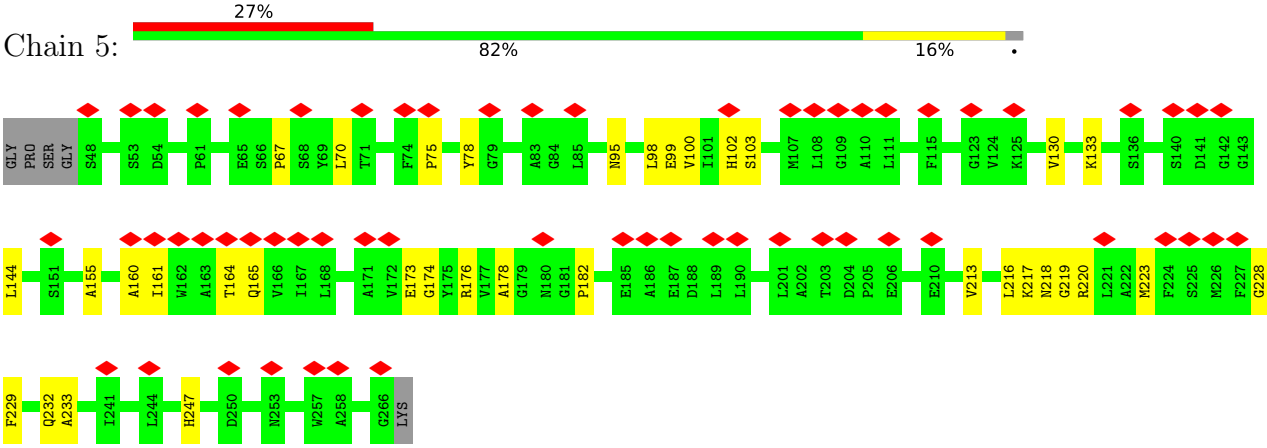
• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 3:



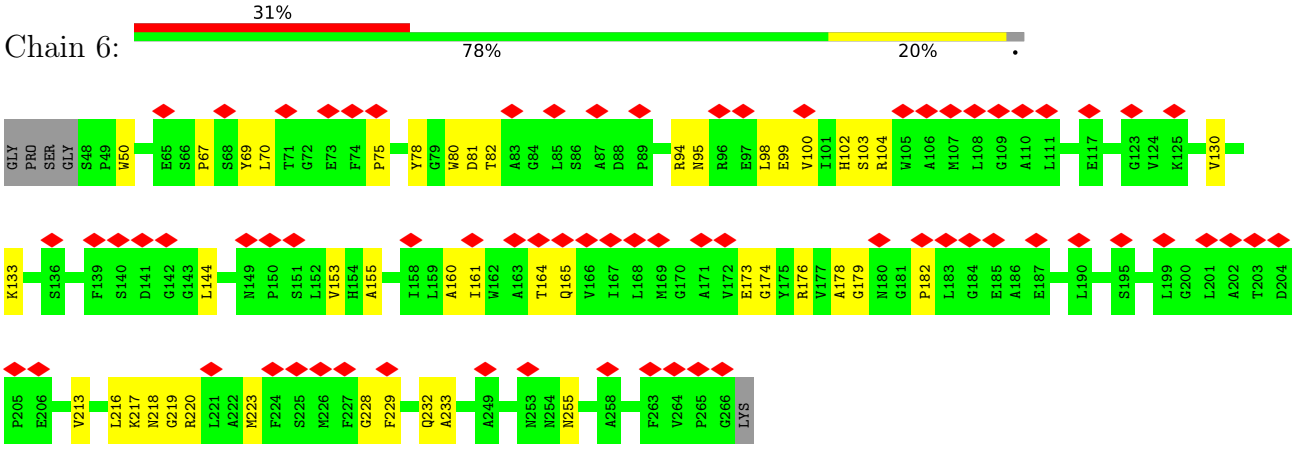
• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 5:



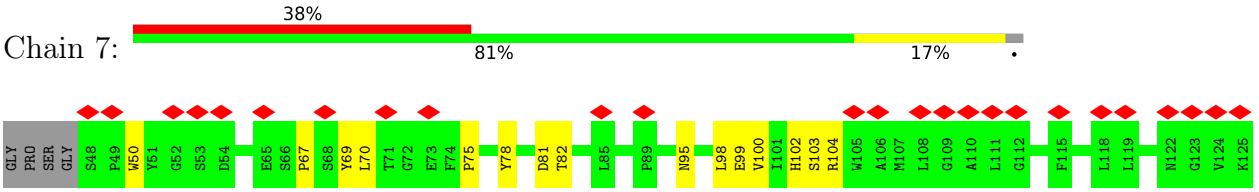
• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

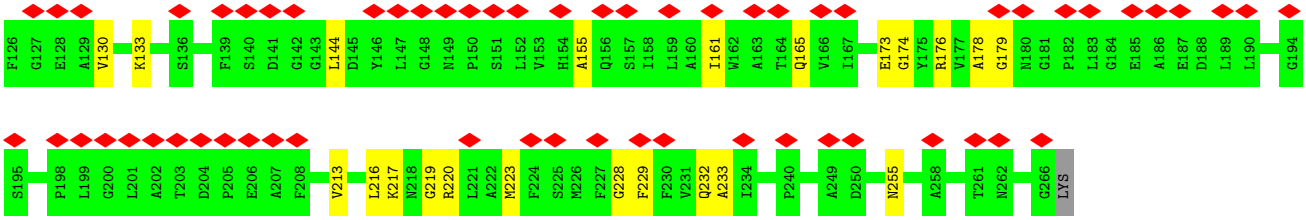
Chain 6:



• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 7:

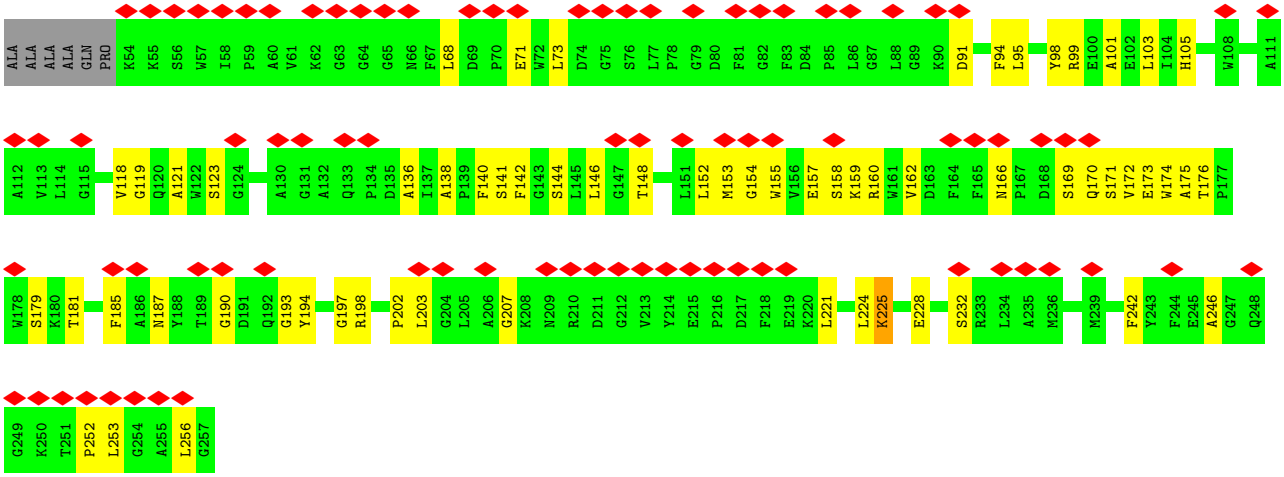




• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 4:

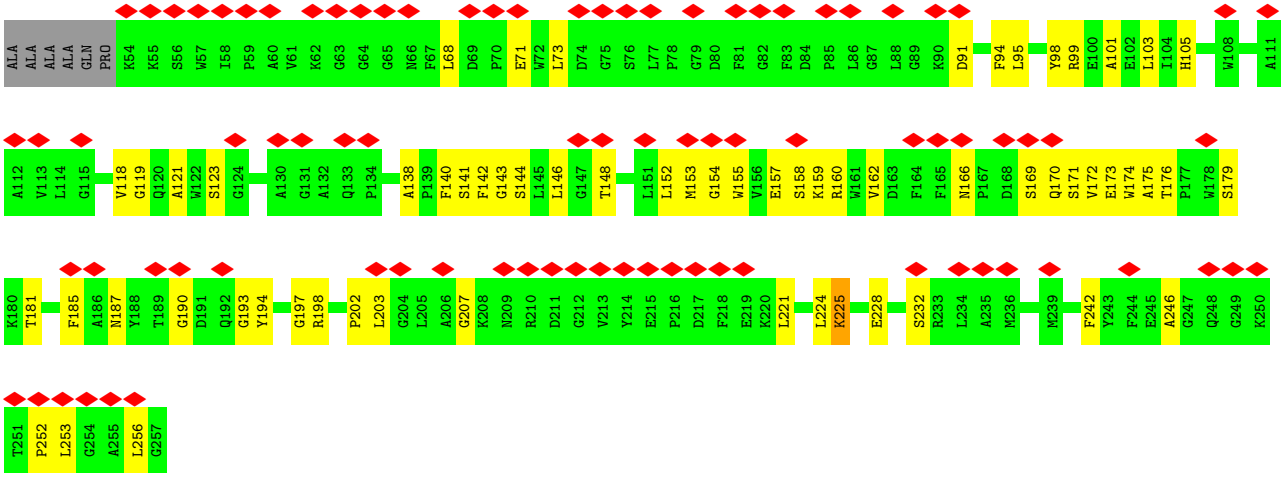




• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 8:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	23434	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.169	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	517.14, 517.14, 517.14	wwPDB
Map dimensions	468, 468, 468	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.105, 1.105, 1.105	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: CLA, PHO, FE2, CHL, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.30	0/2458	0.70	0/3348
1	a	0.30	0/2665	0.70	0/3634
2	B	0.28	0/3881	0.70	0/5286
2	b	0.28	0/3881	0.70	0/5286
3	C	0.29	0/3487	0.72	2/4750 (0.0%)
3	c	0.29	0/3487	0.72	2/4750 (0.0%)
4	D	0.30	0/2768	0.74	1/3774 (0.0%)
4	d	0.30	0/2768	0.74	1/3774 (0.0%)
5	E	0.34	0/603	0.90	2/819 (0.2%)
5	e	0.34	0/603	0.90	2/819 (0.2%)
6	F	0.31	0/229	0.78	0/311
6	f	0.31	0/229	0.78	0/311
7	H	0.30	0/398	0.70	0/541
7	h	0.30	0/398	0.70	0/541
8	I	0.35	0/294	0.87	0/397
8	i	0.35	0/294	0.87	0/397
9	K	0.37	0/301	0.93	0/414
9	k	0.37	0/301	0.93	0/414
10	L	0.32	0/310	0.86	0/421
10	l	0.32	0/310	0.86	0/421
11	M	0.37	0/230	0.79	0/315
11	m	0.37	0/230	0.79	0/315
12	O	0.28	0/1518	0.72	2/2049 (0.1%)
12	o	0.28	0/1518	0.72	2/2049 (0.1%)
13	T	0.29	0/246	0.72	0/333
13	t	0.29	0/246	0.72	0/333
14	W	0.27	0/383	0.76	0/519
14	w	0.27	0/383	0.76	0/519
15	X	0.29	0/228	0.60	0/310
15	x	0.28	0/228	0.59	0/310
16	Z	0.27	0/468	0.67	0/641
16	z	0.28	0/468	0.68	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	R	0.26	0/1502	0.58	0/2047
17	r	0.26	0/1502	0.58	0/2047
18	S	0.32	0/1698	0.96	11/2305 (0.5%)
18	s	0.32	0/1698	0.96	11/2305 (0.5%)
19	1	0.23	0/1716	0.60	0/2336
19	2	0.23	0/1716	0.60	0/2336
19	3	0.23	0/1716	0.60	0/2336
19	5	0.23	0/1716	0.60	0/2336
19	6	0.23	0/1716	0.60	0/2336
19	7	0.23	0/1716	0.60	0/2336
19	G	0.27	0/1716	0.63	0/2336
19	N	0.27	0/1716	0.63	0/2336
19	Y	0.27	0/1716	0.63	0/2336
19	g	0.27	0/1716	0.63	0/2336
19	n	0.27	0/1716	0.63	0/2336
19	y	0.27	0/1716	0.63	0/2336
20	4	0.29	0/1652	1.10	5/2242 (0.2%)
20	8	0.29	0/1652	1.10	5/2242 (0.2%)
All	All	0.28	0/66107	0.73	46/89962 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	b	0	1
17	R	0	1
17	r	0	1
18	S	0	1
18	s	0	1
20	4	0	1
20	8	0	1
All	All	0	8

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	207	GLY	CA-C-O	28.04	152.19	121.90
20	8	207	GLY	CA-C-O	28.04	152.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	207	GLY	O-C-N	-27.56	87.76	122.76
20	8	207	GLY	O-C-N	-27.56	87.76	122.76
20	4	207	GLY	CA-C-N	6.29	131.37	122.05
20	4	207	GLY	C-N-CA	6.29	131.37	122.05
20	8	207	GLY	CA-C-N	6.29	131.37	122.05
20	8	207	GLY	C-N-CA	6.29	131.37	122.05
18	S	166	ASN	CA-C-N	6.12	124.10	120.24
18	S	166	ASN	C-N-CA	6.12	124.10	120.24
18	s	166	ASN	CA-C-N	6.12	124.10	120.24
18	s	166	ASN	C-N-CA	6.12	124.10	120.24
18	S	167	ILE	CA-C-N	6.08	141.58	127.00
18	S	167	ILE	C-N-CA	6.08	141.58	127.00
18	s	167	ILE	CA-C-N	6.08	141.58	127.00
18	s	167	ILE	C-N-CA	6.08	141.58	127.00
12	O	192	ASP	CA-C-N	6.00	132.49	121.70
12	O	192	ASP	C-N-CA	6.00	132.49	121.70
3	c	266	TRP	N-CA-C	5.99	117.62	110.44
12	o	192	ASP	CA-C-N	5.98	132.47	121.70
12	o	192	ASP	C-N-CA	5.98	132.47	121.70
3	C	266	TRP	N-CA-C	5.96	117.59	110.44
18	S	138	GLY	N-CA-C	5.90	127.15	113.18
18	s	138	GLY	N-CA-C	5.90	127.15	113.18
18	S	139	ALA	CA-C-N	5.65	132.11	123.47
18	S	139	ALA	C-N-CA	5.65	132.11	123.47
18	s	139	ALA	CA-C-N	5.65	132.11	123.47
18	s	139	ALA	C-N-CA	5.65	132.11	123.47
5	E	59	SER	CA-C-N	5.63	132.28	121.54
5	E	59	SER	C-N-CA	5.63	132.28	121.54
5	e	59	SER	CA-C-N	5.60	132.24	121.54
5	e	59	SER	C-N-CA	5.60	132.24	121.54
4	d	100	GLY	N-CA-C	-5.56	100.00	113.18
4	D	100	GLY	N-CA-C	-5.55	100.02	113.18
18	S	167	ILE	C-N-CD	-5.29	108.97	120.60
18	s	167	ILE	C-N-CD	-5.29	108.97	120.60
20	4	225	LYS	N-CA-C	-5.19	105.53	111.14
20	8	225	LYS	N-CA-C	-5.19	105.53	111.14
18	S	178	GLU	CA-CB-CG	-5.19	103.73	114.10
18	s	178	GLU	CA-CB-CG	-5.19	103.73	114.10
18	S	142	GLY	CA-C-N	5.06	139.14	127.00
18	S	142	GLY	C-N-CA	5.06	139.14	127.00
18	s	142	GLY	CA-C-N	5.06	139.14	127.00
18	s	142	GLY	C-N-CA	5.06	139.14	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	223	TRP	N-CA-C	-5.01	101.31	108.23
3	c	223	TRP	N-CA-C	-5.00	101.33	108.23

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	4	176	THR	Peptide
20	8	176	THR	Peptide
2	B	179	GLN	Peptide
17	R	59	TYR	Peptide
18	S	71	LEU	Peptide
2	b	179	GLN	Peptide
17	r	59	TYR	Peptide
18	s	71	LEU	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	A	2388	0	2309	59	0
1	a	2584	0	2490	55	0
2	B	3752	0	3636	109	0
2	b	3752	0	3636	115	0
3	C	3373	0	3302	127	0
3	c	3373	0	3302	111	0
4	D	2675	0	2565	86	0
4	d	2675	0	2565	64	0
5	E	586	0	566	13	0
5	e	586	0	566	12	0
6	F	224	0	233	4	0
6	f	224	0	233	6	0
7	H	389	0	411	8	0
7	h	389	0	411	4	0
8	I	286	0	295	2	0
8	i	286	0	295	8	0
9	K	290	0	300	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	k	290	0	300	5	0
10	L	302	0	291	13	0
10	l	302	0	291	7	0
11	M	226	0	252	6	0
11	m	226	0	252	9	0
12	O	1487	0	1462	36	0
12	o	1487	0	1462	35	0
13	T	239	0	255	9	0
13	t	239	0	255	3	0
14	W	372	0	346	7	0
14	w	372	0	346	6	0
15	X	226	0	244	6	0
15	x	226	0	244	6	0
16	Z	458	0	490	32	0
16	z	458	0	489	23	0
17	R	1459	0	1428	132	0
17	r	1459	0	1428	127	0
18	S	1653	0	1639	79	0
18	s	1653	0	1639	73	0
19	1	1666	0	1593	29	0
19	2	1666	0	1593	33	0
19	3	1666	0	1593	29	0
19	5	1666	0	1593	28	0
19	6	1666	0	1593	37	0
19	7	1666	0	1593	30	0
19	G	1666	0	1593	33	0
19	N	1666	0	1593	33	0
19	Y	1666	0	1593	36	0
19	g	1666	0	1593	31	0
19	n	1666	0	1593	33	0
19	y	1666	0	1593	35	0
20	4	1597	0	1526	159	0
20	8	1597	0	1526	162	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	1	360	0	264	3	0
22	2	360	0	264	22	0
22	3	360	0	264	2	0
22	4	270	0	196	43	0
22	5	360	0	264	3	0
22	6	360	0	264	22	0
22	7	360	0	264	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	8	270	0	196	45	0
22	A	135	0	99	4	0
22	B	720	0	528	23	0
22	C	540	0	396	15	0
22	D	135	0	99	3	0
22	G	360	0	264	7	0
22	N	360	0	264	4	0
22	R	360	0	264	27	0
22	S	450	0	330	13	0
22	Y	360	0	264	8	0
22	a	135	0	99	3	0
22	b	720	0	528	19	0
22	c	540	0	396	13	0
22	d	135	0	99	4	0
22	g	360	0	264	6	0
22	n	360	0	264	4	0
22	r	360	0	264	8	0
22	s	450	0	330	23	0
22	y	360	0	264	5	0
23	A	44	0	35	2	0
23	D	44	0	35	1	0
23	a	44	0	35	2	0
23	d	44	0	35	2	0
24	F	43	0	30	3	0
24	e	43	0	30	3	0
25	1	318	0	213	9	0
25	2	226	0	151	13	0
25	3	272	0	182	6	0
25	4	230	0	155	14	0
25	5	318	0	213	7	0
25	6	226	0	151	13	0
25	7	272	0	182	7	0
25	8	230	0	155	15	0
25	G	272	0	182	11	0
25	N	272	0	182	9	0
25	R	138	0	93	6	0
25	S	184	0	124	4	0
25	Y	272	0	182	12	0
25	g	272	0	182	11	0
25	n	272	0	182	8	0
25	r	138	0	93	3	0
25	s	184	0	124	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	y	272	0	182	11	0
All	All	78324	0	72516	1876	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 12.

All (1876) 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)
3:C:182:PHE:CZ	18:S:261:PRO:HG2	1.17	1.70
16:Z:59:SER:CB	18:S:267:LEU:CD2	1.74	1.58
17:r:280:HIS:HA	20:4:141:SER:N	1.20	1.48
16:Z:59:SER:CB	18:S:267:LEU:HD23	1.02	1.47
2:b:214:LEU:HD22	22:R:302:CLA:CED	1.42	1.47
3:C:182:PHE:CE1	18:S:261:PRO:HG2	1.47	1.46
17:R:280:HIS:HA	20:8:141:SER:N	1.20	1.44
3:C:182:PHE:CE1	18:S:261:PRO:CG	2.02	1.43
2:b:214:LEU:HB3	22:R:302:CLA:CED	1.51	1.40
18:s:74:GLY:N	22:s:301:CLA:HED2	1.25	1.40
16:z:60:LEU:CD2	18:s:270:ILE:HG21	1.52	1.39
3:C:182:PHE:CZ	18:S:261:PRO:CG	2.07	1.38
2:b:214:LEU:CG	22:R:302:CLA:HED1	1.55	1.37
20:8:173:GLU:HG2	22:8:301:CLA:C1B	1.37	1.35
2:b:214:LEU:CB	22:R:302:CLA:HED1	1.55	1.34
17:R:285:ASP:CB	20:8:141:SER:HB3	1.45	1.32
3:C:131:TYR:OH	18:S:74:GLY:HA3	1.21	1.30
3:C:131:TYR:OH	18:S:74:GLY:CA	1.80	1.29
17:r:285:ASP:CB	20:4:141:SER:HB3	1.45	1.29
20:8:174:TRP:O	22:8:301:CLA:CHC	1.80	1.29
16:Z:59:SER:OG	18:S:267:LEU:CD2	1.71	1.28
20:4:174:TRP:O	22:4:301:CLA:CHC	1.80	1.28
20:4:174:TRP:O	22:4:301:CLA:HHC	1.13	1.28
20:4:173:GLU:HG2	22:4:301:CLA:C1B	1.37	1.27
18:s:73:ASP:C	22:s:301:CLA:HED2	1.58	1.27
2:b:214:LEU:CD2	22:R:302:CLA:CED	2.09	1.27
17:R:280:HIS:CA	20:8:141:SER:N	1.98	1.26
18:s:74:GLY:N	22:s:301:CLA:CED	1.98	1.26
17:r:280:HIS:CA	20:4:141:SER:N	1.98	1.26
20:8:173:GLU:CG	22:8:301:CLA:C1B	2.09	1.26
20:4:148:THR:OG1	25:4:302:CHL:CED	1.85	1.25
17:R:62:ALA:CB	20:8:172:VAL:CG2	2.15	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:8:148:THR:OG1	25:8:302:CHL:CED	1.85	1.24
17:r:62:ALA:CB	20:4:172:VAL:CG2	2.15	1.24
20:8:174:TRP:O	22:8:301:CLA:HHC	1.13	1.24
20:8:173:GLU:HG2	22:8:301:CLA:NB	1.52	1.22
17:R:285:ASP:OD1	20:8:142:PHE:N	1.71	1.21
20:4:173:GLU:HG2	22:4:301:CLA:NB	1.52	1.21
2:b:214:LEU:HD22	22:R:302:CLA:O2D	1.37	1.20
17:r:285:ASP:OD1	20:4:142:PHE:N	1.71	1.20
16:z:60:LEU:HD22	18:s:270:ILE:HG21	1.21	1.19
2:b:162:TYR:CE1	17:R:193:TRP:HZ2	1.59	1.19
20:4:173:GLU:CG	22:4:301:CLA:C1B	2.09	1.19
17:R:285:ASP:CB	20:8:141:SER:CB	2.18	1.19
16:Z:59:SER:HB3	18:S:267:LEU:CD2	1.48	1.18
17:r:62:ALA:CB	20:4:172:VAL:HG23	1.71	1.18
17:r:280:HIS:CA	20:4:141:SER:H	1.55	1.17
2:b:162:TYR:HE1	17:R:193:TRP:CZ2	1.60	1.17
17:r:285:ASP:CB	20:4:141:SER:CB	2.18	1.17
17:r:285:ASP:HB2	20:4:141:SER:CB	1.75	1.17
20:4:173:GLU:CG	22:4:301:CLA:NB	2.07	1.17
17:R:285:ASP:HB2	20:8:141:SER:CB	1.75	1.16
17:r:56:PRO:N	20:4:174:TRP:HE1	1.43	1.16
17:R:280:HIS:CA	20:8:141:SER:H	1.55	1.15
17:R:59:TYR:HE1	20:8:170:GLN:N	1.42	1.15
17:r:59:TYR:HE1	20:4:170:GLN:N	1.42	1.15
17:R:62:ALA:CB	20:8:172:VAL:HG23	1.71	1.14
2:b:214:LEU:CG	22:R:302:CLA:CED	2.24	1.14
2:b:214:LEU:CD1	22:R:302:CLA:HED1	1.78	1.14
17:R:56:PRO:N	20:8:174:TRP:HE1	1.43	1.14
2:b:214:LEU:CB	22:R:302:CLA:CED	2.17	1.13
20:8:173:GLU:CG	22:8:301:CLA:NB	2.07	1.13
17:R:280:HIS:CE1	20:8:138:ALA:O	2.01	1.13
17:r:280:HIS:CE1	20:4:138:ALA:O	2.01	1.12
17:R:62:ALA:HB2	20:8:172:VAL:HG23	1.16	1.12
20:4:159:LYS:CE	22:4:301:CLA:HMA1	1.80	1.11
20:8:173:GLU:O	22:8:301:CLA:HBB1	1.37	1.11
20:8:159:LYS:CE	22:8:301:CLA:HMA1	1.80	1.11
2:b:214:LEU:HD22	22:R:302:CLA:HED3	1.29	1.10
17:r:285:ASP:HB2	20:4:141:SER:HB3	1.31	1.10
22:2:613:CLA:HAB	25:4:302:CHL:HAB	1.29	1.10
17:r:62:ALA:HB2	20:4:172:VAL:HG23	1.16	1.09
20:8:175:ALA:HB2	22:8:301:CLA:C3B	1.83	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:60:LEU:CD2	18:S:270:ILE:HG21	1.83	1.08
22:6:613:CLA:HAB	25:8:302:CHL:HAB	1.29	1.08
20:4:173:GLU:O	22:4:301:CLA:HBB1	1.37	1.08
16:Z:60:LEU:HD22	18:S:270:ILE:CG2	1.82	1.07
17:r:280:HIS:HE1	20:4:138:ALA:O	1.33	1.07
16:z:60:LEU:CD2	18:s:270:ILE:CG2	2.33	1.06
20:4:175:ALA:HB2	22:4:301:CLA:C3B	1.83	1.06
3:c:182:PHE:HZ	18:s:261:PRO:HG2	1.17	1.06
3:C:206:PRO:HG3	22:Y:614:CLA:HBB2	1.12	1.06
20:4:148:THR:OG1	25:4:302:CHL:HED3	1.54	1.06
17:R:59:TYR:CE1	20:8:170:GLN:HA	1.91	1.05
17:R:62:ALA:HB2	20:8:172:VAL:CG2	1.82	1.05
17:r:62:ALA:HB1	20:4:172:VAL:CG2	1.85	1.05
3:C:182:PHE:CE1	18:S:261:PRO:CD	2.37	1.05
16:Z:59:SER:OG	18:S:267:LEU:HD21	1.41	1.05
17:r:59:TYR:CE1	20:4:170:GLN:HA	1.91	1.04
17:R:285:ASP:HB2	20:8:141:SER:HB3	1.31	1.04
17:r:56:PRO:N	20:4:174:TRP:NE1	2.05	1.03
20:4:162:VAL:HG21	22:4:301:CLA:O2A	1.58	1.03
20:8:148:THR:OG1	25:8:302:CHL:HED3	1.54	1.03
17:R:56:PRO:N	20:8:174:TRP:NE1	2.05	1.03
20:8:159:LYS:HE2	22:8:301:CLA:HMA1	1.37	1.02
17:R:62:ALA:HB1	20:8:172:VAL:CG2	1.85	1.02
17:r:62:ALA:HB2	20:4:172:VAL:CG2	1.82	1.02
20:4:159:LYS:HE2	22:4:301:CLA:HMA1	1.37	1.01
20:8:162:VAL:HG21	22:8:301:CLA:O2A	1.58	1.01
16:Z:60:LEU:CD2	18:S:270:ILE:CG2	2.38	1.01
3:c:182:PHE:CZ	18:s:261:PRO:HG2	1.94	1.01
17:R:62:ALA:HB1	20:8:172:VAL:HG21	1.40	1.01
17:R:280:HIS:HE1	20:8:138:ALA:O	1.33	1.01
17:r:62:ALA:HB1	20:4:172:VAL:HG21	1.40	1.01
15:X:82:SER:O	15:X:86:PHE:HB3	1.61	1.01
15:x:82:SER:O	15:x:86:PHE:HB3	1.60	1.01
16:Z:60:LEU:HD22	18:S:270:ILE:HG21	1.01	1.00
3:C:182:PHE:HE1	18:S:261:PRO:CG	1.67	1.00
18:s:74:GLY:CA	22:s:301:CLA:HED2	1.91	0.99
20:4:175:ALA:CB	22:4:301:CLA:C3B	2.38	0.99
3:c:131:TYR:OH	18:s:74:GLY:HA3	1.63	0.99
17:R:62:ALA:CB	20:8:172:VAL:HG21	1.90	0.98
3:C:182:PHE:CE1	18:S:261:PRO:HD2	1.97	0.98
16:Z:59:SER:CB	18:S:267:LEU:HD21	1.85	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:8:148:THR:OG1	25:8:302:CHL:HED1	1.61	0.97
20:4:173:GLU:O	22:4:301:CLA:CBB	2.13	0.97
20:8:175:ALA:CB	22:8:301:CLA:C3B	2.38	0.97
3:C:182:PHE:CE1	18:S:261:PRO:CB	2.48	0.96
3:c:260:ALA:O	3:c:264:LEU:HB2	1.66	0.96
2:b:214:LEU:HD13	22:R:302:CLA:HED1	1.47	0.96
18:s:177:ALA:O	18:s:181:LEU:HB2	1.66	0.96
20:8:173:GLU:O	22:8:301:CLA:CBB	2.13	0.96
2:b:214:LEU:CD2	22:R:302:CLA:HED3	1.86	0.95
20:8:173:GLU:HG2	22:8:301:CLA:C2B	1.96	0.95
22:6:613:CLA:CAB	25:8:302:CHL:HAB	1.97	0.95
20:4:173:GLU:HG2	22:4:301:CLA:C2B	1.96	0.95
20:8:162:VAL:HG21	22:8:301:CLA:CGA	1.96	0.95
3:C:260:ALA:O	3:C:264:LEU:HB2	1.66	0.95
20:4:148:THR:OG1	25:4:302:CHL:HED1	1.61	0.95
17:r:62:ALA:CB	20:4:172:VAL:HG21	1.90	0.95
17:r:191:LEU:O	17:r:195:GLU:HB2	1.67	0.95
17:r:285:ASP:HB2	20:4:141:SER:OG	1.67	0.95
22:2:613:CLA:CAB	25:4:302:CHL:HAB	1.97	0.94
20:4:162:VAL:HG21	22:4:301:CLA:CGA	1.96	0.94
20:4:159:LYS:CE	22:4:301:CLA:CMA	2.45	0.94
18:S:177:ALA:O	18:S:181:LEU:HB2	1.66	0.94
17:r:278:PRO:CG	22:2:613:CLA:HBB2	1.98	0.94
20:8:173:GLU:HG2	22:8:301:CLA:C4B	1.98	0.93
2:B:345:VAL:O	2:B:399:VAL:HA	1.69	0.93
20:8:159:LYS:CE	22:8:301:CLA:CMA	2.45	0.93
15:x:84:LYS:O	15:x:88:LEU:HB2	1.68	0.93
17:R:191:LEU:O	17:R:195:GLU:HB2	1.67	0.93
16:Z:36:ASN:O	16:Z:40:VAL:HB	1.68	0.93
20:4:173:GLU:HG2	22:4:301:CLA:C4B	1.98	0.93
2:B:346:PHE:O	2:B:354:LEU:HB2	1.69	0.92
17:R:285:ASP:HB2	20:8:141:SER:OG	1.67	0.92
17:R:278:PRO:CG	22:6:613:CLA:HBB2	1.98	0.92
18:s:74:GLY:CA	22:s:301:CLA:CED	2.46	0.92
20:8:148:THR:HG1	25:8:302:CHL:CED	1.76	0.92
17:r:59:TYR:CE1	20:4:170:GLN:N	2.35	0.92
17:r:59:TYR:CE1	20:4:170:GLN:CA	2.53	0.92
20:8:159:LYS:HE3	22:8:301:CLA:CMA	2.00	0.92
2:b:345:VAL:O	2:b:399:VAL:HA	1.69	0.92
16:z:36:ASN:O	16:z:40:VAL:HB	1.68	0.91
17:R:61:GLY:O	20:8:166:ASN:ND2	2.03	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:159:LYS:HE3	22:4:301:CLA:CMA	2.00	0.91
16:Z:59:SER:HB2	18:S:267:LEU:CD2	1.99	0.91
17:R:59:TYR:CE1	20:8:170:GLN:CA	2.53	0.91
15:X:84:LYS:O	15:X:88:LEU:HB2	1.68	0.91
2:b:346:PHE:O	2:b:354:LEU:HB2	1.69	0.91
17:r:61:GLY:O	20:4:166:ASN:ND2	2.03	0.91
3:C:182:PHE:HZ	18:S:261:PRO:HG2	1.15	0.90
17:R:278:PRO:CD	22:6:613:CLA:HBB2	2.01	0.90
17:r:278:PRO:CD	22:2:613:CLA:HBB2	2.01	0.90
17:r:61:GLY:HA2	20:4:169:SER:HB2	1.52	0.90
17:R:61:GLY:HA2	20:8:169:SER:HB2	1.52	0.90
17:R:280:HIS:HA	20:8:140:PHE:C	1.96	0.90
17:R:288:SER:OG	20:8:142:PHE:HD2	1.56	0.89
17:r:280:HIS:HA	20:4:140:PHE:C	1.96	0.89
17:r:280:HIS:CA	20:4:140:PHE:C	2.44	0.89
3:C:206:PRO:CG	22:Y:614:CLA:HBB2	2.02	0.89
17:R:59:TYR:CE1	20:8:170:GLN:N	2.35	0.89
3:C:182:PHE:HE1	18:S:261:PRO:CD	1.80	0.89
1:A:51:ALA:O	1:A:55:ALA:HB2	1.73	0.88
17:r:255:GLY:O	17:r:259:GLN:HB3	1.73	0.88
17:R:280:HIS:CA	20:8:140:PHE:C	2.44	0.88
3:C:131:TYR:OH	18:S:74:GLY:HA2	1.70	0.88
1:a:51:ALA:O	1:a:55:ALA:HB2	1.73	0.88
3:c:182:PHE:HZ	18:s:261:PRO:CG	1.87	0.87
17:r:58:TRP:C	20:4:173:GLU:HG3	1.98	0.87
17:R:58:TRP:C	20:8:173:GLU:HG3	1.98	0.87
17:r:288:SER:OG	20:4:142:PHE:HD2	1.56	0.87
20:4:148:THR:HG1	25:4:302:CHL:HED3	1.35	0.87
2:b:110:ALA:O	2:b:114:HIS:HB2	1.74	0.86
17:R:255:GLY:O	17:R:259:GLN:HB3	1.73	0.86
20:4:94:PHE:O	20:4:98:TYR:HB3	1.74	0.86
20:8:94:PHE:O	20:8:98:TYR:HB3	1.74	0.86
3:c:182:PHE:CE1	18:s:261:PRO:HD2	2.11	0.86
2:B:110:ALA:O	2:B:114:HIS:HB2	1.74	0.86
2:b:214:LEU:HB3	22:R:302:CLA:HED1	1.15	0.86
3:C:182:PHE:CE1	18:S:261:PRO:HB2	2.11	0.85
20:8:159:LYS:HE2	22:8:301:CLA:CMA	2.07	0.85
2:b:64:PRO:O	2:b:68:ARG:HB2	1.76	0.85
3:C:182:PHE:HE1	18:S:261:PRO:CB	1.85	0.85
2:b:214:LEU:CD2	22:R:302:CLA:O2D	2.19	0.84
17:R:284:ILE:HG12	20:8:146:LEU:N	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:159:LYS:HE2	22:4:301:CLA:CMA	2.07	0.84
17:r:287:PHE:CZ	20:4:146:LEU:HD23	2.13	0.84
17:R:278:PRO:HD3	22:6:613:CLA:HBB2	1.59	0.84
2:B:64:PRO:O	2:B:68:ARG:HB2	1.77	0.84
17:R:59:TYR:HE1	20:8:170:GLN:CA	1.91	0.84
17:R:287:PHE:CZ	20:8:146:LEU:HD23	2.13	0.83
17:R:56:PRO:N	20:8:174:TRP:CD1	2.47	0.83
2:b:214:LEU:HD13	22:R:302:CLA:CED	2.08	0.83
2:B:346:PHE:HB2	2:B:354:LEU:O	1.78	0.83
17:r:278:PRO:HD3	22:2:613:CLA:HBB2	1.59	0.83
2:b:346:PHE:HB2	2:b:354:LEU:O	1.78	0.83
17:r:56:PRO:N	20:4:174:TRP:CD1	2.47	0.83
17:r:284:ILE:HG12	20:4:146:LEU:N	1.92	0.82
17:r:285:ASP:CA	20:4:141:SER:HB3	2.09	0.82
3:C:130:ILE:O	3:C:134:LEU:HB2	1.78	0.82
20:4:144:SER:O	25:4:302:CHL:CED	2.28	0.82
20:8:144:SER:O	25:8:302:CHL:CED	2.28	0.81
3:c:130:ILE:O	3:c:134:LEU:HB2	1.78	0.81
17:R:285:ASP:CA	20:8:141:SER:HB3	2.09	0.81
18:S:178:GLU:O	18:S:182:LEU:HB3	1.81	0.81
2:B:247:PHE:HB2	22:B:608:CLA:HBC1	1.61	0.81
17:R:59:TYR:HE1	20:8:170:GLN:H	0.81	0.81
18:s:178:GLU:O	18:s:182:LEU:HB3	1.81	0.80
17:r:58:TRP:O	20:4:173:GLU:HG3	1.82	0.80
15:x:83:LEU:O	15:x:87:LEU:HB2	1.82	0.80
15:X:83:LEU:O	15:X:87:LEU:HB2	1.82	0.80
17:R:284:ILE:HG12	20:8:146:LEU:H	1.47	0.80
17:r:285:ASP:CG	20:4:142:PHE:H	1.88	0.79
2:B:114:HIS:HE1	22:B:616:CLA:ND	1.79	0.79
16:z:60:LEU:HD23	18:s:270:ILE:HG21	1.63	0.79
17:R:58:TRP:O	20:8:173:GLU:HG3	1.82	0.79
17:R:285:ASP:CG	20:8:142:PHE:N	2.41	0.79
20:8:148:THR:HG1	25:8:302:CHL:HED3	1.34	0.79
5:E:72:SER:O	5:E:76:LEU:HB2	1.83	0.79
2:b:214:LEU:CB	22:R:302:CLA:HED3	2.12	0.78
20:4:159:LYS:HE3	22:4:301:CLA:HMA1	1.61	0.78
17:r:280:HIS:CB	20:4:141:SER:N	2.42	0.78
3:C:182:PHE:CZ	18:S:261:PRO:CB	2.66	0.78
3:C:182:PHE:HZ	18:S:261:PRO:CG	1.78	0.78
13:T:20:ALA:O	13:T:24:ARG:HB3	1.84	0.78
5:e:72:SER:O	5:e:76:LEU:HB2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:280:HIS:CA	20:8:140:PHE:CA	2.47	0.78
17:r:284:ILE:HG12	20:4:146:LEU:H	1.47	0.78
17:r:285:ASP:CG	20:4:142:PHE:N	2.41	0.78
20:4:148:THR:HG1	25:4:302:CHL:CED	1.89	0.78
2:b:214:LEU:CD1	22:R:302:CLA:CED	2.57	0.78
13:t:20:ALA:O	13:t:24:ARG:HB3	1.84	0.78
17:r:59:TYR:HE1	20:4:170:GLN:CA	1.91	0.78
22:B:604:CLA:HBB1	22:B:607:CLA:HBB2	1.65	0.77
4:D:154:PHE:O	4:D:158:PHE:HB2	1.84	0.77
1:a:48:PHE:O	1:a:52:PHE:HB2	1.84	0.77
17:R:285:ASP:CG	20:8:142:PHE:H	1.88	0.77
1:A:48:PHE:O	1:A:52:PHE:HB2	1.84	0.77
17:r:287:PHE:HZ	20:4:146:LEU:HD23	1.49	0.77
18:S:250:PRO:O	18:S:254:LEU:HB2	1.84	0.77
4:D:186:PHE:O	4:D:190:HIS:HB2	1.85	0.77
22:2:613:CLA:HAB	25:4:302:CHL:CAB	2.13	0.77
4:d:154:PHE:O	4:d:158:PHE:HB2	1.84	0.77
2:b:214:LEU:HB3	22:R:302:CLA:HED3	1.61	0.77
18:S:73:ASP:HB3	22:S:301:CLA:O2D	1.84	0.77
4:d:327:ARG:O	4:d:331:ALA:HB2	1.85	0.77
18:s:73:ASP:HB3	22:s:301:CLA:CED	2.15	0.77
3:c:182:PHE:CZ	18:s:261:PRO:CG	2.64	0.76
17:R:288:SER:HG	20:8:142:PHE:HD2	0.78	0.76
5:E:33:ALA:O	5:E:37:PHE:HB2	1.86	0.76
5:e:33:ALA:O	5:e:37:PHE:HB2	1.86	0.76
17:R:287:PHE:HZ	20:8:146:LEU:HD23	1.49	0.76
17:r:59:TYR:HE1	20:4:170:GLN:H	0.81	0.76
18:s:225:GLU:HA	22:s:310:CLA:HBB1	1.67	0.76
18:s:250:PRO:O	18:s:254:LEU:HB2	1.84	0.76
3:C:131:TYR:CZ	18:S:74:GLY:HA3	2.22	0.75
2:b:168:VAL:O	2:b:176:GLY:HA2	1.86	0.75
4:d:186:PHE:O	4:d:190:HIS:HB2	1.85	0.75
22:6:613:CLA:HAB	25:8:302:CHL:CAB	2.13	0.75
20:8:173:GLU:HG3	22:8:301:CLA:NB	2.00	0.75
1:A:186:PHE:O	1:A:190:HIS:HB2	1.87	0.75
1:a:186:PHE:O	1:a:190:HIS:HB2	1.87	0.75
17:R:177:SER:O	17:R:183:PRO:HA	1.87	0.75
16:Z:60:LEU:CD2	18:S:270:ILE:HG22	2.17	0.75
2:B:2:GLY:HA3	10:L:12:GLU:HG2	1.68	0.75
17:R:285:ASP:N	20:8:141:SER:HB3	2.02	0.75
20:8:175:ALA:CB	22:8:301:CLA:C2B	2.65	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:225:GLU:HA	22:S:310:CLA:HBB1	1.67	0.75
18:s:73:ASP:C	22:s:301:CLA:CED	2.49	0.74
20:4:175:ALA:CB	22:4:301:CLA:C2B	2.65	0.74
3:c:182:PHE:CE1	18:s:262:PHE:HD2	2.05	0.74
2:B:168:VAL:O	2:B:176:GLY:HA2	1.87	0.74
16:z:37:LYS:O	16:z:41:PHE:HB2	1.87	0.74
17:R:280:HIS:CB	20:8:141:SER:N	2.42	0.74
4:D:327:ARG:O	4:D:331:ALA:HB2	1.85	0.74
16:Z:37:LYS:O	16:Z:41:PHE:HB2	1.87	0.74
17:r:177:SER:O	17:r:183:PRO:HA	1.87	0.74
4:D:181:ARG:O	4:D:185:PHE:HB2	1.88	0.74
18:S:73:ASP:HB2	22:S:301:CLA:HBD	1.69	0.74
4:d:181:ARG:O	4:d:185:PHE:HB2	1.88	0.74
2:B:282:GLN:O	2:B:286:ARG:HB2	1.88	0.73
9:K:31:ALA:O	9:K:34:ASN:HB2	1.88	0.73
4:d:178:ALA:O	4:d:182:PHE:HB2	1.88	0.73
12:O:136:PHE:HB3	12:O:174:ILE:HB	1.71	0.73
12:O:137:CYS:HB3	12:O:328:TYR:HB3	1.70	0.73
20:4:173:GLU:HG3	22:4:301:CLA:NB	2.00	0.73
19:1:228:GLY:O	19:1:232:GLN:HB3	1.89	0.73
2:b:282:GLN:O	2:b:286:ARG:HB2	1.88	0.73
17:r:285:ASP:N	20:4:141:SER:HB3	2.02	0.73
19:5:228:GLY:O	19:5:232:GLN:HB3	1.89	0.73
16:z:60:LEU:HD21	18:s:270:ILE:CG2	2.18	0.72
19:7:228:GLY:O	19:7:232:GLN:HB3	1.89	0.72
4:D:178:ALA:O	4:D:182:PHE:HB2	1.88	0.72
16:Z:42:SER:O	16:Z:46:LEU:HB2	1.89	0.72
19:3:228:GLY:O	19:3:232:GLN:HB3	1.89	0.72
2:b:247:PHE:HB2	22:b:608:CLA:HBC1	1.71	0.72
16:z:42:SER:O	16:z:46:LEU:HB2	1.90	0.72
16:z:60:LEU:HD21	18:s:270:ILE:HG21	1.68	0.72
4:d:302:GLN:O	4:d:306:ALA:HB3	1.90	0.72
12:o:137:CYS:HB3	12:o:328:TYR:HB3	1.70	0.72
2:B:333:GLY:HA2	2:B:444:ARG:HH11	1.55	0.72
9:k:31:ALA:O	9:k:34:ASN:HB2	1.88	0.72
19:6:228:GLY:O	19:6:232:GLN:HB3	1.89	0.72
1:A:331:MET:HG3	4:D:325:GLY:HA3	1.72	0.71
17:r:288:SER:HG	20:4:142:PHE:HD2	0.78	0.71
3:c:224:ILE:O	3:c:227:VAL:HB	1.90	0.71
2:b:157:HIS:HE1	22:b:606:CLA:NA	1.88	0.71
2:b:333:GLY:HA2	2:b:444:ARG:HH11	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:95:LEU:O	20:4:99:ARG:HB2	1.91	0.71
19:2:228:GLY:O	19:2:232:GLN:HB3	1.89	0.71
10:l:36:PHE:HB3	11:m:7:ALA:HB1	1.72	0.71
2:b:161:LEU:HD21	25:R:305:CHL:HMD2	1.73	0.70
12:o:136:PHE:HB3	12:o:174:ILE:HB	1.70	0.70
4:D:302:GLN:O	4:D:306:ALA:HB3	1.90	0.70
16:z:33:TRP:O	16:z:37:LYS:HB2	1.92	0.70
3:C:224:ILE:O	3:C:227:VAL:HB	1.90	0.70
4:d:330:MET:O	4:d:334:ASP:HB2	1.92	0.70
16:Z:33:TRP:O	16:Z:37:LYS:HB2	1.91	0.70
16:Z:59:SER:OG	18:S:267:LEU:HD23	1.57	0.70
2:b:212:ALA:O	2:b:216:HIS:HB2	1.92	0.70
17:r:280:HIS:CA	20:4:140:PHE:CA	2.47	0.70
20:8:95:LEU:O	20:8:99:ARG:HB2	1.91	0.70
2:B:212:ALA:O	2:B:216:HIS:HB2	1.91	0.70
20:4:187:ASN:HD22	20:4:197:GLY:H	1.40	0.70
20:8:187:ASN:HD22	20:8:197:GLY:H	1.40	0.70
4:D:330:MET:O	4:D:334:ASP:HB2	1.92	0.69
1:A:75:ASN:OD1	4:D:302:GLN:NE2	2.26	0.69
20:4:159:LYS:HE3	22:4:301:CLA:HMA2	1.74	0.69
2:b:162:TYR:CE1	17:R:193:TRP:CZ2	2.49	0.69
1:A:272:HIS:HD2	4:D:215:HIS:NE2	1.90	0.69
3:C:276:LEU:HD21	22:C:508:CLA:HAB	1.75	0.69
20:4:162:VAL:CG2	22:4:301:CLA:O2A	2.40	0.68
3:C:165:LEU:HD21	22:C:506:CLA:HAB	1.74	0.68
17:R:209:GLU:HB2	25:R:306:CHL:HBC1	1.75	0.68
17:r:209:GLU:HB2	25:r:306:CHL:HBC1	1.75	0.68
20:8:159:LYS:HE3	22:8:301:CLA:HMA2	1.74	0.68
17:R:59:TYR:O	20:8:173:GLU:OE1	2.11	0.68
2:B:214:LEU:HB3	22:r:302:CLA:HED1	1.76	0.68
20:4:175:ALA:HB3	22:4:301:CLA:C2B	2.24	0.68
1:a:288:LEU:HD22	3:c:432:VAL:HG22	1.74	0.68
2:b:214:LEU:HD22	22:R:302:CLA:CGD	2.23	0.68
25:R:304:CHL:HBB2	25:R:305:CHL:HAB	1.76	0.68
12:o:227:PHE:HB2	12:o:287:LEU:HB2	1.75	0.68
19:Y:182:PRO:HD2	25:Y:608:CHL:HBB2	1.76	0.68
20:8:144:SER:O	25:8:302:CHL:HED1	1.94	0.68
17:r:59:TYR:O	20:4:173:GLU:OE1	2.11	0.67
25:r:304:CHL:HBB2	25:r:305:CHL:HAB	1.76	0.67
20:8:175:ALA:HB2	22:8:301:CLA:C2B	2.25	0.67
4:D:280:LEU:HD22	23:D:402:PHO:HBC3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:59:SER:HB3	18:S:267:LEU:CG	2.24	0.67
25:G:606:CHL:HBB2	25:G:607:CHL:HBB1	1.77	0.67
17:R:56:PRO:CD	20:8:174:TRP:HE1	2.07	0.67
25:g:606:CHL:HBB2	25:g:607:CHL:HBB1	1.77	0.67
20:8:175:ALA:HB3	22:8:301:CLA:C2B	2.24	0.67
20:8:159:LYS:HE3	22:8:301:CLA:HMA1	1.61	0.67
3:C:466:VAL:HG21	4:D:249:THR:HA	1.77	0.66
12:O:227:PHE:HB2	12:O:287:LEU:HB2	1.75	0.66
17:r:56:PRO:CD	20:4:174:TRP:HE1	2.07	0.66
19:3:161:ILE:HG12	25:3:306:CHL:HAC1	1.78	0.66
4:d:210:LEU:O	4:d:214:ILE:HB	1.96	0.66
18:s:159:THR:O	18:s:166:ASN:ND2	2.29	0.66
20:4:144:SER:O	25:4:302:CHL:HED1	1.94	0.66
19:y:182:PRO:HD2	25:y:608:CHL:HBB2	1.76	0.66
19:n:182:PRO:HD2	25:n:608:CHL:HBB2	1.77	0.66
20:4:175:ALA:HB2	22:4:301:CLA:C2B	2.25	0.66
3:c:251:HIS:CE1	22:c:506:CLA:NA	2.62	0.66
19:N:182:PRO:HD2	25:N:608:CHL:HBB2	1.77	0.66
18:s:74:GLY:H	22:s:301:CLA:CED	2.07	0.66
4:D:210:LEU:O	4:D:214:ILE:HB	1.96	0.66
17:R:275:LEU:O	22:6:613:CLA:CMB	2.44	0.66
3:C:440:GLY:O	3:C:444:HIS:HB2	1.97	0.65
17:r:275:LEU:O	22:2:613:CLA:CMB	2.44	0.65
19:7:161:ILE:HG12	25:7:306:CHL:HAC1	1.78	0.65
12:o:230:LYS:HG2	12:o:284:GLU:HG2	1.78	0.65
17:r:191:LEU:O	17:r:195:GLU:CB	2.44	0.65
18:s:74:GLY:CA	22:s:301:CLA:HED3	2.26	0.65
18:s:256:LYS:HB3	18:s:264:ASN:HD21	1.62	0.65
20:4:121:ALA:HA	20:4:253:LEU:HD22	1.78	0.65
13:T:5:VAL:O	13:T:9:LEU:HB2	1.97	0.65
19:g:182:PRO:HD2	25:g:608:CHL:HBB2	1.79	0.65
3:C:79:LYS:HB2	3:C:84:GLN:HE21	1.61	0.65
20:8:121:ALA:HA	20:8:253:LEU:HD22	1.78	0.65
13:t:5:VAL:O	13:t:9:LEU:HB2	1.97	0.65
20:8:94:PHE:O	20:8:98:TYR:CB	2.45	0.65
3:c:39:ASN:O	3:c:42:LEU:HB2	1.97	0.65
2:B:111:ALA:O	2:B:115:TRP:HB2	1.96	0.65
2:b:111:ALA:O	2:b:115:TRP:HB2	1.96	0.65
3:c:440:GLY:O	3:c:444:HIS:HB2	1.97	0.65
17:r:275:LEU:O	22:2:613:CLA:HMB3	1.97	0.64
1:a:85:THR:HA	1:a:109:GLY:HA3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:273:TYR:O	2:b:277:GLN:HB2	1.97	0.64
2:B:273:TYR:O	2:B:277:GLN:HB2	1.96	0.64
3:c:289:PHE:O	3:c:293:ASN:HB3	1.98	0.64
17:R:275:LEU:O	22:6:613:CLA:HMB3	1.97	0.64
12:O:230:LYS:HG2	12:O:284:GLU:HG2	1.78	0.64
18:S:159:THR:O	18:S:166:ASN:ND2	2.29	0.64
3:C:39:ASN:O	3:C:42:LEU:HB2	1.97	0.64
20:4:174:TRP:C	22:4:301:CLA:HHC	2.10	0.64
2:B:52:LEU:HD21	2:B:307:GLU:HB3	1.80	0.64
18:S:256:LYS:HB3	18:S:264:ASN:HD21	1.62	0.64
1:A:85:THR:HA	1:A:109:GLY:HA3	1.79	0.64
3:C:227:VAL:HG11	3:C:233:ILE:HD11	1.80	0.64
12:O:138:PHE:HB2	12:O:171:LEU:HB2	1.80	0.64
17:R:61:GLY:CA	20:8:169:SER:HB2	2.26	0.64
17:r:61:GLY:CA	20:4:169:SER:HB2	2.26	0.64
1:a:145:VAL:HG22	3:c:442:LEU:HB3	1.78	0.64
3:c:79:LYS:HB2	3:c:84:GLN:HE21	1.61	0.64
20:4:173:GLU:HG2	22:4:301:CLA:C3B	2.28	0.64
20:8:174:TRP:C	22:8:301:CLA:HHC	2.10	0.64
1:a:334:ARG:HB2	4:d:350:GLY:HA2	1.80	0.63
12:o:138:PHE:HB2	12:o:171:LEU:HB2	1.80	0.63
20:8:173:GLU:HG2	22:8:301:CLA:C3B	2.28	0.63
11:M:27:VAL:HG21	11:m:24:ILE:HG23	1.81	0.63
12:o:213:PHE:HA	12:o:307:GLN:HE22	1.64	0.63
19:2:161:ILE:HG12	25:2:605:CHL:HAC1	1.81	0.63
20:4:94:PHE:O	20:4:98:TYR:CB	2.45	0.63
3:c:227:VAL:HG11	3:c:233:ILE:HD11	1.80	0.63
19:G:182:PRO:HD2	25:G:608:CHL:HBB2	1.79	0.63
2:b:329:SER:H	2:b:332:ASN:HD22	1.46	0.63
12:o:216:LYS:H	12:o:231:PHE:HB2	1.63	0.63
4:D:181:ARG:NH2	4:D:334:ASP:OD1	2.32	0.63
2:b:52:LEU:HD21	2:b:307:GLU:HB3	1.80	0.62
3:C:251:HIS:CE1	22:C:506:CLA:NA	2.67	0.62
3:C:345:PRO:HB3	12:O:166:ARG:HE	1.63	0.62
4:d:181:ARG:NH2	4:d:334:ASP:OD1	2.31	0.62
19:6:179:GLY:HA2	25:6:607:CHL:HMC	1.81	0.62
20:8:162:VAL:CG2	22:8:301:CLA:O2A	2.40	0.62
3:C:459:ILE:H	4:D:224:PHE:HA	1.65	0.62
3:c:131:TYR:HH	18:s:74:GLY:HA3	1.63	0.62
19:6:161:ILE:HG12	25:6:605:CHL:HAC1	1.81	0.62
2:b:336:ILE:HB	2:b:433:ASP:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:o:202:GLN:HE21	12:o:206:GLY:HA2	1.65	0.62
17:r:73:VAL:HB	17:r:137:ARG:HH12	1.64	0.62
2:B:357:ARG:NH2	4:D:338:GLU:OE1	2.33	0.62
12:O:216:LYS:H	12:O:231:PHE:HB2	1.63	0.62
3:c:165:LEU:HD21	22:c:506:CLA:HAB	1.81	0.62
17:r:275:LEU:O	22:2:613:CLA:HBB1	2.00	0.62
1:a:97:TRP:HA	8:i:1:MET:HE2	1.82	0.62
17:R:191:LEU:O	17:R:195:GLU:CB	2.44	0.62
3:C:289:PHE:O	3:C:293:ASN:HB3	1.98	0.62
16:Z:37:LYS:O	16:Z:41:PHE:CB	2.47	0.62
1:A:133:LEU:HD23	4:D:257:ILE:HG12	1.82	0.62
2:b:41:GLU:O	2:b:45:PHE:HB2	2.00	0.62
3:c:132:HIS:CE1	22:s:301:CLA:NA	2.67	0.62
17:R:275:LEU:O	22:6:613:CLA:HBB1	2.00	0.62
12:O:213:PHE:HA	12:O:307:GLN:HE22	1.64	0.62
16:z:37:LYS:O	16:z:41:PHE:CB	2.48	0.62
17:R:73:VAL:HB	17:R:137:ARG:HH12	1.64	0.62
2:B:41:GLU:O	2:B:45:PHE:HB2	2.00	0.61
3:C:282:CYS:O	3:C:286:ALA:HB2	2.00	0.61
19:2:179:GLY:HA2	25:2:607:CHL:HMC	1.81	0.61
12:O:202:GLN:HE21	12:O:206:GLY:HA2	1.64	0.61
3:c:282:CYS:O	3:c:286:ALA:HB2	2.00	0.61
2:B:254:GLY:O	2:B:258:TYR:HB2	2.01	0.61
3:C:349:VAL:H	3:C:374:GLY:HA3	1.65	0.61
18:S:192:ASN:HB3	18:S:196:PHE:HB2	1.83	0.61
3:c:150:VAL:HG13	3:c:152:LYS:H	1.66	0.61
3:C:75:PHE:O	9:K:25:LYS:NZ	2.33	0.61
10:L:16:THR:O	10:L:20:TRP:HB3	2.01	0.61
3:c:251:HIS:HE1	22:c:506:CLA:NA	1.99	0.61
20:4:175:ALA:HB3	22:4:301:CLA:CMB	2.31	0.61
3:c:349:VAL:H	3:c:374:GLY:HA3	1.65	0.61
19:1:182:PRO:HD2	25:1:608:CHL:HBB2	1.82	0.61
2:B:329:SER:H	2:B:332:ASN:HD22	1.46	0.61
2:b:254:GLY:O	2:b:258:TYR:HB2	2.01	0.61
4:d:280:LEU:HD22	23:d:402:PHO:HBC3	1.81	0.61
2:B:208:LEU:HD12	22:B:602:CLA:HAC2	1.83	0.61
19:G:82:THR:HG21	25:Y:609:CHL:HAA1	1.83	0.61
20:4:173:GLU:C	22:4:301:CLA:C3B	2.74	0.61
3:C:150:VAL:HG13	3:C:152:LYS:H	1.66	0.61
3:c:160:ILE:HD13	22:c:512:CLA:HAC2	1.83	0.61
19:1:103:SER:HB3	19:1:219:GLY:HA3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:ILE:HB	2:B:433:ASP:HB3	1.81	0.60
1:a:317:TRP:HE3	4:d:181:ARG:HD3	1.66	0.60
2:B:347:ARG:O	2:B:397:VAL:HA	2.02	0.60
3:C:444:HIS:CE1	22:C:508:CLA:NA	2.69	0.60
20:8:175:ALA:HB3	22:8:301:CLA:CMB	2.31	0.60
3:c:441:HIS:O	3:c:445:ALA:HB3	2.01	0.60
25:S:306:CHL:HBA1	25:S:306:CHL:HBD	1.83	0.60
19:3:103:SER:HB3	19:3:219:GLY:HA3	1.83	0.60
3:c:206:PRO:HG3	22:y:614:CLA:HBB2	1.82	0.60
20:8:173:GLU:C	22:8:301:CLA:C3B	2.74	0.60
12:o:107:GLY:HA3	14:w:90:THR:HG22	1.83	0.60
3:c:131:TYR:OH	18:s:74:GLY:CA	2.46	0.60
17:r:72:LEU:HD13	17:r:137:ARG:HD2	1.84	0.60
3:c:361:LEU:O	3:c:370:ARG:NH2	2.35	0.60
18:s:192:ASN:HB3	18:s:196:PHE:HB2	1.83	0.60
19:5:103:SER:HB3	19:5:219:GLY:HA3	1.83	0.60
3:C:361:LEU:O	3:C:370:ARG:NH2	2.35	0.60
2:b:347:ARG:O	2:b:397:VAL:HA	2.02	0.60
19:6:229:PHE:O	19:6:233:ALA:HB3	2.02	0.60
13:T:19:PHE:O	13:T:23:PHE:HB2	2.02	0.60
19:n:94:ARG:NH1	19:y:81:ASP:O	2.35	0.60
3:C:441:HIS:O	3:C:445:ALA:HB3	2.01	0.60
10:l:16:THR:O	10:l:20:TRP:HB3	2.01	0.60
13:t:19:PHE:O	13:t:23:PHE:HB2	2.02	0.60
3:c:444:HIS:CE1	22:c:508:CLA:NA	2.70	0.60
17:r:275:LEU:HB3	22:2:613:CLA:CMB	2.32	0.60
18:s:242:GLN:OE1	22:s:313:CLA:ND	2.35	0.60
19:3:229:PHE:O	19:3:233:ALA:HB3	2.02	0.60
19:7:103:SER:HB3	19:7:219:GLY:HA3	1.83	0.60
16:Z:59:SER:CB	18:S:267:LEU:CG	2.74	0.59
25:s:306:CHL:HBD	25:s:306:CHL:HBA1	1.83	0.59
19:g:82:THR:HG21	25:y:609:CHL:HAA1	1.83	0.59
17:R:275:LEU:HB3	22:6:613:CLA:CMB	2.32	0.59
19:2:229:PHE:O	19:2:233:ALA:HB3	2.02	0.59
19:6:103:SER:HB3	19:6:219:GLY:HA3	1.83	0.59
17:R:72:LEU:HD13	17:R:137:ARG:HD2	1.84	0.59
19:2:103:SER:HB3	19:2:219:GLY:HA3	1.83	0.59
20:4:173:GLU:O	22:4:301:CLA:C3B	2.50	0.59
19:5:182:PRO:HD2	25:5:608:CHL:HBB2	1.82	0.59
19:7:229:PHE:O	19:7:233:ALA:HB3	2.02	0.59
3:C:25:GLY:O	3:C:41:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:25:GLY:O	3:c:41:ARG:NH1	2.35	0.59
20:8:159:LYS:CE	22:8:301:CLA:HMA2	2.32	0.59
20:8:173:GLU:O	22:8:301:CLA:C3B	2.50	0.59
2:B:227:LYS:O	2:B:230:ARG:NH1	2.36	0.59
2:b:256:MET:HA	2:b:263:THR:HG21	1.85	0.59
19:N:94:ARG:NH1	19:Y:81:ASP:O	2.35	0.59
20:8:175:ALA:HB3	22:8:301:CLA:HMB1	1.84	0.59
20:4:171:SER:HA	20:4:179:SER:HB2	1.83	0.59
2:B:256:MET:HA	2:B:263:THR:HG21	1.85	0.59
18:S:176:VAL:O	18:S:180:VAL:HB	2.03	0.59
19:1:229:PHE:O	19:1:233:ALA:HB3	2.02	0.59
18:S:242:GLN:OE1	22:S:313:CLA:ND	2.35	0.59
19:5:229:PHE:O	19:5:233:ALA:HB3	2.02	0.59
3:c:43:ILE:HG12	22:c:509:CLA:HAC2	1.85	0.58
3:c:76:VAL:O	3:c:84:GLN:NE2	2.36	0.58
4:d:327:ARG:O	4:d:331:ALA:CB	2.51	0.58
3:C:76:VAL:O	3:C:84:GLN:NE2	2.36	0.58
2:b:214:LEU:HB3	22:R:302:CLA:HED2	1.72	0.58
3:c:118:HIS:CE1	22:c:502:CLA:NA	2.71	0.58
19:1:78:TYR:OH	19:1:217:LYS:NZ	2.36	0.58
19:3:78:TYR:OH	19:3:217:LYS:NZ	2.36	0.58
4:D:21:ASP:OD1	4:D:24:ARG:NH2	2.37	0.58
2:b:227:LYS:O	2:b:230:ARG:NH1	2.36	0.58
4:d:21:ASP:OD1	4:d:24:ARG:NH2	2.37	0.58
19:2:78:TYR:OH	19:2:217:LYS:NZ	2.36	0.58
19:6:78:TYR:OH	19:6:217:LYS:NZ	2.36	0.58
3:c:276:LEU:HD21	22:c:508:CLA:HAB	1.84	0.58
17:R:285:ASP:CB	20:8:141:SER:OG	2.40	0.58
18:s:176:VAL:O	18:s:180:VAL:HB	2.03	0.58
20:8:171:SER:HA	20:8:179:SER:HB2	1.83	0.58
2:B:79:ASN:H	2:B:83:GLY:H	1.52	0.58
3:C:33:PHE:O	3:C:41:ARG:NH2	2.30	0.58
4:D:217:ALA:O	4:D:221:ASN:HB2	2.03	0.58
16:Z:60:LEU:HD21	18:S:270:ILE:HG22	1.85	0.58
17:r:152:LEU:O	17:r:156:SER:HB3	2.04	0.58
19:g:67:PRO:HG2	19:g:70:LEU:HD12	1.86	0.58
20:4:175:ALA:HB2	22:4:301:CLA:C4B	2.33	0.58
19:7:161:ILE:O	19:7:165:GLN:HB2	2.04	0.58
2:B:368:VAL:HB	2:B:381:VAL:HB	1.84	0.58
4:D:327:ARG:O	4:D:331:ALA:CB	2.51	0.58
2:b:368:VAL:HB	2:b:381:VAL:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:83:GLU:OE2	3:c:398:HIS:NE2	2.37	0.58
17:R:280:HIS:HA	20:8:141:SER:H	0.61	0.58
18:S:71:LEU:HB2	18:S:75:LEU:HD22	1.86	0.58
20:8:175:ALA:HB2	22:8:301:CLA:C4B	2.33	0.58
1:A:307:VAL:HG22	1:A:313:VAL:HG22	1.86	0.58
3:C:307:PRO:HB2	3:C:361:LEU:HD13	1.86	0.58
1:a:307:VAL:HG22	1:a:313:VAL:HG22	1.86	0.58
4:d:217:ALA:O	4:d:221:ASN:HB2	2.03	0.58
17:R:152:LEU:O	17:R:156:SER:HB3	2.04	0.58
19:5:161:ILE:O	19:5:165:GLN:HB2	2.04	0.58
19:7:78:TYR:OH	19:7:217:LYS:NZ	2.36	0.58
3:c:297:TYR:O	3:c:423:ARG:NH2	2.35	0.57
19:6:161:ILE:O	19:6:165:GLN:HB2	2.04	0.57
3:C:131:TYR:O	3:C:136:GLY:N	2.36	0.57
2:b:158:VAL:HG22	2:b:166:ILE:HD11	1.86	0.57
3:c:365:TRP:HB2	3:c:388:GLN:HG2	1.86	0.57
19:3:161:ILE:O	19:3:165:GLN:HB2	2.04	0.57
1:A:225:ARG:NH2	2:B:477:ASP:O	2.37	0.57
16:Z:59:SER:HB3	18:S:267:LEU:HD23	0.58	0.57
1:A:245:THR:OG1	4:D:266:ARG:NH2	2.37	0.57
19:1:161:ILE:O	19:1:165:GLN:HB2	2.04	0.57
19:5:78:TYR:OH	19:5:217:LYS:NZ	2.36	0.57
4:D:36:LEU:HD21	15:X:104:VAL:HG11	1.86	0.57
17:r:236:ALA:O	17:r:240:LEU:HB2	2.05	0.57
1:A:225:ARG:HH21	2:B:478:VAL:HA	1.70	0.57
3:C:83:GLU:OE2	3:C:398:HIS:NE2	2.37	0.57
3:C:365:TRP:HB2	3:C:388:GLN:HG2	1.86	0.57
2:b:474:LEU:O	4:d:135:ARG:NH1	2.38	0.57
1:A:317:TRP:HE1	4:D:66:SER:HB3	1.70	0.57
3:C:346:THR:OG1	3:C:348:GLU:OE1	2.23	0.57
3:c:131:TYR:O	3:c:136:GLY:N	2.36	0.57
18:s:250:PRO:O	18:s:254:LEU:CB	2.53	0.57
2:B:158:VAL:HG22	2:B:166:ILE:HD11	1.86	0.57
2:b:79:ASN:H	2:b:83:GLY:H	1.52	0.57
17:R:267:PRO:O	17:R:271:TRP:CB	2.53	0.57
25:6:606:CHL:HBB2	25:7:301:CHL:HBB1	1.87	0.57
3:C:441:HIS:O	3:C:445:ALA:CB	2.53	0.56
17:r:62:ALA:CA	20:4:172:VAL:HG21	2.35	0.56
19:2:161:ILE:O	19:2:165:GLN:HB2	2.04	0.56
3:c:307:PRO:HB2	3:c:361:LEU:HD13	1.86	0.56
19:1:100:VAL:HG22	19:1:216:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:175:ALA:HB3	22:4:301:CLA:HMB2	1.87	0.56
1:a:217:SER:O	1:a:221:SER:CB	2.54	0.56
2:b:355:PHE:O	2:b:370:LEU:HA	2.04	0.56
17:r:267:PRO:O	17:r:271:TRP:CB	2.53	0.56
18:s:71:LEU:HB2	18:s:75:LEU:HD22	1.86	0.56
19:n:67:PRO:HG2	19:n:70:LEU:HD12	1.86	0.56
19:2:100:VAL:HG22	19:2:216:LEU:HD21	1.88	0.56
19:6:104:ARG:NH1	25:6:607:CHL:OBD	2.38	0.56
3:C:132:HIS:CE1	22:S:301:CLA:NA	2.74	0.56
5:E:19:TYR:O	5:E:23:HIS:ND1	2.39	0.56
2:b:41:GLU:O	2:b:45:PHE:CB	2.54	0.56
18:S:250:PRO:O	18:S:254:LEU:CB	2.53	0.56
19:G:67:PRO:HG2	19:G:70:LEU:HD12	1.86	0.56
19:Y:67:PRO:HG2	19:Y:70:LEU:HD12	1.86	0.56
2:B:355:PHE:O	2:B:370:LEU:HA	2.04	0.56
14:W:97:SER:H	14:W:101:LEU:HD22	1.71	0.56
19:N:67:PRO:HG2	19:N:70:LEU:HD12	1.86	0.56
2:B:384:ARG:HH21	4:D:345:GLU:HA	1.70	0.56
1:a:53:ILE:HG12	1:a:71:LEU:HD12	1.88	0.56
4:d:59:TRP:CE2	5:e:64:PRO:HG3	2.40	0.56
18:S:113:PHE:O	18:S:117:HIS:HB2	2.06	0.56
19:Y:179:GLY:HA3	19:Y:186:ALA:HB2	1.87	0.56
18:s:74:GLY:HA3	22:s:301:CLA:CED	2.33	0.56
19:n:179:GLY:HA3	19:n:186:ALA:HB2	1.87	0.56
19:y:179:GLY:HA3	19:y:186:ALA:HB2	1.87	0.56
3:C:297:TYR:O	3:C:423:ARG:NH2	2.35	0.56
12:o:293:LYS:HD3	12:o:298:GLU:HB2	1.88	0.56
17:R:62:ALA:CA	20:8:172:VAL:HG21	2.35	0.56
19:N:179:GLY:HA3	19:N:186:ALA:HB2	1.87	0.56
25:2:608:CHL:HAA1	19:3:82:THR:HG21	1.88	0.56
20:8:148:THR:HG1	25:8:302:CHL:HED1	1.53	0.56
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.87	0.56
1:a:234:ASN:O	4:d:264:ASN:ND2	2.38	0.56
14:w:97:SER:H	14:w:101:LEU:HD22	1.71	0.56
3:c:441:HIS:O	3:c:445:ALA:CB	2.53	0.56
19:n:176:ARG:NH1	25:n:608:CHL:O1D	2.39	0.56
19:y:67:PRO:HG2	19:y:70:LEU:HD12	1.86	0.56
1:A:53:ILE:HG12	1:A:71:LEU:HD12	1.88	0.56
3:C:148:GLY:O	3:C:156:LYS:NZ	2.39	0.56
3:C:256:PRO:O	3:C:261:ARG:NH1	2.39	0.56
12:o:298:GLU:HG2	12:o:330:GLN:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:236:ALA:O	17:R:240:LEU:HB2	2.05	0.56
18:s:68:ARG:HH11	25:s:302:CHL:HBC1	1.71	0.56
19:g:179:GLY:HA3	19:g:186:ALA:HB2	1.87	0.56
2:B:321:LYS:NZ	2:B:363:PHE:O	2.39	0.56
17:r:63:ILE:HG13	20:4:166:ASN:ND2	2.21	0.56
2:B:167:TRP:HA	2:B:177:LYS:O	2.07	0.55
7:H:20:GLY:O	7:H:24:LYS:HB2	2.06	0.55
2:b:167:TRP:HA	2:b:177:LYS:O	2.06	0.55
10:l:15:ARG:NH2	11:m:26:TYR:OH	2.38	0.55
17:r:275:LEU:HB3	22:2:613:CLA:HMB3	1.87	0.55
19:n:103:SER:HB3	19:n:219:GLY:HA3	1.88	0.55
1:A:56:PRO:HB2	12:O:208:ARG:HH22	1.71	0.55
12:O:293:LYS:HD3	12:O:298:GLU:HB2	1.88	0.55
17:R:168:ALA:O	17:R:172:GLU:HB2	2.06	0.55
25:6:608:CHL:HAA1	19:7:82:THR:HG21	1.88	0.55
7:H:39:THR:HG22	7:H:42:LEU:HB3	1.89	0.55
3:c:148:GLY:O	3:c:156:LYS:NZ	2.39	0.55
1:A:217:SER:O	1:A:221:SER:CB	2.54	0.55
3:C:187:ASP:O	3:C:194:GLY:HA2	2.06	0.55
1:a:225:ARG:NH2	2:b:477:ASP:O	2.40	0.55
2:b:321:LYS:NZ	2:b:363:PHE:O	2.39	0.55
18:S:68:ARG:HH11	25:S:302:CHL:HBC1	1.71	0.55
18:s:74:GLY:N	22:s:301:CLA:HED1	2.14	0.55
18:s:113:PHE:O	18:s:117:HIS:HB2	2.06	0.55
25:n:606:CHL:HBB2	25:n:607:CHL:HBB1	1.88	0.55
19:5:100:VAL:HG22	19:5:216:LEU:HD21	1.88	0.55
1:A:150:PRO:HD3	23:A:404:PHO:HBC2	1.89	0.55
1:a:217:SER:O	1:a:221:SER:HB2	2.06	0.55
3:c:33:PHE:O	3:c:41:ARG:NH2	2.30	0.55
25:2:606:CHL:HBB2	25:3:301:CHL:HBB1	1.87	0.55
19:6:100:VAL:HG22	19:6:216:LEU:HD21	1.88	0.55
19:7:100:VAL:HG22	19:7:216:LEU:HD21	1.88	0.55
11:M:22:LEU:HD23	11:M:25:ILE:HD12	1.89	0.55
17:R:63:ILE:HG13	20:8:166:ASN:ND2	2.21	0.55
19:3:100:VAL:HG22	19:3:216:LEU:HD21	1.88	0.55
19:7:67:PRO:HG2	19:7:70:LEU:HD12	1.89	0.55
2:B:41:GLU:O	2:B:45:PHE:CB	2.54	0.55
16:Z:8:ALA:O	16:Z:12:LEU:HB2	2.07	0.55
7:h:20:GLY:O	7:h:24:LYS:HB2	2.06	0.55
17:R:58:TRP:C	20:8:173:GLU:CG	2.77	0.55
19:G:179:GLY:HA3	19:G:186:ALA:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:344:SER:OG	3:C:348:GLU:N	2.40	0.55
16:z:8:ALA:O	16:z:12:LEU:HB2	2.07	0.55
17:r:168:ALA:O	17:r:172:GLU:HB2	2.06	0.55
19:5:67:PRO:HG2	19:5:70:LEU:HD12	1.89	0.55
1:A:217:SER:O	1:A:221:SER:HB2	2.07	0.55
14:W:93:PRO:HB2	14:W:96:LEU:HB2	1.88	0.55
14:W:99:ASN:ND2	19:Y:122:ASN:O	2.40	0.55
1:a:48:PHE:O	1:a:52:PHE:CB	2.55	0.55
11:m:22:LEU:HD23	11:m:25:ILE:HD12	1.89	0.55
14:w:93:PRO:HB2	14:w:96:LEU:HB2	1.88	0.55
3:c:346:THR:OG1	3:c:348:GLU:OE1	2.23	0.55
17:R:275:LEU:HB3	22:6:613:CLA:HMB3	1.87	0.55
18:S:218:GLY:O	18:S:222:LYS:HB2	2.07	0.55
19:N:176:ARG:NH1	25:N:608:CHL:O1D	2.39	0.55
19:y:229:PHE:O	19:y:233:ALA:CB	2.55	0.55
12:O:298:GLU:HG2	12:O:330:GLN:HG2	1.88	0.55
4:d:297:TYR:O	4:d:316:TYR:OH	2.25	0.55
3:c:256:PRO:O	3:c:261:ARG:NH1	2.39	0.55
17:R:63:ILE:HD11	20:8:166:ASN:ND2	2.22	0.55
19:g:229:PHE:O	19:g:233:ALA:CB	2.55	0.55
19:n:229:PHE:O	19:n:233:ALA:CB	2.55	0.55
2:B:8:VAL:HG12	10:L:11:VAL:HG21	1.89	0.54
4:D:259:GLY:O	13:T:24:ARG:NH1	2.40	0.54
17:r:280:HIS:HA	20:4:141:SER:H	0.61	0.54
7:h:39:THR:HG22	7:h:42:LEU:HB3	1.89	0.54
25:G:601:CHL:HED3	25:G:601:CHL:HBA1	1.89	0.54
19:g:103:SER:HB3	19:g:219:GLY:HA3	1.88	0.54
4:D:297:TYR:O	4:D:316:TYR:OH	2.25	0.54
19:2:67:PRO:HG2	19:2:70:LEU:HD12	1.89	0.54
19:2:104:ARG:NH1	25:2:607:CHL:OBD	2.38	0.54
19:2:229:PHE:O	19:2:233:ALA:CB	2.56	0.54
19:5:229:PHE:O	19:5:233:ALA:CB	2.56	0.54
4:D:195:ASN:HD21	4:D:286:GLY:HA3	1.73	0.54
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.87	0.54
3:c:456:GLU:HG2	3:c:457:LYS:HD2	1.90	0.54
19:N:246:ASP:O	19:N:254:ASN:ND2	2.40	0.54
19:3:179:GLY:HA2	25:3:308:CHL:HMC	1.89	0.54
25:N:606:CHL:HBB2	25:N:607:CHL:HBB1	1.88	0.54
18:s:218:GLY:O	18:s:222:LYS:HB2	2.07	0.54
19:3:67:PRO:HG2	19:3:70:LEU:HD12	1.89	0.54
1:A:238:ARG:NH1	1:A:239:PHE:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:195:ASN:HD21	4:d:286:GLY:HA3	1.73	0.54
18:S:119:ARG:NH1	25:S:308:CHL:OBD	2.41	0.54
19:Y:103:SER:HB3	19:Y:219:GLY:HA3	1.88	0.54
19:Y:229:PHE:O	19:Y:233:ALA:CB	2.55	0.54
2:B:162:TYR:HD2	22:B:606:CLA:HAC2	1.73	0.54
4:D:337:HIS:HA	5:E:65:LEU:HD21	1.90	0.54
12:O:136:PHE:HA	12:O:329:GLY:HA2	1.90	0.54
4:d:330:MET:O	4:d:334:ASP:CB	2.56	0.54
3:c:187:ASP:O	3:c:194:GLY:HA2	2.06	0.54
19:G:103:SER:HB3	19:G:219:GLY:HA3	1.88	0.54
19:N:103:SER:HB3	19:N:219:GLY:HA3	1.88	0.54
19:N:228:GLY:O	19:N:232:GLN:HB3	2.08	0.54
19:3:229:PHE:O	19:3:233:ALA:CB	2.56	0.54
19:6:182:PRO:HD2	25:6:607:CHL:HBB2	1.89	0.54
17:R:280:HIS:CE1	20:8:138:ALA:C	2.85	0.54
19:g:228:GLY:O	19:g:232:GLN:HB3	2.08	0.54
19:3:75:PRO:HB3	19:3:213:VAL:HG22	1.90	0.54
20:4:95:LEU:O	20:4:99:ARG:CB	2.56	0.54
20:8:252:PRO:O	20:8:256:LEU:HB3	2.07	0.54
3:C:456:GLU:HG2	3:C:457:LYS:HD2	1.90	0.54
1:a:238:ARG:NH1	1:a:239:PHE:O	2.40	0.54
17:r:63:ILE:HD11	20:4:166:ASN:ND2	2.22	0.54
18:s:73:ASP:HB3	22:s:301:CLA:HED1	1.89	0.54
19:7:229:PHE:O	19:7:233:ALA:CB	2.56	0.54
2:B:153:PHE:HB2	22:B:606:CLA:HAB	1.89	0.54
1:a:103:ASP:O	1:a:107:TYR:HB2	2.08	0.54
3:c:344:SER:OG	3:c:348:GLU:N	2.40	0.54
17:R:58:TRP:O	20:8:173:GLU:CG	2.55	0.54
19:N:229:PHE:O	19:N:233:ALA:CB	2.55	0.54
18:s:119:ARG:NH1	25:s:308:CHL:OBD	2.41	0.54
19:2:182:PRO:HD2	25:2:607:CHL:HBB2	1.89	0.54
19:6:67:PRO:HG2	19:6:70:LEU:HD12	1.89	0.54
19:6:229:PHE:O	19:6:233:ALA:CB	2.56	0.54
19:7:176:ARG:HH22	25:7:308:CHL:HED2	1.73	0.54
2:B:122:ILE:HG12	7:H:24:LYS:HA	1.90	0.53
19:G:229:PHE:O	19:G:233:ALA:CB	2.55	0.53
19:y:103:SER:HB3	19:y:219:GLY:HA3	1.88	0.53
19:3:176:ARG:HH22	25:3:308:CHL:HED2	1.73	0.53
2:B:73:ASN:HB3	2:B:88:PRO:HB3	1.89	0.53
3:C:87:ILE:O	3:C:91:HIS:ND1	2.38	0.53
1:a:23:SER:OG	1:a:24:THR:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:73:ASN:HB3	2:b:88:PRO:HB3	1.89	0.53
19:G:228:GLY:O	19:G:232:GLN:HB3	2.08	0.53
25:G:601:CHL:O1A	25:G:601:CHL:HBD	2.09	0.53
19:Y:228:GLY:O	19:Y:232:GLN:HB3	2.08	0.53
19:7:75:PRO:HB3	19:7:213:VAL:HG22	1.90	0.53
3:C:230:LEU:HA	3:C:233:ILE:HB	1.90	0.53
3:c:230:LEU:HA	3:c:233:ILE:HB	1.90	0.53
25:N:606:CHL:HBC2	25:N:607:CHL:HAC2	1.90	0.53
19:Y:247:HIS:NE2	22:Y:614:CLA:ND	2.56	0.53
19:g:99:GLU:OE2	19:g:220:ARG:NE	2.33	0.53
25:g:601:CHL:O1A	25:g:601:CHL:HBD	2.09	0.53
20:8:91:ASP:HB2	20:8:94:PHE:HD2	1.73	0.53
17:r:58:TRP:C	20:4:173:GLU:CG	2.77	0.53
19:y:228:GLY:O	19:y:232:GLN:HB3	2.08	0.53
19:1:75:PRO:HB3	19:1:213:VAL:HG22	1.90	0.53
19:1:229:PHE:O	19:1:233:ALA:CB	2.56	0.53
1:A:103:ASP:O	1:A:107:TYR:HB2	2.08	0.53
2:B:299:SER:O	2:B:303:ALA:HB2	2.09	0.53
3:C:160:ILE:HD13	22:C:512:CLA:HAC2	1.89	0.53
3:C:303:GLY:O	3:C:423:ARG:NE	2.37	0.53
4:d:34:SER:O	4:d:38:LEU:HB3	2.08	0.53
12:o:312:ASP:HB3	12:o:315:ALA:HB3	1.90	0.53
17:r:278:PRO:HG2	22:2:613:CLA:HBB2	1.90	0.53
19:1:67:PRO:HG2	19:1:70:LEU:HD12	1.89	0.53
19:7:179:GLY:HA2	25:7:308:CHL:HMC	1.89	0.53
4:D:189:PHE:HE1	4:D:327:ARG:HA	1.74	0.53
25:n:606:CHL:HBC2	25:n:607:CHL:HAC2	1.90	0.53
19:6:75:PRO:HB3	19:6:213:VAL:HG22	1.90	0.53
3:C:43:ILE:HG12	22:C:509:CLA:HAC2	1.91	0.53
4:D:34:SER:O	4:D:38:LEU:HB3	2.08	0.53
4:D:302:GLN:O	4:D:306:ALA:CB	2.57	0.53
19:5:75:PRO:HB3	19:5:213:VAL:HG22	1.90	0.53
17:r:58:TRP:O	20:4:173:GLU:CG	2.55	0.53
17:r:285:ASP:CB	20:4:141:SER:OG	2.40	0.53
20:4:91:ASP:HB2	20:4:94:PHE:HD2	1.73	0.53
20:4:252:PRO:O	20:4:256:LEU:HB3	2.07	0.53
20:8:153:MET:HE2	25:8:309:CHL:HBC3	1.91	0.53
2:B:281:GLN:O	2:B:285:TYR:HB3	2.09	0.53
3:C:178:LYS:NZ	3:C:182:PHE:O	2.42	0.53
17:R:256:PHE:O	17:R:260:ALA:HB3	2.09	0.53
18:s:178:GLU:O	18:s:182:LEU:CB	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:n:228:GLY:O	19:n:232:GLN:HB3	2.08	0.53
19:y:99:GLU:OE2	19:y:220:ARG:NE	2.33	0.53
19:y:247:HIS:NE2	22:y:614:CLA:ND	2.56	0.53
20:4:153:MET:HE2	25:4:309:CHL:HBC3	1.91	0.53
3:C:130:ILE:HA	3:C:134:LEU:HD13	1.91	0.53
12:o:136:PHE:HA	12:o:329:GLY:HA2	1.90	0.53
3:c:303:GLY:O	3:c:423:ARG:NE	2.37	0.53
25:g:601:CHL:HED3	25:g:601:CHL:HBA1	1.89	0.53
2:B:216:HIS:CE1	22:B:609:CLA:NA	2.76	0.52
2:B:225:LEU:O	2:B:229:LEU:HB2	2.09	0.52
12:O:312:ASP:HB3	12:O:315:ALA:HB3	1.90	0.52
3:c:45:LEU:O	3:c:49:LEU:HB2	2.10	0.52
2:B:201:HIS:CE1	22:B:602:CLA:ND	2.77	0.52
10:L:30:VAL:HG22	13:T:9:LEU:HG	1.90	0.52
2:b:299:SER:O	2:b:303:ALA:HB2	2.09	0.52
12:o:122:GLU:HG2	12:o:291:LYS:HG2	1.90	0.52
17:r:284:ILE:CG1	20:4:146:LEU:H	2.21	0.52
12:O:122:GLU:HG2	12:O:291:LYS:HG2	1.90	0.52
12:o:312:ASP:HB2	12:o:316:LYS:HG2	1.91	0.52
3:c:289:PHE:O	3:c:293:ASN:CB	2.58	0.52
17:r:256:PHE:O	17:r:260:ALA:HB3	2.09	0.52
19:y:246:ASP:O	19:y:254:ASN:ND2	2.40	0.52
2:B:111:ALA:O	2:B:115:TRP:CB	2.56	0.52
12:O:312:ASP:HB2	12:O:316:LYS:HG2	1.91	0.52
2:b:281:GLN:O	2:b:285:TYR:HB3	2.09	0.52
20:8:174:TRP:O	22:8:301:CLA:C4B	2.42	0.52
1:A:279:PRO:HG2	4:D:213:ALA:HB2	1.91	0.52
3:C:45:LEU:O	3:C:49:LEU:HB2	2.10	0.52
3:C:212:TYR:HB3	3:C:224:ILE:HG22	1.91	0.52
4:D:255:SER:HB3	13:T:24:ARG:HH22	1.73	0.52
5:E:33:ALA:O	5:E:37:PHE:CB	2.58	0.52
2:b:197:GLY:O	2:b:201:HIS:CB	2.58	0.52
19:2:98:LEU:O	19:2:102:HIS:ND1	2.42	0.52
20:8:95:LEU:O	20:8:99:ARG:CB	2.56	0.52
1:a:93:PHE:HB2	3:c:218:PHE:CG	2.45	0.52
3:c:130:ILE:HA	3:c:134:LEU:HD13	1.91	0.52
3:c:250:TRP:O	3:c:254:THR:OG1	2.25	0.52
19:2:75:PRO:HB3	19:2:213:VAL:HG22	1.90	0.52
20:8:68:LEU:HB3	20:8:71:GLU:HB2	1.92	0.52
16:z:60:LEU:HD23	18:s:270:ILE:CG2	2.28	0.52
3:c:349:VAL:HB	3:c:375:LEU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:n:176:ARG:HH22	25:n:608:CHL:HED2	1.75	0.52
2:B:400:GLU:HA	2:B:410:SER:HA	1.92	0.52
4:D:262:PHE:HB2	4:D:268:LEU:HD12	1.91	0.52
4:D:330:MET:O	4:D:334:ASP:CB	2.56	0.52
2:b:111:ALA:O	2:b:115:TRP:CB	2.56	0.52
3:c:178:LYS:NZ	3:c:182:PHE:O	2.42	0.52
17:r:56:PRO:CA	20:4:174:TRP:CD1	2.93	0.52
2:B:193:PHE:HA	2:B:261:ALA:HB2	1.91	0.52
2:b:400:GLU:HA	2:b:410:SER:HA	1.92	0.52
4:d:262:PHE:HB2	4:d:268:LEU:HD12	1.92	0.52
5:e:19:TYR:O	5:e:23:HIS:ND1	2.39	0.52
19:G:246:ASP:O	19:G:254:ASN:ND2	2.40	0.52
3:C:118:HIS:CE1	22:C:502:CLA:NA	2.78	0.52
4:D:148:SER:HA	4:D:151:ILE:HD12	1.91	0.52
12:O:140:PRO:HD2	12:O:170:THR:HG22	1.92	0.52
1:a:245:THR:OG1	4:d:266:ARG:NH2	2.43	0.52
10:l:13:LEU:HD23	10:l:14:ASN:H	1.76	0.52
3:c:162:GLY:HA3	3:c:252:ILE:HG13	1.92	0.52
3:c:215:LYS:NZ	3:c:226:SER:OG	2.42	0.52
17:R:63:ILE:CD1	20:8:166:ASN:ND2	2.73	0.52
19:n:78:TYR:OH	19:n:217:LYS:NZ	2.43	0.52
20:8:173:GLU:CG	22:8:301:CLA:C4B	2.71	0.52
18:S:167:ILE:HD12	18:S:169:ILE:HG12	1.91	0.51
19:g:78:TYR:OH	19:g:217:LYS:NZ	2.43	0.51
19:1:176:ARG:NH1	25:1:608:CHL:O1D	2.43	0.51
3:C:349:VAL:HB	3:C:375:LEU:H	1.74	0.51
3:C:447:ARG:O	3:C:451:ALA:HB2	2.10	0.51
4:d:189:PHE:HE1	4:d:327:ARG:HA	1.74	0.51
4:d:302:GLN:O	4:d:306:ALA:CB	2.57	0.51
3:c:212:TYR:HB3	3:c:224:ILE:HG22	1.91	0.51
17:R:56:PRO:CA	20:8:174:TRP:CD1	2.93	0.51
17:R:62:ALA:CA	20:8:172:VAL:CG2	2.88	0.51
19:5:176:ARG:NH1	25:5:608:CHL:O1D	2.43	0.51
2:B:197:GLY:O	2:B:201:HIS:CB	2.58	0.51
2:b:161:LEU:CD2	25:R:305:CHL:HMD2	2.39	0.51
19:Y:78:TYR:OH	19:Y:217:LYS:NZ	2.43	0.51
17:r:63:ILE:CD1	20:4:166:ASN:ND2	2.73	0.51
18:s:167:ILE:HD12	18:s:169:ILE:HG12	1.91	0.51
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.93	0.51
2:B:23:HIS:ND1	22:B:615:CLA:OBD	2.39	0.51
3:C:289:PHE:O	3:C:293:ASN:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:4:PRO:HG2	2:b:7:ARG:HD2	1.93	0.51
2:b:225:LEU:O	2:b:229:LEU:HB2	2.09	0.51
9:k:47:PHE:O	9:k:50:LEU:HB3	2.11	0.51
19:y:78:TYR:OH	19:y:217:LYS:NZ	2.43	0.51
19:3:176:ARG:NH1	25:3:308:CHL:O1D	2.44	0.51
9:K:47:PHE:O	9:K:50:LEU:HB3	2.10	0.51
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.93	0.51
19:G:176:ARG:NH1	25:G:608:CHL:O1D	2.44	0.51
19:n:99:GLU:OE2	19:n:220:ARG:NE	2.33	0.51
20:4:119:GLY:O	20:4:123:SER:CB	2.59	0.51
3:C:162:GLY:HA3	3:C:252:ILE:HG13	1.92	0.51
19:N:78:TYR:OH	19:N:217:LYS:NZ	2.43	0.51
20:4:173:GLU:CG	22:4:301:CLA:C4B	2.71	0.51
4:d:97:GLU:OE2	5:e:69:ARG:NH2	2.44	0.51
6:f:24:THR:O	6:f:28:LEU:HB2	2.11	0.51
17:R:265:LYS:HB3	17:R:269:ASN:HB3	1.93	0.51
19:G:78:TYR:OH	19:G:217:LYS:NZ	2.43	0.51
25:Y:601:CHL:HBD	25:Y:601:CHL:CGA	2.41	0.51
20:4:228:GLU:O	20:4:232:SER:OG	2.29	0.51
19:7:176:ARG:NH1	25:7:308:CHL:O1D	2.44	0.51
1:A:55:ALA:HB3	1:A:70:SER:HB3	1.93	0.51
19:G:50:TRP:HE1	22:G:611:CLA:HED2	1.75	0.51
1:A:317:TRP:HE3	4:D:181:ARG:HD3	1.75	0.51
2:B:4:PRO:HG2	2:B:7:ARG:HD2	1.93	0.51
3:C:164:HIS:HD2	3:C:167:LEU:HD21	1.75	0.51
2:b:143:LEU:HD11	22:b:609:CLA:HBB1	1.91	0.51
2:b:403:GLY:H	2:b:407:ASN:HA	1.75	0.51
4:d:148:SER:HA	4:d:151:ILE:HD12	1.91	0.51
10:l:10:SER:OG	11:m:32:GLN:NE2	2.40	0.51
1:A:245:THR:O	4:D:266:ARG:NH2	2.44	0.51
10:L:13:LEU:HD23	10:L:14:ASN:H	1.76	0.51
2:b:193:PHE:HA	2:b:261:ALA:HB2	1.91	0.51
2:b:236:THR:HB	2:b:473:THR:HG21	1.93	0.51
3:c:164:HIS:HD2	3:c:167:LEU:HD21	1.75	0.51
19:G:160:ALA:O	19:G:164:THR:OG1	2.27	0.51
19:g:50:TRP:HE1	22:g:611:CLA:HED2	1.75	0.51
25:g:609:CHL:HAA1	19:n:82:THR:HG21	1.93	0.51
25:y:601:CHL:HBD	25:y:601:CHL:CGA	2.41	0.51
20:4:68:LEU:HB3	20:4:71:GLU:HB2	1.92	0.51
20:4:154:GLY:O	20:4:158:SER:CB	2.59	0.51
1:A:276:ALA:HA	4:D:213:ALA:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:299:SER:HG	3:c:308:GLU:CD	2.19	0.50
19:Y:99:GLU:OE2	19:Y:220:ARG:NE	2.33	0.50
19:Y:146:TYR:HD2	19:Y:152:LEU:HD13	1.76	0.50
17:r:278:PRO:N	20:4:140:PHE:HE1	2.09	0.50
20:4:252:PRO:O	20:4:256:LEU:CB	2.59	0.50
20:8:119:GLY:O	20:8:123:SER:CB	2.59	0.50
20:8:154:GLY:O	20:8:158:SER:CB	2.59	0.50
1:A:48:PHE:O	1:A:52:PHE:CB	2.55	0.50
2:B:222:PRO:HG3	7:H:38:GLY:HA3	1.93	0.50
2:B:236:THR:HB	2:B:473:THR:HG21	1.93	0.50
3:c:447:ARG:O	3:c:451:ALA:HB2	2.10	0.50
17:r:288:SER:OG	20:4:142:PHE:CD2	2.44	0.50
19:2:95:ASN:HA	19:2:98:LEU:HD12	1.94	0.50
19:5:98:LEU:O	19:5:102:HIS:ND1	2.42	0.50
2:B:403:GLY:H	2:B:407:ASN:HA	1.75	0.50
4:D:34:SER:O	4:D:38:LEU:CB	2.60	0.50
6:F:24:THR:O	6:F:28:LEU:HB2	2.11	0.50
1:a:183:MET:HB3	22:a:402:CLA:HBC2	1.93	0.50
4:d:168:TRP:O	4:d:171:ALA:HB3	2.11	0.50
4:d:185:PHE:O	4:d:189:PHE:HB2	2.12	0.50
12:o:140:PRO:HD2	12:o:170:THR:HG22	1.92	0.50
12:o:291:LYS:HB2	12:o:300:ILE:HG22	1.94	0.50
17:R:278:PRO:CA	20:8:140:PHE:HE1	2.02	0.50
19:g:176:ARG:NH1	25:g:608:CHL:O1D	2.44	0.50
19:1:95:ASN:HA	19:1:98:LEU:HD12	1.94	0.50
2:B:151:PHE:O	2:B:155:ALA:HB3	2.12	0.50
4:D:168:TRP:O	4:D:171:ALA:HB3	2.11	0.50
5:e:33:ALA:O	5:e:37:PHE:CB	2.58	0.50
25:G:609:CHL:HAA1	19:N:82:THR:HG21	1.93	0.50
2:b:151:PHE:O	2:b:155:ALA:HB3	2.12	0.50
2:b:392:VAL:HG13	2:b:397:VAL:HB	1.94	0.50
3:c:182:PHE:CZ	18:s:261:PRO:HD2	2.45	0.50
19:g:160:ALA:O	19:g:164:THR:OG1	2.27	0.50
19:6:174:GLY:O	19:6:178:ALA:HB3	2.12	0.50
2:B:139:PHE:O	2:B:143:LEU:HB2	2.12	0.50
2:B:379:ALA:HB2	2:B:395:VAL:HG11	1.94	0.50
1:a:55:ALA:HB3	1:a:70:SER:HB3	1.93	0.50
2:b:205:ALA:HA	22:b:602:CLA:HBC2	1.94	0.50
17:R:278:PRO:N	20:8:140:PHE:HE1	2.09	0.50
17:r:265:LYS:HB3	17:r:269:ASN:HB3	1.93	0.50
4:D:185:PHE:O	4:D:189:PHE:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:139:PHE:O	2:b:143:LEU:HB2	2.12	0.50
4:d:34:SER:O	4:d:38:LEU:CB	2.60	0.50
17:R:256:PHE:O	17:R:260:ALA:CB	2.60	0.50
19:g:146:TYR:HD2	19:g:152:LEU:HD13	1.76	0.50
20:8:118:VAL:HG11	22:8:305:CLA:HAC2	1.94	0.50
2:B:7:ARG:HG2	22:B:611:CLA:HED2	1.93	0.50
2:B:122:ILE:HD11	7:H:20:GLY:HA2	1.93	0.50
12:O:130:LYS:HG2	12:O:179:GLU:HG2	1.94	0.50
22:b:611:CLA:HBB2	22:b:613:CLA:HMB3	1.94	0.50
3:c:182:PHE:CE1	18:s:262:PHE:CD2	2.94	0.50
17:r:144:GLY:HA3	17:r:246:ALA:HB1	1.93	0.50
19:1:174:GLY:O	19:1:178:ALA:HB3	2.12	0.50
20:4:118:VAL:HG11	22:4:305:CLA:HAC2	1.94	0.50
20:4:162:VAL:HG11	22:4:301:CLA:O1A	2.12	0.50
2:b:8:VAL:HB	22:b:614:CLA:HED1	1.93	0.50
4:d:303:GLU:O	4:d:307:ALA:HB2	2.11	0.50
3:c:444:HIS:HE1	22:c:508:CLA:NA	2.10	0.50
19:g:246:ASP:O	19:g:254:ASN:ND2	2.40	0.50
19:1:98:LEU:O	19:1:102:HIS:ND1	2.42	0.50
20:4:119:GLY:O	20:4:123:SER:OG	2.30	0.50
20:4:157:GLU:OE1	20:4:160:ARG:NH2	2.36	0.50
20:4:242:PHE:O	20:4:246:ALA:CB	2.60	0.50
20:8:242:PHE:O	20:8:246:ALA:CB	2.60	0.50
1:A:240:GLY:HA2	13:T:29:ILE:HB	1.94	0.49
3:c:33:PHE:HB2	3:c:41:ARG:HE	1.77	0.49
17:r:279:LEU:HB3	20:4:140:PHE:N	2.27	0.49
1:A:334:ARG:HH22	4:D:321:LEU:HD13	1.76	0.49
3:C:33:PHE:HB2	3:C:41:ARG:HE	1.77	0.49
4:D:303:GLU:O	4:D:307:ALA:HB2	2.11	0.49
17:R:284:ILE:CG1	20:8:146:LEU:H	2.21	0.49
19:N:146:TYR:HD2	19:N:152:LEU:HD13	1.76	0.49
19:Y:157:SER:N	25:Y:605:CHL:OMC	2.36	0.49
25:n:601:CHL:O1A	25:n:601:CHL:HBD	2.13	0.49
19:2:94:ARG:NH1	19:3:81:ASP:O	2.45	0.49
19:2:174:GLY:O	19:2:178:ALA:HB3	2.12	0.49
2:B:372:ASP:OD1	2:B:376:ILE:N	2.46	0.49
3:C:215:LYS:NZ	3:C:226:SER:OG	2.42	0.49
19:N:176:ARG:HH22	25:N:608:CHL:HED2	1.75	0.49
17:r:62:ALA:CA	20:4:172:VAL:CG2	2.88	0.49
18:s:73:ASP:HB3	22:s:301:CLA:O2D	2.11	0.49
19:y:146:TYR:HD2	19:y:152:LEU:HD13	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:174:GLY:O	19:5:178:ALA:HB3	2.12	0.49
19:7:174:GLY:O	19:7:178:ALA:HB3	2.12	0.49
20:8:162:VAL:HG11	22:8:301:CLA:O1A	2.12	0.49
20:8:252:PRO:O	20:8:256:LEU:CB	2.59	0.49
2:B:3:LEU:H	10:L:12:GLU:H	1.59	0.49
4:d:45:ALA:HA	4:d:115:VAL:HG22	1.95	0.49
24:e:101:HEM:HHC	24:e:101:HEM:HBB2	1.94	0.49
17:R:267:PRO:O	17:R:271:TRP:HB2	2.12	0.49
18:s:146:VAL:HG23	18:s:149:LYS:HB2	1.94	0.49
19:6:95:ASN:HA	19:6:98:LEU:HD12	1.94	0.49
3:c:39:ASN:HD21	22:c:511:CLA:C1C	2.26	0.49
18:S:69:ILE:HG21	18:S:76:LEU:HD21	1.95	0.49
18:S:178:GLU:O	18:S:182:LEU:CB	2.55	0.49
19:Y:246:ASP:O	19:Y:254:ASN:ND2	2.40	0.49
17:r:287:PHE:CE2	20:4:146:LEU:HD23	2.48	0.49
18:s:69:ILE:HG21	18:s:76:LEU:HD21	1.95	0.49
20:8:154:GLY:O	20:8:158:SER:OG	2.30	0.49
4:D:45:ALA:HA	4:D:115:VAL:HG22	1.95	0.49
12:O:302:VAL:HG22	12:O:326:VAL:HG12	1.94	0.49
5:e:72:SER:O	5:e:76:LEU:CB	2.58	0.49
12:o:130:LYS:HG2	12:o:179:GLU:HG2	1.94	0.49
16:z:60:LEU:HD21	18:s:270:ILE:HG22	1.95	0.49
3:c:87:ILE:O	3:c:91:HIS:ND1	2.38	0.49
19:G:146:TYR:HD2	19:G:152:LEU:HD13	1.76	0.49
19:N:75:PRO:HB3	19:N:213:VAL:HG22	1.95	0.49
25:Y:601:CHL:HBD	25:Y:601:CHL:O1A	2.13	0.49
19:3:95:ASN:HA	19:3:98:LEU:HD12	1.94	0.49
19:3:174:GLY:O	19:3:178:ALA:HB3	2.12	0.49
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.94	0.49
2:B:3:LEU:HB2	10:L:11:VAL:HG22	1.93	0.49
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.94	0.49
2:B:392:VAL:HG13	2:B:397:VAL:HB	1.94	0.49
3:C:112:PHE:HZ	16:Z:58:ASN:HD21	1.60	0.49
1:a:272:HIS:HA	1:a:275:LEU:HD12	1.95	0.49
2:b:7:ARG:HG2	22:b:611:CLA:HED2	1.95	0.49
10:l:16:THR:O	10:l:20:TRP:CB	2.60	0.49
19:2:50:TRP:HE1	22:2:610:CLA:HED2	1.77	0.49
3:C:178:LYS:HG2	3:C:182:PHE:HB2	1.94	0.49
1:a:29:TYR:O	1:a:129:ARG:NH2	2.42	0.49
2:b:187:VAL:HG12	22:b:601:CLA:HBC3	1.95	0.49
2:b:372:ASP:OD1	2:b:376:ILE:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:w:111:LEU:O	14:w:114:THR:OG1	2.26	0.49
17:R:279:LEU:HB3	20:8:140:PHE:N	2.27	0.49
25:N:601:CHL:O1A	25:N:601:CHL:HBD	2.13	0.49
19:Y:75:PRO:HB3	19:Y:213:VAL:HG22	1.95	0.49
17:r:256:PHE:O	17:r:260:ALA:CB	2.60	0.49
19:n:246:ASP:O	19:n:254:ASN:ND2	2.40	0.49
19:y:75:PRO:HB3	19:y:213:VAL:HG22	1.95	0.49
19:y:176:ARG:NH1	25:y:608:CHL:O1D	2.46	0.49
20:4:159:LYS:CE	22:4:301:CLA:HMA2	2.32	0.49
19:7:98:LEU:O	19:7:102:HIS:ND1	2.42	0.49
20:8:99:ARG:HA	22:8:303:CLA:HMA2	1.95	0.49
20:8:103:LEU:HD13	20:8:193:GLY:HA3	1.95	0.49
3:C:92:LEU:HD21	22:C:502:CLA:H2A	1.93	0.49
12:O:291:LYS:HB2	12:O:300:ILE:HG22	1.94	0.49
17:R:287:PHE:CE2	20:8:146:LEU:HD23	2.48	0.49
18:S:146:VAL:HG23	18:S:149:LYS:HB2	1.94	0.49
17:r:280:HIS:CE1	20:4:138:ALA:C	2.85	0.49
19:5:95:ASN:HA	19:5:98:LEU:HD12	1.94	0.49
2:B:257:TRP:HB2	2:B:452:THR:HG21	1.95	0.49
3:C:356:MET:O	3:C:359:TRP:HB3	2.13	0.49
6:F:12:VAL:O	6:F:16:ALA:HB2	2.13	0.49
2:b:157:HIS:HA	2:b:163:GLY:HA3	1.94	0.49
2:b:257:TRP:HB2	2:b:452:THR:HG21	1.95	0.49
12:o:305:SER:N	12:o:323:ILE:O	2.46	0.49
3:c:178:LYS:HG2	3:c:182:PHE:HB2	1.94	0.49
19:Y:176:ARG:NH1	25:Y:608:CHL:O1D	2.46	0.49
17:r:267:PRO:O	17:r:271:TRP:HB2	2.12	0.49
19:3:98:LEU:O	19:3:102:HIS:ND1	2.42	0.49
1:A:272:HIS:HA	1:A:275:LEU:HD12	1.95	0.48
10:L:16:THR:O	10:L:20:TRP:CB	2.60	0.48
2:b:379:ALA:HB2	2:b:395:VAL:HG11	1.94	0.48
19:g:75:PRO:HB3	19:g:213:VAL:HG22	1.95	0.48
19:n:146:TYR:HD2	19:n:152:LEU:HD13	1.76	0.48
19:6:50:TRP:HE1	22:6:610:CLA:HED2	1.77	0.48
19:7:95:ASN:HA	19:7:98:LEU:HD12	1.94	0.48
20:8:119:GLY:O	20:8:123:SER:OG	2.30	0.48
14:W:111:LEU:O	14:W:114:THR:OG1	2.26	0.48
16:z:40:VAL:O	16:z:44:THR:CB	2.62	0.48
3:c:189:TRP:HZ3	3:c:367:GLU:HG3	1.78	0.48
19:n:91:THR:OG1	19:y:84:GLY:O	2.27	0.48
19:6:94:ARG:NH1	19:7:81:ASP:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:405:CLA:H3A	22:A:405:CLA:HBA1	1.51	0.48
2:B:216:HIS:HE1	22:B:609:CLA:C1A	2.26	0.48
4:D:194:LEU:O	10:L:35:TYR:OH	2.26	0.48
16:Z:40:VAL:O	16:Z:44:THR:CB	2.61	0.48
12:o:302:VAL:HG22	12:o:326:VAL:HG12	1.94	0.48
16:z:40:VAL:O	16:z:44:THR:OG1	2.29	0.48
19:Y:160:ALA:O	19:Y:164:THR:OG1	2.27	0.48
25:y:601:CHL:HBD	25:y:601:CHL:O1A	2.13	0.48
16:Z:24:PRO:O	16:Z:28:ALA:CB	2.62	0.48
15:x:85:ASN:O	15:x:89:SER:OG	2.25	0.48
3:c:182:PHE:CZ	18:s:261:PRO:CD	2.97	0.48
17:R:144:GLY:HA3	17:R:246:ALA:HB1	1.93	0.48
19:n:160:ALA:O	19:n:164:THR:OG1	2.27	0.48
25:1:609:CHL:HAA1	19:2:82:THR:HG21	1.95	0.48
3:C:189:TRP:HZ3	3:C:367:GLU:HG3	1.78	0.48
3:c:182:PHE:HE1	18:s:261:PRO:HD2	1.71	0.48
3:c:356:MET:O	3:c:359:TRP:HB3	2.13	0.48
22:8:310:CLA:HAA1	22:8:310:CLA:HED2	1.95	0.48
2:B:282:GLN:O	2:B:286:ARG:CB	2.61	0.48
2:B:384:ARG:HG2	2:B:386:ALA:H	1.79	0.48
3:C:447:ARG:HD3	22:C:508:CLA:HED3	1.96	0.48
12:o:142:SER:HB2	12:o:324:GLN:HB3	1.95	0.48
19:N:91:THR:OG1	19:Y:84:GLY:O	2.27	0.48
18:s:74:GLY:HA3	22:s:301:CLA:HED2	1.84	0.48
2:B:190:PHE:HB3	7:H:60:ILE:HG21	1.96	0.48
3:C:299:SER:HG	3:C:308:GLU:CD	2.20	0.48
4:D:18:ILE:O	4:D:22:TRP:CB	2.62	0.48
19:G:75:PRO:HB3	19:G:213:VAL:HG22	1.95	0.48
19:n:75:PRO:HB3	19:n:213:VAL:HG22	1.95	0.48
20:4:99:ARG:HA	22:4:303:CLA:HMA2	1.95	0.48
8:i:5:LYS:NZ	8:i:9:TYR:OH	2.46	0.48
14:w:117:PHE:O	14:w:121:SER:OG	2.32	0.48
22:s:303:CLA:H3A	22:s:303:CLA:HBA2	1.66	0.48
19:1:247:HIS:NE2	22:1:614:CLA:ND	2.61	0.48
3:C:39:ASN:ND2	22:C:508:CLA:O2A	2.39	0.48
2:b:469:HIS:O	2:b:473:THR:OG1	2.29	0.48
4:d:187:GLN:HB2	22:d:403:CLA:HBC1	1.95	0.48
17:R:145:ARG:NH2	17:R:216:LEU:O	2.47	0.48
25:5:609:CHL:HAA1	19:6:82:THR:HG21	1.95	0.48
19:6:98:LEU:O	19:6:102:HIS:ND1	2.42	0.48
1:a:217:SER:O	1:a:221:SER:OG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:187:GLN:OE1	4:d:193:THR:N	2.45	0.48
5:e:76:LEU:O	5:e:80:SER:HB2	2.14	0.48
3:c:187:ASP:O	3:c:194:GLY:CA	2.62	0.48
19:Y:247:HIS:HB2	22:Y:613:CLA:HAA2	1.96	0.48
19:y:157:SER:N	25:y:605:CHL:OMC	2.36	0.48
2:B:9:HIS:CE1	22:B:614:CLA:NC	2.82	0.47
2:B:197:GLY:O	2:B:201:HIS:HB2	2.14	0.47
12:O:142:SER:HB2	12:O:324:GLN:HB3	1.95	0.47
12:O:305:SER:HB3	12:O:323:ILE:HB	1.96	0.47
2:b:197:GLY:O	2:b:201:HIS:HB2	2.14	0.47
16:z:24:PRO:O	16:z:28:ALA:CB	2.62	0.47
17:R:278:PRO:HD3	22:6:613:CLA:CBB	2.39	0.47
3:C:187:ASP:O	3:C:194:GLY:CA	2.62	0.47
23:a:404:PHO:HED2	23:a:404:PHO:H2A	1.95	0.47
5:e:69:ARG:NH2	7:h:63:SER:O	2.47	0.47
19:y:160:ALA:O	19:y:164:THR:OG1	2.27	0.47
20:4:103:LEU:HD13	20:4:193:GLY:HA3	1.95	0.47
20:8:228:GLU:O	20:8:232:SER:OG	2.29	0.47
5:E:76:LEU:O	5:E:80:SER:HB2	2.14	0.47
2:b:282:GLN:O	2:b:286:ARG:CB	2.61	0.47
22:b:604:CLA:HMB2	22:b:607:CLA:HAB	1.96	0.47
4:d:18:ILE:O	4:d:22:TRP:CB	2.62	0.47
6:f:12:VAL:O	6:f:16:ALA:HB2	2.13	0.47
3:c:132:HIS:HE1	22:s:301:CLA:NA	2.08	0.47
19:5:247:HIS:NE2	22:5:614:CLA:ND	2.61	0.47
5:E:72:SER:O	5:E:76:LEU:CB	2.58	0.47
12:O:94:TYR:CZ	12:O:135:LYS:HE3	2.50	0.47
19:n:98:LEU:HD23	25:n:609:CHL:HED3	1.97	0.47
19:1:144:LEU:HB3	19:1:155:ALA:HB3	1.97	0.47
19:3:144:LEU:HB3	19:3:155:ALA:HB3	1.97	0.47
19:6:69:TYR:OH	19:6:81:ASP:OD2	2.26	0.47
19:6:80:TRP:NE1	25:6:601:CHL:O2A	2.47	0.47
2:B:469:HIS:O	2:B:473:THR:OG1	2.29	0.47
3:C:66:ALA:HB1	9:K:40:MET:HG3	1.95	0.47
4:D:86:LEU:HD13	4:D:91:LEU:HD11	1.96	0.47
2:b:161:LEU:HD21	25:R:305:CHL:CMD	2.43	0.47
17:R:283:ILE:N	20:8:144:SER:OG	2.20	0.47
19:G:158:ILE:HA	19:G:161:ILE:HD12	1.97	0.47
19:N:98:LEU:HD23	25:N:609:CHL:HED3	1.97	0.47
19:N:158:ILE:HA	19:N:161:ILE:HD12	1.97	0.47
17:r:68:LEU:HD13	17:r:77:GLY:HA2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:145:ARG:NH2	17:r:216:LEU:O	2.47	0.47
19:2:80:TRP:NE1	25:2:601:CHL:O2A	2.47	0.47
19:7:144:LEU:HB3	19:7:155:ALA:HB3	1.97	0.47
3:C:464:GLU:OE2	4:D:249:THR:OG1	2.33	0.47
24:F:101:HEM:HBC2	24:F:101:HEM:HHD	1.97	0.47
12:O:304:GLU:HG2	12:O:324:GLN:HG3	1.96	0.47
1:a:92:HIS:CE1	3:c:220:GLY:HA3	2.49	0.47
1:a:317:TRP:CE3	4:d:181:ARG:HD3	2.49	0.47
24:e:101:HEM:HHD	24:e:101:HEM:HBC2	1.97	0.47
12:o:146:LYS:HE3	12:o:157:GLU:HA	1.97	0.47
16:z:37:LYS:HD2	18:s:75:LEU:O	2.15	0.47
22:4:310:CLA:HAA1	22:4:310:CLA:HED2	1.95	0.47
19:5:161:ILE:HG12	25:5:605:CHL:HAC1	1.97	0.47
19:6:99:GLU:HG3	19:6:223:MET:HE1	1.97	0.47
19:6:176:ARG:HH22	25:6:607:CHL:HED2	1.80	0.47
2:B:381:VAL:HG13	2:B:418:LYS:HD3	1.97	0.47
2:b:151:PHE:O	2:b:155:ALA:CB	2.63	0.47
3:c:48:LYS:HA	3:c:133:ALA:HA	1.96	0.47
3:c:164:HIS:ND1	22:c:507:CLA:OBD	2.41	0.47
3:c:447:ARG:O	3:c:451:ALA:CB	2.63	0.47
18:S:120:TRP:HH2	18:S:182:LEU:HD11	1.80	0.47
19:y:158:ILE:HA	19:y:161:ILE:HD12	1.97	0.47
19:y:247:HIS:HB2	22:y:613:CLA:HAA2	1.96	0.47
20:8:146:LEU:HD13	25:8:307:CHL:HAC2	1.97	0.47
20:8:194:TYR:CZ	20:8:225:LYS:HG2	2.50	0.47
15:x:80:SER:HB3	15:x:83:LEU:HG	1.97	0.47
17:R:288:SER:OG	20:8:142:PHE:CD2	2.44	0.47
19:Y:158:ILE:HA	19:Y:161:ILE:HD12	1.97	0.47
19:5:99:GLU:HG3	19:5:223:MET:HE1	1.97	0.47
2:B:5:TRP:HD1	10:L:13:LEU:HD11	1.79	0.47
3:C:48:LYS:HA	3:C:133:ALA:HA	1.96	0.47
12:o:94:TYR:CZ	12:o:135:LYS:HE3	2.50	0.47
17:R:68:LEU:HD13	17:R:77:GLY:HA2	1.97	0.47
19:N:99:GLU:OE2	19:N:220:ARG:NE	2.33	0.47
18:s:221:LEU:HD23	18:s:224:LYS:HD2	1.97	0.47
18:s:241:ILE:HG21	22:s:313:CLA:HAC2	1.96	0.47
12:o:304:GLU:HG2	12:o:324:GLN:HG3	1.96	0.46
3:c:312:ALA:HB1	3:c:392:SER:HA	1.97	0.46
2:B:315:ILE:HG21	2:B:426:LEU:HD22	1.97	0.46
17:R:275:LEU:O	22:6:613:CLA:HMB2	2.15	0.46
19:2:144:LEU:HB3	19:2:155:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:146:LEU:HD13	25:4:307:CHL:HAC2	1.97	0.46
1:A:41:LEU:O	1:A:45:THR:OG1	2.28	0.46
2:B:384:ARG:HE	4:D:345:GLU:HA	1.80	0.46
3:C:260:ALA:HA	3:C:264:LEU:HD13	1.97	0.46
3:C:294:ASN:HD21	3:C:362:ARG:HB2	1.80	0.46
3:C:430:HIS:CE1	22:C:501:CLA:NA	2.82	0.46
12:O:305:SER:N	12:O:323:ILE:O	2.46	0.46
1:a:19:ASN:OD1	8:i:30:ARG:NH2	2.48	0.46
2:b:384:ARG:HG2	2:b:386:ALA:H	1.79	0.46
3:c:260:ALA:HA	3:c:264:LEU:HD13	1.97	0.46
3:c:294:ASN:HD21	3:c:362:ARG:HB2	1.80	0.46
17:R:146:TRP:CD1	22:R:307:CLA:HMD3	2.51	0.46
19:G:99:GLU:OE2	19:G:220:ARG:NE	2.33	0.46
19:G:176:ARG:HH22	25:G:608:CHL:HED2	1.80	0.46
19:Y:109:GLY:O	19:Y:113:CYS:HB2	2.15	0.46
19:g:109:GLY:O	19:g:113:CYS:HB2	2.14	0.46
19:n:109:GLY:O	19:n:113:CYS:HB2	2.15	0.46
19:n:158:ILE:HA	19:n:161:ILE:HD12	1.97	0.46
19:y:109:GLY:O	19:y:113:CYS:HB2	2.15	0.46
2:B:347:ARG:HG2	2:B:353:GLU:HA	1.98	0.46
3:C:294:ASN:ND2	3:C:362:ARG:O	2.49	0.46
4:D:178:ALA:O	4:D:182:PHE:CB	2.61	0.46
4:d:86:LEU:HD13	4:d:91:LEU:HD11	1.96	0.46
4:d:91:LEU:O	4:d:105:TRP:NE1	2.41	0.46
4:d:156:SER:HA	4:d:160:ILE:HD12	1.98	0.46
18:S:241:ILE:HG21	22:S:313:CLA:HAC2	1.96	0.46
19:g:158:ILE:HA	19:g:161:ILE:HD12	1.97	0.46
19:y:95:ASN:HB3	22:y:602:CLA:HHB	1.98	0.46
20:4:194:TYR:CZ	20:4:225:LYS:HG2	2.50	0.46
3:C:206:PRO:HG3	22:Y:614:CLA:CBB	2.08	0.46
3:C:312:ALA:HB1	3:C:392:SER:HA	1.97	0.46
7:H:59:GLU:HG2	15:X:86:PHE:HZ	1.79	0.46
14:W:117:PHE:O	14:W:121:SER:OG	2.32	0.46
17:R:63:ILE:HG13	20:8:166:ASN:HD21	1.81	0.46
17:r:172:GLU:OE2	17:r:178:SER:N	2.49	0.46
19:2:176:ARG:HH22	25:2:607:CHL:HED2	1.80	0.46
20:8:157:GLU:OE1	20:8:160:ARG:NH2	2.36	0.46
1:A:272:HIS:HD2	4:D:215:HIS:CD2	2.33	0.46
12:O:146:LYS:HE3	12:O:157:GLU:HA	1.97	0.46
14:w:117:PHE:O	14:w:121:SER:CB	2.63	0.46
19:G:109:GLY:O	19:G:113:CYS:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:146:TRP:CD1	22:r:307:CLA:HMD3	2.51	0.46
19:n:69:TYR:OH	19:n:81:ASP:OD2	2.31	0.46
19:3:99:GLU:HG3	19:3:223:MET:HE1	1.97	0.46
25:6:606:CHL:HBA2	25:6:606:CHL:H3A	1.81	0.46
2:B:151:PHE:O	2:B:155:ALA:CB	2.63	0.46
22:B:611:CLA:HBB2	22:B:613:CLA:HMB3	1.96	0.46
3:C:71:GLU:HG2	3:C:86:LEU:HD22	1.98	0.46
1:a:288:LEU:HD13	3:c:432:VAL:HG13	1.98	0.46
12:o:305:SER:HB3	12:o:323:ILE:HB	1.96	0.46
18:S:221:LEU:HD23	18:S:224:LYS:HD2	1.97	0.46
19:N:109:GLY:O	19:N:113:CYS:HB2	2.15	0.46
17:r:168:ALA:HB1	22:r:303:CLA:HED1	1.97	0.46
18:s:120:TRP:HH2	18:s:182:LEU:HD11	1.80	0.46
19:7:255:ASN:HA	22:7:313:CLA:HAA1	1.98	0.46
1:A:308:ASP:HB3	1:A:314:ILE:HD11	1.98	0.46
1:A:334:ARG:HB2	4:D:350:GLY:HA2	1.96	0.46
2:B:205:ALA:HA	22:B:602:CLA:HBC2	1.97	0.46
1:a:308:ASP:HB3	1:a:314:ILE:HD11	1.98	0.46
19:y:69:TYR:OH	19:y:81:ASP:OD2	2.31	0.46
22:y:611:CLA:H3A	22:y:611:CLA:HBA2	1.75	0.46
19:2:99:GLU:HG3	19:2:223:MET:HE1	1.97	0.46
19:6:144:LEU:HB3	19:6:155:ALA:HB3	1.97	0.46
3:C:276:LEU:O	3:C:280:SER:HB2	2.16	0.46
4:D:91:LEU:O	4:D:105:TRP:NE1	2.41	0.46
2:b:315:ILE:HG21	2:b:426:LEU:HD22	1.97	0.46
3:c:276:LEU:O	3:c:280:SER:HB2	2.16	0.46
19:Y:95:ASN:HB3	22:Y:602:CLA:HHB	1.98	0.46
17:r:135:ARG:NH1	22:r:302:CLA:O1A	2.49	0.46
19:1:161:ILE:HG12	25:1:605:CHL:HAC1	1.97	0.46
19:3:104:ARG:NH1	25:3:308:CHL:OBD	2.44	0.46
1:A:216:GLY:O	1:A:220:THR:CB	2.64	0.46
4:D:156:SER:HA	4:D:160:ILE:HD12	1.98	0.46
4:D:187:GLN:HB2	22:D:403:CLA:HBC1	1.96	0.46
4:d:331:ALA:HA	4:d:334:ASP:HB3	1.98	0.46
6:f:23:PRO:O	6:f:27:PHE:HB2	2.16	0.46
17:r:236:ALA:O	17:r:240:LEU:CB	2.64	0.46
19:g:176:ARG:HH22	25:g:608:CHL:HED2	1.80	0.46
19:n:144:LEU:HB3	19:n:155:ALA:HB3	1.98	0.46
19:5:144:LEU:HB3	19:5:155:ALA:HB3	1.97	0.46
3:C:159:THR:HG23	3:C:252:ILE:HG23	1.98	0.45
3:C:447:ARG:O	3:C:451:ALA:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:LEU:O	5:E:80:SER:CB	2.64	0.45
6:F:23:PRO:O	6:F:27:PHE:HB2	2.16	0.45
12:O:146:LYS:HB2	12:O:158:PHE:HB3	1.98	0.45
4:d:178:ALA:O	4:d:182:PHE:CB	2.61	0.45
16:z:42:SER:O	16:z:46:LEU:CB	2.63	0.45
3:c:90:PRO:O	3:c:94:THR:OG1	2.31	0.45
3:c:294:ASN:ND2	3:c:362:ARG:O	2.48	0.45
18:S:103:LYS:HD3	18:S:106:ASN:HD22	1.81	0.45
17:r:267:PRO:O	17:r:271:TRP:HB3	2.16	0.45
18:s:169:ILE:HD13	18:s:173:LEU:HB3	1.98	0.45
2:b:393:GLU:HG3	2:b:414:PRO:HG2	1.98	0.45
4:d:58:SER:HG	4:d:80:SER:HG	1.64	0.45
4:d:193:THR:HG23	22:d:403:CLA:HBC2	1.98	0.45
17:R:275:LEU:O	22:6:613:CLA:CBB	2.63	0.45
18:s:103:LYS:HD3	18:s:106:ASN:HD22	1.81	0.45
19:7:99:GLU:HG3	19:7:223:MET:HE1	1.97	0.45
20:8:119:GLY:O	20:8:123:SER:HB3	2.16	0.45
23:A:404:PHO:HED2	23:A:404:PHO:H2A	1.99	0.45
3:C:233:ILE:HD13	3:C:233:ILE:HA	1.82	0.45
12:O:130:LYS:HA	12:O:179:GLU:HA	1.98	0.45
1:a:216:GLY:O	1:a:220:THR:CB	2.64	0.45
2:b:381:VAL:HG13	2:b:418:LYS:HD3	1.97	0.45
12:o:130:LYS:HA	12:o:179:GLU:HA	1.98	0.45
12:o:146:LYS:HB2	12:o:158:PHE:HB3	1.98	0.45
17:R:59:TYR:N	20:8:173:GLU:CA	2.79	0.45
17:R:278:PRO:HG2	22:6:613:CLA:HBB2	1.90	0.45
19:N:229:PHE:O	19:N:233:ALA:HB3	2.17	0.45
19:y:144:LEU:HB3	19:y:155:ALA:HB3	1.98	0.45
19:1:99:GLU:HG3	19:1:223:MET:HE1	1.97	0.45
19:2:218:ASN:OD1	22:2:611:CLA:NB	2.49	0.45
2:B:64:PRO:O	2:B:68:ARG:CB	2.58	0.45
4:D:254:TRP:O	4:D:259:GLY:N	2.45	0.45
14:W:117:PHE:O	14:W:121:SER:CB	2.63	0.45
1:a:103:ASP:O	1:a:107:TYR:CB	2.65	0.45
2:b:272:ARG:HH12	4:d:293:ASN:ND2	2.15	0.45
17:R:278:PRO:HG3	22:6:613:CLA:HBB2	1.94	0.45
19:6:218:ASN:OD1	22:6:611:CLA:NB	2.49	0.45
20:8:154:GLY:O	20:8:158:SER:HB2	2.16	0.45
2:B:393:GLU:HG3	2:B:414:PRO:HG2	1.98	0.45
3:C:470:THR:O	4:D:252:ARG:NH1	2.49	0.45
15:X:80:SER:HB3	15:X:83:LEU:HG	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:347:ARG:HG2	2:b:353:GLU:HA	1.98	0.45
17:r:63:ILE:HG13	20:4:166:ASN:HD21	1.81	0.45
17:r:278:PRO:CA	20:4:140:PHE:HE1	2.02	0.45
19:n:153:VAL:HA	25:n:605:CHL:C4D	2.47	0.45
19:n:229:PHE:O	19:n:233:ALA:HB3	2.17	0.45
4:D:331:ALA:HA	4:D:334:ASP:HB3	1.98	0.45
22:a:405:CLA:HBA1	22:a:405:CLA:H3A	1.68	0.45
3:c:314:ALA:HA	3:c:317:PHE:HD2	1.82	0.45
17:R:135:ARG:NH1	22:R:302:CLA:O1A	2.49	0.45
18:S:169:ILE:HD13	18:S:173:LEU:HB3	1.98	0.45
19:G:144:LEU:HB3	19:G:155:ALA:HB3	1.98	0.45
19:3:255:ASN:HA	22:3:313:CLA:HAA1	1.98	0.45
1:A:59:ASP:OD2	1:A:63:ILE:N	2.50	0.45
2:b:455:HIS:CD2	22:b:604:CLA:NC	2.84	0.45
5:e:76:LEU:O	5:e:80:SER:CB	2.64	0.45
3:c:86:LEU:HD13	3:c:89:LEU:HD12	1.99	0.45
3:c:159:THR:HG23	3:c:252:ILE:HG23	1.98	0.45
17:R:168:ALA:HB1	22:R:303:CLA:HED1	1.97	0.45
19:N:144:LEU:HB3	19:N:155:ALA:HB3	1.98	0.45
19:Y:144:LEU:HB3	19:Y:155:ALA:HB3	1.98	0.45
20:4:101:ALA:O	20:4:105:HIS:ND1	2.38	0.45
20:4:119:GLY:O	20:4:123:SER:HB3	2.16	0.45
20:4:185:PHE:HA	20:4:190:GLY:HA2	1.98	0.45
19:5:176:ARG:HH22	25:5:608:CHL:HED2	1.81	0.45
25:5:606:CHL:HBA2	25:5:606:CHL:H3A	1.83	0.45
20:8:185:PHE:HA	20:8:190:GLY:HA2	1.98	0.45
8:I:3:THR:HA	8:I:6:LEU:HD12	1.99	0.45
1:a:97:TRP:CG	8:i:5:LYS:HD2	2.52	0.45
4:d:90:LEU:HG	7:h:62:ASN:HD21	1.81	0.45
8:i:15:PHE:O	8:i:19:PHE:HB2	2.17	0.45
17:R:206:ARG:HA	25:R:306:CHL:HBC3	1.98	0.45
19:N:153:VAL:HA	25:N:605:CHL:C4D	2.47	0.45
17:r:275:LEU:O	22:2:613:CLA:HMB2	2.15	0.45
25:2:606:CHL:HBA2	25:2:606:CHL:H3A	1.81	0.45
12:O:131:TYR:HB2	12:O:178:PHE:HB3	1.99	0.45
17:r:146:TRP:CD2	22:r:307:CLA:HAC2	2.52	0.45
19:1:174:GLY:O	19:1:178:ALA:CB	2.65	0.45
19:2:255:ASN:HA	22:2:612:CLA:HAA1	1.99	0.45
1:A:40:THR:O	1:A:44:ALA:HB3	2.17	0.45
2:B:194:VAL:HG12	2:B:196:GLY:H	1.82	0.45
2:b:214:LEU:HD13	22:R:302:CLA:O2D	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:74:GLY:CA	22:S:301:CLA:OBD	2.64	0.45
19:G:229:PHE:O	19:G:233:ALA:HB3	2.17	0.45
2:B:299:SER:O	2:B:303:ALA:CB	2.66	0.44
8:I:15:PHE:O	8:I:19:PHE:HB2	2.17	0.44
22:b:602:CLA:H2A	22:b:602:CLA:HED3	1.99	0.44
19:g:98:LEU:HD23	25:g:609:CHL:HED3	1.99	0.44
19:6:174:GLY:O	19:6:178:ALA:CB	2.65	0.44
20:8:221:LEU:HG	20:8:225:LYS:HE3	1.99	0.44
1:A:334:ARG:HH12	4:D:321:LEU:HD13	1.81	0.44
22:A:403:CLA:HED2	4:D:176:VAL:HG13	1.99	0.44
2:B:238:LEU:HD11	22:B:611:CLA:HMB2	1.98	0.44
2:B:255:THR:HG21	22:B:602:CLA:HED1	1.99	0.44
4:D:303:GLU:O	4:D:307:ALA:CB	2.66	0.44
3:c:199:ILE:HD11	3:c:230:LEU:HB2	1.99	0.44
17:R:236:ALA:O	17:R:240:LEU:CB	2.64	0.44
19:G:214:LYS:HD3	22:G:612:CLA:HAA2	1.99	0.44
17:r:182:GLN:NE2	25:y:605:CHL:HHB	2.33	0.44
19:g:218:ASN:OD1	22:g:612:CLA:NB	2.51	0.44
19:y:229:PHE:O	19:y:233:ALA:HB3	2.17	0.44
19:7:69:TYR:OH	19:7:81:ASP:OD2	2.26	0.44
20:8:144:SER:O	25:8:302:CHL:HED3	2.16	0.44
1:A:103:ASP:O	1:A:107:TYR:CB	2.65	0.44
3:C:69:LEU:HA	3:C:72:VAL:HG12	1.99	0.44
3:C:314:ALA:HA	3:C:317:PHE:HD2	1.81	0.44
3:C:343:ARG:NE	12:O:170:THR:O	2.49	0.44
1:a:59:ASP:OD2	1:a:63:ILE:N	2.50	0.44
3:c:71:GLU:HG2	3:c:86:LEU:HD22	1.98	0.44
17:R:146:TRP:CD2	22:R:307:CLA:HAC2	2.52	0.44
17:R:267:PRO:O	17:R:271:TRP:HB3	2.16	0.44
19:Y:229:PHE:O	19:Y:233:ALA:HB3	2.17	0.44
19:g:214:LYS:HD3	22:g:612:CLA:HAA2	1.99	0.44
19:3:174:GLY:O	19:3:178:ALA:CB	2.65	0.44
20:8:173:GLU:O	22:8:301:CLA:CAB	2.64	0.44
1:A:309:SER:H	5:E:55:TYR:HD2	1.66	0.44
3:C:39:ASN:HD21	22:C:511:CLA:C1C	2.30	0.44
3:C:261:ARG:HA	3:C:266:TRP:HE1	1.82	0.44
12:O:107:GLY:HA3	14:W:90:THR:HG22	1.98	0.44
1:a:40:THR:O	1:a:44:ALA:HB3	2.17	0.44
22:a:403:CLA:HED2	4:d:176:VAL:HG13	1.99	0.44
2:b:66:MET:HG2	22:b:605:CLA:HMA3	2.00	0.44
17:r:59:TYR:N	20:4:173:GLU:CA	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:62:ALA:HB2	20:4:172:VAL:CB	2.45	0.44
17:r:206:ARG:HA	25:r:306:CHL:HBC3	1.98	0.44
19:5:174:GLY:O	19:5:178:ALA:CB	2.65	0.44
19:7:104:ARG:NH1	25:7:308:CHL:OBD	2.44	0.44
19:7:174:GLY:O	19:7:178:ALA:CB	2.65	0.44
2:B:413:ASP:N	2:B:413:ASP:OD1	2.51	0.44
3:C:86:LEU:HD13	3:C:89:LEU:HD12	1.99	0.44
12:o:131:TYR:HB2	12:o:178:PHE:HB3	1.99	0.44
22:S:303:CLA:HBA2	22:S:303:CLA:H3A	1.66	0.44
19:Y:100:VAL:HG22	19:Y:216:LEU:HD21	2.00	0.44
17:r:275:LEU:O	22:2:613:CLA:CBB	2.63	0.44
19:g:144:LEU:HB3	19:g:155:ALA:HB3	1.98	0.44
19:n:100:VAL:HG22	19:n:216:LEU:HD21	2.00	0.44
19:1:176:ARG:HH22	25:1:608:CHL:HED2	1.81	0.44
20:4:154:GLY:O	20:4:158:SER:HB2	2.16	0.44
19:6:75:PRO:HB2	19:6:216:LEU:HD12	2.00	0.44
19:6:255:ASN:HA	22:6:612:CLA:HAA1	1.99	0.44
1:A:267:ASN:HB3	1:A:270:SER:HB3	2.00	0.44
1:a:115:ILE:O	1:a:119:PHE:HB2	2.17	0.44
2:b:208:LEU:HD12	22:b:602:CLA:HAC2	2.00	0.44
2:b:357:ARG:NH1	2:b:358:ARG:O	2.51	0.44
4:d:303:GLU:O	4:d:307:ALA:CB	2.66	0.44
8:i:3:THR:HA	8:i:6:LEU:HD12	1.99	0.44
19:G:98:LEU:HD23	25:G:609:CHL:HED3	1.99	0.44
19:G:218:ASN:OD1	22:G:612:CLA:NB	2.51	0.44
22:G:602:CLA:H3A	22:G:602:CLA:HBA2	1.80	0.44
19:g:229:PHE:O	19:g:233:ALA:HB3	2.17	0.44
2:B:357:ARG:NH1	2:B:358:ARG:O	2.51	0.44
1:a:267:ASN:HB3	1:a:270:SER:HB3	2.00	0.44
2:b:281:GLN:O	2:b:285:TYR:CB	2.66	0.44
2:b:462:PHE:HE2	22:b:604:CLA:HAC2	1.82	0.44
3:c:309:ALA:O	3:c:313:GLN:HB2	2.18	0.44
17:R:182:GLN:NE2	25:Y:605:CHL:HHB	2.33	0.44
18:S:74:GLY:HA3	22:S:301:CLA:OBD	2.18	0.44
19:G:100:VAL:HG22	19:G:216:LEU:HD21	1.99	0.44
22:n:610:CLA:H3A	22:n:610:CLA:HBA2	1.84	0.44
19:6:173:GLU:HA	19:6:176:ARG:HG2	2.00	0.44
2:B:201:HIS:HE1	22:B:602:CLA:ND	2.15	0.44
4:D:208:ALA:HB2	4:D:276:PRO:HB3	1.99	0.44
2:b:7:ARG:O	2:b:10:THR:OG1	2.28	0.44
9:k:35:PRO:O	9:k:38:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:261:ARG:HA	3:c:266:TRP:HE1	1.82	0.44
19:Y:160:ALA:O	19:Y:164:THR:CB	2.66	0.44
18:s:260:ASP:HB3	18:s:263:GLY:HA3	2.00	0.44
1:A:115:ILE:O	1:A:119:PHE:HB2	2.18	0.44
3:C:164:HIS:ND1	22:C:507:CLA:OBD	2.48	0.44
4:D:251:ASN:HD21	13:T:27:PRO:HB2	1.83	0.44
9:K:35:PRO:O	9:K:38:ASP:HB2	2.18	0.44
2:b:194:VAL:HG12	2:b:196:GLY:H	1.82	0.44
2:b:299:SER:O	2:b:303:ALA:CB	2.66	0.44
6:f:12:VAL:O	6:f:16:ALA:CB	2.66	0.44
10:l:30:VAL:O	10:l:33:SER:OG	2.28	0.44
3:c:69:LEU:HA	3:c:72:VAL:HG12	1.99	0.44
19:G:160:ALA:O	19:G:164:THR:CB	2.66	0.44
19:N:160:ALA:O	19:N:164:THR:CB	2.66	0.44
20:8:73:LEU:HD21	22:8:303:CLA:HAA1	2.00	0.44
2:B:257:TRP:NE1	4:D:164:GLY:O	2.52	0.43
6:F:12:VAL:O	6:F:16:ALA:CB	2.66	0.43
16:Z:24:PRO:O	16:Z:28:ALA:HB3	2.18	0.43
4:d:208:ALA:HB2	4:d:276:PRO:HB3	1.99	0.43
12:o:194:ILE:H	12:o:194:ILE:HG13	1.52	0.43
17:R:172:GLU:OE2	17:R:178:SER:N	2.49	0.43
25:G:606:CHL:HBA2	25:G:606:CHL:H3A	1.94	0.43
25:g:606:CHL:HBA2	25:g:606:CHL:H3A	1.94	0.43
19:2:174:GLY:O	19:2:178:ALA:CB	2.65	0.43
3:C:309:ALA:O	3:C:313:GLN:HB2	2.18	0.43
4:D:58:SER:O	4:D:63:GLY:N	2.51	0.43
4:D:266:ARG:O	4:D:270:PHE:HB2	2.19	0.43
17:R:285:ASP:H	20:8:141:SER:HB3	1.81	0.43
19:Y:170:GLY:N	25:Y:609:CHL:HAB	2.33	0.43
19:1:75:PRO:HB2	19:1:216:LEU:HD12	2.00	0.43
19:2:75:PRO:HB2	19:2:216:LEU:HD12	2.00	0.43
22:6:602:CLA:HBA2	22:6:602:CLA:H3A	1.69	0.43
19:7:173:GLU:HA	19:7:176:ARG:HG2	2.00	0.43
1:A:213:ALA:HB1	4:D:146:ALA:HB1	1.98	0.43
2:B:85:ILE:HD11	12:o:204:PRO:HD3	1.99	0.43
2:B:281:GLN:O	2:B:285:TYR:CB	2.66	0.43
3:C:182:PHE:CD1	18:S:261:PRO:HD2	2.48	0.43
12:O:185:SER:HA	12:O:223:LYS:HA	2.00	0.43
17:r:240:LEU:HA	17:r:243:ILE:HG22	2.01	0.43
19:1:173:GLU:HA	19:1:176:ARG:HG2	2.00	0.43
19:5:173:GLU:HA	19:5:176:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:7:75:PRO:HB2	19:7:216:LEU:HD12	2.00	0.43
2:B:109:LEU:HA	2:B:112:ILE:HD12	2.00	0.43
4:D:187:GLN:OE1	4:D:193:THR:N	2.45	0.43
4:d:266:ARG:O	4:d:270:PHE:HB2	2.18	0.43
25:N:606:CHL:HBA2	25:N:606:CHL:H3A	1.83	0.43
19:g:160:ALA:O	19:g:164:THR:CB	2.66	0.43
20:4:221:LEU:HG	20:4:225:LYS:HE3	1.99	0.43
1:A:216:GLY:O	1:A:220:THR:OG1	2.31	0.43
3:C:186:TYR:HA	3:C:196:VAL:HA	2.01	0.43
2:b:141:ILE:HG13	2:b:217:LEU:HD21	2.01	0.43
4:d:58:SER:O	4:d:63:GLY:N	2.51	0.43
17:R:240:LEU:HA	17:R:243:ILE:HG22	2.01	0.43
19:N:100:VAL:HG22	19:N:216:LEU:HD21	2.00	0.43
17:r:62:ALA:HA	20:4:172:VAL:HG21	2.01	0.43
17:r:241:ALA:O	17:r:245:HIS:ND1	2.48	0.43
17:r:283:ILE:N	20:4:144:SER:OG	2.20	0.43
19:n:160:ALA:O	19:n:164:THR:CB	2.66	0.43
19:y:170:GLY:N	25:y:609:CHL:HAB	2.33	0.43
19:1:218:ASN:OD1	22:1:612:CLA:NB	2.51	0.43
19:2:173:GLU:HA	19:2:176:ARG:HG2	2.00	0.43
22:2:609:CLA:H3A	22:2:609:CLA:HBA2	1.82	0.43
19:3:173:GLU:HA	19:3:176:ARG:HG2	2.00	0.43
1:A:77:ILE:HB	10:L:34:ASN:HD21	1.83	0.43
3:C:199:ILE:HD11	3:C:230:LEU:HB2	2.00	0.43
1:a:269:ARG:NH1	4:d:235:ALA:O	2.51	0.43
18:s:110:TYR:HA	18:s:113:PHE:HD2	1.83	0.43
19:g:100:VAL:HG22	19:g:216:LEU:HD21	1.99	0.43
16:z:24:PRO:O	16:z:28:ALA:HB3	2.18	0.43
3:c:447:ARG:HD3	22:c:508:CLA:HED3	2.00	0.43
18:s:114:GLU:O	18:s:118:ALA:CB	2.66	0.43
19:y:100:VAL:HG22	19:y:216:LEU:HD21	2.00	0.43
19:5:75:PRO:HB2	19:5:216:LEU:HD12	2.00	0.43
2:B:384:ARG:HH22	4:D:349:ARG:NE	2.16	0.43
3:C:430:HIS:CD2	22:C:501:CLA:NC	2.87	0.43
17:R:284:ILE:CG2	20:8:141:SER:O	2.67	0.43
18:S:239:PHE:O	18:S:243:ALA:HB3	2.19	0.43
18:S:260:ASP:HB3	18:S:263:GLY:HA3	2.00	0.43
18:s:114:GLU:O	18:s:118:ALA:HB2	2.19	0.43
19:3:50:TRP:HE1	22:3:311:CLA:HED2	1.84	0.43
19:5:218:ASN:OD1	22:5:612:CLA:NB	2.51	0.43
1:A:133:LEU:HD12	1:A:136:ARG:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:23:HIS:CD2	24:F:101:HEM:NC	2.87	0.43
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.53	0.43
19:6:176:ARG:NH1	25:6:607:CHL:O1D	2.52	0.43
1:A:56:PRO:HA	1:A:73:TYR:HE2	1.84	0.43
1:A:91:LEU:HD11	1:A:163:ILE:HA	2.01	0.43
10:L:18:LEU:HD22	11:M:26:TYR:CD1	2.53	0.43
12:o:162:LYS:HE2	12:o:202:GLN:HB3	2.01	0.43
18:S:110:TYR:HA	18:S:113:PHE:HD2	1.83	0.43
22:Y:610:CLA:HBA2	22:Y:610:CLA:H3A	1.81	0.43
18:s:239:PHE:O	18:s:243:ALA:HB3	2.19	0.43
19:y:160:ALA:O	19:y:164:THR:CB	2.66	0.43
20:4:173:GLU:O	22:4:301:CLA:CAB	2.64	0.43
1:a:32:TRP:CE3	8:i:22:GLY:HA3	2.54	0.42
3:c:233:ILE:HD13	3:c:233:ILE:HA	1.81	0.42
18:S:73:ASP:HB2	22:S:301:CLA:CBD	2.45	0.42
18:S:114:GLU:O	18:S:118:ALA:HB2	2.19	0.42
17:r:62:ALA:HA	20:4:172:VAL:HB	2.01	0.42
17:r:284:ILE:CG2	20:4:141:SER:O	2.67	0.42
19:g:104:ARG:NH1	25:g:608:CHL:OBD	2.51	0.42
19:6:160:ALA:O	19:6:164:THR:OG1	2.32	0.42
19:6:216:LEU:HD23	19:6:216:LEU:HA	1.87	0.42
20:8:101:ALA:O	20:8:105:HIS:ND1	2.38	0.42
3:C:308:GLU:O	3:C:312:ALA:CB	2.67	0.42
4:D:52:GLY:HA2	4:D:56:VAL:HB	2.01	0.42
1:a:304:GLN:HA	1:a:313:VAL:HG11	2.02	0.42
2:b:201:HIS:HE2	22:b:603:CLA:C1B	2.31	0.42
6:f:11:THR:OG1	6:f:12:VAL:N	2.51	0.42
16:z:15:THR:HA	16:z:18:ILE:HD12	2.01	0.42
3:c:154:ARG:HB3	3:c:256:PRO:HG2	2.00	0.42
17:R:62:ALA:HB1	20:8:172:VAL:HG23	1.64	0.42
18:S:114:GLU:O	18:S:118:ALA:CB	2.66	0.42
17:r:278:PRO:HD3	22:2:613:CLA:CBB	2.39	0.42
22:s:303:CLA:HBB2	22:s:304:CLA:HHB	2.01	0.42
19:2:176:ARG:NH1	25:2:607:CHL:O1D	2.52	0.42
19:7:50:TRP:HE1	22:7:311:CLA:HED2	1.84	0.42
20:8:152:LEU:HA	20:8:155:TRP:HD1	1.85	0.42
2:B:114:HIS:HE1	22:B:616:CLA:C1D	2.31	0.42
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.53	0.42
3:C:182:PHE:CE2	22:S:314:CLA:HMB1	2.53	0.42
12:O:162:LYS:HE2	12:O:202:GLN:HB3	2.01	0.42
16:Z:42:SER:O	16:Z:46:LEU:CB	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:606:CHL:HBA2	25:Y:606:CHL:H3A	1.66	0.42
19:g:69:TYR:OH	19:g:81:ASP:OD2	2.31	0.42
19:g:99:GLU:HG3	19:g:223:MET:HE1	2.02	0.42
25:6:601:CHL:HBC2	22:6:610:CLA:C4B	2.49	0.42
24:F:101:HEM:HBB2	24:F:101:HEM:HHC	2.01	0.42
16:Z:15:THR:HA	16:Z:18:ILE:HD12	2.01	0.42
1:a:133:LEU:HD12	1:a:136:ARG:HB2	2.01	0.42
2:b:413:ASP:N	2:b:413:ASP:OD1	2.50	0.42
3:c:308:GLU:O	3:c:312:ALA:CB	2.68	0.42
19:N:99:GLU:HG3	19:N:223:MET:HE1	2.02	0.42
20:4:144:SER:O	20:4:148:THR:OG1	2.30	0.42
20:4:152:LEU:HA	20:4:155:TRP:HD1	1.85	0.42
19:6:130:VAL:HB	19:6:133:LYS:HB2	2.02	0.42
9:K:28:GLU:O	9:K:31:ALA:HB3	2.19	0.42
1:a:91:LEU:HD11	1:a:163:ILE:HA	2.01	0.42
2:b:139:PHE:O	2:b:143:LEU:CB	2.68	0.42
19:G:104:ARG:NH1	25:G:608:CHL:OBD	2.51	0.42
19:Y:99:GLU:HG3	19:Y:223:MET:HE1	2.02	0.42
20:4:73:LEU:HD21	22:4:303:CLA:HAA1	2.00	0.42
22:A:402:CLA:HAB	22:A:402:CLA:HHC	1.85	0.42
2:B:141:ILE:HG13	2:B:217:LEU:HD21	2.01	0.42
1:a:126:TYR:OH	23:a:404:PHO:O1D	2.35	0.42
2:b:151:PHE:HB2	2:b:206:GLY:HA3	2.00	0.42
23:d:402:PHO:HED2	23:d:402:PHO:H2A	2.02	0.42
12:o:185:SER:HA	12:o:223:LYS:HA	2.00	0.42
16:z:19:LEU:HD11	16:z:44:THR:HA	2.01	0.42
3:c:42:LEU:HD23	3:c:45:LEU:HD12	2.01	0.42
3:c:186:TYR:HA	3:c:196:VAL:HA	2.01	0.42
17:R:62:ALA:HA	20:8:172:VAL:HB	2.01	0.42
17:R:145:ARG:HD3	22:R:308:CLA:HAC2	2.01	0.42
19:G:99:GLU:HG3	19:G:223:MET:HE1	2.02	0.42
19:N:50:TRP:HE1	22:N:611:CLA:HED2	1.84	0.42
18:s:240:PHE:O	18:s:244:TYR:HB2	2.20	0.42
25:4:306:CHL:HMC	25:4:307:CHL:C4C	2.50	0.42
2:B:151:PHE:HB2	2:B:206:GLY:HA3	2.00	0.42
2:B:348:ASN:OD1	2:B:352:ARG:N	2.53	0.42
11:M:16:LEU:HD23	11:m:16:LEU:HD23	2.02	0.42
2:b:109:LEU:HA	2:b:112:ILE:HD12	2.00	0.42
9:k:52:PHE:O	9:k:55:GLN:HB2	2.20	0.42
3:c:184:GLY:HA3	3:c:197:ARG:O	2.20	0.42
18:S:167:ILE:HB	18:S:169:ILE:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:59:TYR:N	20:4:173:GLU:HA	2.35	0.42
19:n:50:TRP:HE1	22:n:611:CLA:HED2	1.84	0.42
19:y:99:GLU:HG3	19:y:223:MET:HE1	2.02	0.42
25:1:606:CHL:HBA2	25:1:606:CHL:H3A	1.83	0.42
25:2:601:CHL:HBC2	22:2:610:CLA:C4B	2.49	0.42
20:8:202:PRO:HG2	20:8:203:LEU:HD12	2.01	0.42
20:8:224:LEU:HB3	22:8:310:CLA:HHB	2.02	0.42
1:A:304:GLN:HA	1:A:313:VAL:HG11	2.02	0.42
2:B:139:PHE:O	2:B:143:LEU:CB	2.68	0.42
1:a:56:PRO:HA	1:a:73:TYR:HE2	1.84	0.42
5:e:28:PRO:HA	5:e:31:PHE:HB3	2.02	0.42
12:o:309:SER:N	12:o:319:LYS:O	2.49	0.42
3:c:299:SER:OG	3:c:308:GLU:OE1	2.29	0.42
17:r:56:PRO:HA	20:4:174:TRP:CD1	2.55	0.42
18:s:242:GLN:O	18:s:246:THR:OG1	2.25	0.42
19:7:130:VAL:HB	19:7:133:LYS:HB2	2.02	0.42
19:7:228:GLY:O	19:7:232:GLN:CB	2.65	0.42
1:A:140:ARG:HE	1:A:142:TRP:HZ3	1.67	0.42
2:B:252:VAL:HG12	22:B:603:CLA:CGA	2.50	0.42
9:K:52:PHE:O	9:K:55:GLN:HB2	2.20	0.42
9:k:28:GLU:O	9:k:31:ALA:HB3	2.19	0.42
17:R:56:PRO:HA	20:8:174:TRP:CD1	2.55	0.42
18:S:240:PHE:O	18:S:244:TYR:HB2	2.20	0.42
19:G:247:HIS:HB2	22:G:613:CLA:HAA2	2.02	0.42
17:r:63:ILE:CG1	20:4:166:ASN:ND2	2.82	0.42
19:g:247:HIS:HB2	22:g:613:CLA:HAA2	2.02	0.42
19:n:252:VAL:O	19:n:255:ASN:ND2	2.53	0.42
19:y:252:VAL:O	19:y:255:ASN:ND2	2.53	0.42
22:2:602:CLA:H3A	22:2:602:CLA:HBA2	1.69	0.42
25:5:601:CHL:HED3	25:5:601:CHL:HBA1	2.02	0.42
1:A:41:LEU:O	1:A:45:THR:CB	2.68	0.42
2:B:453:PHE:HB2	4:D:292:LEU:HD12	2.01	0.42
3:C:131:TYR:HH	18:S:74:GLY:HA2	1.79	0.42
4:D:107:GLN:HE21	5:E:48:GLY:HA3	1.84	0.42
4:D:299:PHE:HD2	4:D:316:TYR:CZ	2.38	0.42
5:E:28:PRO:HA	5:E:31:PHE:HB3	2.02	0.42
2:b:109:LEU:HD23	2:b:112:ILE:HD12	2.01	0.42
17:R:59:TYR:N	20:8:173:GLU:HA	2.35	0.42
17:R:166:GLN:HE22	17:R:267:PRO:HD3	1.84	0.42
19:N:252:VAL:O	19:N:255:ASN:ND2	2.53	0.42
17:r:255:GLY:O	17:r:259:GLN:CB	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:274:HIS:CG	22:r:311:CLA:HAA2	2.55	0.42
18:s:167:ILE:HB	18:s:169:ILE:H	1.84	0.42
19:2:152:LEU:HD23	19:2:152:LEU:HA	1.90	0.42
19:3:75:PRO:HB2	19:3:216:LEU:HD12	2.00	0.42
19:3:130:VAL:HB	19:3:133:LYS:HB2	2.02	0.42
19:6:228:GLY:O	19:6:232:GLN:CB	2.65	0.42
3:C:42:LEU:HB3	3:C:49:LEU:HD13	2.01	0.41
3:C:154:ARG:HB3	3:C:256:PRO:HG2	2.00	0.41
12:O:145:VAL:HG22	12:O:321:VAL:HG22	2.02	0.41
2:b:464:PHE:HB2	4:d:281:TRP:CZ3	2.55	0.41
4:d:52:GLY:HA2	4:d:56:VAL:HB	2.01	0.41
4:d:58:SER:OG	4:d:80:SER:OG	2.38	0.41
4:d:168:TRP:O	4:d:171:ALA:CB	2.68	0.41
22:N:602:CLA:H3A	22:N:602:CLA:HBA2	1.83	0.41
19:Y:69:TYR:OH	19:Y:81:ASP:OD2	2.31	0.41
17:r:59:TYR:N	20:4:173:GLU:CG	2.79	0.41
19:y:152:LEU:HD23	19:y:152:LEU:HA	1.86	0.41
19:y:161:ILE:HG12	25:y:605:CHL:HAC1	2.02	0.41
20:4:159:LYS:HE2	22:4:301:CLA:HHB	2.02	0.41
20:4:202:PRO:HG2	20:4:203:LEU:HD12	2.01	0.41
1:A:217:SER:O	1:A:221:SER:OG	2.32	0.41
3:C:273:SER:HA	3:C:276:LEU:HD12	2.02	0.41
12:o:145:VAL:HG22	12:o:321:VAL:HG22	2.02	0.41
17:R:63:ILE:CG1	20:8:166:ASN:ND2	2.82	0.41
17:R:255:GLY:O	17:R:259:GLN:CB	2.57	0.41
19:G:252:VAL:O	19:G:255:ASN:ND2	2.53	0.41
22:G:610:CLA:H3A	22:G:610:CLA:HBA2	1.79	0.41
19:Y:161:ILE:HG12	25:Y:605:CHL:HAC1	2.02	0.41
19:Y:252:VAL:O	19:Y:255:ASN:ND2	2.53	0.41
17:r:61:GLY:CA	20:4:169:SER:CB	2.96	0.41
17:r:145:ARG:HA	17:r:148:MET:HE3	2.01	0.41
17:r:145:ARG:HD3	22:r:308:CLA:HAC2	2.01	0.41
19:2:130:VAL:HB	19:2:133:LYS:HB2	2.02	0.41
19:3:99:GLU:OE2	19:3:220:ARG:NE	2.54	0.41
2:B:109:LEU:HD23	2:B:112:ILE:HD12	2.01	0.41
4:D:107:GLN:NE2	5:E:48:GLY:HA3	2.35	0.41
3:c:273:SER:HA	3:c:276:LEU:HD12	2.02	0.41
17:R:59:TYR:N	20:8:173:GLU:CG	2.79	0.41
17:R:145:ARG:HA	17:R:148:MET:HE3	2.01	0.41
17:R:157:VAL:O	17:R:161:THR:OG1	2.34	0.41
22:S:303:CLA:HBB2	22:S:304:CLA:HHB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:141:CYS:HA	18:s:145:ALA:HB2	2.01	0.41
19:g:252:VAL:O	19:g:255:ASN:ND2	2.53	0.41
22:g:610:CLA:H3A	22:g:610:CLA:HBA2	1.79	0.41
20:4:224:LEU:HB3	22:4:310:CLA:HHB	2.02	0.41
19:5:130:VAL:HB	19:5:133:LYS:HB2	2.02	0.41
1:A:59:ASP:OD2	1:A:64:ARG:N	2.53	0.41
2:B:187:VAL:HG12	22:B:601:CLA:HBC3	2.03	0.41
3:C:184:GLY:HA3	3:C:197:ARG:O	2.20	0.41
1:a:41:LEU:O	1:a:45:THR:CB	2.68	0.41
1:a:59:ASP:OD2	1:a:64:ARG:N	2.53	0.41
1:a:269:ARG:O	1:a:273:PHE:HB2	2.21	0.41
4:d:189:PHE:HD1	4:d:327:ARG:HG2	1.86	0.41
4:d:251:ASN:O	4:d:255:SER:OG	2.29	0.41
3:c:228:ASP:HA	3:c:362:ARG:NH2	2.36	0.41
17:R:274:HIS:CG	22:R:311:CLA:HAA2	2.55	0.41
18:S:141:CYS:HA	18:S:145:ALA:HB2	2.01	0.41
17:r:166:GLN:HE22	17:r:267:PRO:HD3	1.84	0.41
25:y:606:CHL:HBA2	25:y:606:CHL:H3A	1.66	0.41
19:6:99:GLU:OE2	19:6:220:ARG:NE	2.54	0.41
3:C:42:LEU:HD23	3:C:45:LEU:HD12	2.01	0.41
4:D:193:THR:HG23	22:D:403:CLA:HBC2	2.03	0.41
13:T:8:PHE:O	13:T:12:SER:OG	2.31	0.41
16:Z:19:LEU:HD11	16:Z:44:THR:HA	2.01	0.41
2:b:137:LYS:HB2	2:b:137:LYS:HE2	1.91	0.41
4:d:299:PHE:HD2	4:d:316:TYR:CZ	2.38	0.41
19:Y:144:LEU:HD23	25:Y:606:CHL:HMD2	2.03	0.41
17:r:285:ASP:H	20:4:141:SER:HB3	1.81	0.41
19:n:173:GLU:HA	19:n:176:ARG:HG2	2.03	0.41
19:1:130:VAL:HB	19:1:133:LYS:HB2	2.02	0.41
19:2:99:GLU:OE2	19:2:220:ARG:NE	2.54	0.41
20:4:242:PHE:O	20:4:246:ALA:HB3	2.21	0.41
22:8:301:CLA:H3A	22:8:301:CLA:HBA2	1.85	0.41
3:C:215:LYS:NZ	3:C:223:TRP:O	2.47	0.41
16:Z:12:LEU:O	16:Z:16:SER:OG	2.34	0.41
1:a:97:TRP:CD1	8:i:5:LYS:HD2	2.56	0.41
1:a:269:ARG:O	1:a:273:PHE:CB	2.69	0.41
2:b:237:VAL:HG22	22:b:610:CLA:HBC2	2.03	0.41
2:b:348:ASN:OD1	2:b:352:ARG:N	2.53	0.41
4:d:254:TRP:O	4:d:259:GLY:N	2.45	0.41
3:c:42:LEU:HB3	3:c:49:LEU:HD13	2.02	0.41
3:c:293:ASN:HD21	3:c:296:ALA:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:89:VAL:HB	18:S:92:ASP:HB2	2.03	0.41
19:G:229:PHE:O	19:G:233:ALA:HB2	2.21	0.41
19:N:229:PHE:O	19:N:233:ALA:HB2	2.21	0.41
17:r:275:LEU:CB	22:2:613:CLA:HMB3	2.51	0.41
19:g:161:ILE:HG12	25:g:605:CHL:HAC1	2.02	0.41
19:1:265:PRO:HD3	25:1:615:CHL:HAA2	2.03	0.41
25:2:601:CHL:O1A	25:2:601:CHL:HBD	2.21	0.41
25:8:306:CHL:HMC	25:8:307:CHL:C4C	2.50	0.41
3:C:100:GLY:N	3:C:104:GLU:O	2.36	0.41
22:b:614:CLA:HHD	11:m:21:PHE:CZ	2.56	0.41
17:R:62:ALA:HA	20:8:172:VAL:HG21	2.01	0.41
18:S:230:ARG:NH2	22:S:303:CLA:O2D	2.54	0.41
19:N:104:ARG:HD3	22:N:610:CLA:HAC2	2.03	0.41
19:Y:229:PHE:O	19:Y:233:ALA:HB2	2.21	0.41
19:7:99:GLU:OE2	19:7:220:ARG:NE	2.54	0.41
1:A:57:PRO:O	12:O:208:ARG:NH1	2.47	0.41
2:B:22:VAL:HG22	22:B:614:CLA:HMB2	2.03	0.41
3:C:119:LEU:O	3:C:122:SER:OG	2.33	0.41
4:D:181:ARG:O	4:D:185:PHE:CB	2.65	0.41
4:D:251:ASN:O	4:D:255:SER:OG	2.29	0.41
17:R:168:ALA:O	17:R:172:GLU:CB	2.67	0.41
22:r:311:CLA:H2A	22:r:311:CLA:HED3	2.03	0.41
19:n:104:ARG:HD3	22:n:610:CLA:HAC2	2.03	0.41
19:5:99:GLU:OE2	19:5:220:ARG:NE	2.53	0.41
25:7:307:CHL:HBA2	25:7:307:CHL:H3A	1.87	0.41
2:B:132:SER:O	7:H:27:ASN:ND2	2.54	0.41
2:B:359:MET:HE2	2:B:366:PHE:HB3	2.03	0.41
22:B:616:CLA:HAB	22:B:616:CLA:HHC	1.86	0.41
3:C:444:HIS:HE1	22:C:508:CLA:NA	2.15	0.41
4:D:257:ILE:HD13	4:D:257:ILE:HA	1.91	0.41
10:L:12:GLU:HA	11:M:29:THR:HA	2.02	0.41
11:M:24:ILE:HG23	11:m:27:VAL:HG21	2.03	0.41
12:O:309:SER:N	12:O:319:LYS:O	2.49	0.41
2:b:434:ARG:HA	2:b:439:SER:HB2	2.03	0.41
5:e:19:TYR:HE1	24:e:101:HEM:C4D	2.39	0.41
17:R:61:GLY:CA	20:8:169:SER:CB	2.96	0.41
18:S:196:PHE:HA	25:S:308:CHL:HBC1	2.03	0.41
22:Y:611:CLA:HBA2	22:Y:611:CLA:H3A	1.75	0.41
17:r:157:VAL:O	17:r:161:THR:OG1	2.34	0.41
17:r:168:ALA:O	17:r:172:GLU:CB	2.67	0.41
19:n:99:GLU:HG3	19:n:223:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:y:144:LEU:HD23	25:y:606:CHL:HMD2	2.03	0.41
19:1:50:TRP:HE1	22:1:611:CLA:HED2	1.86	0.41
25:1:601:CHL:HED3	25:1:601:CHL:HBA1	2.02	0.41
20:4:181:THR:HG21	20:4:198:ARG:HD2	2.02	0.41
1:A:269:ARG:O	1:A:273:PHE:CB	2.69	0.41
2:B:234:ILE:HG23	22:B:612:CLA:HBC1	2.03	0.41
3:C:293:ASN:HD21	3:C:296:ALA:HB3	1.86	0.41
3:C:466:VAL:HG11	4:D:248:VAL:HG12	2.03	0.41
4:D:168:TRP:O	4:D:171:ALA:CB	2.69	0.41
16:Z:40:VAL:O	16:Z:44:THR:HB	2.21	0.41
4:d:94:TRP:CD1	15:x:86:PHE:HA	2.56	0.41
4:d:189:PHE:CD1	4:d:327:ARG:HG2	2.56	0.41
17:R:283:ILE:O	20:8:143:GLY:HA3	2.21	0.41
19:G:173:GLU:HA	19:G:176:ARG:HG2	2.03	0.41
18:s:89:VAL:HB	18:s:92:ASP:HB2	2.03	0.41
18:s:230:ARG:NH2	22:s:303:CLA:O2D	2.54	0.41
19:n:130:VAL:HB	19:n:133:LYS:HB2	2.03	0.41
19:5:160:ALA:O	19:5:164:THR:OG1	2.32	0.41
25:6:601:CHL:O1A	25:6:601:CHL:HBD	2.21	0.41
2:B:434:ARG:HA	2:B:439:SER:HB2	2.03	0.40
3:C:387:TRP:O	3:C:391:ARG:HG2	2.21	0.40
4:d:202:VAL:HG22	22:d:403:CLA:C1B	2.51	0.40
6:f:14:TRP:O	6:f:18:HIS:ND1	2.51	0.40
17:R:275:LEU:CB	22:6:613:CLA:HMB3	2.51	0.40
19:N:52:GLY:H	19:N:72:GLY:HA3	1.86	0.40
19:2:153:VAL:HA	25:2:605:CHL:C4D	2.51	0.40
19:6:153:VAL:HA	25:6:605:CHL:C4D	2.51	0.40
2:B:365:THR:HG21	4:D:324:GLU:HG2	2.02	0.40
3:C:228:ASP:HA	3:C:362:ARG:NH2	2.36	0.40
3:C:457:LYS:HG2	4:D:229:GLY:HA2	2.03	0.40
4:D:202:VAL:HG22	22:D:403:CLA:C1B	2.51	0.40
1:a:140:ARG:HE	1:a:142:TRP:HZ3	1.67	0.40
22:d:403:CLA:HAB	22:d:403:CLA:HHC	1.80	0.40
12:o:135:LYS:O	12:o:330:GLN:N	2.53	0.40
19:G:52:GLY:H	19:G:72:GLY:HA3	1.86	0.40
19:Y:173:GLU:HA	19:Y:176:ARG:HG2	2.03	0.40
18:s:73:ASP:CB	22:s:301:CLA:CED	2.93	0.40
22:n:602:CLA:H3A	22:n:602:CLA:HBA2	1.83	0.40
19:1:264:VAL:HG13	25:1:615:CHL:HED1	2.03	0.40
22:5:610:CLA:H3A	22:5:610:CLA:HBA2	1.82	0.40
20:8:159:LYS:HE2	22:8:301:CLA:HHB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:8:181:THR:HG21	20:8:198:ARG:HD2	2.02	0.40
1:A:269:ARG:O	1:A:273:PHE:HB2	2.21	0.40
1:A:329:GLU:HA	1:A:332:HIS:CE1	2.56	0.40
1:a:227:THR:HG21	1:a:236:GLY:HA3	2.03	0.40
1:a:329:GLU:HA	1:a:332:HIS:CE1	2.56	0.40
3:c:387:TRP:O	3:c:391:ARG:HG2	2.21	0.40
3:c:438:PHE:CE1	22:c:505:CLA:HAB	2.56	0.40
19:G:161:ILE:HG12	25:G:605:CHL:HAC1	2.02	0.40
19:1:67:PRO:HB2	19:1:70:LEU:HB2	2.04	0.40
19:5:67:PRO:HB2	19:5:70:LEU:HB2	2.04	0.40
19:5:216:LEU:HD23	19:5:216:LEU:HA	1.87	0.40
2:b:230:ARG:HH21	4:d:135:ARG:HH21	1.69	0.40
3:c:100:GLY:N	3:c:104:GLU:O	2.36	0.40
17:R:156:SER:O	17:R:160:LEU:HB2	2.22	0.40
19:N:173:GLU:HA	19:N:176:ARG:HG2	2.03	0.40
19:N:247:HIS:HB2	22:N:613:CLA:HAA2	2.04	0.40
19:Y:52:GLY:H	19:Y:72:GLY:HA3	1.86	0.40
18:s:240:PHE:O	18:s:244:TYR:CB	2.70	0.40
22:g:611:CLA:H2A	22:g:611:CLA:HED3	2.04	0.40
19:y:229:PHE:O	19:y:233:ALA:HB2	2.21	0.40
19:1:99:GLU:OE2	19:1:220:ARG:NE	2.53	0.40
19:3:160:ALA:O	19:3:164:THR:OG1	2.32	0.40
20:4:136:ALA:HB1	25:4:306:CHL:HMD1	2.03	0.40
19:6:67:PRO:HB2	19:6:70:LEU:HB2	2.04	0.40
4:D:189:PHE:HD1	4:D:327:ARG:HG2	1.86	0.40
4:D:189:PHE:CD1	4:D:327:ARG:HG2	2.56	0.40
2:b:9:HIS:HB2	22:b:611:CLA:CGA	2.52	0.40
2:b:17:GLY:HA2	2:b:20:LEU:HD12	2.04	0.40
22:b:614:CLA:HHD	11:m:21:PHE:HZ	1.86	0.40
16:z:40:VAL:O	16:z:44:THR:HB	2.21	0.40
18:S:240:PHE:O	18:S:244:TYR:CB	2.70	0.40
18:S:265:ASN:O	18:S:268:THR:OG1	2.39	0.40
22:G:611:CLA:H2A	22:G:611:CLA:HED3	2.04	0.40
19:N:152:LEU:HA	19:N:152:LEU:HD23	1.86	0.40
19:Y:130:VAL:HB	19:Y:133:LYS:HB2	2.03	0.40
25:Y:606:CHL:HBB2	25:Y:607:CHL:HBB1	2.04	0.40
19:n:75:PRO:HB2	19:n:216:LEU:HD12	2.04	0.40
19:y:52:GLY:H	19:y:72:GLY:HA3	1.86	0.40
19:y:130:VAL:HB	19:y:133:LYS:HB2	2.03	0.40
20:8:242:PHE:O	20:8:246:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	303/343 (88%)	282 (93%)	21 (7%)	0	100	100
1	a	328/343 (96%)	306 (93%)	22 (7%)	0	100	100
2	B	476/507 (94%)	448 (94%)	28 (6%)	0	100	100
2	b	476/507 (94%)	448 (94%)	28 (6%)	0	100	100
3	C	429/459 (94%)	401 (94%)	28 (6%)	0	100	100
3	c	429/459 (94%)	402 (94%)	27 (6%)	0	100	100
4	D	334/352 (95%)	308 (92%)	26 (8%)	0	100	100
4	d	334/352 (95%)	307 (92%)	27 (8%)	0	100	100
5	E	68/83 (82%)	59 (87%)	9 (13%)	0	100	100
5	e	68/83 (82%)	59 (87%)	9 (13%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	0	100	100
6	f	27/39 (69%)	27 (100%)	0	0	100	100
7	H	50/72 (69%)	44 (88%)	6 (12%)	0	100	100
7	h	50/72 (69%)	44 (88%)	6 (12%)	0	100	100
8	I	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
8	i	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
9	K	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
9	k	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
10	L	34/38 (90%)	28 (82%)	6 (18%)	0	100	100
10	l	34/38 (90%)	28 (82%)	6 (18%)	0	100	100
11	M	27/34 (79%)	27 (100%)	0	0	100	100
11	m	27/34 (79%)	27 (100%)	0	0	100	100
12	O	187/247 (76%)	162 (87%)	24 (13%)	1 (0%)	24	63
12	o	187/247 (76%)	163 (87%)	23 (12%)	1 (0%)	24	63
13	T	27/33 (82%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	t	27/33 (82%)	27 (100%)	0	0	100	100
14	W	44/54 (82%)	39 (89%)	5 (11%)	0	100	100
14	w	44/54 (82%)	39 (89%)	5 (11%)	0	100	100
15	X	30/116 (26%)	29 (97%)	1 (3%)	0	100	100
15	x	30/116 (26%)	29 (97%)	1 (3%)	0	100	100
16	Z	59/62 (95%)	59 (100%)	0	0	100	100
16	z	59/62 (95%)	59 (100%)	0	0	100	100
17	R	184/250 (74%)	172 (94%)	12 (6%)	0	100	100
17	r	184/250 (74%)	172 (94%)	12 (6%)	0	100	100
18	S	212/232 (91%)	171 (81%)	41 (19%)	0	100	100
18	s	212/232 (91%)	171 (81%)	41 (19%)	0	100	100
19	1	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	2	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	3	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	5	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	6	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	7	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	G	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	N	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	Y	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	g	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	n	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	y	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
20	4	202/210 (96%)	184 (91%)	18 (9%)	0	100	100
20	8	202/210 (96%)	184 (91%)	18 (9%)	0	100	100
All	All	8149/9096 (90%)	7521 (92%)	626 (8%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	O	194	ILE
12	o	194	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/278 (89%)	247 (100%)	0	100	100
1	a	267/278 (96%)	267 (100%)	0	100	100
2	B	379/401 (94%)	379 (100%)	0	100	100
2	b	379/401 (94%)	379 (100%)	0	100	100
3	C	340/359 (95%)	340 (100%)	0	100	100
3	c	340/359 (95%)	340 (100%)	0	100	100
4	D	269/282 (95%)	269 (100%)	0	100	100
4	d	269/282 (95%)	269 (100%)	0	100	100
5	E	63/73 (86%)	63 (100%)	0	100	100
5	e	63/73 (86%)	63 (100%)	0	100	100
6	F	24/34 (71%)	24 (100%)	0	100	100
6	f	24/34 (71%)	24 (100%)	0	100	100
7	H	43/60 (72%)	43 (100%)	0	100	100
7	h	43/60 (72%)	43 (100%)	0	100	100
8	I	32/33 (97%)	32 (100%)	0	100	100
8	i	32/33 (97%)	32 (100%)	0	100	100
9	K	31/32 (97%)	31 (100%)	0	100	100
9	k	31/32 (97%)	31 (100%)	0	100	100
10	L	34/36 (94%)	34 (100%)	0	100	100
10	l	34/36 (94%)	34 (100%)	0	100	100
11	M	25/30 (83%)	25 (100%)	0	100	100
11	m	25/30 (83%)	24 (96%)	1 (4%)	28	48
12	O	164/204 (80%)	164 (100%)	0	100	100
12	o	164/204 (80%)	164 (100%)	0	100	100
13	T	26/30 (87%)	26 (100%)	0	100	100
13	t	26/30 (87%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	W	40/47 (85%)	40 (100%)	0	100	100
14	w	40/47 (85%)	40 (100%)	0	100	100
15	X	27/92 (29%)	27 (100%)	0	100	100
15	x	27/92 (29%)	27 (100%)	0	100	100
16	Z	53/54 (98%)	53 (100%)	0	100	100
16	z	53/54 (98%)	53 (100%)	0	100	100
17	R	150/201 (75%)	149 (99%)	1 (1%)	76	80
17	r	150/201 (75%)	149 (99%)	1 (1%)	76	80
18	S	165/180 (92%)	163 (99%)	2 (1%)	63	74
18	s	165/180 (92%)	163 (99%)	2 (1%)	63	74
19	1	167/170 (98%)	167 (100%)	0	100	100
19	2	167/170 (98%)	167 (100%)	0	100	100
19	3	167/170 (98%)	167 (100%)	0	100	100
19	5	167/170 (98%)	167 (100%)	0	100	100
19	6	167/170 (98%)	167 (100%)	0	100	100
19	7	167/170 (98%)	167 (100%)	0	100	100
19	G	167/170 (98%)	167 (100%)	0	100	100
19	N	167/170 (98%)	167 (100%)	0	100	100
19	Y	167/170 (98%)	167 (100%)	0	100	100
19	g	167/170 (98%)	167 (100%)	0	100	100
19	n	167/170 (98%)	167 (100%)	0	100	100
19	y	167/170 (98%)	167 (100%)	0	100	100
20	4	156/158 (99%)	156 (100%)	0	100	100
20	8	156/158 (99%)	156 (100%)	0	100	100
All	All	6560/7208 (91%)	6553 (100%)	7 (0%)	87	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	m	16	LEU
17	R	199	ILE
18	S	81	ILE
18	S	169	ILE
17	r	199	ILE

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Mol	Chain	Res	Type
18	s	81	ILE
18	s	169	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	303	ASN
1	A	335	ASN
2	B	79	ASN
2	B	332	ASN
3	C	84	GLN
4	D	84	ASN
4	D	88	HIS
4	D	107	GLN
4	D	221	ASN
4	D	251	ASN
4	D	302	GLN
8	I	26	ASN
9	K	55	GLN
10	L	38	ASN
11	M	32	GLN
12	O	202	GLN
12	O	307	GLN
14	W	99	ASN
16	Z	6	GLN
16	Z	58	ASN
1	a	303	ASN
2	b	79	ASN
2	b	332	ASN
4	d	84	ASN
4	d	107	GLN
4	d	293	ASN
4	d	351	ASN
7	h	27	ASN
10	l	34	ASN
12	o	202	GLN
12	o	307	GLN
3	c	84	GLN
3	c	332	GLN
17	R	134	GLN
17	R	182	GLN

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Mol	Chain	Res	Type
17	R	270	ASN
18	S	86	ASN
18	S	106	ASN
18	S	117	HIS
18	S	257	HIS
18	S	264	ASN
19	G	156	GLN
19	G	243	ASN
19	G	255	ASN
19	N	156	GLN
19	N	243	ASN
19	Y	156	GLN
19	Y	243	ASN
19	Y	255	ASN
17	r	134	GLN
17	r	182	GLN
17	r	270	ASN
18	s	86	ASN
18	s	106	ASN
18	s	117	HIS
18	s	253	ASN
18	s	257	HIS
18	s	264	ASN
19	g	156	GLN
19	g	243	ASN
19	g	255	ASN
19	n	156	GLN
19	n	243	ASN
19	n	255	ASN
19	y	156	GLN
19	y	243	ASN
19	y	255	ASN
19	1	243	ASN
19	2	243	ASN
19	3	243	ASN
20	4	133	GLN
20	4	166	ASN
19	6	243	ASN
19	7	243	ASN
20	8	166	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 316 ligands modelled in this entry, 2 are monoatomic - leaving 314 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	$\#\|Z\| > 2$
22	CLA	B	609	2	49,53,73	2.28	17 (34%)	59,89,113	3.01	31 (52%)
25	CHL	6	606	-	50,54,74	1.61	7 (14%)	56,90,114	1.80	12 (21%)
25	CHL	r	305	-	50,54,74	1.63	7 (14%)	56,90,114	1.86	13 (23%)
22	CLA	r	311	17	49,53,73	2.28	17 (34%)	59,89,113	2.92	28 (47%)
22	CLA	s	304	18	49,53,73	2.20	16 (32%)	59,89,113	2.78	27 (45%)
22	CLA	5	612	19	49,53,73	2.29	19 (38%)	59,89,113	2.89	28 (47%)
22	CLA	g	602	19	49,53,73	2.27	19 (38%)	59,89,113	2.91	27 (45%)
25	CHL	n	605	19	46,50,74	1.48	6 (13%)	51,85,114	1.84	6 (11%)
22	CLA	G	611	-	49,53,73	2.23	15 (30%)	59,89,113	2.97	29 (49%)
22	CLA	7	312	19	49,53,73	2.27	19 (38%)	59,89,113	2.87	27 (45%)
22	CLA	r	302	17	49,53,73	2.29	16 (32%)	59,89,113	2.87	25 (42%)
25	CHL	G	609	19	50,54,74	1.62	7 (14%)	56,90,114	2.16	12 (21%)
22	CLA	g	614	19	49,53,73	2.29	18 (36%)	59,89,113	2.88	27 (45%)
22	CLA	R	302	17	49,53,73	2.29	16 (32%)	59,89,113	2.87	25 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	4	305	-	49,53,73	2.28	20 (40%)	59,89,113	2.92	28 (47%)
22	CLA	b	606	2	49,53,73	2.38	19 (38%)	59,89,113	2.89	28 (47%)
25	CHL	4	302	17	50,54,74	1.60	7 (14%)	56,90,114	1.77	12 (21%)
22	CLA	R	310	17	49,53,73	2.24	17 (34%)	59,89,113	2.85	26 (44%)
22	CLA	C	509	3	49,53,73	2.29	18 (36%)	59,89,113	2.88	29 (49%)
25	CHL	4	309	20	50,54,74	1.58	7 (14%)	56,90,114	1.90	8 (14%)
22	CLA	a	405	1	49,53,73	2.28	16 (32%)	59,89,113	3.02	28 (47%)
22	CLA	b	607	-	49,53,73	2.24	16 (32%)	59,89,113	2.95	31 (52%)
25	CHL	s	307	-	50,54,74	1.63	7 (14%)	56,90,114	5.85	12 (21%)
22	CLA	6	613	19	49,53,73	2.32	19 (38%)	59,89,113	2.80	26 (44%)
22	CLA	S	312	18	49,53,73	2.28	17 (34%)	59,89,113	3.03	32 (54%)
22	CLA	4	311	20	49,53,73	2.30	19 (38%)	59,89,113	2.80	27 (45%)
22	CLA	Y	614	19	49,53,73	2.25	15 (30%)	59,89,113	3.00	28 (47%)
22	CLA	3	305	-	49,53,73	2.29	20 (40%)	59,89,113	2.90	26 (44%)
22	CLA	b	611	2	49,53,73	2.23	15 (30%)	59,89,113	3.04	29 (49%)
22	CLA	b	610	-	49,53,73	2.30	19 (38%)	59,89,113	2.91	26 (44%)
25	CHL	2	606	-	50,54,74	1.61	7 (14%)	56,90,114	1.80	12 (21%)
22	CLA	B	614	2	49,53,73	2.30	15 (30%)	59,89,113	2.90	30 (50%)
22	CLA	c	504	-	49,53,73	2.29	17 (34%)	59,89,113	2.88	28 (47%)
22	CLA	2	604	-	49,53,73	2.30	20 (40%)	59,89,113	2.91	27 (45%)
22	CLA	2	610	-	49,53,73	2.28	18 (36%)	59,89,113	2.87	26 (44%)
22	CLA	R	309	-	49,53,73	2.24	16 (32%)	59,89,113	2.92	28 (47%)
22	CLA	N	603	19	49,53,73	2.24	15 (30%)	59,89,113	2.96	32 (54%)
22	CLA	N	614	19	49,53,73	2.30	20 (40%)	59,89,113	2.85	25 (42%)
25	CHL	Y	608	-	50,54,74	1.61	7 (14%)	56,90,114	1.75	9 (16%)
22	CLA	C	507	-	49,53,73	2.22	16 (32%)	59,89,113	2.96	30 (50%)
22	CLA	y	612	19	49,53,73	2.24	16 (32%)	59,89,113	3.00	31 (52%)
22	CLA	C	511	3	49,53,73	2.29	19 (38%)	59,89,113	2.98	30 (50%)
22	CLA	1	610	19	49,53,73	2.28	17 (34%)	59,89,113	2.88	25 (42%)
25	CHL	4	306	20	50,54,74	1.60	7 (14%)	56,90,114	1.90	13 (23%)
22	CLA	c	503	3	49,53,73	2.24	15 (30%)	59,89,113	2.94	27 (45%)
22	CLA	R	308	17	49,53,73	2.28	16 (32%)	59,89,113	2.91	28 (47%)
22	CLA	r	307	17	49,53,73	2.27	17 (34%)	59,89,113	2.89	27 (45%)
25	CHL	4	308	-	50,54,74	1.61	8 (16%)	56,90,114	5.82	10 (17%)
22	CLA	8	305	-	49,53,73	2.28	20 (40%)	59,89,113	2.92	28 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CHL	N	606	-	50,54,74	1.61	7 (14%)	56,90,114	1.88	12 (21%)
22	CLA	C	506	3	49,53,73	2.26	18 (36%)	59,89,113	2.99	28 (47%)
23	PHO	d	402	-	38,49,69	2.78	13 (34%)	32,75,99	3.41	14 (43%)
24	HEM	F	101	5,6	50,50,50	1.43	4 (8%)	66,82,82	1.37	14 (21%)
22	CLA	N	604	-	49,53,73	2.28	15 (30%)	59,89,113	2.95	29 (49%)
22	CLA	5	603	19	49,53,73	2.26	19 (38%)	59,89,113	2.86	28 (47%)
25	CHL	Y	605	19	46,50,74	1.55	6 (13%)	51,85,114	1.95	10 (19%)
25	CHL	R	304	-	50,54,74	1.64	7 (14%)	56,90,114	1.85	12 (21%)
22	CLA	Y	604	-	49,53,73	2.28	16 (32%)	59,89,113	3.07	28 (47%)
22	CLA	6	612	19	49,53,73	2.28	18 (36%)	59,89,113	2.87	26 (44%)
22	CLA	b	609	2	49,53,73	2.24	17 (34%)	59,89,113	3.03	31 (52%)
22	CLA	C	512	3	49,53,73	2.31	18 (36%)	59,89,113	2.84	27 (45%)
22	CLA	5	613	19	49,53,73	2.29	19 (38%)	59,89,113	2.87	28 (47%)
25	CHL	3	308	-	50,54,74	1.61	7 (14%)	56,90,114	1.69	11 (19%)
22	CLA	b	608	2	49,53,73	2.32	17 (34%)	59,89,113	2.89	29 (49%)
25	CHL	Y	601	19	50,54,74	1.58	6 (12%)	56,90,114	1.84	13 (23%)
22	CLA	s	312	18	49,53,73	2.28	17 (34%)	59,89,113	3.03	32 (54%)
25	CHL	R	306	-	50,54,74	1.61	7 (14%)	56,90,114	1.72	9 (16%)
22	CLA	B	611	2	49,53,73	2.26	15 (30%)	59,89,113	2.96	28 (47%)
25	CHL	g	607	-	50,54,74	1.62	7 (14%)	56,90,114	1.86	13 (23%)
25	CHL	y	607	-	50,54,74	1.62	7 (14%)	56,90,114	1.90	13 (23%)
22	CLA	d	403	4	49,53,73	2.29	16 (32%)	59,89,113	3.08	33 (55%)
22	CLA	3	313	19	49,53,73	2.29	19 (38%)	59,89,113	2.85	26 (44%)
25	CHL	Y	606	-	50,54,74	1.63	6 (12%)	56,90,114	1.80	11 (19%)
23	PHO	a	404	-	38,49,69	2.78	14 (36%)	32,75,99	3.48	14 (43%)
25	CHL	N	605	19	46,50,74	1.48	6 (13%)	51,85,114	1.84	6 (11%)
22	CLA	r	303	-	49,53,73	2.25	15 (30%)	59,89,113	3.06	32 (54%)
22	CLA	c	501	3	49,53,73	2.27	15 (30%)	59,89,113	2.97	26 (44%)
22	CLA	b	616	2	49,53,73	2.25	18 (36%)	59,89,113	3.27	30 (50%)
22	CLA	Y	611	-	49,53,73	2.25	15 (30%)	59,89,113	3.01	25 (42%)
22	CLA	Y	602	19	49,53,73	2.27	17 (34%)	59,89,113	2.94	27 (45%)
25	CHL	8	306	20	50,54,74	1.60	7 (14%)	56,90,114	1.90	13 (23%)
25	CHL	7	301	-	50,54,74	1.62	7 (14%)	56,90,114	1.83	12 (21%)
25	CHL	8	309	20	50,54,74	1.58	7 (14%)	56,90,114	1.90	8 (14%)
22	CLA	5	610	19	49,53,73	2.28	17 (34%)	59,89,113	2.88	25 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	3	304	19	49,53,73	2.28	19 (38%)	59,89,113	2.90	28 (47%)
22	CLA	S	301	3	49,53,73	2.29	16 (32%)	59,89,113	2.94	30 (50%)
22	CLA	y	603	19	49,53,73	2.21	15 (30%)	59,89,113	2.98	30 (50%)
25	CHL	4	307	-	50,54,74	1.61	7 (14%)	56,90,114	1.74	10 (17%)
22	CLA	b	601	-	49,53,73	2.26	16 (32%)	59,89,113	2.85	29 (49%)
22	CLA	a	403	-	49,53,73	2.28	15 (30%)	59,89,113	3.00	28 (47%)
25	CHL	5	615	-	50,54,74	1.61	7 (14%)	56,90,114	1.80	12 (21%)
22	CLA	c	512	3	49,53,73	2.24	18 (36%)	59,89,113	3.00	30 (50%)
25	CHL	R	305	-	50,54,74	1.63	7 (14%)	56,90,114	1.86	13 (23%)
22	CLA	D	403	4	49,53,73	2.27	14 (28%)	59,89,113	3.05	30 (50%)
22	CLA	1	604	-	49,53,73	2.28	19 (38%)	59,89,113	2.89	25 (42%)
25	CHL	6	601	19	50,54,74	1.59	7 (14%)	56,90,114	1.87	10 (17%)
22	CLA	1	603	19	49,53,73	2.26	19 (38%)	59,89,113	2.86	28 (47%)
22	CLA	6	603	19	49,53,73	2.27	19 (38%)	59,89,113	2.84	28 (47%)
22	CLA	4	301	17,20	49,53,73	2.29	18 (36%)	59,89,113	2.88	28 (47%)
25	CHL	S	302	18	50,54,74	1.64	7 (14%)	56,90,114	1.65	9 (16%)
22	CLA	3	311	-	49,53,73	2.29	19 (38%)	59,89,113	2.87	29 (49%)
25	CHL	5	607	-	50,54,74	1.60	7 (14%)	56,90,114	1.85	9 (16%)
22	CLA	R	307	17	49,53,73	2.27	17 (34%)	59,89,113	2.89	27 (45%)
25	CHL	N	608	-	50,54,74	1.62	6 (12%)	56,90,114	1.71	10 (17%)
22	CLA	C	508	3	49,53,73	2.27	18 (36%)	59,89,113	3.04	26 (44%)
22	CLA	G	604	-	49,53,73	2.26	18 (36%)	59,89,113	2.96	30 (50%)
25	CHL	1	609	19	50,54,74	1.61	7 (14%)	56,90,114	2.03	11 (19%)
25	CHL	G	606	-	50,54,74	1.63	7 (14%)	56,90,114	1.82	9 (16%)
22	CLA	2	609	19	49,53,73	2.28	16 (32%)	59,89,113	2.87	24 (40%)
22	CLA	N	612	19	49,53,73	2.23	16 (32%)	59,89,113	2.93	29 (49%)
22	CLA	r	301	17	49,53,73	2.27	16 (32%)	59,89,113	2.91	28 (47%)
22	CLA	7	314	19	49,53,73	2.33	20 (40%)	59,89,113	2.80	27 (45%)
25	CHL	1	607	-	50,54,74	1.60	7 (14%)	56,90,114	1.85	9 (16%)
22	CLA	5	602	19	49,53,73	2.26	19 (38%)	59,89,113	2.85	26 (44%)
22	CLA	n	604	-	49,53,73	2.28	15 (30%)	59,89,113	2.95	29 (49%)
22	CLA	n	603	19	49,53,73	2.24	15 (30%)	59,89,113	2.96	32 (54%)
22	CLA	B	613	2	49,53,73	2.28	17 (34%)	59,89,113	2.96	29 (49%)
22	CLA	7	305	-	49,53,73	2.29	20 (40%)	59,89,113	2.90	26 (44%)
25	CHL	n	608	-	50,54,74	1.62	6 (12%)	56,90,114	1.71	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	Y	603	19	49,53,73	2.21	15 (30%)	59,89,113	2.98	30 (50%)
22	CLA	B	615	2	49,53,73	2.21	16 (32%)	59,89,113	3.13	28 (47%)
24	HEM	e	101	5,6	50,50,50	1.43	5 (10%)	66,82,82	1.42	9 (13%)
22	CLA	B	607	-	49,53,73	2.26	16 (32%)	59,89,113	2.94	28 (47%)
22	CLA	G	602	19	49,53,73	2.27	19 (38%)	59,89,113	2.91	27 (45%)
22	CLA	y	614	19	49,53,73	2.25	15 (30%)	59,89,113	3.00	28 (47%)
25	CHL	1	615	-	50,54,74	1.61	7 (14%)	56,90,114	1.80	12 (21%)
23	PHO	D	402	-	38,49,69	2.78	13 (34%)	32,75,99	3.52	15 (46%)
25	CHL	7	306	19	46,50,74	1.44	6 (13%)	51,85,114	1.87	8 (15%)
22	CLA	Y	613	19	49,53,73	2.26	16 (32%)	59,89,113	3.00	29 (49%)
22	CLA	4	310	20	49,53,73	2.27	18 (36%)	59,89,113	2.80	28 (47%)
25	CHL	6	607	-	50,54,74	1.59	7 (14%)	56,90,114	1.72	9 (16%)
22	CLA	3	314	19	49,53,73	2.33	20 (40%)	59,89,113	2.80	27 (45%)
22	CLA	S	309	18	49,53,73	2.23	16 (32%)	59,89,113	2.84	29 (49%)
25	CHL	7	308	-	50,54,74	1.61	7 (14%)	56,90,114	1.69	11 (19%)
22	CLA	1	614	19	49,53,73	2.29	20 (40%)	59,89,113	3.04	30 (50%)
22	CLA	7	313	19	49,53,73	2.29	19 (38%)	59,89,113	2.85	26 (44%)
22	CLA	d	404	4	49,53,73	2.29	17 (34%)	59,89,113	2.83	28 (47%)
25	CHL	1	608	-	50,54,74	1.61	7 (14%)	56,90,114	1.68	9 (16%)
22	CLA	8	301	17,20	49,53,73	2.29	18 (36%)	59,89,113	2.88	28 (47%)
22	CLA	c	502	3	49,53,73	2.23	17 (34%)	59,89,113	2.90	29 (49%)
25	CHL	1	606	-	50,54,74	1.61	7 (14%)	56,90,114	1.72	11 (19%)
22	CLA	S	311	-	49,53,73	2.28	15 (30%)	59,89,113	2.98	27 (45%)
25	CHL	5	606	-	50,54,74	1.61	7 (14%)	56,90,114	1.72	11 (19%)
22	CLA	d	401	-	49,53,73	2.26	16 (32%)	59,89,113	2.91	29 (49%)
25	CHL	8	302	17	50,54,74	1.60	7 (14%)	56,90,114	1.77	12 (21%)
25	CHL	n	609	19	50,54,74	1.63	7 (14%)	56,90,114	2.11	11 (19%)
25	CHL	n	606	-	50,54,74	1.61	7 (14%)	56,90,114	1.88	12 (21%)
22	CLA	s	303	18	49,53,73	2.26	15 (30%)	59,89,113	2.91	26 (44%)
25	CHL	r	306	-	50,54,74	1.61	7 (14%)	56,90,114	1.72	9 (16%)
22	CLA	1	611	-	49,53,73	2.27	19 (38%)	59,89,113	2.89	26 (44%)
25	CHL	3	307	-	50,54,74	1.61	7 (14%)	56,90,114	1.74	8 (14%)
22	CLA	G	610	19	49,53,73	2.26	15 (30%)	59,89,113	2.89	27 (45%)
22	CLA	B	608	2	49,53,73	2.26	17 (34%)	59,89,113	3.07	28 (47%)
22	CLA	C	503	3	49,53,73	2.27	15 (30%)	59,89,113	2.88	30 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CHL	n	607	-	50,54,74	1.61	6 (12%)	56,90,114	1.99	12 (21%)
25	CHL	r	304	-	50,54,74	1.64	7 (14%)	56,90,114	1.85	12 (21%)
22	CLA	B	616	2	49,53,73	2.26	18 (36%)	59,89,113	2.93	28 (47%)
22	CLA	s	305	-	49,53,73	2.28	16 (32%)	59,89,113	3.02	28 (47%)
22	CLA	c	510	3	49,53,73	2.29	18 (36%)	59,89,113	2.86	26 (44%)
22	CLA	3	312	19	49,53,73	2.27	19 (38%)	59,89,113	2.87	27 (45%)
22	CLA	c	509	3	49,53,73	2.28	14 (28%)	59,89,113	2.83	24 (40%)
22	CLA	2	611	19	49,53,73	2.29	18 (36%)	59,89,113	2.84	26 (44%)
25	CHL	G	607	-	50,54,74	1.62	7 (14%)	56,90,114	1.86	13 (23%)
22	CLA	G	612	19	49,53,73	2.27	16 (32%)	59,89,113	2.93	28 (47%)
22	CLA	Y	612	19	49,53,73	2.24	16 (32%)	59,89,113	3.00	31 (52%)
22	CLA	G	613	19	49,53,73	2.25	15 (30%)	59,89,113	2.93	27 (45%)
22	CLA	1	613	19	49,53,73	2.29	19 (38%)	59,89,113	2.87	28 (47%)
22	CLA	8	310	20	49,53,73	2.27	18 (36%)	59,89,113	2.80	28 (47%)
25	CHL	g	605	19	46,50,74	1.46	6 (13%)	51,85,114	1.81	7 (13%)
22	CLA	B	601	-	49,53,73	2.26	15 (30%)	59,89,113	2.85	26 (44%)
22	CLA	S	313	18	49,53,73	2.27	16 (32%)	59,89,113	2.99	31 (52%)
22	CLA	y	604	-	49,53,73	2.28	16 (32%)	59,89,113	3.07	28 (47%)
22	CLA	c	507	-	49,53,73	2.18	14 (28%)	59,89,113	2.93	31 (52%)
25	CHL	1	601	19	50,54,74	1.58	7 (14%)	56,90,114	1.82	12 (21%)
22	CLA	c	506	3	49,53,73	2.28	19 (38%)	59,89,113	2.99	29 (49%)
23	PHO	A	404	-	38,49,69	2.74	14 (36%)	32,75,99	3.78	14 (43%)
22	CLA	b	605	2	49,53,73	2.33	17 (34%)	59,89,113	2.92	28 (47%)
25	CHL	6	608	19	50,54,74	1.59	7 (14%)	56,90,114	2.04	13 (23%)
25	CHL	8	308	-	50,54,74	1.61	8 (16%)	56,90,114	5.82	10 (17%)
22	CLA	N	611	-	49,53,73	2.25	16 (32%)	59,89,113	2.99	31 (52%)
25	CHL	3	301	-	50,54,74	1.62	7 (14%)	56,90,114	1.83	12 (21%)
22	CLA	1	612	19	49,53,73	2.29	19 (38%)	59,89,113	2.89	28 (47%)
22	CLA	s	314	18	49,53,73	2.25	15 (30%)	59,89,113	2.97	27 (45%)
22	CLA	6	604	-	49,53,73	2.30	20 (40%)	59,89,113	2.91	27 (45%)
25	CHL	6	605	19	46,50,74	1.43	6 (13%)	51,85,114	1.86	8 (15%)
22	CLA	R	301	17	49,53,73	2.27	16 (32%)	59,89,113	2.91	28 (47%)
22	CLA	s	311	-	49,53,73	2.28	15 (30%)	59,89,113	2.98	27 (45%)
22	CLA	4	303	20	49,53,73	2.25	20 (40%)	59,89,113	3.02	29 (49%)
22	CLA	c	511	3	49,53,73	2.27	18 (36%)	59,89,113	2.93	27 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CHL	3	302	19	50,54,74	1.59	7 (14%)	56,90,114	1.82	9 (16%)
25	CHL	3	309	19	50,54,74	1.61	7 (14%)	56,90,114	2.17	11 (19%)
22	CLA	g	611	-	49,53,73	2.23	15 (30%)	59,89,113	2.97	29 (49%)
22	CLA	y	611	-	49,53,73	2.25	15 (30%)	59,89,113	3.01	25 (42%)
22	CLA	C	504	-	49,53,73	2.26	17 (34%)	59,89,113	2.94	29 (49%)
25	CHL	5	605	19	46,50,74	1.49	6 (13%)	51,85,114	1.77	8 (15%)
22	CLA	2	612	19	49,53,73	2.28	18 (36%)	59,89,113	2.87	26 (44%)
22	CLA	B	602	2	49,53,73	2.22	16 (32%)	59,89,113	2.85	27 (45%)
25	CHL	g	601	19	50,54,74	1.59	6 (12%)	56,90,114	1.90	12 (21%)
25	CHL	2	607	-	50,54,74	1.59	7 (14%)	56,90,114	1.72	9 (16%)
22	CLA	c	508	3	49,53,73	2.29	18 (36%)	59,89,113	2.99	26 (44%)
22	CLA	8	303	20	49,53,73	2.25	20 (40%)	59,89,113	3.02	29 (49%)
25	CHL	2	601	19	50,54,74	1.59	7 (14%)	56,90,114	1.87	10 (17%)
22	CLA	a	402	1	49,53,73	2.29	17 (34%)	59,89,113	2.89	28 (47%)
25	CHL	2	608	19	50,54,74	1.59	7 (14%)	56,90,114	2.04	13 (23%)
22	CLA	1	602	19	49,53,73	2.26	19 (38%)	59,89,113	2.85	26 (44%)
25	CHL	g	609	19	50,54,74	1.62	7 (14%)	56,90,114	2.16	12 (21%)
25	CHL	7	302	19	50,54,74	1.59	7 (14%)	56,90,114	1.82	9 (16%)
22	CLA	C	505	3	49,53,73	2.26	16 (32%)	59,89,113	2.99	30 (50%)
22	CLA	n	613	19	49,53,73	2.25	17 (34%)	59,89,113	2.94	25 (42%)
22	CLA	6	610	-	49,53,73	2.28	18 (36%)	59,89,113	2.87	26 (44%)
25	CHL	s	306	18	50,54,74	1.58	7 (14%)	56,90,114	1.86	12 (21%)
22	CLA	S	310	18	49,53,73	2.26	16 (32%)	59,89,113	2.94	31 (52%)
25	CHL	g	608	-	50,54,74	1.61	7 (14%)	56,90,114	1.70	11 (19%)
25	CHL	s	308	-	50,54,74	1.59	7 (14%)	56,90,114	1.78	8 (14%)
22	CLA	R	311	17	49,53,73	2.28	17 (34%)	59,89,113	2.92	28 (47%)
22	CLA	s	313	18	49,53,73	2.27	16 (32%)	59,89,113	2.99	31 (52%)
25	CHL	N	609	19	50,54,74	1.63	7 (14%)	56,90,114	2.11	11 (19%)
22	CLA	r	310	17	49,53,73	2.24	17 (34%)	59,89,113	2.85	26 (44%)
22	CLA	y	602	19	49,53,73	2.27	17 (34%)	59,89,113	2.94	27 (45%)
22	CLA	5	604	-	49,53,73	2.28	19 (38%)	59,89,113	2.89	25 (42%)
25	CHL	N	607	-	50,54,74	1.61	6 (12%)	56,90,114	1.99	12 (21%)
25	CHL	y	601	19	50,54,74	1.58	6 (12%)	56,90,114	1.84	13 (23%)
22	CLA	G	603	19	49,53,73	2.25	19 (38%)	59,89,113	2.93	31 (52%)
22	CLA	8	311	20	49,53,73	2.30	19 (38%)	59,89,113	2.80	27 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	r	309	-	49,53,73	2.24	16 (32%)	59,89,113	2.92	28 (47%)
22	CLA	Y	610	19	49,53,73	2.24	15 (30%)	59,89,113	2.92	26 (44%)
25	CHL	s	302	18	50,54,74	1.64	7 (14%)	56,90,114	1.65	9 (16%)
25	CHL	y	609	19	50,54,74	1.62	7 (14%)	56,90,114	2.14	11 (19%)
22	CLA	C	510	3	49,53,73	2.25	18 (36%)	59,89,113	3.03	27 (45%)
25	CHL	g	606	-	50,54,74	1.63	7 (14%)	56,90,114	1.82	9 (16%)
22	CLA	D	401	-	49,53,73	2.27	16 (32%)	59,89,113	2.92	29 (49%)
22	CLA	C	502	3	49,53,73	2.28	15 (30%)	59,89,113	2.78	28 (47%)
22	CLA	n	612	19	49,53,73	2.23	16 (32%)	59,89,113	2.93	29 (49%)
22	CLA	3	310	19	49,53,73	2.29	17 (34%)	59,89,113	2.87	25 (42%)
22	CLA	n	602	19	49,53,73	2.25	16 (32%)	59,89,113	2.90	27 (45%)
25	CHL	7	309	19	50,54,74	1.61	7 (14%)	56,90,114	2.17	11 (19%)
22	CLA	B	610	-	49,53,73	2.27	18 (36%)	59,89,113	2.89	26 (44%)
22	CLA	6	602	19	49,53,73	2.27	20 (40%)	59,89,113	2.86	27 (45%)
25	CHL	5	609	19	50,54,74	1.61	7 (14%)	56,90,114	2.03	11 (19%)
25	CHL	S	308	-	50,54,74	1.59	7 (14%)	56,90,114	1.78	8 (14%)
25	CHL	3	306	19	46,50,74	1.44	6 (13%)	51,85,114	1.87	8 (15%)
22	CLA	b	614	2	49,53,73	2.25	18 (36%)	59,89,113	2.99	30 (50%)
22	CLA	2	602	19	49,53,73	2.27	20 (40%)	59,89,113	2.86	27 (45%)
22	CLA	s	310	18	49,53,73	2.26	16 (32%)	59,89,113	2.94	31 (52%)
22	CLA	C	501	3	49,53,73	2.27	17 (34%)	59,89,113	3.01	30 (50%)
22	CLA	S	314	18	49,53,73	2.25	15 (30%)	59,89,113	2.97	27 (45%)
25	CHL	N	601	19	50,54,74	1.58	7 (14%)	56,90,114	1.89	11 (19%)
22	CLA	G	614	19	49,53,73	2.29	18 (36%)	59,89,113	2.88	27 (45%)
22	CLA	7	310	19	49,53,73	2.29	17 (34%)	59,89,113	2.87	25 (42%)
25	CHL	n	601	19	50,54,74	1.58	7 (14%)	56,90,114	1.89	11 (19%)
22	CLA	g	603	19	49,53,73	2.25	19 (38%)	59,89,113	2.93	31 (52%)
22	CLA	y	610	19	49,53,73	2.24	15 (30%)	59,89,113	2.92	26 (44%)
22	CLA	3	303	19	49,53,73	2.28	19 (38%)	59,89,113	2.89	28 (47%)
22	CLA	b	612	2	49,53,73	2.38	19 (38%)	59,89,113	2.93	29 (49%)
22	CLA	b	613	2	49,53,73	2.23	17 (34%)	59,89,113	3.10	32 (54%)
22	CLA	2	603	19	49,53,73	2.27	19 (38%)	59,89,113	2.84	28 (47%)
22	CLA	A	403	-	49,53,73	2.33	18 (36%)	59,89,113	2.93	30 (50%)
22	CLA	s	301	3	49,53,73	2.31	18 (36%)	59,89,113	2.85	30 (50%)
22	CLA	2	613	19	49,53,73	2.32	19 (38%)	59,89,113	2.80	26 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	g	610	19	49,53,73	2.26	15 (30%)	59,89,113	2.89	27 (45%)
25	CHL	8	307	-	50,54,74	1.61	7 (14%)	56,90,114	1.74	10 (17%)
22	CLA	y	613	19	49,53,73	2.26	16 (32%)	59,89,113	3.00	29 (49%)
22	CLA	4	304	20	49,53,73	2.28	19 (38%)	59,89,113	2.80	26 (44%)
22	CLA	6	611	19	49,53,73	2.29	18 (36%)	59,89,113	2.84	26 (44%)
22	CLA	R	303	-	49,53,73	2.25	15 (30%)	59,89,113	3.06	32 (54%)
25	CHL	Y	607	-	50,54,74	1.62	7 (14%)	56,90,114	1.90	13 (23%)
22	CLA	A	405	1	49,53,73	2.31	17 (34%)	59,89,113	3.00	27 (45%)
22	CLA	c	505	3	49,53,73	2.28	16 (32%)	59,89,113	3.05	29 (49%)
22	CLA	N	602	19	49,53,73	2.25	16 (32%)	59,89,113	2.90	27 (45%)
25	CHL	2	605	19	46,50,74	1.43	6 (13%)	51,85,114	1.86	8 (15%)
22	CLA	g	613	19	49,53,73	2.25	15 (30%)	59,89,113	2.93	27 (45%)
25	CHL	y	608	-	50,54,74	1.61	7 (14%)	56,90,114	1.75	9 (16%)
22	CLA	s	309	18	49,53,73	2.23	16 (32%)	59,89,113	2.84	29 (49%)
22	CLA	N	610	19	49,53,73	2.25	15 (30%)	59,89,113	2.89	25 (42%)
22	CLA	n	614	19	49,53,73	2.30	20 (40%)	59,89,113	2.85	25 (42%)
22	CLA	b	604	2	49,53,73	2.25	17 (34%)	59,89,113	2.91	27 (45%)
22	CLA	N	613	19	49,53,73	2.25	17 (34%)	59,89,113	2.94	25 (42%)
22	CLA	7	303	19	49,53,73	2.28	19 (38%)	59,89,113	2.89	28 (47%)
22	CLA	B	604	2	49,53,73	2.22	18 (36%)	59,89,113	3.10	28 (47%)
25	CHL	G	608	-	50,54,74	1.61	7 (14%)	56,90,114	1.70	11 (19%)
22	CLA	B	603	2	49,53,73	2.28	15 (30%)	59,89,113	2.88	31 (52%)
22	CLA	n	610	19	49,53,73	2.25	15 (30%)	59,89,113	2.89	25 (42%)
22	CLA	b	615	2	49,53,73	2.31	18 (36%)	59,89,113	2.95	27 (45%)
22	CLA	n	611	-	49,53,73	2.25	16 (32%)	59,89,113	2.99	31 (52%)
22	CLA	7	311	-	49,53,73	2.29	19 (38%)	59,89,113	2.87	29 (49%)
22	CLA	b	602	2	49,53,73	2.22	15 (30%)	59,89,113	2.94	30 (50%)
22	CLA	8	304	20	49,53,73	2.28	19 (38%)	59,89,113	2.80	26 (44%)
22	CLA	A	402	1	49,53,73	2.24	15 (30%)	59,89,113	2.97	27 (45%)
25	CHL	5	608	-	50,54,74	1.61	7 (14%)	56,90,114	1.68	9 (16%)
22	CLA	S	304	18	49,53,73	2.20	16 (32%)	59,89,113	2.78	27 (45%)
25	CHL	7	307	-	50,54,74	1.61	7 (14%)	56,90,114	1.74	8 (14%)
22	CLA	r	308	17	49,53,73	2.28	16 (32%)	59,89,113	2.91	28 (47%)
22	CLA	B	606	2	49,53,73	2.18	15 (30%)	59,89,113	3.02	29 (49%)
22	CLA	B	612	2	49,53,73	2.29	15 (30%)	59,89,113	3.00	28 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CHL	G	605	19	46,50,74	1.46	6 (13%)	51,85,114	1.81	7 (13%)
25	CHL	1	605	19	46,50,74	1.49	6 (13%)	51,85,114	1.77	8 (15%)
25	CHL	G	601	19	50,54,74	1.59	6 (12%)	56,90,114	1.90	12 (21%)
22	CLA	B	605	2	49,53,73	2.24	16 (32%)	59,89,113	2.91	26 (44%)
22	CLA	S	305	-	49,53,73	2.28	16 (32%)	59,89,113	3.02	28 (47%)
25	CHL	y	606	-	50,54,74	1.63	6 (12%)	56,90,114	1.80	11 (19%)
22	CLA	7	304	19	49,53,73	2.28	19 (38%)	59,89,113	2.90	28 (47%)
25	CHL	Y	609	19	50,54,74	1.62	7 (14%)	56,90,114	2.14	11 (19%)
25	CHL	y	605	19	46,50,74	1.55	6 (13%)	51,85,114	1.95	10 (19%)
22	CLA	b	603	2	49,53,73	2.30	18 (36%)	59,89,113	3.00	32 (54%)
22	CLA	g	604	-	49,53,73	2.26	18 (36%)	59,89,113	2.96	30 (50%)
22	CLA	D	404	4	49,53,73	2.28	17 (34%)	59,89,113	2.90	29 (49%)
22	CLA	5	611	-	49,53,73	2.27	19 (38%)	59,89,113	2.89	26 (44%)
25	CHL	S	307	-	50,54,74	1.63	7 (14%)	56,90,114	5.85	12 (21%)
22	CLA	5	614	19	49,53,73	2.29	20 (40%)	59,89,113	3.04	30 (50%)
25	CHL	5	601	19	50,54,74	1.58	7 (14%)	56,90,114	1.82	12 (21%)
22	CLA	g	612	19	49,53,73	2.27	16 (32%)	59,89,113	2.93	28 (47%)
25	CHL	S	306	18	50,54,74	1.58	7 (14%)	56,90,114	1.86	12 (21%)
22	CLA	S	303	18	49,53,73	2.26	15 (30%)	59,89,113	2.91	26 (44%)
22	CLA	6	609	19	49,53,73	2.28	16 (32%)	59,89,113	2.87	24 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	609	2	-	6/15/91/115	-
25	CHL	6	606	-	-	9/17/93/117	-
25	CHL	r	305	-	-	10/17/93/117	-
22	CLA	r	311	17	-	7/15/91/115	-
22	CLA	s	304	18	-	8/15/91/115	-
22	CLA	5	612	19	-	9/15/91/115	-
22	CLA	g	602	19	-	11/15/91/115	-
25	CHL	n	605	19	-	9/12/88/117	-
22	CLA	G	611	-	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	7	312	19	-	9/15/91/115	-
22	CLA	r	302	17	-	11/15/91/115	-
25	CHL	G	609	19	-	14/17/93/117	-
22	CLA	g	614	19	-	6/15/91/115	-
22	CLA	R	302	17	-	11/15/91/115	-
22	CLA	4	305	-	-	7/15/91/115	-
22	CLA	b	606	2	-	4/15/91/115	-
25	CHL	4	302	17	-	10/17/93/117	-
22	CLA	R	310	17	-	9/15/91/115	-
22	CLA	C	509	3	-	8/15/91/115	-
25	CHL	4	309	20	-	10/17/93/117	-
22	CLA	a	405	1	-	4/15/91/115	-
22	CLA	b	607	-	-	8/15/91/115	-
25	CHL	s	307	-	-	9/17/93/117	-
22	CLA	6	613	19	-	6/15/91/115	-
22	CLA	S	312	18	-	8/15/91/115	-
22	CLA	4	311	20	-	4/15/91/115	-
22	CLA	Y	614	19	-	7/15/91/115	-
22	CLA	3	305	-	-	6/15/91/115	-
22	CLA	b	611	2	-	3/15/91/115	-
22	CLA	b	610	-	-	10/15/91/115	-
25	CHL	2	606	-	-	9/17/93/117	-
22	CLA	B	614	2	-	10/15/91/115	-
22	CLA	c	504	-	-	5/15/91/115	-
22	CLA	2	604	-	-	8/15/91/115	-
22	CLA	2	610	-	-	3/15/91/115	-
22	CLA	R	309	-	-	10/15/91/115	-
22	CLA	N	603	19	-	7/15/91/115	-
22	CLA	N	614	19	-	7/15/91/115	-
25	CHL	Y	608	-	-	7/17/93/117	-
22	CLA	C	507	-	-	10/15/91/115	-
22	CLA	y	612	19	-	11/15/91/115	-
22	CLA	C	511	3	-	8/15/91/115	-
22	CLA	1	610	19	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	4	306	20	-	7/17/93/117	-
22	CLA	c	503	3	-	11/15/91/115	-
22	CLA	R	308	17	-	7/15/91/115	-
22	CLA	r	307	17	-	10/15/91/115	-
25	CHL	4	308	-	-	12/17/93/117	-
22	CLA	8	305	-	-	7/15/91/115	-
25	CHL	N	606	-	-	8/17/93/117	-
22	CLA	C	506	3	-	8/15/91/115	-
23	PHO	d	402	-	-	6/13/79/103	0/5/6/6
24	HEM	F	101	5,6	-	4/14/54/54	-
22	CLA	N	604	-	-	10/15/91/115	-
22	CLA	5	603	19	-	7/15/91/115	-
25	CHL	Y	605	19	-	9/12/88/117	-
25	CHL	R	304	-	-	12/17/93/117	-
22	CLA	Y	604	-	-	8/15/91/115	-
22	CLA	6	612	19	-	7/15/91/115	-
22	CLA	b	609	2	-	6/15/91/115	-
22	CLA	C	512	3	-	5/15/91/115	-
22	CLA	5	613	19	-	6/15/91/115	-
25	CHL	3	308	-	-	7/17/93/117	-
22	CLA	b	608	2	-	4/15/91/115	-
25	CHL	Y	601	19	-	9/17/93/117	-
22	CLA	s	312	18	-	8/15/91/115	-
25	CHL	R	306	-	-	15/17/93/117	-
22	CLA	B	611	2	-	4/15/91/115	-
25	CHL	g	607	-	-	7/17/93/117	-
25	CHL	y	607	-	-	7/17/93/117	-
22	CLA	d	403	4	-	8/15/91/115	-
22	CLA	3	313	19	-	7/15/91/115	-
25	CHL	Y	606	-	-	10/17/93/117	-
23	PHO	a	404	-	-	3/13/79/103	0/5/6/6
25	CHL	N	605	19	-	9/12/88/117	-
22	CLA	r	303	-	-	6/15/91/115	-
22	CLA	c	501	3	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	616	2	-	12/15/91/115	-
22	CLA	Y	611	-	-	7/15/91/115	-
22	CLA	Y	602	19	-	11/15/91/115	-
25	CHL	8	306	20	-	7/17/93/117	-
25	CHL	7	301	-	-	9/17/93/117	-
25	CHL	8	309	20	-	10/17/93/117	-
22	CLA	5	610	19	-	6/15/91/115	-
22	CLA	3	304	19	-	6/15/91/115	-
22	CLA	S	301	3	-	4/15/91/115	-
22	CLA	y	603	19	-	10/15/91/115	-
25	CHL	4	307	-	-	14/17/93/117	-
22	CLA	b	601	-	-	11/15/91/115	-
22	CLA	a	403	-	-	10/15/91/115	-
25	CHL	5	615	-	-	11/17/93/117	-
22	CLA	c	512	3	-	4/15/91/115	-
25	CHL	R	305	-	-	10/17/93/117	-
22	CLA	D	403	4	-	6/15/91/115	-
22	CLA	1	604	-	-	4/15/91/115	-
25	CHL	6	601	19	-	10/17/93/117	-
22	CLA	1	603	19	-	7/15/91/115	-
22	CLA	6	603	19	-	8/15/91/115	-
22	CLA	4	301	17,20	-	6/15/91/115	-
25	CHL	S	302	18	-	8/17/93/117	-
22	CLA	3	311	-	-	6/15/91/115	-
25	CHL	5	607	-	-	8/17/93/117	-
22	CLA	R	307	17	-	10/15/91/115	-
25	CHL	N	608	-	-	8/17/93/117	-
22	CLA	C	508	3	-	5/15/91/115	-
22	CLA	G	604	-	-	10/15/91/115	-
25	CHL	1	609	19	-	14/17/93/117	-
25	CHL	G	606	-	-	10/17/93/117	-
22	CLA	2	609	19	-	6/15/91/115	-
22	CLA	N	612	19	-	10/15/91/115	-
22	CLA	r	301	17	-	11/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	7	314	19	-	6/15/91/115	-
25	CHL	1	607	-	-	8/17/93/117	-
22	CLA	5	602	19	-	10/15/91/115	-
22	CLA	n	604	-	-	10/15/91/115	-
22	CLA	n	603	19	-	7/15/91/115	-
22	CLA	B	613	2	-	5/15/91/115	-
22	CLA	7	305	-	-	6/15/91/115	-
25	CHL	n	608	-	-	8/17/93/117	-
22	CLA	Y	603	19	-	10/15/91/115	-
22	CLA	B	615	2	-	12/15/91/115	-
24	HEM	e	101	5,6	-	6/14/54/54	-
22	CLA	B	607	-	-	6/15/91/115	-
22	CLA	G	602	19	-	11/15/91/115	-
22	CLA	y	614	19	-	7/15/91/115	-
25	CHL	1	615	-	-	11/17/93/117	-
23	PHO	D	402	-	-	4/13/79/103	0/5/6/6
25	CHL	7	306	19	-	9/12/88/117	-
22	CLA	Y	613	19	-	7/15/91/115	-
22	CLA	4	310	20	-	8/15/91/115	-
25	CHL	6	607	-	-	7/17/93/117	-
22	CLA	3	314	19	-	6/15/91/115	-
22	CLA	S	309	18	-	6/15/91/115	-
25	CHL	7	308	-	-	7/17/93/117	-
22	CLA	1	614	19	-	8/15/91/115	-
22	CLA	7	313	19	-	7/15/91/115	-
22	CLA	d	404	4	-	8/15/91/115	-
25	CHL	1	608	-	-	7/17/93/117	-
22	CLA	8	301	17,20	-	6/15/91/115	-
22	CLA	c	502	3	-	8/15/91/115	-
25	CHL	1	606	-	-	8/17/93/117	-
22	CLA	S	311	-	-	4/15/91/115	-
25	CHL	5	606	-	-	8/17/93/117	-
22	CLA	d	401	-	-	8/15/91/115	-
25	CHL	8	302	17	-	10/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	n	609	19	-	15/17/93/117	-
25	CHL	n	606	-	-	8/17/93/117	-
22	CLA	s	303	18	-	11/15/91/115	-
25	CHL	r	306	-	-	15/17/93/117	-
22	CLA	1	611	-	-	7/15/91/115	-
25	CHL	3	307	-	-	8/17/93/117	-
22	CLA	G	610	19	-	7/15/91/115	-
22	CLA	B	608	2	-	4/15/91/115	-
22	CLA	C	503	3	-	11/15/91/115	-
25	CHL	n	607	-	-	7/17/93/117	-
25	CHL	r	304	-	-	12/17/93/117	-
22	CLA	B	616	2	-	6/15/91/115	-
22	CLA	s	305	-	-	9/15/91/115	-
22	CLA	c	510	3	-	5/15/91/115	-
22	CLA	3	312	19	-	9/15/91/115	-
22	CLA	c	509	3	-	8/15/91/115	-
22	CLA	2	611	19	-	10/15/91/115	-
25	CHL	G	607	-	-	7/17/93/117	-
22	CLA	G	612	19	-	10/15/91/115	-
22	CLA	Y	612	19	-	11/15/91/115	-
22	CLA	G	613	19	-	7/15/91/115	-
22	CLA	1	613	19	-	6/15/91/115	-
22	CLA	8	310	20	-	8/15/91/115	-
25	CHL	g	605	19	-	9/12/88/117	-
22	CLA	B	601	-	-	9/15/91/115	-
22	CLA	S	313	18	-	7/15/91/115	-
22	CLA	y	604	-	-	8/15/91/115	-
22	CLA	c	507	-	-	10/15/91/115	-
25	CHL	1	601	19	-	9/17/93/117	-
22	CLA	c	506	3	-	8/15/91/115	-
23	PHO	A	404	-	-	4/13/79/103	0/5/6/6
22	CLA	b	605	2	-	2/15/91/115	-
25	CHL	6	608	19	-	14/17/93/117	-
25	CHL	8	308	-	-	12/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	N	611	-	-	6/15/91/115	-
25	CHL	3	301	-	-	9/17/93/117	-
22	CLA	1	612	19	-	9/15/91/115	-
22	CLA	s	314	18	-	7/15/91/115	-
22	CLA	6	604	-	-	8/15/91/115	-
25	CHL	6	605	19	-	8/12/88/117	-
22	CLA	R	301	17	-	11/15/91/115	-
22	CLA	s	311	-	-	4/15/91/115	-
22	CLA	4	303	20	-	7/15/91/115	-
22	CLA	c	511	3	-	8/15/91/115	-
25	CHL	3	302	19	-	9/17/93/117	-
25	CHL	3	309	19	-	14/17/93/117	-
22	CLA	g	611	-	-	5/15/91/115	-
22	CLA	y	611	-	-	7/15/91/115	-
22	CLA	C	504	-	-	8/15/91/115	-
25	CHL	5	605	19	-	9/12/88/117	-
22	CLA	2	612	19	-	7/15/91/115	-
22	CLA	B	602	2	-	9/15/91/115	-
25	CHL	g	601	19	-	9/17/93/117	-
25	CHL	2	607	-	-	7/17/93/117	-
22	CLA	c	508	3	-	5/15/91/115	-
22	CLA	8	303	20	-	7/15/91/115	-
25	CHL	2	601	19	-	10/17/93/117	-
22	CLA	a	402	1	-	5/15/91/115	-
25	CHL	2	608	19	-	14/17/93/117	-
22	CLA	1	602	19	-	10/15/91/115	-
25	CHL	g	609	19	-	14/17/93/117	-
25	CHL	7	302	19	-	9/17/93/117	-
22	CLA	C	505	3	-	10/15/91/115	-
22	CLA	n	613	19	-	7/15/91/115	-
22	CLA	6	610	-	-	3/15/91/115	-
25	CHL	s	306	18	-	11/17/93/117	-
22	CLA	S	310	18	-	10/15/91/115	-
25	CHL	g	608	-	-	8/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	s	308	-	-	9/17/93/117	-
22	CLA	R	311	17	-	7/15/91/115	-
22	CLA	s	313	18	-	7/15/91/115	-
25	CHL	N	609	19	-	15/17/93/117	-
22	CLA	r	310	17	-	9/15/91/115	-
22	CLA	y	602	19	-	11/15/91/115	-
22	CLA	5	604	-	-	4/15/91/115	-
25	CHL	N	607	-	-	7/17/93/117	-
25	CHL	y	601	19	-	9/17/93/117	-
22	CLA	G	603	19	-	8/15/91/115	-
22	CLA	8	311	20	-	4/15/91/115	-
22	CLA	r	309	-	-	10/15/91/115	-
22	CLA	Y	610	19	-	6/15/91/115	-
25	CHL	s	302	18	-	8/17/93/117	-
25	CHL	y	609	19	-	15/17/93/117	-
22	CLA	C	510	3	-	5/15/91/115	-
25	CHL	g	606	-	-	10/17/93/117	-
22	CLA	D	401	-	-	8/15/91/115	-
22	CLA	C	502	3	-	9/15/91/115	-
22	CLA	n	612	19	-	10/15/91/115	-
22	CLA	3	310	19	-	7/15/91/115	-
22	CLA	n	602	19	-	11/15/91/115	-
25	CHL	7	309	19	-	14/17/93/117	-
22	CLA	B	610	-	-	10/15/91/115	-
22	CLA	6	602	19	-	9/15/91/115	-
25	CHL	5	609	19	-	14/17/93/117	-
25	CHL	S	308	-	-	9/17/93/117	-
25	CHL	3	306	19	-	9/12/88/117	-
22	CLA	b	614	2	-	5/15/91/115	-
22	CLA	2	602	19	-	9/15/91/115	-
22	CLA	s	310	18	-	10/15/91/115	-
22	CLA	C	501	3	-	5/15/91/115	-
22	CLA	S	314	18	-	7/15/91/115	-
25	CHL	N	601	19	-	9/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	G	614	19	-	6/15/91/115	-
22	CLA	7	310	19	-	7/15/91/115	-
25	CHL	n	601	19	-	9/17/93/117	-
22	CLA	g	603	19	-	8/15/91/115	-
22	CLA	y	610	19	-	6/15/91/115	-
22	CLA	3	303	19	-	11/15/91/115	-
22	CLA	b	612	2	-	9/15/91/115	-
22	CLA	b	613	2	-	5/15/91/115	-
22	CLA	2	603	19	-	8/15/91/115	-
22	CLA	A	403	-	-	8/15/91/115	-
22	CLA	s	301	3	-	5/15/91/115	-
22	CLA	2	613	19	-	6/15/91/115	-
22	CLA	g	610	19	-	7/15/91/115	-
25	CHL	8	307	-	-	14/17/93/117	-
22	CLA	y	613	19	-	7/15/91/115	-
22	CLA	4	304	20	-	10/15/91/115	-
22	CLA	6	611	19	-	10/15/91/115	-
22	CLA	R	303	-	-	6/15/91/115	-
25	CHL	Y	607	-	-	7/17/93/117	-
22	CLA	A	405	1	-	4/15/91/115	-
22	CLA	c	505	3	-	11/15/91/115	-
22	CLA	N	602	19	-	11/15/91/115	-
25	CHL	2	605	19	-	8/12/88/117	-
22	CLA	g	613	19	-	7/15/91/115	-
25	CHL	y	608	-	-	7/17/93/117	-
22	CLA	s	309	18	-	6/15/91/115	-
22	CLA	N	610	19	-	7/15/91/115	-
22	CLA	n	614	19	-	7/15/91/115	-
22	CLA	b	604	2	-	11/15/91/115	-
22	CLA	N	613	19	-	7/15/91/115	-
22	CLA	7	303	19	-	11/15/91/115	-
22	CLA	B	604	2	-	9/15/91/115	-
25	CHL	G	608	-	-	8/17/93/117	-
22	CLA	B	603	2	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	n	610	19	-	7/15/91/115	-
22	CLA	b	615	2	-	9/15/91/115	-
22	CLA	n	611	-	-	6/15/91/115	-
22	CLA	7	311	-	-	6/15/91/115	-
22	CLA	b	602	2	-	7/15/91/115	-
22	CLA	8	304	20	-	10/15/91/115	-
22	CLA	A	402	1	-	5/15/91/115	-
25	CHL	5	608	-	-	7/17/93/117	-
22	CLA	S	304	18	-	8/15/91/115	-
25	CHL	7	307	-	-	8/17/93/117	-
22	CLA	r	308	17	-	7/15/91/115	-
22	CLA	B	606	2	-	5/15/91/115	-
22	CLA	B	612	2	-	8/15/91/115	-
25	CHL	G	605	19	-	9/12/88/117	-
25	CHL	1	605	19	-	9/12/88/117	-
25	CHL	G	601	19	-	9/17/93/117	-
22	CLA	B	605	2	-	4/15/91/115	-
22	CLA	S	305	-	-	9/15/91/115	-
25	CHL	y	606	-	-	10/17/93/117	-
22	CLA	7	304	19	-	6/15/91/115	-
25	CHL	Y	609	19	-	15/17/93/117	-
25	CHL	y	605	19	-	9/12/88/117	-
22	CLA	b	603	2	-	7/15/91/115	-
22	CLA	g	604	-	-	10/15/91/115	-
22	CLA	D	404	4	-	8/15/91/115	-
22	CLA	5	611	-	-	7/15/91/115	-
25	CHL	S	307	-	-	9/17/93/117	-
22	CLA	5	614	19	-	8/15/91/115	-
25	CHL	5	601	19	-	9/17/93/117	-
22	CLA	g	612	19	-	10/15/91/115	-
25	CHL	S	306	18	-	11/17/93/117	-
22	CLA	S	303	18	-	11/15/91/115	-
22	CLA	6	609	19	-	6/15/91/115	-

All (4336) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	402	PHO	C1D-C2D	8.59	1.49	1.39
23	d	402	PHO	C1D-C2D	8.55	1.49	1.39
23	a	404	PHO	C1D-C2D	8.28	1.48	1.39
23	A	404	PHO	C1D-C2D	7.35	1.47	1.39
23	D	402	PHO	C1B-C2B	6.99	1.47	1.39
23	a	404	PHO	C1B-C2B	6.82	1.47	1.39
23	d	402	PHO	C1B-C2B	6.75	1.47	1.39
23	A	404	PHO	C1B-C2B	6.47	1.46	1.39
22	c	501	CLA	C4B-NB	-6.11	1.30	1.37
22	c	505	CLA	C4B-NB	-6.04	1.30	1.37
25	G	609	CHL	O2A-CGA	6.01	1.51	1.30
25	g	609	CHL	O2A-CGA	6.01	1.51	1.30
25	N	609	CHL	O2A-CGA	6.00	1.50	1.30
25	n	609	CHL	O2A-CGA	6.00	1.50	1.30
22	N	604	CLA	C4B-NB	-5.99	1.30	1.37
22	n	604	CLA	C4B-NB	-5.99	1.30	1.37
25	3	309	CHL	O2A-CGA	5.97	1.50	1.30
25	7	309	CHL	O2A-CGA	5.97	1.50	1.30
25	Y	609	CHL	O2A-CGA	5.96	1.50	1.30
25	y	609	CHL	O2A-CGA	5.96	1.50	1.30
25	S	302	CHL	O2A-CGA	5.95	1.50	1.30
25	s	302	CHL	O2A-CGA	5.95	1.50	1.30
25	1	609	CHL	O2A-CGA	5.95	1.50	1.30
25	5	609	CHL	O2A-CGA	5.95	1.50	1.30
25	3	307	CHL	O2A-CGA	5.94	1.50	1.30
25	7	307	CHL	O2A-CGA	5.94	1.50	1.30
22	Y	604	CLA	C4B-NB	-5.94	1.30	1.37
22	y	604	CLA	C4B-NB	-5.94	1.30	1.37
25	1	615	CHL	O2A-CGA	5.94	1.50	1.30
25	5	615	CHL	O2A-CGA	5.94	1.50	1.30
25	1	606	CHL	O2A-CGA	5.94	1.50	1.30
25	5	606	CHL	O2A-CGA	5.94	1.50	1.30
25	S	308	CHL	O2A-CGA	5.93	1.50	1.30
25	s	308	CHL	O2A-CGA	5.93	1.50	1.30
22	B	604	CLA	C4B-NB	-5.93	1.30	1.37
25	2	606	CHL	O2A-CGA	5.93	1.50	1.30
25	6	606	CHL	O2A-CGA	5.93	1.50	1.30
25	Y	606	CHL	O2A-CGA	5.93	1.50	1.30
25	y	606	CHL	O2A-CGA	5.93	1.50	1.30
25	4	309	CHL	O2A-CGA	5.93	1.50	1.30
25	8	309	CHL	O2A-CGA	5.93	1.50	1.30
25	4	302	CHL	O2A-CGA	5.93	1.50	1.30
25	8	302	CHL	O2A-CGA	5.93	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	608	CHL	O2A-CGA	5.92	1.50	1.30
25	6	608	CHL	O2A-CGA	5.92	1.50	1.30
25	Y	607	CHL	O2A-CGA	5.92	1.50	1.30
25	y	607	CHL	O2A-CGA	5.92	1.50	1.30
25	1	607	CHL	O2A-CGA	5.92	1.50	1.30
25	5	607	CHL	O2A-CGA	5.92	1.50	1.30
25	Y	608	CHL	O2A-CGA	5.92	1.50	1.30
25	y	608	CHL	O2A-CGA	5.92	1.50	1.30
25	4	306	CHL	O2A-CGA	5.92	1.50	1.30
25	8	306	CHL	O2A-CGA	5.92	1.50	1.30
22	S	312	CLA	C4B-NB	-5.92	1.30	1.37
22	s	312	CLA	C4B-NB	-5.92	1.30	1.37
25	3	301	CHL	O2A-CGA	5.92	1.50	1.30
25	7	301	CHL	O2A-CGA	5.92	1.50	1.30
25	4	307	CHL	O2A-CGA	5.92	1.50	1.30
25	8	307	CHL	O2A-CGA	5.92	1.50	1.30
25	1	601	CHL	O2A-CGA	5.92	1.50	1.30
25	5	601	CHL	O2A-CGA	5.92	1.50	1.30
25	G	607	CHL	O2A-CGA	5.91	1.50	1.30
25	g	607	CHL	O2A-CGA	5.91	1.50	1.30
25	S	307	CHL	O2A-CGA	5.91	1.50	1.30
25	s	307	CHL	O2A-CGA	5.91	1.50	1.30
25	R	304	CHL	O2A-CGA	5.91	1.50	1.30
25	R	306	CHL	O2A-CGA	5.91	1.50	1.30
25	r	304	CHL	O2A-CGA	5.91	1.50	1.30
25	r	306	CHL	O2A-CGA	5.91	1.50	1.30
25	G	608	CHL	O2A-CGA	5.91	1.50	1.30
25	g	608	CHL	O2A-CGA	5.91	1.50	1.30
25	G	606	CHL	O2A-CGA	5.91	1.50	1.30
25	g	606	CHL	O2A-CGA	5.91	1.50	1.30
25	R	305	CHL	O2A-CGA	5.91	1.50	1.30
25	r	305	CHL	O2A-CGA	5.91	1.50	1.30
25	N	606	CHL	O2A-CGA	5.91	1.50	1.30
25	n	606	CHL	O2A-CGA	5.91	1.50	1.30
25	2	601	CHL	O2A-CGA	5.91	1.50	1.30
25	6	601	CHL	O2A-CGA	5.91	1.50	1.30
25	4	308	CHL	O2A-CGA	5.90	1.50	1.30
25	8	308	CHL	O2A-CGA	5.90	1.50	1.30
25	1	608	CHL	O2A-CGA	5.89	1.50	1.30
25	5	608	CHL	O2A-CGA	5.89	1.50	1.30
25	N	607	CHL	O2A-CGA	5.89	1.50	1.30
25	n	607	CHL	O2A-CGA	5.89	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	302	CHL	O2A-CGA	5.87	1.50	1.30
25	7	302	CHL	O2A-CGA	5.87	1.50	1.30
25	2	607	CHL	O2A-CGA	5.85	1.50	1.30
25	6	607	CHL	O2A-CGA	5.85	1.50	1.30
25	3	308	CHL	O2A-CGA	5.85	1.50	1.30
25	7	308	CHL	O2A-CGA	5.85	1.50	1.30
25	N	608	CHL	O2A-CGA	5.84	1.50	1.30
25	n	608	CHL	O2A-CGA	5.84	1.50	1.30
22	C	501	CLA	C4B-NB	-5.84	1.30	1.37
22	D	403	CLA	C1D-ND	-5.83	1.30	1.37
25	G	601	CHL	O2A-CGA	5.83	1.50	1.30
25	g	601	CHL	O2A-CGA	5.83	1.50	1.30
25	N	601	CHL	O2A-CGA	5.83	1.50	1.30
25	n	601	CHL	O2A-CGA	5.83	1.50	1.30
22	D	403	CLA	C4B-NB	-5.83	1.30	1.37
22	d	403	CLA	C1D-ND	-5.82	1.30	1.37
22	d	403	CLA	C4B-NB	-5.79	1.30	1.37
22	D	401	CLA	C4B-NB	-5.79	1.30	1.37
25	Y	601	CHL	O2A-CGA	5.78	1.50	1.30
25	y	601	CHL	O2A-CGA	5.78	1.50	1.30
22	C	505	CLA	C4B-NB	-5.78	1.30	1.37
22	B	611	CLA	C4B-NB	-5.77	1.30	1.37
22	B	612	CLA	C1D-ND	-5.76	1.30	1.37
22	c	503	CLA	C4B-NB	-5.75	1.30	1.37
22	b	608	CLA	C4B-NB	-5.73	1.30	1.37
25	S	306	CHL	O2A-CGA	5.72	1.50	1.30
25	s	306	CHL	O2A-CGA	5.72	1.50	1.30
22	A	405	CLA	C4B-NB	-5.72	1.30	1.37
22	Y	604	CLA	C1D-ND	-5.70	1.30	1.37
22	y	604	CLA	C1D-ND	-5.70	1.30	1.37
22	b	604	CLA	C4B-NB	-5.70	1.30	1.37
22	C	506	CLA	C1D-ND	-5.69	1.30	1.37
22	A	402	CLA	C4B-NB	-5.68	1.30	1.37
22	a	402	CLA	C4B-NB	-5.68	1.30	1.37
22	b	611	CLA	C4B-NB	-5.68	1.30	1.37
22	a	405	CLA	C4B-NB	-5.67	1.30	1.37
22	B	616	CLA	C4B-NB	-5.66	1.30	1.37
22	B	605	CLA	C4B-NB	-5.64	1.30	1.37
22	b	608	CLA	C1D-ND	-5.63	1.30	1.37
22	G	602	CLA	C4B-NB	-5.62	1.30	1.37
22	g	602	CLA	C4B-NB	-5.62	1.30	1.37
22	S	314	CLA	C4B-NB	-5.61	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	314	CLA	C4B-NB	-5.61	1.30	1.37
22	B	608	CLA	C4B-NB	-5.61	1.30	1.37
22	S	313	CLA	C1D-ND	-5.59	1.30	1.37
22	s	313	CLA	C1D-ND	-5.59	1.30	1.37
22	B	613	CLA	C4B-NB	-5.59	1.30	1.37
22	Y	614	CLA	C4B-NB	-5.58	1.30	1.37
22	y	614	CLA	C4B-NB	-5.58	1.30	1.37
22	S	311	CLA	C4B-NB	-5.57	1.30	1.37
22	s	311	CLA	C4B-NB	-5.57	1.30	1.37
22	c	508	CLA	C1D-ND	-5.57	1.30	1.37
22	C	502	CLA	C4B-NB	-5.57	1.30	1.37
22	C	506	CLA	C4B-NB	-5.56	1.30	1.37
22	C	503	CLA	C4B-NB	-5.56	1.30	1.37
22	B	607	CLA	C4B-NB	-5.56	1.30	1.37
22	C	510	CLA	C4B-NB	-5.56	1.31	1.37
22	c	510	CLA	C4B-NB	-5.55	1.31	1.37
22	C	508	CLA	C4B-NB	-5.55	1.31	1.37
22	c	505	CLA	C1D-ND	-5.54	1.31	1.37
22	B	603	CLA	C4B-NB	-5.53	1.31	1.37
22	S	313	CLA	C4B-NB	-5.53	1.31	1.37
22	s	313	CLA	C4B-NB	-5.53	1.31	1.37
22	N	602	CLA	C4B-NB	-5.53	1.31	1.37
22	Y	602	CLA	C4B-NB	-5.53	1.31	1.37
22	n	602	CLA	C4B-NB	-5.53	1.31	1.37
22	y	602	CLA	C4B-NB	-5.53	1.31	1.37
22	Y	611	CLA	C4B-NB	-5.53	1.31	1.37
22	y	611	CLA	C4B-NB	-5.53	1.31	1.37
22	G	604	CLA	C4B-NB	-5.52	1.31	1.37
22	g	604	CLA	C4B-NB	-5.52	1.31	1.37
22	B	609	CLA	C1D-ND	-5.51	1.31	1.37
22	Y	610	CLA	C4B-NB	-5.51	1.31	1.37
22	y	610	CLA	C4B-NB	-5.51	1.31	1.37
22	Y	612	CLA	C4B-NB	-5.51	1.31	1.37
22	y	612	CLA	C4B-NB	-5.51	1.31	1.37
22	Y	613	CLA	C1D-ND	-5.51	1.31	1.37
22	y	613	CLA	C1D-ND	-5.51	1.31	1.37
22	d	401	CLA	C4B-NB	-5.51	1.31	1.37
22	b	603	CLA	C1D-ND	-5.50	1.31	1.37
22	b	605	CLA	C4B-NB	-5.50	1.31	1.37
22	b	612	CLA	C1D-ND	-5.50	1.31	1.37
22	b	607	CLA	C4B-NB	-5.49	1.31	1.37
22	Y	611	CLA	C1D-ND	-5.49	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	y	611	CLA	C1D-ND	-5.49	1.31	1.37
22	R	303	CLA	C4B-NB	-5.48	1.31	1.37
22	r	303	CLA	C4B-NB	-5.48	1.31	1.37
22	c	506	CLA	C1D-ND	-5.48	1.31	1.37
22	S	310	CLA	C4B-NB	-5.47	1.31	1.37
22	s	310	CLA	C4B-NB	-5.47	1.31	1.37
22	b	615	CLA	C4B-NB	-5.47	1.31	1.37
22	b	612	CLA	C4B-NB	-5.47	1.31	1.37
22	A	403	CLA	C4B-NB	-5.46	1.31	1.37
22	c	508	CLA	C4B-NB	-5.46	1.31	1.37
22	S	305	CLA	C4B-NB	-5.46	1.31	1.37
22	s	305	CLA	C4B-NB	-5.46	1.31	1.37
22	c	501	CLA	C1D-ND	-5.45	1.31	1.37
22	G	613	CLA	C4B-NB	-5.45	1.31	1.37
22	g	613	CLA	C4B-NB	-5.45	1.31	1.37
22	b	614	CLA	C1D-ND	-5.45	1.31	1.37
22	A	405	CLA	C1D-ND	-5.45	1.31	1.37
22	b	606	CLA	C1D-ND	-5.44	1.31	1.37
22	C	504	CLA	C4B-NB	-5.44	1.31	1.37
22	B	608	CLA	C1D-ND	-5.44	1.31	1.37
22	a	405	CLA	C1D-ND	-5.43	1.31	1.37
22	R	311	CLA	C1D-ND	-5.42	1.31	1.37
22	r	311	CLA	C1D-ND	-5.42	1.31	1.37
22	N	604	CLA	C1D-ND	-5.41	1.31	1.37
22	n	604	CLA	C1D-ND	-5.41	1.31	1.37
23	A	404	PHO	C3B-C2B	5.41	1.47	1.40
22	c	502	CLA	C4B-NB	-5.41	1.31	1.37
22	Y	613	CLA	C4B-NB	-5.41	1.31	1.37
22	y	613	CLA	C4B-NB	-5.41	1.31	1.37
22	B	612	CLA	C4B-NB	-5.40	1.31	1.37
22	c	504	CLA	C4B-NB	-5.40	1.31	1.37
22	b	611	CLA	C1D-ND	-5.39	1.31	1.37
22	G	613	CLA	C1D-ND	-5.39	1.31	1.37
22	g	613	CLA	C1D-ND	-5.39	1.31	1.37
22	G	612	CLA	C4B-NB	-5.38	1.31	1.37
22	g	612	CLA	C4B-NB	-5.38	1.31	1.37
22	C	508	CLA	C1D-ND	-5.38	1.31	1.37
22	b	602	CLA	C4B-NB	-5.37	1.31	1.37
22	N	613	CLA	C4B-NB	-5.37	1.31	1.37
22	n	613	CLA	C4B-NB	-5.37	1.31	1.37
22	R	302	CLA	C4B-NB	-5.36	1.31	1.37
22	R	307	CLA	C1D-ND	-5.36	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	302	CLA	C4B-NB	-5.36	1.31	1.37
22	r	307	CLA	C1D-ND	-5.36	1.31	1.37
22	S	301	CLA	C1D-ND	-5.36	1.31	1.37
22	N	612	CLA	C4B-NB	-5.36	1.31	1.37
22	n	612	CLA	C4B-NB	-5.36	1.31	1.37
22	b	613	CLA	C4B-NB	-5.36	1.31	1.37
25	Y	605	CHL	MG-ND	-5.35	1.95	2.05
25	y	605	CHL	MG-ND	-5.35	1.95	2.05
22	C	504	CLA	C1D-ND	-5.35	1.31	1.37
22	N	603	CLA	C4B-NB	-5.35	1.31	1.37
22	n	603	CLA	C4B-NB	-5.35	1.31	1.37
22	C	502	CLA	C1D-ND	-5.35	1.31	1.37
22	b	607	CLA	C1D-ND	-5.35	1.31	1.37
22	b	610	CLA	C4B-NB	-5.34	1.31	1.37
22	a	403	CLA	C4B-NB	-5.34	1.31	1.37
22	B	615	CLA	C4B-NB	-5.34	1.31	1.37
22	S	311	CLA	C1D-ND	-5.34	1.31	1.37
22	s	311	CLA	C1D-ND	-5.34	1.31	1.37
22	B	607	CLA	C1D-ND	-5.32	1.31	1.37
22	R	307	CLA	C4B-NB	-5.32	1.31	1.37
22	r	307	CLA	C4B-NB	-5.32	1.31	1.37
22	B	610	CLA	C4B-NB	-5.32	1.31	1.37
22	G	602	CLA	C1D-ND	-5.32	1.31	1.37
22	g	602	CLA	C1D-ND	-5.32	1.31	1.37
22	B	611	CLA	C1D-ND	-5.31	1.31	1.37
22	s	301	CLA	C1D-ND	-5.31	1.31	1.37
25	N	608	CHL	MG-ND	-5.30	1.95	2.05
25	n	608	CHL	MG-ND	-5.30	1.95	2.05
22	C	505	CLA	C1D-ND	-5.30	1.31	1.37
23	d	402	PHO	C3B-C2B	5.30	1.47	1.40
22	S	305	CLA	C1D-ND	-5.29	1.31	1.37
22	G	611	CLA	C4B-NB	-5.29	1.31	1.37
22	s	305	CLA	C1D-ND	-5.29	1.31	1.37
22	g	611	CLA	C4B-NB	-5.29	1.31	1.37
22	c	506	CLA	C4B-NB	-5.29	1.31	1.37
25	S	302	CHL	MG-ND	-5.29	1.95	2.05
25	s	302	CHL	MG-ND	-5.29	1.95	2.05
25	N	607	CHL	MG-ND	-5.28	1.95	2.05
25	n	607	CHL	MG-ND	-5.28	1.95	2.05
22	c	509	CLA	C1D-ND	-5.28	1.31	1.37
22	c	502	CLA	C1D-ND	-5.28	1.31	1.37
22	c	504	CLA	C1D-ND	-5.27	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	303	CLA	C4B-NB	-5.27	1.31	1.37
22	s	303	CLA	C4B-NB	-5.27	1.31	1.37
22	R	311	CLA	C4B-NB	-5.27	1.31	1.37
22	Y	612	CLA	C1D-ND	-5.27	1.31	1.37
22	r	311	CLA	C4B-NB	-5.27	1.31	1.37
22	y	612	CLA	C1D-ND	-5.27	1.31	1.37
22	C	512	CLA	C4B-NB	-5.26	1.31	1.37
22	N	613	CLA	C1D-ND	-5.26	1.31	1.37
22	n	613	CLA	C1D-ND	-5.26	1.31	1.37
22	c	510	CLA	C1D-ND	-5.26	1.31	1.37
25	N	606	CHL	MG-ND	-5.26	1.95	2.05
25	n	606	CHL	MG-ND	-5.26	1.95	2.05
22	N	611	CLA	C4B-NB	-5.25	1.31	1.37
22	n	611	CLA	C4B-NB	-5.25	1.31	1.37
22	C	511	CLA	C4B-NB	-5.25	1.31	1.37
22	B	603	CLA	C1D-ND	-5.24	1.31	1.37
22	b	616	CLA	C4B-NB	-5.24	1.31	1.37
22	R	308	CLA	C4B-NB	-5.24	1.31	1.37
22	r	308	CLA	C4B-NB	-5.24	1.31	1.37
25	Y	609	CHL	MG-ND	-5.24	1.95	2.05
25	y	609	CHL	MG-ND	-5.24	1.95	2.05
23	a	404	PHO	C3B-C2B	5.24	1.47	1.40
22	c	511	CLA	C4B-NB	-5.23	1.31	1.37
22	Y	614	CLA	C1D-ND	-5.22	1.31	1.37
22	y	614	CLA	C1D-ND	-5.22	1.31	1.37
22	R	308	CLA	C1D-ND	-5.22	1.31	1.37
22	r	308	CLA	C1D-ND	-5.22	1.31	1.37
22	d	404	CLA	C4B-NB	-5.21	1.31	1.37
22	Y	603	CLA	C4B-NB	-5.21	1.31	1.37
22	y	603	CLA	C4B-NB	-5.21	1.31	1.37
25	Y	608	CHL	MG-ND	-5.20	1.95	2.05
25	y	608	CHL	MG-ND	-5.20	1.95	2.05
25	Y	607	CHL	MG-ND	-5.20	1.95	2.05
25	y	607	CHL	MG-ND	-5.20	1.95	2.05
22	c	503	CLA	C1D-ND	-5.20	1.31	1.37
22	s	301	CLA	C4B-NB	-5.20	1.31	1.37
25	N	609	CHL	MG-ND	-5.20	1.95	2.05
25	n	609	CHL	MG-ND	-5.20	1.95	2.05
22	b	603	CLA	C4B-NB	-5.20	1.31	1.37
22	b	616	CLA	C1D-ND	-5.19	1.31	1.37
22	R	301	CLA	C4B-NB	-5.19	1.31	1.37
22	r	301	CLA	C4B-NB	-5.19	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	614	CLA	C4B-NB	-5.18	1.31	1.37
22	g	614	CLA	C4B-NB	-5.18	1.31	1.37
22	C	510	CLA	C1D-ND	-5.18	1.31	1.37
22	B	613	CLA	C1D-ND	-5.18	1.31	1.37
22	N	610	CLA	C4B-NB	-5.17	1.31	1.37
22	n	610	CLA	C4B-NB	-5.17	1.31	1.37
22	G	603	CLA	C4B-NB	-5.17	1.31	1.37
22	g	603	CLA	C4B-NB	-5.17	1.31	1.37
22	C	503	CLA	C1D-ND	-5.17	1.31	1.37
22	d	401	CLA	C1D-ND	-5.17	1.31	1.37
22	1	604	CLA	C4B-NB	-5.17	1.31	1.37
22	5	604	CLA	C4B-NB	-5.17	1.31	1.37
22	c	509	CLA	C4B-NB	-5.17	1.31	1.37
22	c	512	CLA	C4B-NB	-5.17	1.31	1.37
22	R	302	CLA	C1D-ND	-5.17	1.31	1.37
22	r	302	CLA	C1D-ND	-5.17	1.31	1.37
22	R	309	CLA	C4B-NB	-5.16	1.31	1.37
22	r	309	CLA	C4B-NB	-5.16	1.31	1.37
22	R	303	CLA	C1D-ND	-5.16	1.31	1.37
22	r	303	CLA	C1D-ND	-5.16	1.31	1.37
25	G	606	CHL	MG-ND	-5.16	1.95	2.05
25	g	606	CHL	MG-ND	-5.16	1.95	2.05
22	B	606	CLA	C4B-NB	-5.16	1.31	1.37
22	A	403	CLA	C1D-ND	-5.16	1.31	1.37
22	C	507	CLA	C4B-NB	-5.16	1.31	1.37
22	b	605	CLA	C1D-ND	-5.15	1.31	1.37
22	B	614	CLA	C1D-ND	-5.15	1.31	1.37
25	R	304	CHL	MG-ND	-5.15	1.95	2.05
25	r	304	CHL	MG-ND	-5.15	1.95	2.05
22	c	507	CLA	C1D-ND	-5.15	1.31	1.37
22	S	304	CLA	C1D-ND	-5.15	1.31	1.37
22	s	304	CLA	C1D-ND	-5.15	1.31	1.37
22	3	303	CLA	C4B-NB	-5.15	1.31	1.37
22	7	303	CLA	C4B-NB	-5.15	1.31	1.37
22	d	404	CLA	C1D-ND	-5.15	1.31	1.37
22	D	404	CLA	C4B-NB	-5.14	1.31	1.37
22	G	603	CLA	C1D-ND	-5.14	1.31	1.37
22	g	603	CLA	C1D-ND	-5.14	1.31	1.37
22	C	507	CLA	C1D-ND	-5.14	1.31	1.37
22	S	312	CLA	C1D-ND	-5.14	1.31	1.37
22	s	312	CLA	C1D-ND	-5.14	1.31	1.37
22	N	602	CLA	C1D-ND	-5.14	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	n	602	CLA	C1D-ND	-5.14	1.31	1.37
22	D	404	CLA	C1D-ND	-5.14	1.31	1.37
22	B	605	CLA	C1D-ND	-5.14	1.31	1.37
22	b	604	CLA	C1D-ND	-5.14	1.31	1.37
22	S	305	CLA	OBD-CAD	5.13	1.31	1.22
22	s	305	CLA	OBD-CAD	5.13	1.31	1.22
22	G	604	CLA	C1D-ND	-5.13	1.31	1.37
22	N	603	CLA	C1D-ND	-5.13	1.31	1.37
22	g	604	CLA	C1D-ND	-5.13	1.31	1.37
22	n	603	CLA	C1D-ND	-5.13	1.31	1.37
25	S	307	CHL	MG-ND	-5.12	1.95	2.05
25	s	307	CHL	MG-ND	-5.12	1.95	2.05
25	Y	606	CHL	MG-ND	-5.12	1.95	2.05
25	y	606	CHL	MG-ND	-5.12	1.95	2.05
22	S	304	CLA	OBD-CAD	5.12	1.31	1.22
22	s	304	CLA	OBD-CAD	5.12	1.31	1.22
22	b	601	CLA	C1D-ND	-5.12	1.31	1.37
22	b	609	CLA	C4B-NB	-5.12	1.31	1.37
25	1	605	CHL	MG-ND	-5.12	1.95	2.05
25	5	605	CHL	MG-ND	-5.12	1.95	2.05
22	4	303	CLA	C4B-NB	-5.12	1.31	1.37
22	8	303	CLA	C4B-NB	-5.12	1.31	1.37
22	3	314	CLA	C4B-NB	-5.12	1.31	1.37
22	7	314	CLA	C4B-NB	-5.12	1.31	1.37
22	2	612	CLA	C4B-NB	-5.11	1.31	1.37
22	6	612	CLA	C4B-NB	-5.11	1.31	1.37
22	c	507	CLA	C4B-NB	-5.11	1.31	1.37
22	S	301	CLA	C4B-NB	-5.11	1.31	1.37
22	G	610	CLA	C4B-NB	-5.11	1.31	1.37
22	g	610	CLA	C4B-NB	-5.11	1.31	1.37
22	b	610	CLA	C1D-ND	-5.11	1.31	1.37
22	a	403	CLA	C1D-ND	-5.11	1.31	1.37
23	A	404	PHO	CBD-CGD	-5.10	1.45	1.52
22	N	610	CLA	C1D-ND	-5.10	1.31	1.37
22	n	610	CLA	C1D-ND	-5.10	1.31	1.37
22	S	314	CLA	C1D-ND	-5.10	1.31	1.37
22	s	314	CLA	C1D-ND	-5.10	1.31	1.37
22	b	602	CLA	C1D-ND	-5.09	1.31	1.37
22	Y	603	CLA	C1D-ND	-5.09	1.31	1.37
22	y	603	CLA	C1D-ND	-5.09	1.31	1.37
25	R	305	CHL	MG-ND	-5.09	1.95	2.05
25	r	305	CHL	MG-ND	-5.09	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	605	CHL	MG-ND	-5.09	1.95	2.05
25	n	605	CHL	MG-ND	-5.09	1.95	2.05
22	S	309	CLA	C4B-NB	-5.08	1.31	1.37
22	s	309	CLA	C4B-NB	-5.08	1.31	1.37
22	B	602	CLA	C4B-NB	-5.08	1.31	1.37
25	G	601	CHL	MG-ND	-5.07	1.95	2.05
25	g	601	CHL	MG-ND	-5.07	1.95	2.05
22	2	602	CLA	C4B-NB	-5.07	1.31	1.37
22	6	602	CLA	C4B-NB	-5.07	1.31	1.37
25	G	607	CHL	MG-ND	-5.07	1.95	2.05
25	g	607	CHL	MG-ND	-5.07	1.95	2.05
22	C	509	CLA	C4B-NB	-5.06	1.31	1.37
22	N	614	CLA	C4B-NB	-5.06	1.31	1.37
22	n	614	CLA	C4B-NB	-5.06	1.31	1.37
22	B	601	CLA	C4B-NB	-5.05	1.31	1.37
22	b	614	CLA	C4B-NB	-5.05	1.31	1.37
22	1	604	CLA	C1D-ND	-5.05	1.31	1.37
22	5	604	CLA	C1D-ND	-5.05	1.31	1.37
22	b	609	CLA	C1D-ND	-5.05	1.31	1.37
22	b	613	CLA	C1D-ND	-5.05	1.31	1.37
22	2	604	CLA	OBD-CAD	5.05	1.31	1.22
22	6	604	CLA	OBD-CAD	5.05	1.31	1.22
22	C	511	CLA	C1D-ND	-5.05	1.31	1.37
22	b	606	CLA	OBD-CAD	5.04	1.31	1.22
23	D	402	PHO	C3B-C2B	5.04	1.47	1.40
22	B	614	CLA	C4B-NB	-5.04	1.31	1.37
25	G	608	CHL	MG-ND	-5.03	1.95	2.05
25	g	608	CHL	MG-ND	-5.03	1.95	2.05
25	R	306	CHL	MG-ND	-5.03	1.95	2.05
25	r	306	CHL	MG-ND	-5.03	1.95	2.05
22	C	501	CLA	C1D-ND	-5.03	1.31	1.37
22	S	310	CLA	C1D-ND	-5.03	1.31	1.37
22	s	310	CLA	C1D-ND	-5.03	1.31	1.37
22	b	601	CLA	C4B-NB	-5.03	1.31	1.37
22	B	610	CLA	C1D-ND	-5.02	1.31	1.37
22	1	612	CLA	C4B-NB	-5.02	1.31	1.37
22	5	612	CLA	C4B-NB	-5.02	1.31	1.37
22	D	401	CLA	C1D-ND	-5.01	1.31	1.37
22	S	303	CLA	C1D-ND	-5.01	1.31	1.37
22	s	303	CLA	C1D-ND	-5.01	1.31	1.37
22	B	609	CLA	C4B-NB	-5.01	1.31	1.37
22	1	614	CLA	OBD-CAD	5.01	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	614	CLA	OBD-CAD	5.01	1.31	1.22
22	G	612	CLA	C1D-ND	-5.01	1.31	1.37
22	g	612	CLA	C1D-ND	-5.01	1.31	1.37
22	c	512	CLA	C1D-ND	-5.00	1.31	1.37
22	2	611	CLA	C4B-NB	-5.00	1.31	1.37
22	2	613	CLA	C4B-NB	-5.00	1.31	1.37
22	6	611	CLA	C4B-NB	-5.00	1.31	1.37
22	6	613	CLA	C4B-NB	-5.00	1.31	1.37
25	N	601	CHL	MG-ND	-5.00	1.95	2.05
25	n	601	CHL	MG-ND	-5.00	1.95	2.05
22	C	509	CLA	C1D-ND	-5.00	1.31	1.37
22	B	606	CLA	C1D-ND	-5.00	1.31	1.37
22	c	511	CLA	C1D-ND	-4.99	1.31	1.37
22	R	302	CLA	OBD-CAD	4.99	1.31	1.22
22	r	302	CLA	OBD-CAD	4.99	1.31	1.22
22	1	613	CLA	C4B-NB	-4.99	1.31	1.37
22	5	613	CLA	C4B-NB	-4.99	1.31	1.37
22	B	615	CLA	OBD-CAD	4.99	1.31	1.22
22	1	604	CLA	OBD-CAD	4.98	1.31	1.22
22	5	604	CLA	OBD-CAD	4.98	1.31	1.22
22	3	313	CLA	C4B-NB	-4.98	1.31	1.37
22	7	313	CLA	C4B-NB	-4.98	1.31	1.37
22	s	301	CLA	OBD-CAD	4.98	1.31	1.22
22	2	611	CLA	OBD-CAD	4.98	1.31	1.22
22	6	611	CLA	OBD-CAD	4.98	1.31	1.22
22	4	301	CLA	C4B-NB	-4.98	1.31	1.37
22	8	301	CLA	C4B-NB	-4.98	1.31	1.37
22	4	305	CLA	C4B-NB	-4.98	1.31	1.37
22	8	305	CLA	C4B-NB	-4.98	1.31	1.37
22	3	312	CLA	OBD-CAD	4.97	1.31	1.22
22	7	312	CLA	OBD-CAD	4.97	1.31	1.22
22	a	402	CLA	C1D-ND	-4.96	1.31	1.37
25	S	308	CHL	MG-ND	-4.96	1.95	2.05
25	s	308	CHL	MG-ND	-4.96	1.95	2.05
22	b	601	CLA	OBD-CAD	4.96	1.31	1.22
22	3	310	CLA	OBD-CAD	4.96	1.31	1.22
22	7	310	CLA	OBD-CAD	4.96	1.31	1.22
22	1	613	CLA	C1D-ND	-4.96	1.31	1.37
22	5	613	CLA	C1D-ND	-4.96	1.31	1.37
22	A	402	CLA	C1D-ND	-4.95	1.31	1.37
22	B	615	CLA	C1D-ND	-4.95	1.31	1.37
22	3	311	CLA	OBD-CAD	4.95	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	311	CLA	OBD-CAD	4.95	1.31	1.22
22	4	311	CLA	C4B-NB	-4.95	1.31	1.37
22	8	311	CLA	C4B-NB	-4.95	1.31	1.37
22	N	614	CLA	OBD-CAD	4.95	1.31	1.22
22	n	614	CLA	OBD-CAD	4.95	1.31	1.22
22	G	614	CLA	C1D-ND	-4.95	1.31	1.37
22	g	614	CLA	C1D-ND	-4.95	1.31	1.37
22	R	311	CLA	OBD-CAD	4.94	1.31	1.22
22	r	311	CLA	OBD-CAD	4.94	1.31	1.22
22	1	603	CLA	OBD-CAD	4.94	1.31	1.22
22	5	603	CLA	OBD-CAD	4.94	1.31	1.22
22	3	313	CLA	OBD-CAD	4.94	1.31	1.22
22	7	313	CLA	OBD-CAD	4.94	1.31	1.22
22	1	611	CLA	OBD-CAD	4.94	1.31	1.22
22	5	611	CLA	OBD-CAD	4.94	1.31	1.22
25	G	609	CHL	MG-ND	-4.93	1.96	2.05
25	g	609	CHL	MG-ND	-4.93	1.96	2.05
22	R	310	CLA	C1D-ND	-4.93	1.31	1.37
22	r	310	CLA	C1D-ND	-4.93	1.31	1.37
22	2	603	CLA	OBD-CAD	4.93	1.31	1.22
22	6	603	CLA	OBD-CAD	4.93	1.31	1.22
22	2	613	CLA	OBD-CAD	4.93	1.31	1.22
22	6	613	CLA	OBD-CAD	4.93	1.31	1.22
22	S	301	CLA	OBD-CAD	4.93	1.31	1.22
22	4	310	CLA	OBD-CAD	4.93	1.31	1.22
22	8	310	CLA	OBD-CAD	4.93	1.31	1.22
22	B	603	CLA	C1B-NB	-4.93	1.31	1.37
22	4	305	CLA	OBD-CAD	4.92	1.31	1.22
22	8	305	CLA	OBD-CAD	4.92	1.31	1.22
22	G	611	CLA	C1D-ND	-4.92	1.31	1.37
22	g	611	CLA	C1D-ND	-4.92	1.31	1.37
22	C	505	CLA	OBD-CAD	4.92	1.31	1.22
25	3	301	CHL	MG-ND	-4.92	1.96	2.05
25	7	301	CHL	MG-ND	-4.92	1.96	2.05
22	Y	610	CLA	C1D-ND	-4.92	1.31	1.37
22	y	610	CLA	C1D-ND	-4.92	1.31	1.37
22	B	601	CLA	C1D-ND	-4.92	1.31	1.37
22	1	610	CLA	C4B-NB	-4.91	1.31	1.37
22	5	610	CLA	C4B-NB	-4.91	1.31	1.37
22	S	309	CLA	OBD-CAD	4.91	1.30	1.22
22	s	309	CLA	OBD-CAD	4.91	1.30	1.22
22	b	609	CLA	OBD-CAD	4.91	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	611	CLA	OBD-CAD	4.91	1.30	1.22
22	n	611	CLA	OBD-CAD	4.91	1.30	1.22
22	Y	602	CLA	C1D-ND	-4.90	1.31	1.37
22	y	602	CLA	C1D-ND	-4.90	1.31	1.37
22	c	504	CLA	OBD-CAD	4.90	1.30	1.22
22	4	311	CLA	OBD-CAD	4.90	1.30	1.22
22	8	311	CLA	OBD-CAD	4.90	1.30	1.22
22	G	610	CLA	C1D-ND	-4.90	1.31	1.37
22	g	610	CLA	C1D-ND	-4.90	1.31	1.37
22	3	314	CLA	OBD-CAD	4.90	1.30	1.22
22	7	314	CLA	OBD-CAD	4.90	1.30	1.22
22	R	307	CLA	OBD-CAD	4.90	1.30	1.22
22	r	307	CLA	OBD-CAD	4.90	1.30	1.22
22	B	604	CLA	C1D-ND	-4.90	1.31	1.37
22	3	305	CLA	C4B-NB	-4.90	1.31	1.37
22	7	305	CLA	C4B-NB	-4.90	1.31	1.37
22	B	610	CLA	OBD-CAD	4.90	1.30	1.22
22	1	602	CLA	C4B-NB	-4.89	1.31	1.37
22	5	602	CLA	C4B-NB	-4.89	1.31	1.37
22	B	601	CLA	OBD-CAD	4.89	1.30	1.22
22	2	610	CLA	OBD-CAD	4.89	1.30	1.22
22	6	610	CLA	OBD-CAD	4.89	1.30	1.22
22	1	613	CLA	OBD-CAD	4.89	1.30	1.22
22	5	613	CLA	OBD-CAD	4.89	1.30	1.22
22	1	611	CLA	C4B-NB	-4.89	1.31	1.37
22	5	611	CLA	C4B-NB	-4.89	1.31	1.37
22	2	604	CLA	C4B-NB	-4.89	1.31	1.37
22	6	604	CLA	C4B-NB	-4.89	1.31	1.37
22	d	404	CLA	OBD-CAD	4.88	1.30	1.22
22	N	604	CLA	OBD-CAD	4.88	1.30	1.22
22	n	604	CLA	OBD-CAD	4.88	1.30	1.22
22	3	305	CLA	OBD-CAD	4.88	1.30	1.22
22	7	305	CLA	OBD-CAD	4.88	1.30	1.22
22	b	610	CLA	OBD-CAD	4.88	1.30	1.22
22	D	404	CLA	OBD-CAD	4.87	1.30	1.22
22	4	301	CLA	OBD-CAD	4.87	1.30	1.22
22	8	301	CLA	OBD-CAD	4.87	1.30	1.22
22	B	609	CLA	OBD-CAD	4.87	1.30	1.22
22	3	312	CLA	C4B-NB	-4.87	1.31	1.37
22	7	312	CLA	C4B-NB	-4.87	1.31	1.37
22	b	603	CLA	OBD-CAD	4.87	1.30	1.22
22	3	311	CLA	C4B-NB	-4.87	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	311	CLA	C4B-NB	-4.87	1.31	1.37
24	F	101	HEM	FE-NC	4.87	2.11	1.95
22	N	611	CLA	C1D-ND	-4.86	1.31	1.37
22	n	611	CLA	C1D-ND	-4.86	1.31	1.37
22	3	304	CLA	OBD-CAD	4.86	1.30	1.22
22	7	304	CLA	OBD-CAD	4.86	1.30	1.22
22	C	511	CLA	OBD-CAD	4.86	1.30	1.22
22	b	615	CLA	OBD-CAD	4.86	1.30	1.22
22	c	506	CLA	OBD-CAD	4.86	1.30	1.22
22	b	615	CLA	C1D-ND	-4.86	1.31	1.37
25	Y	601	CHL	MG-ND	-4.85	1.96	2.05
25	y	601	CHL	MG-ND	-4.85	1.96	2.05
22	G	614	CLA	OBD-CAD	4.85	1.30	1.22
22	g	614	CLA	OBD-CAD	4.85	1.30	1.22
22	R	309	CLA	C1D-ND	-4.85	1.31	1.37
22	r	309	CLA	C1D-ND	-4.85	1.31	1.37
22	C	512	CLA	OBD-CAD	4.85	1.30	1.22
22	R	309	CLA	OBD-CAD	4.85	1.30	1.22
22	r	309	CLA	OBD-CAD	4.85	1.30	1.22
22	1	610	CLA	OBD-CAD	4.84	1.30	1.22
22	5	610	CLA	OBD-CAD	4.84	1.30	1.22
22	3	310	CLA	C4B-NB	-4.84	1.31	1.37
22	7	310	CLA	C4B-NB	-4.84	1.31	1.37
22	G	604	CLA	OBD-CAD	4.84	1.30	1.22
22	g	604	CLA	OBD-CAD	4.84	1.30	1.22
22	R	301	CLA	C1D-ND	-4.84	1.31	1.37
22	r	301	CLA	C1D-ND	-4.84	1.31	1.37
22	1	614	CLA	C1D-ND	-4.84	1.31	1.37
22	5	614	CLA	C1D-ND	-4.84	1.31	1.37
25	2	606	CHL	MG-ND	-4.84	1.96	2.05
25	6	606	CHL	MG-ND	-4.84	1.96	2.05
22	1	612	CLA	C1D-ND	-4.83	1.31	1.37
22	5	612	CLA	C1D-ND	-4.83	1.31	1.37
22	2	612	CLA	OBD-CAD	4.83	1.30	1.22
22	6	612	CLA	OBD-CAD	4.83	1.30	1.22
22	2	609	CLA	OBD-CAD	4.82	1.30	1.22
22	6	609	CLA	OBD-CAD	4.82	1.30	1.22
22	N	614	CLA	C1D-ND	-4.82	1.31	1.37
22	n	614	CLA	C1D-ND	-4.82	1.31	1.37
22	1	612	CLA	OBD-CAD	4.81	1.30	1.22
22	5	612	CLA	OBD-CAD	4.81	1.30	1.22
22	d	401	CLA	OBD-CAD	4.81	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	504	CLA	OBD-CAD	4.81	1.30	1.22
22	c	510	CLA	OBD-CAD	4.81	1.30	1.22
22	B	607	CLA	OBD-CAD	4.81	1.30	1.22
22	4	305	CLA	C1D-ND	-4.81	1.31	1.37
22	8	305	CLA	C1D-ND	-4.81	1.31	1.37
22	D	403	CLA	OBD-CAD	4.80	1.30	1.22
25	3	308	CHL	MG-ND	-4.80	1.96	2.05
25	7	308	CHL	MG-ND	-4.80	1.96	2.05
22	d	403	CLA	OBD-CAD	4.80	1.30	1.22
22	C	509	CLA	OBD-CAD	4.80	1.30	1.22
22	4	301	CLA	C1D-ND	-4.80	1.31	1.37
22	4	304	CLA	C4B-NB	-4.80	1.31	1.37
22	8	301	CLA	C1D-ND	-4.80	1.31	1.37
22	8	304	CLA	C4B-NB	-4.80	1.31	1.37
25	1	606	CHL	MG-ND	-4.80	1.96	2.05
25	5	606	CHL	MG-ND	-4.80	1.96	2.05
22	4	303	CLA	C1D-ND	-4.79	1.31	1.37
22	8	303	CLA	C1D-ND	-4.79	1.31	1.37
22	c	512	CLA	OBD-CAD	4.79	1.30	1.22
25	1	607	CHL	MG-ND	-4.79	1.96	2.05
25	5	607	CHL	MG-ND	-4.79	1.96	2.05
22	2	612	CLA	C1D-ND	-4.79	1.31	1.37
22	6	612	CLA	C1D-ND	-4.79	1.31	1.37
22	a	405	CLA	OBD-CAD	4.79	1.30	1.22
25	Y	605	CHL	C3A-C2A	-4.79	1.50	1.54
25	y	605	CHL	C3A-C2A	-4.79	1.50	1.54
22	b	612	CLA	OBD-CAD	4.79	1.30	1.22
22	2	610	CLA	C4B-NB	-4.79	1.31	1.37
22	6	610	CLA	C4B-NB	-4.79	1.31	1.37
22	4	310	CLA	C4B-NB	-4.79	1.31	1.37
22	8	310	CLA	C4B-NB	-4.79	1.31	1.37
22	2	609	CLA	C4B-NB	-4.79	1.31	1.37
22	6	609	CLA	C4B-NB	-4.79	1.31	1.37
22	C	507	CLA	OBD-CAD	4.78	1.30	1.22
22	b	614	CLA	OBD-CAD	4.78	1.30	1.22
22	G	611	CLA	OBD-CAD	4.78	1.30	1.22
22	g	611	CLA	OBD-CAD	4.78	1.30	1.22
22	b	606	CLA	C4B-NB	-4.78	1.31	1.37
22	c	505	CLA	OBD-CAD	4.78	1.30	1.22
22	Y	604	CLA	OBD-CAD	4.78	1.30	1.22
22	y	604	CLA	OBD-CAD	4.78	1.30	1.22
22	3	304	CLA	C1D-ND	-4.78	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	304	CLA	C1D-ND	-4.78	1.31	1.37
22	2	602	CLA	C1D-ND	-4.77	1.31	1.37
22	6	602	CLA	C1D-ND	-4.77	1.31	1.37
22	C	506	CLA	OBD-CAD	4.77	1.30	1.22
22	B	606	CLA	OBD-CAD	4.77	1.30	1.22
25	1	615	CHL	MG-ND	-4.77	1.96	2.05
25	5	615	CHL	MG-ND	-4.77	1.96	2.05
22	N	612	CLA	C1D-ND	-4.77	1.31	1.37
22	n	612	CLA	C1D-ND	-4.77	1.31	1.37
22	C	510	CLA	OBD-CAD	4.77	1.30	1.22
22	b	616	CLA	OBD-CAD	4.76	1.30	1.22
25	2	601	CHL	MG-ND	-4.76	1.96	2.05
25	6	601	CHL	MG-ND	-4.76	1.96	2.05
22	G	612	CLA	OBD-CAD	4.76	1.30	1.22
22	g	612	CLA	OBD-CAD	4.76	1.30	1.22
22	Y	614	CLA	OBD-CAD	4.76	1.30	1.22
22	y	614	CLA	OBD-CAD	4.76	1.30	1.22
22	S	311	CLA	OBD-CAD	4.76	1.30	1.22
22	s	311	CLA	OBD-CAD	4.76	1.30	1.22
25	4	308	CHL	MG-ND	-4.75	1.96	2.05
25	8	308	CHL	MG-ND	-4.75	1.96	2.05
22	1	614	CLA	C4B-NB	-4.75	1.31	1.37
22	5	614	CLA	C4B-NB	-4.75	1.31	1.37
22	S	314	CLA	OBD-CAD	4.75	1.30	1.22
22	s	314	CLA	OBD-CAD	4.75	1.30	1.22
22	3	313	CLA	C1D-ND	-4.75	1.31	1.37
22	7	313	CLA	C1D-ND	-4.75	1.31	1.37
22	B	608	CLA	OBD-CAD	4.75	1.30	1.22
25	4	302	CHL	MG-ND	-4.74	1.96	2.05
25	8	302	CHL	MG-ND	-4.74	1.96	2.05
25	4	307	CHL	MG-ND	-4.74	1.96	2.05
25	8	307	CHL	MG-ND	-4.74	1.96	2.05
22	R	303	CLA	OBD-CAD	4.73	1.30	1.22
22	r	303	CLA	OBD-CAD	4.73	1.30	1.22
22	B	614	CLA	OBD-CAD	4.73	1.30	1.22
22	C	512	CLA	C1D-ND	-4.73	1.32	1.37
22	1	611	CLA	C1D-ND	-4.73	1.32	1.37
22	5	611	CLA	C1D-ND	-4.73	1.32	1.37
22	B	602	CLA	C1D-ND	-4.73	1.32	1.37
22	b	602	CLA	OBD-CAD	4.73	1.30	1.22
22	C	508	CLA	OBD-CAD	4.72	1.30	1.22
22	A	402	CLA	OBD-CAD	4.72	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Y	602	CLA	OBD-CAD	4.72	1.30	1.22
22	y	602	CLA	OBD-CAD	4.72	1.30	1.22
22	2	613	CLA	C1D-ND	-4.72	1.32	1.37
22	6	613	CLA	C1D-ND	-4.72	1.32	1.37
22	c	509	CLA	OBD-CAD	4.71	1.30	1.22
22	b	605	CLA	OBD-CAD	4.71	1.30	1.22
23	a	404	PHO	CBD-CGD	-4.71	1.46	1.52
22	2	603	CLA	C4B-NB	-4.71	1.32	1.37
22	6	603	CLA	C4B-NB	-4.71	1.32	1.37
22	2	604	CLA	C1D-ND	-4.71	1.32	1.37
22	6	604	CLA	C1D-ND	-4.71	1.32	1.37
22	B	602	CLA	OBD-CAD	4.70	1.30	1.22
25	S	306	CHL	MG-ND	-4.70	1.96	2.05
25	s	306	CHL	MG-ND	-4.70	1.96	2.05
22	3	314	CLA	C1D-ND	-4.70	1.32	1.37
22	7	314	CLA	C1D-ND	-4.70	1.32	1.37
25	3	302	CHL	MG-ND	-4.70	1.96	2.05
25	7	302	CHL	MG-ND	-4.70	1.96	2.05
22	b	607	CLA	OBD-CAD	4.70	1.30	1.22
22	b	612	CLA	CHC-C1C	4.70	1.48	1.38
22	Y	611	CLA	OBD-CAD	4.69	1.30	1.22
22	y	611	CLA	OBD-CAD	4.69	1.30	1.22
22	3	303	CLA	OBD-CAD	4.69	1.30	1.22
22	7	303	CLA	OBD-CAD	4.69	1.30	1.22
22	S	312	CLA	OBD-CAD	4.69	1.30	1.22
22	s	312	CLA	OBD-CAD	4.69	1.30	1.22
22	4	304	CLA	OBD-CAD	4.69	1.30	1.22
22	8	304	CLA	OBD-CAD	4.69	1.30	1.22
22	B	612	CLA	OBD-CAD	4.69	1.30	1.22
22	3	305	CLA	C1D-ND	-4.68	1.32	1.37
22	7	305	CLA	C1D-ND	-4.68	1.32	1.37
22	4	311	CLA	C1D-ND	-4.68	1.32	1.37
22	8	311	CLA	C1D-ND	-4.68	1.32	1.37
25	1	608	CHL	MG-ND	-4.68	1.96	2.05
25	5	608	CHL	MG-ND	-4.68	1.96	2.05
22	c	508	CLA	OBD-CAD	4.67	1.30	1.22
22	A	403	CLA	OBD-CAD	4.67	1.30	1.22
22	2	609	CLA	CHC-C1C	4.66	1.48	1.38
22	6	609	CLA	CHC-C1C	4.66	1.48	1.38
22	4	304	CLA	C1D-ND	-4.66	1.32	1.37
22	8	304	CLA	C1D-ND	-4.66	1.32	1.37
22	S	309	CLA	C1D-ND	-4.66	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	309	CLA	C1D-ND	-4.66	1.32	1.37
22	B	603	CLA	OBD-CAD	4.65	1.30	1.22
22	N	612	CLA	OBD-CAD	4.65	1.30	1.22
22	n	612	CLA	OBD-CAD	4.65	1.30	1.22
25	1	609	CHL	MG-ND	-4.65	1.96	2.05
25	5	609	CHL	MG-ND	-4.65	1.96	2.05
22	2	610	CLA	C1D-ND	-4.65	1.32	1.37
22	6	610	CLA	C1D-ND	-4.65	1.32	1.37
25	3	307	CHL	MG-ND	-4.65	1.96	2.05
25	7	307	CHL	MG-ND	-4.65	1.96	2.05
22	R	310	CLA	OBD-CAD	4.64	1.30	1.22
22	r	310	CLA	OBD-CAD	4.64	1.30	1.22
25	2	607	CHL	MG-ND	-4.64	1.96	2.05
25	6	607	CHL	MG-ND	-4.64	1.96	2.05
22	a	402	CLA	OBD-CAD	4.64	1.30	1.22
22	A	405	CLA	OBD-CAD	4.64	1.30	1.22
22	1	603	CLA	C1D-ND	-4.63	1.32	1.37
22	5	603	CLA	C1D-ND	-4.63	1.32	1.37
22	3	311	CLA	C1D-ND	-4.63	1.32	1.37
22	7	311	CLA	C1D-ND	-4.63	1.32	1.37
22	G	610	CLA	OBD-CAD	4.62	1.30	1.22
22	N	610	CLA	OBD-CAD	4.62	1.30	1.22
22	g	610	CLA	OBD-CAD	4.62	1.30	1.22
22	n	610	CLA	OBD-CAD	4.62	1.30	1.22
22	D	401	CLA	OBD-CAD	4.62	1.30	1.22
22	G	603	CLA	OBD-CAD	4.62	1.30	1.22
22	g	603	CLA	OBD-CAD	4.62	1.30	1.22
25	2	608	CHL	MG-ND	-4.62	1.96	2.05
25	6	608	CHL	MG-ND	-4.62	1.96	2.05
22	3	303	CLA	C1D-ND	-4.61	1.32	1.37
22	7	303	CLA	C1D-ND	-4.61	1.32	1.37
22	2	603	CLA	C1D-ND	-4.61	1.32	1.37
22	6	603	CLA	C1D-ND	-4.61	1.32	1.37
22	3	310	CLA	CHC-C1C	4.61	1.47	1.38
22	7	310	CLA	CHC-C1C	4.61	1.47	1.38
25	4	309	CHL	MG-ND	-4.60	1.96	2.05
25	8	309	CHL	MG-ND	-4.60	1.96	2.05
22	2	602	CLA	OBD-CAD	4.60	1.30	1.22
22	6	602	CLA	OBD-CAD	4.60	1.30	1.22
22	N	602	CLA	OBD-CAD	4.60	1.30	1.22
22	n	602	CLA	OBD-CAD	4.60	1.30	1.22
22	1	603	CLA	C4B-NB	-4.60	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	603	CLA	C4B-NB	-4.60	1.32	1.37
22	b	606	CLA	CHC-C1C	4.60	1.47	1.38
23	d	402	PHO	C4D-CHA	4.59	1.46	1.39
22	R	301	CLA	OBD-CAD	4.59	1.30	1.22
22	r	301	CLA	OBD-CAD	4.59	1.30	1.22
22	3	304	CLA	C4B-NB	-4.58	1.32	1.37
22	7	304	CLA	C4B-NB	-4.58	1.32	1.37
23	D	402	PHO	C4D-CHA	4.58	1.46	1.39
25	G	606	CHL	MG-NA	4.58	2.17	2.06
25	g	606	CHL	MG-NA	4.58	2.17	2.06
22	B	605	CLA	OBD-CAD	4.58	1.30	1.22
22	4	310	CLA	C1D-ND	-4.58	1.32	1.37
22	8	310	CLA	C1D-ND	-4.58	1.32	1.37
22	R	310	CLA	C4B-NB	-4.57	1.32	1.37
22	r	310	CLA	C4B-NB	-4.57	1.32	1.37
22	R	308	CLA	OBD-CAD	4.56	1.30	1.22
22	r	308	CLA	OBD-CAD	4.56	1.30	1.22
22	b	604	CLA	OBD-CAD	4.56	1.30	1.22
22	4	303	CLA	OBD-CAD	4.56	1.30	1.22
22	8	303	CLA	OBD-CAD	4.56	1.30	1.22
25	3	309	CHL	MG-ND	-4.56	1.96	2.05
25	7	309	CHL	MG-ND	-4.56	1.96	2.05
22	1	602	CLA	C1D-ND	-4.55	1.32	1.37
22	5	602	CLA	C1D-ND	-4.55	1.32	1.37
22	Y	610	CLA	OBD-CAD	4.55	1.30	1.22
22	y	610	CLA	OBD-CAD	4.55	1.30	1.22
22	b	608	CLA	OBD-CAD	4.55	1.30	1.22
22	S	312	CLA	C1B-NB	-4.55	1.32	1.37
22	s	312	CLA	C1B-NB	-4.55	1.32	1.37
22	Y	612	CLA	OBD-CAD	4.54	1.30	1.22
22	y	612	CLA	OBD-CAD	4.54	1.30	1.22
25	4	306	CHL	MG-ND	-4.54	1.96	2.05
25	8	306	CHL	MG-ND	-4.54	1.96	2.05
22	G	602	CLA	OBD-CAD	4.53	1.30	1.22
22	g	602	CLA	OBD-CAD	4.53	1.30	1.22
22	3	314	CLA	CHC-C1C	4.53	1.47	1.38
22	7	314	CLA	CHC-C1C	4.53	1.47	1.38
25	2	606	CHL	MG-NA	4.52	2.17	2.06
25	6	606	CHL	MG-NA	4.52	2.17	2.06
24	e	101	HEM	FE-NB	4.52	2.08	1.94
22	4	311	CLA	C3C-C2C	4.52	1.46	1.36
22	8	311	CLA	C3C-C2C	4.52	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	507	CLA	OBD-CAD	4.52	1.30	1.22
22	G	613	CLA	OBD-CAD	4.52	1.30	1.22
22	g	613	CLA	OBD-CAD	4.52	1.30	1.22
22	3	310	CLA	CHC-C4B	4.52	1.49	1.39
22	7	310	CLA	CHC-C4B	4.52	1.49	1.39
25	3	301	CHL	MG-NA	4.51	2.17	2.06
25	7	301	CHL	MG-NA	4.51	2.17	2.06
25	3	307	CHL	MG-NA	4.51	2.17	2.06
25	7	307	CHL	MG-NA	4.51	2.17	2.06
23	A	404	PHO	C3C-C2C	4.51	1.46	1.36
25	3	308	CHL	MG-NA	4.51	2.17	2.06
25	7	308	CHL	MG-NA	4.51	2.17	2.06
22	C	503	CLA	OBD-CAD	4.51	1.30	1.22
22	1	610	CLA	C1D-ND	-4.50	1.32	1.37
22	5	610	CLA	C1D-ND	-4.50	1.32	1.37
22	S	313	CLA	OBD-CAD	4.50	1.30	1.22
22	s	313	CLA	OBD-CAD	4.50	1.30	1.22
22	2	611	CLA	C1D-ND	-4.50	1.32	1.37
22	6	611	CLA	C1D-ND	-4.50	1.32	1.37
22	2	609	CLA	CHC-C4B	4.50	1.49	1.39
22	6	609	CLA	CHC-C4B	4.50	1.49	1.39
25	1	608	CHL	MG-NA	4.50	2.17	2.06
25	5	608	CHL	MG-NA	4.50	2.17	2.06
22	b	613	CLA	OBD-CAD	4.49	1.30	1.22
22	B	614	CLA	CHC-C1C	4.49	1.47	1.38
22	B	611	CLA	OBD-CAD	4.49	1.30	1.22
22	2	609	CLA	C1D-ND	-4.49	1.32	1.37
22	6	609	CLA	C1D-ND	-4.49	1.32	1.37
25	2	608	CHL	MG-NA	4.49	2.16	2.06
25	6	608	CHL	MG-NA	4.49	2.16	2.06
22	N	613	CLA	OBD-CAD	4.48	1.30	1.22
22	n	613	CLA	OBD-CAD	4.48	1.30	1.22
22	c	501	CLA	OBD-CAD	4.48	1.30	1.22
25	1	606	CHL	MG-NA	4.48	2.16	2.06
25	5	606	CHL	MG-NA	4.48	2.16	2.06
25	2	607	CHL	MG-NA	4.47	2.16	2.06
25	6	607	CHL	MG-NA	4.47	2.16	2.06
22	2	611	CLA	CHC-C1C	4.47	1.47	1.38
22	6	611	CLA	CHC-C1C	4.47	1.47	1.38
22	b	611	CLA	OBD-CAD	4.47	1.30	1.22
22	3	310	CLA	C1D-ND	-4.47	1.32	1.37
22	7	310	CLA	C1D-ND	-4.47	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	304	CHL	MG-NA	4.47	2.16	2.06
25	r	304	CHL	MG-NA	4.47	2.16	2.06
22	c	503	CLA	OBD-CAD	4.46	1.30	1.22
22	Y	613	CLA	OBD-CAD	4.46	1.30	1.22
22	y	613	CLA	OBD-CAD	4.46	1.30	1.22
25	G	605	CHL	MG-ND	-4.46	1.96	2.05
25	g	605	CHL	MG-ND	-4.46	1.96	2.05
22	B	614	CLA	CHC-C4B	4.46	1.49	1.39
22	b	606	CLA	C3C-C2C	4.46	1.46	1.36
22	b	612	CLA	C3C-C2C	4.46	1.46	1.36
25	4	306	CHL	MG-NA	4.45	2.16	2.06
25	8	306	CHL	MG-NA	4.45	2.16	2.06
22	b	610	CLA	C3C-C2C	4.45	1.46	1.36
22	c	511	CLA	OBD-CAD	4.45	1.30	1.22
22	S	310	CLA	OBD-CAD	4.44	1.30	1.22
22	s	310	CLA	OBD-CAD	4.44	1.30	1.22
25	4	307	CHL	MG-NA	4.43	2.16	2.06
25	8	307	CHL	MG-NA	4.43	2.16	2.06
22	1	602	CLA	OBD-CAD	4.43	1.30	1.22
22	5	602	CLA	OBD-CAD	4.43	1.30	1.22
25	1	615	CHL	MG-NA	4.43	2.16	2.06
25	5	615	CHL	MG-NA	4.43	2.16	2.06
25	4	302	CHL	MG-NA	4.43	2.16	2.06
25	8	302	CHL	MG-NA	4.43	2.16	2.06
22	4	310	CLA	CHC-C1C	4.42	1.47	1.38
22	8	310	CLA	CHC-C1C	4.42	1.47	1.38
22	1	612	CLA	C3C-C2C	4.42	1.46	1.36
22	5	612	CLA	C3C-C2C	4.42	1.46	1.36
25	3	306	CHL	MG-ND	-4.41	1.97	2.05
25	7	306	CHL	MG-ND	-4.41	1.97	2.05
22	c	508	CLA	C1B-NB	-4.41	1.32	1.37
22	B	601	CLA	CHC-C1C	4.41	1.47	1.38
25	3	306	CHL	MG-NA	4.41	2.16	2.06
25	7	306	CHL	MG-NA	4.41	2.16	2.06
22	C	512	CLA	CHC-C1C	4.40	1.47	1.38
22	R	302	CLA	CHC-C1C	4.40	1.47	1.38
22	r	302	CLA	CHC-C1C	4.40	1.47	1.38
22	1	610	CLA	CHC-C1C	4.40	1.47	1.38
22	5	610	CLA	CHC-C1C	4.40	1.47	1.38
22	b	612	CLA	CHC-C4B	4.40	1.49	1.39
22	2	613	CLA	CHC-C1C	4.40	1.47	1.38
22	6	613	CLA	CHC-C1C	4.40	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	603	CLA	CHC-C1C	4.40	1.47	1.38
22	6	603	CLA	CHC-C1C	4.40	1.47	1.38
22	S	309	CLA	C3C-C2C	4.40	1.46	1.36
22	s	309	CLA	C3C-C2C	4.40	1.46	1.36
25	G	605	CHL	MG-NA	4.39	2.16	2.06
25	g	605	CHL	MG-NA	4.39	2.16	2.06
22	b	605	CLA	CHC-C1C	4.39	1.47	1.38
22	G	610	CLA	CHC-C1C	4.39	1.47	1.38
22	g	610	CLA	CHC-C1C	4.39	1.47	1.38
22	R	302	CLA	C3C-C2C	4.39	1.46	1.36
22	r	302	CLA	C3C-C2C	4.39	1.46	1.36
22	Y	603	CLA	OBD-CAD	4.39	1.30	1.22
22	y	603	CLA	OBD-CAD	4.39	1.30	1.22
22	C	512	CLA	C3C-C2C	4.39	1.46	1.36
22	4	301	CLA	CHC-C1C	4.39	1.47	1.38
22	8	301	CLA	CHC-C1C	4.39	1.47	1.38
22	2	611	CLA	C3C-C2C	4.39	1.46	1.36
22	6	611	CLA	C3C-C2C	4.39	1.46	1.36
23	a	404	PHO	C4D-CHA	4.39	1.46	1.39
22	4	311	CLA	CHC-C1C	4.38	1.47	1.38
22	8	311	CLA	CHC-C1C	4.38	1.47	1.38
25	1	607	CHL	MG-NA	4.38	2.16	2.06
25	5	607	CHL	MG-NA	4.38	2.16	2.06
22	B	604	CLA	OBD-CAD	4.38	1.30	1.22
22	c	507	CLA	C3C-C2C	4.37	1.46	1.36
22	C	502	CLA	CHC-C1C	4.37	1.47	1.38
22	1	612	CLA	CHC-C1C	4.37	1.47	1.38
22	5	612	CLA	CHC-C1C	4.37	1.47	1.38
25	3	309	CHL	MG-NA	4.37	2.16	2.06
25	7	309	CHL	MG-NA	4.37	2.16	2.06
25	2	605	CHL	MG-ND	-4.37	1.97	2.05
25	6	605	CHL	MG-ND	-4.37	1.97	2.05
22	3	314	CLA	C3C-C2C	4.37	1.46	1.36
22	7	314	CLA	C3C-C2C	4.37	1.46	1.36
22	b	615	CLA	CHC-C1C	4.36	1.47	1.38
22	B	616	CLA	OBD-CAD	4.36	1.30	1.22
25	2	605	CHL	MG-NA	4.36	2.16	2.06
25	6	605	CHL	MG-NA	4.36	2.16	2.06
22	3	311	CLA	CHC-C1C	4.35	1.47	1.38
22	7	311	CLA	CHC-C1C	4.35	1.47	1.38
22	S	303	CLA	OBD-CAD	4.35	1.30	1.22
22	s	303	CLA	OBD-CAD	4.35	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	501	CLA	C3C-C2C	4.35	1.46	1.36
22	N	614	CLA	C3C-C2C	4.35	1.46	1.36
22	n	614	CLA	C3C-C2C	4.35	1.46	1.36
25	4	308	CHL	MG-NA	4.35	2.16	2.06
25	8	308	CHL	MG-NA	4.35	2.16	2.06
22	B	613	CLA	OBD-CAD	4.35	1.30	1.22
22	A	403	CLA	CHC-C1C	4.35	1.47	1.38
22	2	613	CLA	C3C-C2C	4.35	1.46	1.36
22	6	613	CLA	C3C-C2C	4.35	1.46	1.36
22	R	310	CLA	CHC-C1C	4.35	1.47	1.38
22	r	310	CLA	CHC-C1C	4.35	1.47	1.38
22	2	610	CLA	CHC-C1C	4.34	1.47	1.38
22	6	610	CLA	CHC-C1C	4.34	1.47	1.38
22	N	603	CLA	OBD-CAD	4.34	1.30	1.22
22	n	603	CLA	OBD-CAD	4.34	1.30	1.22
22	4	304	CLA	CHC-C1C	4.34	1.47	1.38
22	8	304	CLA	CHC-C1C	4.34	1.47	1.38
25	G	607	CHL	MG-NA	4.33	2.16	2.06
25	g	607	CHL	MG-NA	4.33	2.16	2.06
22	4	304	CLA	C3C-C2C	4.33	1.45	1.36
22	8	304	CLA	C3C-C2C	4.33	1.45	1.36
22	S	304	CLA	CHC-C1C	4.33	1.47	1.38
22	s	304	CLA	CHC-C1C	4.33	1.47	1.38
22	1	603	CLA	CHC-C1C	4.33	1.47	1.38
22	5	603	CLA	CHC-C1C	4.33	1.47	1.38
25	Y	606	CHL	MG-NA	4.33	2.16	2.06
25	y	606	CHL	MG-NA	4.33	2.16	2.06
22	b	604	CLA	C3C-C2C	4.33	1.45	1.36
22	R	301	CLA	CHC-C1C	4.33	1.47	1.38
22	r	301	CLA	CHC-C1C	4.33	1.47	1.38
22	b	606	CLA	C3B-C4B	4.33	1.52	1.42
22	a	402	CLA	C3C-C2C	4.32	1.45	1.36
22	c	509	CLA	CHC-C1C	4.32	1.47	1.38
22	S	312	CLA	C3C-C2C	4.32	1.45	1.36
22	s	312	CLA	C3C-C2C	4.32	1.45	1.36
22	C	501	CLA	OBD-CAD	4.32	1.29	1.22
22	3	312	CLA	C1D-ND	-4.32	1.32	1.37
22	7	312	CLA	C1D-ND	-4.32	1.32	1.37
22	3	304	CLA	CHC-C1C	4.31	1.47	1.38
22	7	304	CLA	CHC-C1C	4.31	1.47	1.38
22	3	305	CLA	C3C-C2C	4.31	1.45	1.36
22	7	305	CLA	C3C-C2C	4.31	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	CHC-C4B	4.31	1.49	1.39
22	G	614	CLA	CHC-C1C	4.31	1.47	1.38
22	g	614	CLA	CHC-C1C	4.31	1.47	1.38
22	2	602	CLA	CHC-C1C	4.31	1.47	1.38
22	6	602	CLA	CHC-C1C	4.31	1.47	1.38
22	3	303	CLA	CHC-C1C	4.31	1.47	1.38
22	7	303	CLA	CHC-C1C	4.31	1.47	1.38
22	C	509	CLA	C3C-C2C	4.30	1.45	1.36
22	4	305	CLA	C3C-C2C	4.30	1.45	1.36
22	8	305	CLA	C3C-C2C	4.30	1.45	1.36
22	2	604	CLA	C3C-C2C	4.30	1.45	1.36
22	6	604	CLA	C3C-C2C	4.30	1.45	1.36
22	b	615	CLA	C3C-C2C	4.30	1.45	1.36
22	3	305	CLA	CHC-C1C	4.30	1.47	1.38
22	7	305	CLA	CHC-C1C	4.30	1.47	1.38
25	1	609	CHL	MG-NA	4.30	2.16	2.06
25	5	609	CHL	MG-NA	4.30	2.16	2.06
25	1	601	CHL	MG-NA	4.30	2.16	2.06
25	5	601	CHL	MG-NA	4.30	2.16	2.06
22	2	610	CLA	C3C-C2C	4.29	1.45	1.36
22	6	610	CLA	C3C-C2C	4.29	1.45	1.36
22	d	404	CLA	C3C-C2C	4.29	1.45	1.36
25	G	608	CHL	MG-NA	4.29	2.16	2.06
25	g	608	CHL	MG-NA	4.29	2.16	2.06
22	4	301	CLA	C3C-C2C	4.29	1.45	1.36
22	8	301	CLA	C3C-C2C	4.29	1.45	1.36
22	3	312	CLA	CHC-C1C	4.29	1.47	1.38
22	7	312	CLA	CHC-C1C	4.29	1.47	1.38
22	3	304	CLA	C3C-C2C	4.29	1.45	1.36
22	7	304	CLA	C3C-C2C	4.29	1.45	1.36
22	1	610	CLA	CHC-C4B	4.29	1.49	1.39
22	5	610	CLA	CHC-C4B	4.29	1.49	1.39
22	3	313	CLA	C3C-C2C	4.29	1.45	1.36
22	7	313	CLA	C3C-C2C	4.29	1.45	1.36
22	1	604	CLA	C3C-C2C	4.29	1.45	1.36
22	5	604	CLA	C3C-C2C	4.29	1.45	1.36
22	D	401	CLA	C3C-C2C	4.29	1.45	1.36
25	R	305	CHL	MG-NA	4.29	2.16	2.06
25	r	305	CHL	MG-NA	4.29	2.16	2.06
22	1	602	CLA	CHC-C1C	4.28	1.47	1.38
22	5	602	CLA	CHC-C1C	4.28	1.47	1.38
22	c	509	CLA	C3C-C2C	4.28	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	310	CLA	C3C-C2C	4.28	1.45	1.36
22	r	310	CLA	C3C-C2C	4.28	1.45	1.36
22	3	312	CLA	C3C-C2C	4.28	1.45	1.36
22	7	312	CLA	C3C-C2C	4.28	1.45	1.36
25	1	601	CHL	MG-ND	-4.28	1.97	2.05
25	5	601	CHL	MG-ND	-4.28	1.97	2.05
22	s	301	CLA	CHC-C1C	4.28	1.47	1.38
22	C	502	CLA	C3C-C2C	4.28	1.45	1.36
22	c	505	CLA	C1B-NB	-4.28	1.32	1.37
22	3	311	CLA	C3C-C2C	4.27	1.45	1.36
22	7	311	CLA	C3C-C2C	4.27	1.45	1.36
22	R	311	CLA	CHC-C1C	4.27	1.47	1.38
22	r	311	CLA	CHC-C1C	4.27	1.47	1.38
22	A	403	CLA	C3C-C2C	4.27	1.45	1.36
22	3	314	CLA	CHC-C4B	4.27	1.49	1.39
22	7	314	CLA	CHC-C4B	4.27	1.49	1.39
25	R	306	CHL	MG-NA	4.27	2.16	2.06
25	r	306	CHL	MG-NA	4.27	2.16	2.06
22	3	313	CLA	CHC-C1C	4.27	1.47	1.38
22	7	313	CLA	CHC-C1C	4.27	1.47	1.38
22	2	604	CLA	CHC-C1C	4.27	1.47	1.38
22	6	604	CLA	CHC-C1C	4.27	1.47	1.38
22	2	611	CLA	CHC-C4B	4.27	1.49	1.39
22	6	611	CLA	CHC-C4B	4.27	1.49	1.39
22	3	312	CLA	CHC-C4B	4.27	1.49	1.39
22	7	312	CLA	CHC-C4B	4.27	1.49	1.39
22	b	601	CLA	CHC-C1C	4.26	1.47	1.38
22	4	305	CLA	CHC-C1C	4.26	1.47	1.38
22	8	305	CLA	CHC-C1C	4.26	1.47	1.38
22	2	603	CLA	C3C-C2C	4.26	1.45	1.36
22	6	603	CLA	C3C-C2C	4.26	1.45	1.36
22	1	613	CLA	CHC-C1C	4.26	1.47	1.38
22	5	613	CLA	CHC-C1C	4.26	1.47	1.38
22	C	511	CLA	C3C-C2C	4.26	1.45	1.36
22	C	508	CLA	C1B-NB	-4.26	1.32	1.37
22	a	403	CLA	CHC-C1C	4.26	1.47	1.38
22	N	614	CLA	CHC-C1C	4.25	1.47	1.38
22	n	614	CLA	CHC-C1C	4.25	1.47	1.38
22	G	610	CLA	CHC-C4B	4.25	1.48	1.39
22	g	610	CLA	CHC-C4B	4.25	1.48	1.39
22	b	612	CLA	C3B-C4B	4.25	1.52	1.42
22	1	611	CLA	CHC-C1C	4.24	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	611	CLA	CHC-C1C	4.24	1.47	1.38
22	C	509	CLA	CHC-C1C	4.24	1.47	1.38
22	3	303	CLA	C3C-C2C	4.24	1.45	1.36
22	7	303	CLA	C3C-C2C	4.24	1.45	1.36
22	a	403	CLA	C3C-C2C	4.24	1.45	1.36
22	1	611	CLA	C3C-C2C	4.24	1.45	1.36
22	5	611	CLA	C3C-C2C	4.24	1.45	1.36
22	B	613	CLA	CHC-C1C	4.23	1.47	1.38
22	1	613	CLA	C3C-C2C	4.23	1.45	1.36
22	5	613	CLA	C3C-C2C	4.23	1.45	1.36
25	1	605	CHL	MG-NA	4.23	2.16	2.06
25	5	605	CHL	MG-NA	4.23	2.16	2.06
22	B	610	CLA	C3C-C2C	4.22	1.45	1.36
22	B	607	CLA	C3C-C2C	4.22	1.45	1.36
23	a	404	PHO	C3D-C4D	-4.22	1.35	1.41
22	S	303	CLA	CHC-C1C	4.22	1.47	1.38
22	s	303	CLA	CHC-C1C	4.22	1.47	1.38
23	d	402	PHO	CBD-CGD	-4.22	1.46	1.52
22	B	613	CLA	C3C-C2C	4.22	1.45	1.36
22	3	311	CLA	CHC-C4B	4.21	1.48	1.39
22	7	311	CLA	CHC-C4B	4.21	1.48	1.39
22	3	303	CLA	CHC-C4B	4.21	1.48	1.39
22	7	303	CLA	CHC-C4B	4.21	1.48	1.39
22	2	613	CLA	CHC-C4B	4.21	1.48	1.39
22	6	613	CLA	CHC-C4B	4.21	1.48	1.39
22	s	301	CLA	C3C-C2C	4.21	1.45	1.36
22	a	405	CLA	C1B-NB	-4.21	1.32	1.37
22	a	403	CLA	OBD-CAD	4.21	1.29	1.22
22	G	614	CLA	C3C-C2C	4.21	1.45	1.36
22	g	614	CLA	C3C-C2C	4.21	1.45	1.36
22	1	603	CLA	C3C-C2C	4.21	1.45	1.36
22	5	603	CLA	C3C-C2C	4.21	1.45	1.36
22	B	601	CLA	CHC-C4B	4.20	1.48	1.39
22	Y	612	CLA	C3C-C2C	4.20	1.45	1.36
22	y	612	CLA	C3C-C2C	4.20	1.45	1.36
22	N	610	CLA	CHC-C1C	4.20	1.47	1.38
22	n	610	CLA	CHC-C1C	4.20	1.47	1.38
25	S	306	CHL	MG-NA	4.20	2.16	2.06
25	s	306	CHL	MG-NA	4.20	2.16	2.06
22	3	313	CLA	CHC-C4B	4.20	1.48	1.39
22	7	313	CLA	CHC-C4B	4.20	1.48	1.39
22	R	308	CLA	CHC-C4B	4.20	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	308	CLA	CHC-C4B	4.20	1.48	1.39
25	3	302	CHL	MG-NA	4.20	2.16	2.06
25	7	302	CHL	MG-NA	4.20	2.16	2.06
22	1	602	CLA	CHC-C4B	4.19	1.48	1.39
22	2	610	CLA	CHC-C4B	4.19	1.48	1.39
22	4	304	CLA	CHC-C4B	4.19	1.48	1.39
22	5	602	CLA	CHC-C4B	4.19	1.48	1.39
22	6	610	CLA	CHC-C4B	4.19	1.48	1.39
22	8	304	CLA	CHC-C4B	4.19	1.48	1.39
22	4	310	CLA	CHC-C4B	4.19	1.48	1.39
22	8	310	CLA	CHC-C4B	4.19	1.48	1.39
22	B	604	CLA	C3C-C2C	4.19	1.45	1.36
22	c	504	CLA	C3C-C2C	4.19	1.45	1.36
22	R	301	CLA	CHC-C4B	4.19	1.48	1.39
22	r	301	CLA	CHC-C4B	4.19	1.48	1.39
22	1	602	CLA	C3C-C2C	4.19	1.45	1.36
22	5	602	CLA	C3C-C2C	4.19	1.45	1.36
22	B	604	CLA	C1B-NB	-4.19	1.32	1.37
25	2	601	CHL	MG-NA	4.19	2.16	2.06
25	6	601	CHL	MG-NA	4.19	2.16	2.06
22	2	602	CLA	C3C-C2C	4.19	1.45	1.36
22	6	602	CLA	C3C-C2C	4.19	1.45	1.36
22	R	303	CLA	C3C-C2C	4.18	1.45	1.36
22	r	303	CLA	C3C-C2C	4.18	1.45	1.36
22	D	404	CLA	C3C-C2C	4.18	1.45	1.36
22	A	403	CLA	CHC-C4B	4.18	1.48	1.39
22	S	311	CLA	C3C-C2C	4.18	1.45	1.36
22	s	311	CLA	C3C-C2C	4.18	1.45	1.36
22	b	603	CLA	C3C-C2C	4.18	1.45	1.36
22	A	405	CLA	C1B-NB	-4.18	1.32	1.37
22	B	602	CLA	CHC-C4B	4.18	1.48	1.39
22	2	612	CLA	CHC-C1C	4.18	1.47	1.38
22	6	612	CLA	CHC-C1C	4.18	1.47	1.38
22	C	503	CLA	CHC-C1C	4.18	1.47	1.38
22	b	605	CLA	CHC-C4B	4.18	1.48	1.39
22	c	511	CLA	C3C-C2C	4.17	1.45	1.36
25	S	302	CHL	MG-NA	4.17	2.16	2.06
25	s	302	CHL	MG-NA	4.17	2.16	2.06
22	2	612	CLA	C3C-C2C	4.17	1.45	1.36
22	6	612	CLA	C3C-C2C	4.17	1.45	1.36
23	A	404	PHO	C4D-CHA	4.16	1.46	1.39
22	G	612	CLA	C3C-C2C	4.16	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	g	612	CLA	C3C-C2C	4.16	1.45	1.36
22	R	308	CLA	CHC-C1C	4.16	1.47	1.38
22	r	308	CLA	CHC-C1C	4.16	1.47	1.38
22	C	506	CLA	C1B-NB	-4.16	1.32	1.37
22	4	311	CLA	CHC-C4B	4.16	1.48	1.39
22	8	311	CLA	CHC-C4B	4.16	1.48	1.39
22	B	616	CLA	CHC-C1C	4.16	1.47	1.38
22	2	612	CLA	CHC-C4B	4.16	1.48	1.39
22	6	612	CLA	CHC-C4B	4.16	1.48	1.39
22	N	610	CLA	CHC-C4B	4.16	1.48	1.39
22	n	610	CLA	CHC-C4B	4.16	1.48	1.39
22	2	602	CLA	CHC-C4B	4.15	1.48	1.39
22	6	602	CLA	CHC-C4B	4.15	1.48	1.39
22	b	608	CLA	C3C-C2C	4.15	1.45	1.36
22	b	615	CLA	CHC-C4B	4.15	1.48	1.39
22	G	604	CLA	C3C-C2C	4.15	1.45	1.36
22	g	604	CLA	C3C-C2C	4.15	1.45	1.36
22	C	512	CLA	CHC-C4B	4.15	1.48	1.39
22	R	302	CLA	CHC-C4B	4.15	1.48	1.39
22	r	302	CLA	CHC-C4B	4.15	1.48	1.39
22	1	610	CLA	C3C-C2C	4.15	1.45	1.36
22	5	610	CLA	C3C-C2C	4.15	1.45	1.36
22	c	512	CLA	C3C-C2C	4.15	1.45	1.36
22	S	311	CLA	CHC-C1C	4.15	1.46	1.38
22	s	311	CLA	CHC-C1C	4.15	1.46	1.38
22	c	510	CLA	C3C-C2C	4.14	1.45	1.36
22	a	403	CLA	CHC-C4B	4.14	1.48	1.39
22	c	509	CLA	CHC-C4B	4.14	1.48	1.39
22	4	301	CLA	CHC-C4B	4.14	1.48	1.39
22	8	301	CLA	CHC-C4B	4.14	1.48	1.39
22	C	502	CLA	CHC-C4B	4.14	1.48	1.39
22	Y	610	CLA	C1B-NB	-4.14	1.32	1.37
22	y	610	CLA	C1B-NB	-4.14	1.32	1.37
22	4	303	CLA	C3C-C2C	4.13	1.45	1.36
22	8	303	CLA	C3C-C2C	4.13	1.45	1.36
22	S	305	CLA	C3C-C2C	4.13	1.45	1.36
22	s	305	CLA	C3C-C2C	4.13	1.45	1.36
22	A	402	CLA	C1B-NB	-4.13	1.32	1.37
22	b	601	CLA	C3C-C2C	4.13	1.45	1.36
22	G	614	CLA	CHC-C4B	4.13	1.48	1.39
22	g	614	CLA	CHC-C4B	4.13	1.48	1.39
22	1	612	CLA	CHC-C4B	4.13	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	612	CLA	CHC-C4B	4.13	1.48	1.39
22	R	307	CLA	CHC-C1C	4.13	1.46	1.38
22	r	307	CLA	CHC-C1C	4.13	1.46	1.38
22	G	613	CLA	C3C-C2C	4.13	1.45	1.36
22	g	613	CLA	C3C-C2C	4.13	1.45	1.36
22	R	309	CLA	CHC-C1C	4.13	1.46	1.38
22	r	309	CLA	CHC-C1C	4.13	1.46	1.38
22	b	613	CLA	C1B-NB	-4.13	1.32	1.37
22	b	605	CLA	C3C-C2C	4.13	1.45	1.36
22	d	404	CLA	CHC-C1C	4.12	1.46	1.38
22	2	603	CLA	CHC-C4B	4.12	1.48	1.39
22	6	603	CLA	CHC-C4B	4.12	1.48	1.39
22	1	613	CLA	CHC-C4B	4.12	1.48	1.39
22	5	613	CLA	CHC-C4B	4.12	1.48	1.39
22	c	508	CLA	C3C-C2C	4.12	1.45	1.36
22	b	601	CLA	CHC-C4B	4.12	1.48	1.39
23	D	402	PHO	C3C-C2C	4.12	1.45	1.36
22	C	507	CLA	C3C-C2C	4.12	1.45	1.36
25	N	606	CHL	MG-NA	4.12	2.16	2.06
25	n	606	CHL	MG-NA	4.12	2.16	2.06
22	C	508	CLA	C3C-C2C	4.12	1.45	1.36
25	N	605	CHL	C3A-C2A	-4.11	1.50	1.54
25	n	605	CHL	C3A-C2A	-4.11	1.50	1.54
22	B	611	CLA	CHC-C1C	4.11	1.46	1.38
22	R	310	CLA	CHC-C4B	4.11	1.48	1.39
22	r	310	CLA	CHC-C4B	4.11	1.48	1.39
22	d	401	CLA	C3C-C2C	4.11	1.45	1.36
22	R	301	CLA	C3C-C2C	4.10	1.45	1.36
22	r	301	CLA	C3C-C2C	4.10	1.45	1.36
22	N	612	CLA	C3C-C2C	4.10	1.45	1.36
22	n	612	CLA	C3C-C2C	4.10	1.45	1.36
22	1	604	CLA	CHC-C1C	4.10	1.46	1.38
22	5	604	CLA	CHC-C1C	4.10	1.46	1.38
22	b	608	CLA	CHC-C1C	4.10	1.46	1.38
22	B	602	CLA	CHC-C1C	4.10	1.46	1.38
22	N	610	CLA	C1B-NB	-4.10	1.32	1.37
22	n	610	CLA	C1B-NB	-4.10	1.32	1.37
22	1	614	CLA	CHC-C1C	4.10	1.46	1.38
22	5	614	CLA	CHC-C1C	4.10	1.46	1.38
22	4	305	CLA	CHC-C4B	4.10	1.48	1.39
22	8	305	CLA	CHC-C4B	4.10	1.48	1.39
22	S	310	CLA	C3C-C2C	4.10	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	310	CLA	C3C-C2C	4.10	1.45	1.36
23	d	402	PHO	C3C-C2C	4.09	1.45	1.36
22	C	502	CLA	OBD-CAD	4.09	1.29	1.22
23	d	402	PHO	C3D-C4D	-4.09	1.35	1.41
25	N	608	CHL	MG-NA	4.09	2.16	2.06
25	n	608	CHL	MG-NA	4.09	2.16	2.06
22	S	313	CLA	CHC-C1C	4.09	1.46	1.38
22	s	313	CLA	CHC-C1C	4.09	1.46	1.38
22	1	614	CLA	C3C-C2C	4.09	1.45	1.36
22	5	614	CLA	C3C-C2C	4.09	1.45	1.36
22	B	612	CLA	CHC-C1C	4.09	1.46	1.38
22	N	604	CLA	C3C-C2C	4.09	1.45	1.36
22	n	604	CLA	C3C-C2C	4.09	1.45	1.36
22	B	601	CLA	C3C-C2C	4.09	1.45	1.36
22	a	402	CLA	CHC-C1C	4.09	1.46	1.38
25	Y	607	CHL	MG-NA	4.09	2.16	2.06
25	y	607	CHL	MG-NA	4.09	2.16	2.06
22	1	603	CLA	CHC-C4B	4.08	1.48	1.39
22	5	603	CLA	CHC-C4B	4.08	1.48	1.39
22	S	301	CLA	CHC-C1C	4.08	1.46	1.38
22	G	603	CLA	C3C-C2C	4.08	1.45	1.36
22	g	603	CLA	C3C-C2C	4.08	1.45	1.36
22	C	509	CLA	CHC-C4B	4.08	1.48	1.39
22	1	611	CLA	CHC-C4B	4.08	1.48	1.39
22	5	611	CLA	CHC-C4B	4.08	1.48	1.39
22	b	602	CLA	CHC-C4B	4.08	1.48	1.39
22	C	510	CLA	C1B-NB	-4.07	1.32	1.37
22	G	602	CLA	C1B-NB	-4.07	1.32	1.37
22	g	602	CLA	C1B-NB	-4.07	1.32	1.37
22	S	301	CLA	C3C-C2C	4.07	1.45	1.36
25	S	307	CHL	MG-NA	4.07	2.15	2.06
25	s	307	CHL	MG-NA	4.07	2.15	2.06
22	R	309	CLA	C3C-C2C	4.07	1.45	1.36
22	Y	602	CLA	C3C-C2C	4.07	1.45	1.36
22	r	309	CLA	C3C-C2C	4.07	1.45	1.36
22	y	602	CLA	C3C-C2C	4.07	1.45	1.36
22	S	304	CLA	CHC-C4B	4.07	1.48	1.39
22	s	304	CLA	CHC-C4B	4.07	1.48	1.39
22	G	610	CLA	C3C-C2C	4.07	1.45	1.36
22	g	610	CLA	C3C-C2C	4.07	1.45	1.36
22	Y	603	CLA	C3C-C2C	4.07	1.45	1.36
22	y	603	CLA	C3C-C2C	4.07	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	613	CLA	C3C-C2C	4.07	1.45	1.36
22	S	310	CLA	CHC-C1C	4.06	1.46	1.38
22	s	310	CLA	CHC-C1C	4.06	1.46	1.38
22	R	311	CLA	CHC-C4B	4.06	1.48	1.39
22	S	303	CLA	CHC-C4B	4.06	1.48	1.39
22	r	311	CLA	CHC-C4B	4.06	1.48	1.39
22	s	303	CLA	CHC-C4B	4.06	1.48	1.39
25	Y	608	CHL	MG-NA	4.06	2.15	2.06
25	y	608	CHL	MG-NA	4.06	2.15	2.06
22	s	301	CLA	CHC-C4B	4.06	1.48	1.39
22	b	607	CLA	C3C-C2C	4.06	1.45	1.36
23	a	404	PHO	C3C-C2C	4.06	1.45	1.36
22	Y	613	CLA	C3C-C2C	4.06	1.45	1.36
22	y	613	CLA	C3C-C2C	4.06	1.45	1.36
22	R	308	CLA	C3C-C2C	4.05	1.45	1.36
22	r	308	CLA	C3C-C2C	4.05	1.45	1.36
22	b	609	CLA	C1B-NB	-4.05	1.32	1.37
22	B	613	CLA	CHC-C4B	4.05	1.48	1.39
22	R	307	CLA	C3C-C2C	4.05	1.45	1.36
22	r	307	CLA	C3C-C2C	4.05	1.45	1.36
22	b	616	CLA	C3C-C2C	4.04	1.45	1.36
22	B	614	CLA	C3C-C2C	4.04	1.45	1.36
22	C	503	CLA	CHC-C4B	4.04	1.48	1.39
22	3	304	CLA	CHC-C4B	4.04	1.48	1.39
22	7	304	CLA	CHC-C4B	4.04	1.48	1.39
25	4	309	CHL	MG-NA	4.04	2.15	2.06
25	8	309	CHL	MG-NA	4.04	2.15	2.06
22	G	612	CLA	CHC-C4B	4.04	1.48	1.39
22	g	612	CLA	CHC-C4B	4.04	1.48	1.39
22	R	311	CLA	C3C-C2C	4.04	1.45	1.36
22	r	311	CLA	C3C-C2C	4.04	1.45	1.36
22	3	305	CLA	CHC-C4B	4.04	1.48	1.39
22	7	305	CLA	CHC-C4B	4.04	1.48	1.39
22	4	301	CLA	C3B-C4B	4.04	1.52	1.42
22	8	301	CLA	C3B-C4B	4.04	1.52	1.42
22	S	305	CLA	CHC-C1C	4.04	1.46	1.38
22	s	305	CLA	CHC-C1C	4.04	1.46	1.38
22	c	506	CLA	C1B-NB	-4.04	1.32	1.37
22	N	613	CLA	C3C-C2C	4.03	1.45	1.36
22	n	613	CLA	C3C-C2C	4.03	1.45	1.36
22	b	612	CLA	C1B-NB	-4.03	1.32	1.37
23	A	404	PHO	C3D-C4D	-4.03	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	612	CLA	CHC-C1C	4.03	1.46	1.38
22	g	612	CLA	CHC-C1C	4.03	1.46	1.38
22	S	310	CLA	CHC-C4B	4.03	1.48	1.39
22	s	310	CLA	CHC-C4B	4.03	1.48	1.39
22	c	510	CLA	C1B-NB	-4.02	1.32	1.37
22	S	304	CLA	C3C-C2C	4.02	1.45	1.36
22	s	304	CLA	C3C-C2C	4.02	1.45	1.36
22	B	603	CLA	CHC-C1C	4.02	1.46	1.38
22	D	404	CLA	CHC-C1C	4.02	1.46	1.38
22	B	612	CLA	C3C-C2C	4.02	1.45	1.36
22	N	603	CLA	C3C-C2C	4.02	1.45	1.36
22	n	603	CLA	C3C-C2C	4.02	1.45	1.36
22	S	303	CLA	C3C-C2C	4.02	1.45	1.36
22	N	610	CLA	C3C-C2C	4.02	1.45	1.36
22	s	303	CLA	C3C-C2C	4.02	1.45	1.36
22	n	610	CLA	C3C-C2C	4.02	1.45	1.36
22	Y	610	CLA	C3C-C2C	4.02	1.45	1.36
22	y	610	CLA	C3C-C2C	4.02	1.45	1.36
22	c	511	CLA	CHC-C1C	4.01	1.46	1.38
22	A	405	CLA	C3C-C2C	4.01	1.45	1.36
22	C	509	CLA	C1B-NB	-4.01	1.32	1.37
22	c	510	CLA	CHC-C1C	4.01	1.46	1.38
22	B	609	CLA	CHC-C1C	4.01	1.46	1.38
22	c	502	CLA	C3C-C2C	4.01	1.45	1.36
22	b	602	CLA	CHC-C1C	4.01	1.46	1.38
22	4	310	CLA	C3C-C2C	4.00	1.45	1.36
22	8	310	CLA	C3C-C2C	4.00	1.45	1.36
23	D	402	PHO	CBD-CGD	-4.00	1.47	1.52
22	S	311	CLA	CHC-C4B	4.00	1.48	1.39
22	s	311	CLA	CHC-C4B	4.00	1.48	1.39
22	b	604	CLA	C1B-NB	-4.00	1.32	1.37
22	B	602	CLA	C3C-C2C	4.00	1.45	1.36
22	A	402	CLA	CHC-C1C	4.00	1.46	1.38
22	b	602	CLA	C3C-C2C	4.00	1.45	1.36
22	G	603	CLA	CHC-C1C	4.00	1.46	1.38
22	g	603	CLA	CHC-C1C	4.00	1.46	1.38
22	B	606	CLA	CHC-C1C	3.99	1.46	1.38
22	N	611	CLA	C3C-C2C	3.99	1.45	1.36
22	n	611	CLA	C3C-C2C	3.99	1.45	1.36
22	G	611	CLA	C3C-C2C	3.99	1.45	1.36
22	g	611	CLA	C3C-C2C	3.99	1.45	1.36
22	c	507	CLA	C1B-NB	-3.99	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	403	CLA	C1B-NB	-3.99	1.32	1.37
22	3	310	CLA	C3C-C2C	3.99	1.45	1.36
22	7	310	CLA	C3C-C2C	3.99	1.45	1.36
22	c	501	CLA	C3C-C2C	3.99	1.45	1.36
22	G	602	CLA	C3C-C2C	3.99	1.45	1.36
22	g	602	CLA	C3C-C2C	3.99	1.45	1.36
22	c	503	CLA	CHC-C1C	3.99	1.46	1.38
22	S	314	CLA	C3C-C2C	3.98	1.45	1.36
22	s	314	CLA	C3C-C2C	3.98	1.45	1.36
22	d	401	CLA	CHC-C1C	3.98	1.46	1.38
22	d	404	CLA	CHC-C4B	3.98	1.48	1.39
22	Y	610	CLA	CHC-C1C	3.98	1.46	1.38
22	y	610	CLA	CHC-C1C	3.98	1.46	1.38
22	G	611	CLA	CHC-C1C	3.98	1.46	1.38
22	g	611	CLA	CHC-C1C	3.98	1.46	1.38
22	B	616	CLA	CHC-C4B	3.98	1.48	1.39
22	Y	603	CLA	CHC-C1C	3.98	1.46	1.38
22	y	603	CLA	CHC-C1C	3.98	1.46	1.38
22	3	314	CLA	C3B-C4B	3.98	1.52	1.42
22	7	314	CLA	C3B-C4B	3.98	1.52	1.42
22	2	603	CLA	C3B-C4B	3.98	1.52	1.42
22	6	603	CLA	C3B-C4B	3.98	1.52	1.42
22	N	603	CLA	CHC-C1C	3.98	1.46	1.38
22	n	603	CLA	CHC-C1C	3.98	1.46	1.38
22	a	402	CLA	C1B-NB	-3.98	1.32	1.37
22	4	303	CLA	CHC-C4B	3.97	1.48	1.39
22	8	303	CLA	CHC-C4B	3.97	1.48	1.39
22	3	310	CLA	C3B-C4B	3.97	1.52	1.42
22	7	310	CLA	C3B-C4B	3.97	1.52	1.42
22	N	614	CLA	CHC-C4B	3.97	1.48	1.39
22	n	614	CLA	CHC-C4B	3.97	1.48	1.39
22	N	611	CLA	CHC-C1C	3.97	1.46	1.38
22	n	611	CLA	CHC-C1C	3.97	1.46	1.38
22	b	609	CLA	C3C-C2C	3.97	1.45	1.36
22	C	510	CLA	C3C-C2C	3.97	1.45	1.36
22	Y	604	CLA	C1B-NB	-3.97	1.32	1.37
22	y	604	CLA	C1B-NB	-3.97	1.32	1.37
22	3	304	CLA	C3B-C4B	3.97	1.52	1.42
22	7	304	CLA	C3B-C4B	3.97	1.52	1.42
22	2	604	CLA	CHC-C4B	3.97	1.48	1.39
22	6	604	CLA	CHC-C4B	3.97	1.48	1.39
22	N	602	CLA	C3C-C2C	3.97	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	n	602	CLA	C3C-C2C	3.97	1.45	1.36
22	B	609	CLA	C3C-C2C	3.96	1.45	1.36
23	D	402	PHO	C3D-C4D	-3.96	1.35	1.41
22	G	602	CLA	CHC-C4B	3.96	1.48	1.39
22	g	602	CLA	CHC-C4B	3.96	1.48	1.39
22	R	303	CLA	CHC-C1C	3.96	1.46	1.38
22	r	303	CLA	CHC-C1C	3.96	1.46	1.38
22	c	511	CLA	CHC-C4B	3.96	1.48	1.39
22	2	609	CLA	C3B-C4B	3.96	1.52	1.42
22	6	609	CLA	C3B-C4B	3.96	1.52	1.42
22	c	502	CLA	OBD-CAD	3.95	1.29	1.22
22	b	603	CLA	CHC-C1C	3.95	1.46	1.38
22	B	608	CLA	C3C-C2C	3.95	1.45	1.36
22	Y	602	CLA	CHC-C1C	3.95	1.46	1.38
22	y	602	CLA	CHC-C1C	3.95	1.46	1.38
22	B	609	CLA	CHC-C4B	3.95	1.48	1.39
22	C	512	CLA	C3B-C4B	3.95	1.52	1.42
22	2	609	CLA	C3C-C2C	3.95	1.45	1.36
22	6	609	CLA	C3C-C2C	3.95	1.45	1.36
22	B	610	CLA	CHC-C1C	3.95	1.46	1.38
22	Y	614	CLA	C3C-C2C	3.95	1.45	1.36
22	y	614	CLA	C3C-C2C	3.95	1.45	1.36
25	N	605	CHL	MG-NA	3.95	2.15	2.06
25	n	605	CHL	MG-NA	3.95	2.15	2.06
22	c	512	CLA	CHC-C1C	3.95	1.46	1.38
22	C	503	CLA	C3C-C2C	3.95	1.45	1.36
22	Y	613	CLA	CHC-C4B	3.95	1.48	1.39
22	y	613	CLA	CHC-C4B	3.95	1.48	1.39
23	A	404	PHO	C4D-ND	-3.95	1.33	1.38
22	N	604	CLA	CHC-C1C	3.94	1.46	1.38
22	n	604	CLA	CHC-C1C	3.94	1.46	1.38
22	a	402	CLA	CHC-C4B	3.94	1.48	1.39
22	S	301	CLA	CHC-C4B	3.94	1.48	1.39
22	R	307	CLA	C1B-NB	-3.94	1.32	1.37
22	r	307	CLA	C1B-NB	-3.94	1.32	1.37
22	c	505	CLA	C3C-C2C	3.94	1.45	1.36
22	C	504	CLA	C3C-C2C	3.94	1.45	1.36
22	c	506	CLA	C3C-C2C	3.94	1.45	1.36
23	a	404	PHO	O2A-CGA	3.94	1.44	1.30
22	S	305	CLA	C1B-NB	-3.94	1.32	1.37
22	s	305	CLA	C1B-NB	-3.94	1.32	1.37
23	d	402	PHO	O2A-CGA	3.94	1.44	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	304	CLA	C3B-C4B	3.93	1.51	1.42
22	8	304	CLA	C3B-C4B	3.93	1.51	1.42
22	b	610	CLA	CHC-C1C	3.93	1.46	1.38
22	b	608	CLA	C1B-NB	-3.93	1.32	1.37
23	A	404	PHO	O2A-CGA	3.93	1.44	1.30
22	Y	602	CLA	C1B-NB	-3.93	1.33	1.37
22	y	602	CLA	C1B-NB	-3.93	1.33	1.37
22	4	311	CLA	C3B-C4B	3.92	1.51	1.42
22	8	311	CLA	C3B-C4B	3.92	1.51	1.42
22	R	309	CLA	CHC-C4B	3.92	1.48	1.39
22	r	309	CLA	CHC-C4B	3.92	1.48	1.39
22	A	405	CLA	CHC-C4B	3.92	1.48	1.39
22	B	615	CLA	C1B-NB	-3.92	1.33	1.37
22	c	509	CLA	C1B-NB	-3.92	1.33	1.37
22	G	602	CLA	CHC-C1C	3.92	1.46	1.38
22	g	602	CLA	CHC-C1C	3.92	1.46	1.38
22	b	615	CLA	C3B-C4B	3.92	1.51	1.42
22	G	613	CLA	CHC-C1C	3.92	1.46	1.38
22	g	613	CLA	CHC-C1C	3.92	1.46	1.38
22	N	602	CLA	C1B-NB	-3.92	1.33	1.37
22	n	602	CLA	C1B-NB	-3.92	1.33	1.37
25	S	308	CHL	MG-NA	3.92	2.15	2.06
25	s	308	CHL	MG-NA	3.92	2.15	2.06
22	C	505	CLA	C3C-C2C	3.92	1.45	1.36
22	Y	610	CLA	CHC-C4B	3.92	1.48	1.39
22	y	610	CLA	CHC-C4B	3.92	1.48	1.39
22	R	307	CLA	CHC-C4B	3.92	1.48	1.39
22	r	307	CLA	CHC-C4B	3.92	1.48	1.39
22	c	504	CLA	CHC-C1C	3.92	1.46	1.38
22	c	509	CLA	C3B-C4B	3.91	1.51	1.42
22	A	405	CLA	CHC-C1C	3.91	1.46	1.38
22	c	502	CLA	CHC-C1C	3.91	1.46	1.38
22	C	506	CLA	C3C-C2C	3.91	1.45	1.36
22	b	610	CLA	C1B-NB	-3.91	1.33	1.37
22	4	303	CLA	CHC-C1C	3.91	1.46	1.38
22	8	303	CLA	CHC-C1C	3.91	1.46	1.38
22	D	401	CLA	CHC-C1C	3.91	1.46	1.38
23	D	402	PHO	O2A-CGA	3.91	1.43	1.30
22	1	603	CLA	C3B-C4B	3.91	1.51	1.42
22	5	603	CLA	C3B-C4B	3.91	1.51	1.42
22	B	611	CLA	CHC-C4B	3.91	1.48	1.39
22	b	608	CLA	CHC-C4B	3.91	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Y	614	CLA	CHC-C1C	3.90	1.46	1.38
22	y	614	CLA	CHC-C1C	3.90	1.46	1.38
22	b	614	CLA	CHC-C1C	3.90	1.46	1.38
22	G	614	CLA	C3B-C4B	3.90	1.51	1.42
22	g	614	CLA	C3B-C4B	3.90	1.51	1.42
22	B	609	CLA	C1B-NB	-3.90	1.33	1.37
22	D	404	CLA	CHC-C4B	3.90	1.48	1.39
22	A	403	CLA	C3B-C4B	3.90	1.51	1.42
22	Y	611	CLA	CHC-C1C	3.90	1.46	1.38
22	y	611	CLA	CHC-C1C	3.90	1.46	1.38
22	N	613	CLA	CHC-C1C	3.89	1.46	1.38
22	n	613	CLA	CHC-C1C	3.89	1.46	1.38
22	B	610	CLA	C1B-NB	-3.89	1.33	1.37
22	G	613	CLA	CHC-C4B	3.89	1.48	1.39
22	g	613	CLA	CHC-C4B	3.89	1.48	1.39
22	N	613	CLA	CHC-C4B	3.89	1.48	1.39
22	Y	602	CLA	CHC-C4B	3.89	1.48	1.39
22	n	613	CLA	CHC-C4B	3.89	1.48	1.39
22	y	602	CLA	CHC-C4B	3.89	1.48	1.39
22	C	505	CLA	C1B-NB	-3.88	1.33	1.37
22	B	612	CLA	CHC-C4B	3.88	1.48	1.39
22	1	614	CLA	CHC-C4B	3.88	1.48	1.39
22	5	614	CLA	CHC-C4B	3.88	1.48	1.39
22	2	610	CLA	C3B-C4B	3.88	1.51	1.42
22	6	610	CLA	C3B-C4B	3.88	1.51	1.42
22	c	512	CLA	C1B-NB	-3.88	1.33	1.37
22	b	605	CLA	MG-NA	3.88	2.15	2.06
22	2	613	CLA	C3B-C4B	3.88	1.51	1.42
22	6	613	CLA	C3B-C4B	3.88	1.51	1.42
22	b	611	CLA	CHC-C1C	3.87	1.46	1.38
22	N	612	CLA	C1B-NB	-3.87	1.33	1.37
22	n	612	CLA	C1B-NB	-3.87	1.33	1.37
22	N	612	CLA	CHC-C1C	3.87	1.46	1.38
22	n	612	CLA	CHC-C1C	3.87	1.46	1.38
22	N	602	CLA	CHC-C1C	3.87	1.46	1.38
22	n	602	CLA	CHC-C1C	3.87	1.46	1.38
22	Y	613	CLA	CHC-C1C	3.87	1.46	1.38
22	y	613	CLA	CHC-C1C	3.87	1.46	1.38
22	1	604	CLA	CHC-C4B	3.87	1.48	1.39
22	5	604	CLA	CHC-C4B	3.87	1.48	1.39
22	B	612	CLA	C3B-C4B	3.87	1.51	1.42
22	N	602	CLA	CHC-C4B	3.87	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	n	602	CLA	CHC-C4B	3.87	1.48	1.39
22	b	610	CLA	CHC-C4B	3.87	1.48	1.39
22	3	311	CLA	C3B-C4B	3.86	1.51	1.42
22	7	311	CLA	C3B-C4B	3.86	1.51	1.42
22	b	607	CLA	CHC-C1C	3.86	1.46	1.38
22	N	604	CLA	C1B-NB	-3.86	1.33	1.37
22	n	604	CLA	C1B-NB	-3.86	1.33	1.37
22	c	503	CLA	C1B-NB	-3.86	1.33	1.37
22	B	603	CLA	C3C-C2C	3.86	1.44	1.36
22	d	401	CLA	CHC-C4B	3.86	1.48	1.39
25	N	607	CHL	MG-NA	3.86	2.15	2.06
25	n	607	CHL	MG-NA	3.86	2.15	2.06
22	C	511	CLA	CHC-C1C	3.86	1.46	1.38
22	B	616	CLA	C3C-C2C	3.85	1.44	1.36
22	b	603	CLA	CHC-C4B	3.85	1.48	1.39
22	2	611	CLA	C3B-C4B	3.85	1.51	1.42
22	6	611	CLA	C3B-C4B	3.85	1.51	1.42
22	S	313	CLA	C1B-NB	-3.85	1.33	1.37
22	s	313	CLA	C1B-NB	-3.85	1.33	1.37
22	G	611	CLA	CHC-C4B	3.85	1.48	1.39
22	g	611	CLA	CHC-C4B	3.85	1.48	1.39
22	C	511	CLA	CHC-C4B	3.84	1.48	1.39
22	S	309	CLA	CHC-C1C	3.84	1.46	1.38
22	s	309	CLA	CHC-C1C	3.84	1.46	1.38
22	c	510	CLA	CHC-C4B	3.84	1.48	1.39
22	N	611	CLA	CHC-C4B	3.84	1.48	1.39
22	n	611	CLA	CHC-C4B	3.84	1.48	1.39
22	G	604	CLA	CHC-C1C	3.83	1.46	1.38
22	g	604	CLA	CHC-C1C	3.83	1.46	1.38
25	Y	601	CHL	MG-NA	3.83	2.15	2.06
25	y	601	CHL	MG-NA	3.83	2.15	2.06
22	c	505	CLA	CHC-C1C	3.83	1.46	1.38
22	b	609	CLA	CHC-C1C	3.83	1.46	1.38
22	Y	611	CLA	C1B-NB	-3.83	1.33	1.37
22	y	611	CLA	C1B-NB	-3.83	1.33	1.37
22	3	313	CLA	C3B-C4B	3.83	1.51	1.42
22	7	313	CLA	C3B-C4B	3.83	1.51	1.42
22	1	614	CLA	C3B-C4B	3.82	1.51	1.42
22	5	614	CLA	C3B-C4B	3.82	1.51	1.42
22	b	602	CLA	C1B-NB	-3.82	1.33	1.37
22	S	314	CLA	CHC-C1C	3.82	1.46	1.38
22	s	314	CLA	CHC-C1C	3.82	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	403	CLA	C1B-NB	-3.82	1.33	1.37
22	C	502	CLA	C3B-C4B	3.82	1.51	1.42
22	1	602	CLA	C3B-C4B	3.82	1.51	1.42
22	5	602	CLA	C3B-C4B	3.82	1.51	1.42
22	S	310	CLA	C1B-NB	-3.82	1.33	1.37
22	s	310	CLA	C1B-NB	-3.82	1.33	1.37
22	S	314	CLA	C1B-NB	-3.82	1.33	1.37
22	s	314	CLA	C1B-NB	-3.82	1.33	1.37
25	N	601	CHL	MG-NA	3.81	2.15	2.06
25	n	601	CHL	MG-NA	3.81	2.15	2.06
22	3	312	CLA	C3B-C4B	3.81	1.51	1.42
22	7	312	CLA	C3B-C4B	3.81	1.51	1.42
22	B	613	CLA	C1B-NB	-3.81	1.33	1.37
22	c	502	CLA	CHC-C4B	3.81	1.48	1.39
22	1	612	CLA	C3B-C4B	3.81	1.51	1.42
22	5	612	CLA	C3B-C4B	3.81	1.51	1.42
22	b	616	CLA	MG-NA	3.81	2.15	2.06
22	c	504	CLA	C1B-NB	-3.81	1.33	1.37
22	a	405	CLA	C3C-C2C	3.81	1.44	1.36
22	B	605	CLA	C1B-NB	-3.81	1.33	1.37
22	Y	611	CLA	CHC-C4B	3.81	1.47	1.39
22	y	611	CLA	CHC-C4B	3.81	1.47	1.39
22	Y	613	CLA	C4D-ND	-3.81	1.32	1.37
22	y	613	CLA	C4D-ND	-3.81	1.32	1.37
22	a	405	CLA	CHC-C1C	3.81	1.46	1.38
22	A	402	CLA	C3C-C2C	3.81	1.44	1.36
22	1	610	CLA	C3B-C4B	3.80	1.51	1.42
22	5	610	CLA	C3B-C4B	3.80	1.51	1.42
22	C	509	CLA	C3B-C4B	3.80	1.51	1.42
22	C	502	CLA	C1B-NB	-3.80	1.33	1.37
22	A	402	CLA	CHC-C4B	3.80	1.47	1.39
22	N	612	CLA	CHC-C4B	3.80	1.47	1.39
22	n	612	CLA	CHC-C4B	3.80	1.47	1.39
22	N	614	CLA	C3B-C4B	3.80	1.51	1.42
22	n	614	CLA	C3B-C4B	3.80	1.51	1.42
22	b	614	CLA	CHC-C4B	3.80	1.47	1.39
22	B	610	CLA	CHC-C4B	3.80	1.47	1.39
22	R	301	CLA	C3B-C4B	3.79	1.51	1.42
22	r	301	CLA	C3B-C4B	3.79	1.51	1.42
22	S	313	CLA	CHC-C4B	3.79	1.47	1.39
22	s	313	CLA	CHC-C4B	3.79	1.47	1.39
25	1	605	CHL	C3A-C2A	-3.79	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	605	CHL	C3A-C2A	-3.79	1.51	1.54
22	b	613	CLA	CHC-C1C	3.79	1.46	1.38
22	a	405	CLA	CHC-C4B	3.79	1.47	1.39
22	2	604	CLA	C3B-C4B	3.79	1.51	1.42
22	6	604	CLA	C3B-C4B	3.79	1.51	1.42
25	G	601	CHL	MG-NA	3.79	2.15	2.06
25	g	601	CHL	MG-NA	3.79	2.15	2.06
22	B	605	CLA	CHC-C1C	3.79	1.46	1.38
22	d	403	CLA	C1B-NB	-3.78	1.33	1.37
22	B	608	CLA	C1B-NB	-3.78	1.33	1.37
22	b	605	CLA	C3B-C4B	3.78	1.51	1.42
22	B	607	CLA	CHC-C1C	3.78	1.46	1.38
22	3	303	CLA	C3B-C4B	3.78	1.51	1.42
22	7	303	CLA	C3B-C4B	3.78	1.51	1.42
22	c	512	CLA	CHC-C4B	3.78	1.47	1.39
22	G	612	CLA	C1B-NB	-3.78	1.33	1.37
22	g	612	CLA	C1B-NB	-3.78	1.33	1.37
22	2	612	CLA	C3B-C4B	3.78	1.51	1.42
22	6	612	CLA	C3B-C4B	3.78	1.51	1.42
22	b	615	CLA	MG-NA	3.78	2.15	2.06
22	S	312	CLA	CHC-C1C	3.78	1.46	1.38
22	s	312	CLA	CHC-C1C	3.78	1.46	1.38
22	Y	612	CLA	CHC-C1C	3.78	1.46	1.38
22	y	612	CLA	CHC-C1C	3.78	1.46	1.38
22	S	305	CLA	CHC-C4B	3.78	1.47	1.39
22	s	305	CLA	CHC-C4B	3.78	1.47	1.39
22	D	401	CLA	C1B-NB	-3.77	1.33	1.37
22	C	501	CLA	C1B-NB	-3.77	1.33	1.37
22	S	303	CLA	C3B-C4B	3.77	1.51	1.42
22	s	303	CLA	C3B-C4B	3.77	1.51	1.42
22	S	314	CLA	CHC-C4B	3.77	1.47	1.39
22	s	314	CLA	CHC-C4B	3.77	1.47	1.39
22	Y	603	CLA	C1B-NB	-3.77	1.33	1.37
22	y	603	CLA	C1B-NB	-3.77	1.33	1.37
22	1	613	CLA	C3B-C4B	3.77	1.51	1.42
22	5	613	CLA	C3B-C4B	3.77	1.51	1.42
22	c	508	CLA	CHC-C1C	3.77	1.46	1.38
22	Y	604	CLA	C4D-ND	-3.77	1.32	1.37
22	y	604	CLA	C4D-ND	-3.77	1.32	1.37
22	1	611	CLA	C3B-C4B	3.77	1.51	1.42
22	5	611	CLA	C3B-C4B	3.77	1.51	1.42
22	B	601	CLA	C3B-C4B	3.77	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	313	CLA	C3C-C2C	3.77	1.44	1.36
22	s	313	CLA	C3C-C2C	3.77	1.44	1.36
22	c	506	CLA	CHC-C4B	3.77	1.47	1.39
22	c	504	CLA	CHC-C4B	3.76	1.47	1.39
22	D	401	CLA	CHC-C4B	3.76	1.47	1.39
22	G	610	CLA	C3B-C4B	3.76	1.51	1.42
22	g	610	CLA	C3B-C4B	3.76	1.51	1.42
22	3	305	CLA	C3B-C4B	3.76	1.51	1.42
22	7	305	CLA	C3B-C4B	3.76	1.51	1.42
22	C	507	CLA	CHC-C4B	3.76	1.47	1.39
22	Y	611	CLA	C3C-C2C	3.76	1.44	1.36
22	y	611	CLA	C3C-C2C	3.76	1.44	1.36
22	B	611	CLA	C3C-C2C	3.76	1.44	1.36
22	3	304	CLA	MG-NA	3.76	2.15	2.06
22	7	304	CLA	MG-NA	3.76	2.15	2.06
25	G	609	CHL	MG-NA	3.76	2.15	2.06
25	g	609	CHL	MG-NA	3.76	2.15	2.06
22	G	604	CLA	C1B-NB	-3.76	1.33	1.37
22	g	604	CLA	C1B-NB	-3.76	1.33	1.37
22	Y	604	CLA	C3C-C2C	3.76	1.44	1.36
22	y	604	CLA	C3C-C2C	3.76	1.44	1.36
22	S	311	CLA	C4D-ND	-3.75	1.32	1.37
22	s	311	CLA	C4D-ND	-3.75	1.32	1.37
22	c	503	CLA	CHC-C4B	3.75	1.47	1.39
22	D	404	CLA	C1B-NB	-3.75	1.33	1.37
22	4	310	CLA	C3B-C4B	3.75	1.51	1.42
22	8	310	CLA	C3B-C4B	3.75	1.51	1.42
22	D	403	CLA	CHC-C1C	3.75	1.46	1.38
22	B	605	CLA	CHC-C4B	3.74	1.47	1.39
22	Y	612	CLA	C1B-NB	-3.74	1.33	1.37
22	y	612	CLA	C1B-NB	-3.74	1.33	1.37
22	S	313	CLA	C3B-C4B	3.74	1.51	1.42
22	s	313	CLA	C3B-C4B	3.74	1.51	1.42
22	B	603	CLA	CHC-C4B	3.74	1.47	1.39
22	B	615	CLA	CHC-C1C	3.74	1.46	1.38
22	c	511	CLA	C3B-C4B	3.74	1.51	1.42
22	c	506	CLA	CHC-C1C	3.74	1.46	1.38
25	Y	605	CHL	MG-NA	3.74	2.15	2.06
25	y	605	CHL	MG-NA	3.74	2.15	2.06
22	b	607	CLA	CHC-C4B	3.73	1.47	1.39
22	2	602	CLA	C3B-C4B	3.73	1.51	1.42
22	6	602	CLA	C3B-C4B	3.73	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Y	603	CLA	CHC-C4B	3.73	1.47	1.39
22	y	603	CLA	CHC-C4B	3.73	1.47	1.39
22	G	603	CLA	CHC-C4B	3.73	1.47	1.39
22	g	603	CLA	CHC-C4B	3.73	1.47	1.39
22	Y	614	CLA	CHC-C4B	3.73	1.47	1.39
22	y	614	CLA	CHC-C4B	3.73	1.47	1.39
22	C	512	CLA	C1B-NB	-3.73	1.33	1.37
22	b	611	CLA	C1B-NB	-3.73	1.33	1.37
22	N	603	CLA	CHC-C4B	3.73	1.47	1.39
22	n	603	CLA	CHC-C4B	3.73	1.47	1.39
22	s	301	CLA	C3B-C4B	3.73	1.51	1.42
22	S	304	CLA	C3B-C4B	3.73	1.51	1.42
22	s	304	CLA	C3B-C4B	3.73	1.51	1.42
22	B	612	CLA	C1B-NB	-3.72	1.33	1.37
22	B	602	CLA	C1B-NB	-3.72	1.33	1.37
23	D	402	PHO	C4D-ND	-3.72	1.33	1.38
22	B	611	CLA	C1B-NB	-3.72	1.33	1.37
22	R	310	CLA	C3B-C4B	3.72	1.51	1.42
22	r	310	CLA	C3B-C4B	3.72	1.51	1.42
22	C	505	CLA	CHC-C1C	3.71	1.46	1.38
22	S	309	CLA	C1B-NB	-3.71	1.33	1.37
22	s	309	CLA	C1B-NB	-3.71	1.33	1.37
22	d	403	CLA	CHC-C1C	3.71	1.46	1.38
22	S	303	CLA	C4D-ND	-3.71	1.32	1.37
22	s	303	CLA	C4D-ND	-3.71	1.32	1.37
22	d	404	CLA	C3B-C4B	3.71	1.51	1.42
22	d	403	CLA	C3C-C2C	3.71	1.44	1.36
22	b	601	CLA	C1B-NB	-3.71	1.33	1.37
22	S	311	CLA	C3B-C4B	3.71	1.51	1.42
22	s	311	CLA	C3B-C4B	3.71	1.51	1.42
22	Y	604	CLA	CHC-C1C	3.71	1.46	1.38
22	y	604	CLA	CHC-C1C	3.71	1.46	1.38
22	B	607	CLA	C1B-NB	-3.71	1.33	1.37
22	b	611	CLA	C3C-C2C	3.71	1.44	1.36
22	N	603	CLA	C1B-NB	-3.71	1.33	1.37
22	n	603	CLA	C1B-NB	-3.71	1.33	1.37
22	C	511	CLA	C3B-C4B	3.71	1.51	1.42
22	B	606	CLA	CHC-C4B	3.71	1.47	1.39
22	R	303	CLA	CHC-C4B	3.70	1.47	1.39
22	r	303	CLA	CHC-C4B	3.70	1.47	1.39
22	R	303	CLA	C1B-NB	-3.70	1.33	1.37
22	r	303	CLA	C1B-NB	-3.70	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	608	CLA	C3B-C4B	3.70	1.51	1.42
22	a	403	CLA	C1B-NB	-3.70	1.33	1.37
22	N	613	CLA	C1B-NB	-3.70	1.33	1.37
22	n	613	CLA	C1B-NB	-3.70	1.33	1.37
22	R	308	CLA	C3B-C4B	3.70	1.51	1.42
22	r	308	CLA	C3B-C4B	3.70	1.51	1.42
22	c	503	CLA	C3C-C2C	3.70	1.44	1.36
22	Y	614	CLA	C1B-NB	-3.70	1.33	1.37
22	y	614	CLA	C1B-NB	-3.70	1.33	1.37
22	b	601	CLA	C3B-C4B	3.70	1.51	1.42
22	S	312	CLA	CHC-C4B	3.70	1.47	1.39
22	s	312	CLA	CHC-C4B	3.70	1.47	1.39
22	R	309	CLA	C3B-C4B	3.70	1.51	1.42
22	r	309	CLA	C3B-C4B	3.70	1.51	1.42
22	b	602	CLA	MG-NA	3.69	2.15	2.06
22	S	311	CLA	C1B-NB	-3.69	1.33	1.37
22	s	311	CLA	C1B-NB	-3.69	1.33	1.37
22	Y	611	CLA	C3B-C4B	3.69	1.51	1.42
22	y	611	CLA	C3B-C4B	3.69	1.51	1.42
22	c	501	CLA	C1B-NB	-3.69	1.33	1.37
22	G	610	CLA	C1B-NB	-3.69	1.33	1.37
22	g	610	CLA	C1B-NB	-3.69	1.33	1.37
22	4	305	CLA	C3B-C4B	3.69	1.51	1.42
22	8	305	CLA	C3B-C4B	3.69	1.51	1.42
22	G	613	CLA	C1B-NB	-3.69	1.33	1.37
22	g	613	CLA	C1B-NB	-3.69	1.33	1.37
22	b	609	CLA	CHC-C4B	3.69	1.47	1.39
22	2	604	CLA	MG-NA	3.69	2.15	2.06
22	6	604	CLA	MG-NA	3.69	2.15	2.06
22	d	401	CLA	C1B-NB	-3.69	1.33	1.37
22	R	309	CLA	C1B-NB	-3.68	1.33	1.37
22	r	309	CLA	C1B-NB	-3.68	1.33	1.37
22	C	507	CLA	C1B-NB	-3.68	1.33	1.37
22	C	503	CLA	C1B-NB	-3.68	1.33	1.37
22	G	603	CLA	C3B-C4B	3.68	1.51	1.42
22	g	603	CLA	C3B-C4B	3.68	1.51	1.42
25	G	605	CHL	C3A-C2A	-3.68	1.51	1.54
25	g	605	CHL	C3A-C2A	-3.68	1.51	1.54
22	3	314	CLA	MG-NA	3.68	2.15	2.06
22	7	314	CLA	MG-NA	3.68	2.15	2.06
22	C	505	CLA	CHC-C4B	3.67	1.47	1.39
22	B	616	CLA	C3B-C4B	3.67	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	612	CLA	C3B-C4B	3.67	1.51	1.42
22	g	612	CLA	C3B-C4B	3.67	1.51	1.42
22	B	614	CLA	C3B-C4B	3.67	1.51	1.42
22	C	510	CLA	CHC-C1C	3.67	1.46	1.38
22	a	403	CLA	C3B-C4B	3.67	1.51	1.42
22	c	512	CLA	C3B-C4B	3.67	1.51	1.42
22	C	507	CLA	CHC-C1C	3.67	1.46	1.38
22	1	612	CLA	MG-NA	3.67	2.15	2.06
22	5	612	CLA	MG-NA	3.67	2.15	2.06
22	S	309	CLA	C3B-C4B	3.67	1.51	1.42
22	s	309	CLA	C3B-C4B	3.67	1.51	1.42
22	R	307	CLA	C3B-C4B	3.66	1.51	1.42
22	r	307	CLA	C3B-C4B	3.66	1.51	1.42
22	c	511	CLA	C1B-NB	-3.66	1.33	1.37
22	b	603	CLA	C1B-NB	-3.66	1.33	1.37
22	D	404	CLA	C3B-C4B	3.66	1.51	1.42
22	G	611	CLA	C3B-C4B	3.65	1.51	1.42
22	g	611	CLA	C3B-C4B	3.65	1.51	1.42
22	D	403	CLA	CHC-C4B	3.65	1.47	1.39
22	c	505	CLA	CHC-C4B	3.65	1.47	1.39
22	N	611	CLA	C3B-C4B	3.65	1.51	1.42
22	n	611	CLA	C3B-C4B	3.65	1.51	1.42
22	b	614	CLA	C3C-C2C	3.65	1.44	1.36
22	C	504	CLA	C1B-NB	-3.65	1.33	1.37
23	a	404	PHO	C4D-ND	-3.65	1.33	1.38
22	Y	613	CLA	C1B-NB	-3.65	1.33	1.37
22	y	613	CLA	C1B-NB	-3.65	1.33	1.37
22	b	604	CLA	CHC-C1C	3.65	1.45	1.38
22	C	501	CLA	MG-NA	3.65	2.14	2.06
25	N	609	CHL	MG-NA	3.64	2.14	2.06
25	n	609	CHL	MG-NA	3.64	2.14	2.06
22	B	614	CLA	C1B-NB	-3.64	1.33	1.37
22	3	305	CLA	MG-NA	3.64	2.14	2.06
22	7	305	CLA	MG-NA	3.64	2.14	2.06
22	b	603	CLA	MG-NA	3.63	2.14	2.06
22	S	301	CLA	C3B-C4B	3.63	1.51	1.42
22	C	510	CLA	CHC-C4B	3.63	1.47	1.39
22	C	504	CLA	CHC-C1C	3.63	1.45	1.38
22	b	605	CLA	C1B-NB	-3.63	1.33	1.37
22	C	511	CLA	C1B-NB	-3.63	1.33	1.37
22	b	613	CLA	CHC-C4B	3.63	1.47	1.39
22	2	613	CLA	MG-NA	3.63	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	613	CLA	MG-NA	3.63	2.14	2.06
22	Y	614	CLA	C4D-ND	-3.63	1.32	1.37
22	y	614	CLA	C4D-ND	-3.63	1.32	1.37
22	b	611	CLA	CHC-C4B	3.63	1.47	1.39
22	d	403	CLA	CHC-C4B	3.62	1.47	1.39
22	N	610	CLA	C3B-C4B	3.62	1.51	1.42
22	n	610	CLA	C3B-C4B	3.62	1.51	1.42
22	S	303	CLA	C1B-NB	-3.62	1.33	1.37
22	s	303	CLA	C1B-NB	-3.62	1.33	1.37
22	R	302	CLA	C1B-NB	-3.62	1.33	1.37
22	r	302	CLA	C1B-NB	-3.62	1.33	1.37
22	c	504	CLA	C3B-C4B	3.62	1.51	1.42
22	B	611	CLA	C4D-ND	-3.62	1.32	1.37
22	b	611	CLA	C4D-ND	-3.62	1.32	1.37
22	d	404	CLA	C1B-NB	-3.62	1.33	1.37
22	C	501	CLA	CHC-C1C	3.62	1.45	1.38
22	b	607	CLA	C1B-NB	-3.62	1.33	1.37
22	s	301	CLA	C1B-NB	-3.62	1.33	1.37
22	N	604	CLA	C4D-ND	-3.62	1.32	1.37
22	n	604	CLA	C4D-ND	-3.62	1.32	1.37
22	b	604	CLA	CHC-C4B	3.62	1.47	1.39
22	S	301	CLA	C1B-NB	-3.61	1.33	1.37
22	R	302	CLA	C3B-C4B	3.61	1.51	1.42
22	r	302	CLA	C3B-C4B	3.61	1.51	1.42
22	1	611	CLA	MG-NA	3.61	2.14	2.06
22	5	611	CLA	MG-NA	3.61	2.14	2.06
22	S	309	CLA	CHC-C4B	3.61	1.47	1.39
22	s	309	CLA	CHC-C4B	3.61	1.47	1.39
22	N	603	CLA	C3B-C4B	3.61	1.51	1.42
22	n	603	CLA	C3B-C4B	3.61	1.51	1.42
22	A	402	CLA	C4D-ND	-3.61	1.32	1.37
22	1	604	CLA	C3B-C4B	3.61	1.51	1.42
22	5	604	CLA	C3B-C4B	3.61	1.51	1.42
22	B	615	CLA	C3C-C2C	3.61	1.44	1.36
22	b	616	CLA	CHC-C1C	3.61	1.45	1.38
22	c	502	CLA	C3B-C4B	3.61	1.51	1.42
22	B	615	CLA	CHC-C4B	3.60	1.47	1.39
22	b	615	CLA	C1B-NB	-3.60	1.33	1.37
22	a	402	CLA	C3B-C4B	3.60	1.51	1.42
22	4	305	CLA	MG-NA	3.59	2.14	2.06
22	8	305	CLA	MG-NA	3.59	2.14	2.06
22	B	616	CLA	C1D-ND	-3.59	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	311	CLA	MG-NA	3.59	2.14	2.06
22	7	311	CLA	MG-NA	3.59	2.14	2.06
22	R	311	CLA	C1B-NB	-3.59	1.33	1.37
22	r	311	CLA	C1B-NB	-3.59	1.33	1.37
22	4	310	CLA	MG-NA	3.59	2.14	2.06
22	8	310	CLA	MG-NA	3.59	2.14	2.06
22	B	615	CLA	C4D-ND	-3.59	1.32	1.37
22	Y	611	CLA	C4D-ND	-3.59	1.32	1.37
22	y	611	CLA	C4D-ND	-3.59	1.32	1.37
22	B	606	CLA	C3C-C2C	3.59	1.44	1.36
22	c	502	CLA	C1B-NB	-3.59	1.33	1.37
22	C	512	CLA	MG-NA	3.59	2.14	2.06
22	2	611	CLA	MG-NA	3.59	2.14	2.06
22	6	611	CLA	MG-NA	3.59	2.14	2.06
22	b	616	CLA	C3B-C4B	3.59	1.51	1.42
22	R	301	CLA	C1B-NB	-3.59	1.33	1.37
22	r	301	CLA	C1B-NB	-3.59	1.33	1.37
22	c	508	CLA	CHC-C4B	3.58	1.47	1.39
22	C	503	CLA	MG-NA	3.58	2.14	2.06
22	4	303	CLA	C3B-C4B	3.58	1.51	1.42
22	8	303	CLA	C3B-C4B	3.58	1.51	1.42
22	S	314	CLA	C4D-ND	-3.58	1.32	1.37
22	s	314	CLA	C4D-ND	-3.58	1.32	1.37
22	1	614	CLA	MG-NA	3.58	2.14	2.06
22	5	614	CLA	MG-NA	3.58	2.14	2.06
22	Y	603	CLA	C3B-C4B	3.58	1.51	1.42
22	y	603	CLA	C3B-C4B	3.58	1.51	1.42
22	G	604	CLA	CHC-C4B	3.58	1.47	1.39
22	g	604	CLA	CHC-C4B	3.58	1.47	1.39
22	S	310	CLA	C3B-C4B	3.58	1.51	1.42
22	s	310	CLA	C3B-C4B	3.58	1.51	1.42
22	d	401	CLA	C3B-C4B	3.57	1.51	1.42
22	B	605	CLA	C3C-C2C	3.57	1.44	1.36
22	N	604	CLA	CHC-C4B	3.57	1.47	1.39
22	n	604	CLA	CHC-C4B	3.57	1.47	1.39
22	B	607	CLA	CHC-C4B	3.57	1.47	1.39
22	R	308	CLA	C1B-NB	-3.57	1.33	1.37
22	r	308	CLA	C1B-NB	-3.57	1.33	1.37
22	S	313	CLA	C4D-ND	-3.57	1.32	1.37
22	s	313	CLA	C4D-ND	-3.57	1.32	1.37
22	B	603	CLA	C3B-C4B	3.57	1.51	1.42
22	a	405	CLA	C4D-ND	-3.56	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	603	CLA	C1B-NB	-3.56	1.33	1.37
22	g	603	CLA	C1B-NB	-3.56	1.33	1.37
22	Y	612	CLA	CHC-C4B	3.56	1.47	1.39
22	y	612	CLA	CHC-C4B	3.56	1.47	1.39
22	B	602	CLA	MG-NA	3.56	2.14	2.06
22	G	602	CLA	C3B-C4B	3.56	1.51	1.42
22	g	602	CLA	C3B-C4B	3.56	1.51	1.42
22	B	608	CLA	CHC-C1C	3.55	1.45	1.38
22	4	304	CLA	MG-NA	3.55	2.14	2.06
22	8	304	CLA	MG-NA	3.55	2.14	2.06
22	2	610	CLA	MG-NA	3.55	2.14	2.06
22	6	610	CLA	MG-NA	3.55	2.14	2.06
23	d	402	PHO	C4D-ND	-3.55	1.33	1.38
22	B	606	CLA	C3B-C4B	3.55	1.51	1.42
22	C	506	CLA	CHC-C1C	3.54	1.45	1.38
22	S	305	CLA	C3B-C4B	3.54	1.51	1.42
22	s	305	CLA	C3B-C4B	3.54	1.51	1.42
22	b	614	CLA	C1B-NB	-3.54	1.33	1.37
22	G	613	CLA	C3B-C4B	3.54	1.51	1.42
22	g	613	CLA	C3B-C4B	3.54	1.51	1.42
22	b	603	CLA	C3B-C4B	3.54	1.51	1.42
22	C	504	CLA	CHC-C4B	3.54	1.47	1.39
22	b	610	CLA	MG-NA	3.54	2.14	2.06
22	c	509	CLA	C4D-ND	-3.53	1.32	1.37
22	B	608	CLA	CHC-C4B	3.53	1.47	1.39
25	Y	609	CHL	MG-NA	3.53	2.14	2.06
25	y	609	CHL	MG-NA	3.53	2.14	2.06
22	2	603	CLA	MG-NA	3.53	2.14	2.06
22	6	603	CLA	MG-NA	3.53	2.14	2.06
22	2	602	CLA	C1B-NB	-3.53	1.33	1.37
22	6	602	CLA	C1B-NB	-3.53	1.33	1.37
22	N	611	CLA	C1B-NB	-3.53	1.33	1.37
22	n	611	CLA	C1B-NB	-3.53	1.33	1.37
22	C	508	CLA	CHC-C1C	3.53	1.45	1.38
22	1	610	CLA	MG-NA	3.53	2.14	2.06
22	5	610	CLA	MG-NA	3.53	2.14	2.06
22	1	610	CLA	C1B-NB	-3.52	1.33	1.37
22	5	610	CLA	C1B-NB	-3.52	1.33	1.37
22	B	601	CLA	C1B-NB	-3.52	1.33	1.37
22	4	310	CLA	C1B-NB	-3.52	1.33	1.37
22	8	310	CLA	C1B-NB	-3.52	1.33	1.37
22	c	510	CLA	C3B-C4B	3.52	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	609	CLA	MG-NA	3.51	2.14	2.06
22	6	609	CLA	MG-NA	3.51	2.14	2.06
22	3	312	CLA	MG-NA	3.51	2.14	2.06
22	7	312	CLA	MG-NA	3.51	2.14	2.06
22	C	503	CLA	C3B-C4B	3.51	1.51	1.42
22	1	604	CLA	C1B-NB	-3.51	1.33	1.37
22	5	604	CLA	C1B-NB	-3.51	1.33	1.37
22	B	605	CLA	C3B-C4B	3.51	1.51	1.42
22	B	614	CLA	MG-NA	3.51	2.14	2.06
22	D	403	CLA	C4D-ND	-3.51	1.32	1.37
22	c	503	CLA	C4D-ND	-3.51	1.32	1.37
22	4	303	CLA	C1B-NB	-3.50	1.33	1.37
22	8	303	CLA	C1B-NB	-3.50	1.33	1.37
22	D	401	CLA	C3B-C4B	3.50	1.50	1.42
22	b	604	CLA	C3B-C4B	3.50	1.50	1.42
22	b	606	CLA	MG-NA	3.50	2.14	2.06
22	4	311	CLA	MG-NA	3.50	2.14	2.06
22	8	311	CLA	MG-NA	3.50	2.14	2.06
22	D	401	CLA	C4D-ND	-3.50	1.32	1.37
22	N	613	CLA	C3B-C4B	3.50	1.50	1.42
22	n	613	CLA	C3B-C4B	3.50	1.50	1.42
22	Y	604	CLA	CHC-C4B	3.50	1.47	1.39
22	y	604	CLA	CHC-C4B	3.50	1.47	1.39
22	4	301	CLA	C1B-NB	-3.49	1.33	1.37
22	8	301	CLA	C1B-NB	-3.49	1.33	1.37
22	B	605	CLA	C4D-ND	-3.49	1.32	1.37
22	d	403	CLA	C4D-ND	-3.49	1.32	1.37
22	b	610	CLA	C3B-C4B	3.49	1.50	1.42
22	b	616	CLA	CHC-C4B	3.49	1.47	1.39
22	b	614	CLA	C3B-C4B	3.49	1.50	1.42
22	D	403	CLA	C3C-C2C	3.49	1.44	1.36
22	C	501	CLA	CHC-C4B	3.49	1.47	1.39
22	B	610	CLA	C3B-C4B	3.49	1.50	1.42
22	B	606	CLA	C1B-NB	-3.49	1.33	1.37
22	Y	613	CLA	C3B-C4B	3.49	1.50	1.42
22	y	613	CLA	C3B-C4B	3.49	1.50	1.42
22	c	511	CLA	MG-NA	3.49	2.14	2.06
22	N	603	CLA	C4D-ND	-3.49	1.32	1.37
22	n	603	CLA	C4D-ND	-3.49	1.32	1.37
22	B	602	CLA	C3B-C4B	3.48	1.50	1.42
22	c	501	CLA	CHC-C1C	3.48	1.45	1.38
22	c	501	CLA	CHC-C4B	3.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	616	CLA	C4D-ND	-3.48	1.32	1.37
22	c	508	CLA	C4D-ND	-3.48	1.32	1.37
22	2	604	CLA	C1B-NB	-3.48	1.33	1.37
22	6	604	CLA	C1B-NB	-3.48	1.33	1.37
22	B	610	CLA	MG-NA	3.47	2.14	2.06
22	B	613	CLA	C3B-C4B	3.47	1.50	1.42
22	R	311	CLA	C3B-C4B	3.47	1.50	1.42
22	r	311	CLA	C3B-C4B	3.47	1.50	1.42
22	B	604	CLA	C4D-ND	-3.47	1.32	1.37
22	S	304	CLA	C1B-NB	-3.47	1.33	1.37
22	s	304	CLA	C1B-NB	-3.47	1.33	1.37
22	R	310	CLA	MG-NA	3.47	2.14	2.06
22	r	310	CLA	MG-NA	3.47	2.14	2.06
22	S	314	CLA	C3B-C4B	3.46	1.50	1.42
22	s	314	CLA	C3B-C4B	3.46	1.50	1.42
22	C	506	CLA	CHC-C4B	3.46	1.47	1.39
22	N	613	CLA	C4D-ND	-3.46	1.32	1.37
22	n	613	CLA	C4D-ND	-3.46	1.32	1.37
22	a	403	CLA	C4D-ND	-3.46	1.32	1.37
22	R	311	CLA	C4D-ND	-3.46	1.32	1.37
22	r	311	CLA	C4D-ND	-3.46	1.32	1.37
22	B	616	CLA	C1B-C2B	3.46	1.51	1.43
22	Y	612	CLA	C4D-ND	-3.45	1.32	1.37
22	y	612	CLA	C4D-ND	-3.45	1.32	1.37
22	C	505	CLA	MG-NA	3.45	2.14	2.06
22	3	305	CLA	C1B-NB	-3.45	1.33	1.37
22	7	305	CLA	C1B-NB	-3.45	1.33	1.37
22	2	611	CLA	C1B-NB	-3.45	1.33	1.37
22	6	611	CLA	C1B-NB	-3.45	1.33	1.37
22	A	403	CLA	C4D-ND	-3.44	1.33	1.37
22	C	507	CLA	C4D-ND	-3.44	1.33	1.37
22	c	505	CLA	C3B-C4B	3.44	1.50	1.42
22	N	612	CLA	C3B-C4B	3.43	1.50	1.42
22	n	612	CLA	C3B-C4B	3.43	1.50	1.42
22	C	508	CLA	C4D-ND	-3.43	1.33	1.37
22	C	510	CLA	C4D-ND	-3.43	1.33	1.37
22	Y	602	CLA	C3B-C4B	3.43	1.50	1.42
22	y	602	CLA	C3B-C4B	3.43	1.50	1.42
22	G	611	CLA	C1B-NB	-3.43	1.33	1.37
22	g	611	CLA	C1B-NB	-3.43	1.33	1.37
25	2	605	CHL	C3A-C2A	-3.43	1.51	1.54
25	6	605	CHL	C3A-C2A	-3.43	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	603	CLA	O2A-CGA	3.43	1.42	1.30
22	n	603	CLA	O2A-CGA	3.43	1.42	1.30
22	S	304	CLA	C4B-NB	-3.43	1.33	1.37
22	s	304	CLA	C4B-NB	-3.43	1.33	1.37
22	B	611	CLA	C3B-C4B	3.43	1.50	1.42
22	c	507	CLA	CHC-C4B	3.42	1.47	1.39
22	B	616	CLA	O2A-CGA	3.42	1.42	1.30
22	c	506	CLA	MG-NA	3.42	2.14	2.06
22	B	612	CLA	C4D-ND	-3.42	1.33	1.37
22	R	303	CLA	C3B-C4B	3.41	1.50	1.42
22	r	303	CLA	C3B-C4B	3.41	1.50	1.42
22	3	312	CLA	C1B-NB	-3.41	1.33	1.37
22	7	312	CLA	C1B-NB	-3.41	1.33	1.37
22	b	614	CLA	MG-NA	3.41	2.14	2.06
22	A	405	CLA	C4D-ND	-3.41	1.33	1.37
22	G	613	CLA	C4D-ND	-3.41	1.33	1.37
22	g	613	CLA	C4D-ND	-3.41	1.33	1.37
25	3	306	CHL	C3A-C2A	-3.41	1.51	1.54
25	7	306	CHL	C3A-C2A	-3.41	1.51	1.54
22	N	602	CLA	C3B-C4B	3.41	1.50	1.42
22	n	602	CLA	C3B-C4B	3.41	1.50	1.42
22	c	502	CLA	O2A-CGA	3.41	1.42	1.30
22	2	609	CLA	C1B-NB	-3.41	1.33	1.37
22	3	310	CLA	C1B-NB	-3.41	1.33	1.37
22	6	609	CLA	C1B-NB	-3.41	1.33	1.37
22	7	310	CLA	C1B-NB	-3.41	1.33	1.37
22	b	609	CLA	C3B-C4B	3.41	1.50	1.42
22	B	605	CLA	O2A-CGA	3.40	1.42	1.30
22	b	606	CLA	C1B-NB	-3.40	1.33	1.37
22	b	608	CLA	O2A-CGA	3.40	1.42	1.30
22	G	604	CLA	C3B-C4B	3.40	1.50	1.42
22	g	604	CLA	C3B-C4B	3.40	1.50	1.42
22	C	503	CLA	C4D-ND	-3.40	1.33	1.37
22	Y	610	CLA	C3B-C4B	3.40	1.50	1.42
22	y	610	CLA	C3B-C4B	3.40	1.50	1.42
22	a	402	CLA	C4D-ND	-3.40	1.33	1.37
22	B	601	CLA	O2A-CGA	3.40	1.42	1.30
22	s	301	CLA	MG-NA	3.39	2.14	2.06
22	A	402	CLA	C3B-C4B	3.39	1.50	1.42
22	A	405	CLA	C3B-C4B	3.39	1.50	1.42
22	B	608	CLA	O2A-CGA	3.39	1.42	1.30
22	Y	614	CLA	C3B-C4B	3.39	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	y	614	CLA	C3B-C4B	3.39	1.50	1.42
22	N	614	CLA	O2A-CGA	3.39	1.42	1.30
22	n	614	CLA	O2A-CGA	3.39	1.42	1.30
22	1	603	CLA	MG-NA	3.39	2.14	2.06
22	5	603	CLA	MG-NA	3.39	2.14	2.06
22	D	404	CLA	C4D-ND	-3.39	1.33	1.37
22	Y	603	CLA	C4D-ND	-3.39	1.33	1.37
22	y	603	CLA	C4D-ND	-3.39	1.33	1.37
22	b	605	CLA	O2A-CGA	3.39	1.42	1.30
22	c	512	CLA	C4D-ND	-3.39	1.33	1.37
22	N	612	CLA	O2A-CGA	3.39	1.42	1.30
22	n	612	CLA	O2A-CGA	3.39	1.42	1.30
22	G	614	CLA	C1B-NB	-3.39	1.33	1.37
22	g	614	CLA	C1B-NB	-3.39	1.33	1.37
22	3	310	CLA	MG-NA	3.39	2.14	2.06
22	7	310	CLA	MG-NA	3.39	2.14	2.06
22	N	614	CLA	MG-NA	3.38	2.14	2.06
22	n	614	CLA	MG-NA	3.38	2.14	2.06
22	N	611	CLA	O2A-CGA	3.38	1.42	1.30
22	n	611	CLA	O2A-CGA	3.38	1.42	1.30
22	B	607	CLA	C4D-ND	-3.38	1.33	1.37
22	N	604	CLA	C3B-C4B	3.38	1.50	1.42
22	n	604	CLA	C3B-C4B	3.38	1.50	1.42
22	B	606	CLA	MG-NA	3.38	2.14	2.06
22	A	405	CLA	O2A-CGA	3.38	1.42	1.30
22	C	505	CLA	C3B-C4B	3.38	1.50	1.42
22	s	301	CLA	O2A-CGA	3.37	1.42	1.30
22	2	613	CLA	C1B-NB	-3.37	1.33	1.37
22	6	613	CLA	C1B-NB	-3.37	1.33	1.37
22	c	508	CLA	C3B-C4B	3.37	1.50	1.42
22	S	301	CLA	O2A-CGA	3.37	1.42	1.30
22	c	506	CLA	O2A-CGA	3.37	1.42	1.30
22	b	601	CLA	O2A-CGA	3.37	1.42	1.30
22	G	612	CLA	O2A-CGA	3.37	1.42	1.30
22	g	612	CLA	O2A-CGA	3.37	1.42	1.30
22	c	508	CLA	MG-NA	3.37	2.14	2.06
22	C	504	CLA	O2A-CGA	3.37	1.42	1.30
22	C	508	CLA	CHC-C4B	3.36	1.47	1.39
22	1	604	CLA	O2A-CGA	3.36	1.42	1.30
22	5	604	CLA	O2A-CGA	3.36	1.42	1.30
22	A	402	CLA	O2A-CGA	3.36	1.42	1.30
22	3	312	CLA	O2A-CGA	3.36	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	312	CLA	O2A-CGA	3.36	1.42	1.30
22	A	403	CLA	O2A-CGA	3.36	1.42	1.30
22	c	512	CLA	O2A-CGA	3.36	1.42	1.30
22	C	512	CLA	O2A-CGA	3.36	1.42	1.30
22	a	403	CLA	O2A-CGA	3.36	1.42	1.30
22	B	603	CLA	O2A-CGA	3.36	1.42	1.30
22	B	609	CLA	C3B-C4B	3.36	1.50	1.42
22	B	602	CLA	O2A-CGA	3.36	1.42	1.30
22	Y	612	CLA	C3B-C4B	3.36	1.50	1.42
22	y	612	CLA	C3B-C4B	3.36	1.50	1.42
22	1	614	CLA	O2A-CGA	3.36	1.42	1.30
22	5	614	CLA	O2A-CGA	3.36	1.42	1.30
22	C	506	CLA	O2A-CGA	3.36	1.42	1.30
22	R	310	CLA	O2A-CGA	3.36	1.42	1.30
22	r	310	CLA	O2A-CGA	3.36	1.42	1.30
22	2	612	CLA	C1B-NB	-3.36	1.33	1.37
22	6	612	CLA	C1B-NB	-3.36	1.33	1.37
22	B	608	CLA	C4D-ND	-3.36	1.33	1.37
22	B	614	CLA	O2A-CGA	3.35	1.42	1.30
22	S	305	CLA	O2A-CGA	3.35	1.42	1.30
22	s	305	CLA	O2A-CGA	3.35	1.42	1.30
22	G	611	CLA	O2A-CGA	3.35	1.42	1.30
22	g	611	CLA	O2A-CGA	3.35	1.42	1.30
22	Y	612	CLA	O2A-CGA	3.35	1.42	1.30
22	y	612	CLA	O2A-CGA	3.35	1.42	1.30
22	2	610	CLA	O2A-CGA	3.35	1.42	1.30
22	6	610	CLA	O2A-CGA	3.35	1.42	1.30
22	b	614	CLA	O2A-CGA	3.35	1.42	1.30
22	3	311	CLA	O2A-CGA	3.35	1.42	1.30
22	7	311	CLA	O2A-CGA	3.35	1.42	1.30
22	C	502	CLA	O2A-CGA	3.35	1.42	1.30
22	Y	614	CLA	O2A-CGA	3.35	1.42	1.30
22	y	614	CLA	O2A-CGA	3.35	1.42	1.30
22	2	611	CLA	O2A-CGA	3.35	1.42	1.30
22	6	611	CLA	O2A-CGA	3.35	1.42	1.30
22	d	401	CLA	O2A-CGA	3.35	1.42	1.30
22	d	403	CLA	O2A-CGA	3.35	1.42	1.30
22	2	613	CLA	O2A-CGA	3.35	1.42	1.30
22	6	613	CLA	O2A-CGA	3.35	1.42	1.30
22	d	404	CLA	O2A-CGA	3.34	1.42	1.30
22	c	504	CLA	O2A-CGA	3.34	1.42	1.30
22	B	607	CLA	O2A-CGA	3.34	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	O2A-CGA	3.34	1.42	1.30
22	a	402	CLA	O2A-CGA	3.34	1.42	1.30
22	B	609	CLA	O2A-CGA	3.34	1.42	1.30
22	B	615	CLA	O2A-CGA	3.34	1.42	1.30
22	B	609	CLA	MG-NA	3.34	2.14	2.06
22	D	403	CLA	O2A-CGA	3.34	1.42	1.30
22	D	401	CLA	O2A-CGA	3.34	1.42	1.30
22	R	311	CLA	O2A-CGA	3.34	1.42	1.30
22	r	311	CLA	O2A-CGA	3.34	1.42	1.30
22	S	314	CLA	O2A-CGA	3.34	1.42	1.30
22	s	314	CLA	O2A-CGA	3.34	1.42	1.30
22	3	304	CLA	O2A-CGA	3.34	1.42	1.30
22	7	304	CLA	O2A-CGA	3.34	1.42	1.30
22	R	308	CLA	O2A-CGA	3.33	1.42	1.30
22	r	308	CLA	O2A-CGA	3.33	1.42	1.30
22	S	309	CLA	O2A-CGA	3.33	1.42	1.30
22	s	309	CLA	O2A-CGA	3.33	1.42	1.30
22	S	312	CLA	O2A-CGA	3.33	1.42	1.30
22	s	312	CLA	O2A-CGA	3.33	1.42	1.30
22	C	507	CLA	MG-NA	3.33	2.14	2.06
22	1	612	CLA	O2A-CGA	3.33	1.41	1.30
22	5	612	CLA	O2A-CGA	3.33	1.41	1.30
22	b	616	CLA	O2A-CGA	3.33	1.41	1.30
22	S	311	CLA	O2A-CGA	3.33	1.41	1.30
22	s	311	CLA	O2A-CGA	3.33	1.41	1.30
22	c	503	CLA	C3B-C4B	3.33	1.50	1.42
22	c	507	CLA	C3B-C4B	3.33	1.50	1.42
22	R	309	CLA	O2A-CGA	3.33	1.41	1.30
22	r	309	CLA	O2A-CGA	3.33	1.41	1.30
22	3	314	CLA	O2A-CGA	3.33	1.41	1.30
22	7	314	CLA	O2A-CGA	3.33	1.41	1.30
22	b	609	CLA	C4D-ND	-3.33	1.33	1.37
22	c	502	CLA	C4D-ND	-3.33	1.33	1.37
22	S	310	CLA	C4D-ND	-3.33	1.33	1.37
22	s	310	CLA	C4D-ND	-3.33	1.33	1.37
22	G	612	CLA	MG-NA	3.33	2.14	2.06
22	g	612	CLA	MG-NA	3.33	2.14	2.06
22	4	305	CLA	C1B-NB	-3.33	1.33	1.37
22	8	305	CLA	C1B-NB	-3.33	1.33	1.37
22	1	603	CLA	O2A-CGA	3.33	1.41	1.30
22	5	603	CLA	O2A-CGA	3.33	1.41	1.30
22	R	310	CLA	C1B-NB	-3.33	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	310	CLA	C1B-NB	-3.33	1.33	1.37
22	C	503	CLA	O2A-CGA	3.33	1.41	1.30
22	C	510	CLA	O2A-CGA	3.33	1.41	1.30
22	c	507	CLA	CHC-C1C	3.33	1.45	1.38
22	G	614	CLA	O2A-CGA	3.32	1.41	1.30
22	g	614	CLA	O2A-CGA	3.32	1.41	1.30
22	4	303	CLA	O2A-CGA	3.32	1.41	1.30
22	8	303	CLA	O2A-CGA	3.32	1.41	1.30
22	a	405	CLA	O2A-CGA	3.32	1.41	1.30
22	b	602	CLA	O2A-CGA	3.32	1.41	1.30
22	D	404	CLA	O2A-CGA	3.32	1.41	1.30
22	3	313	CLA	O2A-CGA	3.32	1.41	1.30
22	7	313	CLA	O2A-CGA	3.32	1.41	1.30
22	C	505	CLA	O2A-CGA	3.32	1.41	1.30
22	b	616	CLA	C1B-NB	-3.32	1.33	1.37
22	c	511	CLA	O2A-CGA	3.32	1.41	1.30
22	G	603	CLA	O2A-CGA	3.32	1.41	1.30
22	g	603	CLA	O2A-CGA	3.32	1.41	1.30
22	2	609	CLA	O2A-CGA	3.32	1.41	1.30
22	6	609	CLA	O2A-CGA	3.32	1.41	1.30
22	C	511	CLA	O2A-CGA	3.32	1.41	1.30
22	4	304	CLA	O2A-CGA	3.32	1.41	1.30
22	8	304	CLA	O2A-CGA	3.32	1.41	1.30
22	Y	603	CLA	O2A-CGA	3.32	1.41	1.30
22	y	603	CLA	O2A-CGA	3.32	1.41	1.30
22	1	613	CLA	O2A-CGA	3.32	1.41	1.30
22	5	613	CLA	O2A-CGA	3.32	1.41	1.30
22	G	604	CLA	MG-NA	3.32	2.14	2.06
22	g	604	CLA	MG-NA	3.32	2.14	2.06
22	G	610	CLA	O2A-CGA	3.32	1.41	1.30
22	g	610	CLA	O2A-CGA	3.32	1.41	1.30
22	b	614	CLA	C4D-ND	-3.32	1.33	1.37
22	2	603	CLA	O2A-CGA	3.31	1.41	1.30
22	6	603	CLA	O2A-CGA	3.31	1.41	1.30
22	c	507	CLA	C4D-ND	-3.31	1.33	1.37
22	c	501	CLA	C4D-ND	-3.31	1.33	1.37
22	C	507	CLA	O2A-CGA	3.31	1.41	1.30
22	1	612	CLA	C1B-NB	-3.31	1.33	1.37
22	5	612	CLA	C1B-NB	-3.31	1.33	1.37
22	4	311	CLA	O2A-CGA	3.31	1.41	1.30
22	8	311	CLA	O2A-CGA	3.31	1.41	1.30
22	b	607	CLA	O2A-CGA	3.31	1.41	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	612	CLA	O2A-CGA	3.31	1.41	1.30
22	6	612	CLA	O2A-CGA	3.31	1.41	1.30
22	b	615	CLA	O2A-CGA	3.31	1.41	1.30
22	Y	611	CLA	O2A-CGA	3.31	1.41	1.30
22	y	611	CLA	O2A-CGA	3.31	1.41	1.30
22	c	510	CLA	O2A-CGA	3.31	1.41	1.30
22	S	313	CLA	O2A-CGA	3.31	1.41	1.30
22	s	313	CLA	O2A-CGA	3.31	1.41	1.30
22	R	302	CLA	O2A-CGA	3.31	1.41	1.30
22	r	302	CLA	O2A-CGA	3.31	1.41	1.30
22	3	310	CLA	O2A-CGA	3.31	1.41	1.30
22	7	310	CLA	O2A-CGA	3.31	1.41	1.30
22	B	607	CLA	C3B-C4B	3.31	1.50	1.42
22	B	615	CLA	C3B-C4B	3.31	1.50	1.42
22	C	505	CLA	C4D-ND	-3.31	1.33	1.37
22	G	604	CLA	O2A-CGA	3.31	1.41	1.30
22	g	604	CLA	O2A-CGA	3.31	1.41	1.30
22	4	310	CLA	O2A-CGA	3.31	1.41	1.30
22	8	310	CLA	O2A-CGA	3.31	1.41	1.30
22	1	602	CLA	O2A-CGA	3.30	1.41	1.30
22	5	602	CLA	O2A-CGA	3.30	1.41	1.30
22	4	305	CLA	O2A-CGA	3.30	1.41	1.30
22	8	305	CLA	O2A-CGA	3.30	1.41	1.30
22	3	303	CLA	C1B-NB	-3.30	1.33	1.37
22	7	303	CLA	C1B-NB	-3.30	1.33	1.37
22	d	401	CLA	C4D-ND	-3.30	1.33	1.37
22	S	310	CLA	O2A-CGA	3.30	1.41	1.30
22	s	310	CLA	O2A-CGA	3.30	1.41	1.30
22	C	504	CLA	C3B-C4B	3.30	1.50	1.42
22	D	403	CLA	C3B-C4B	3.30	1.50	1.42
22	1	602	CLA	MG-NA	3.30	2.14	2.06
22	5	602	CLA	MG-NA	3.30	2.14	2.06
22	R	307	CLA	O2A-CGA	3.30	1.41	1.30
22	r	307	CLA	O2A-CGA	3.30	1.41	1.30
22	B	601	CLA	MG-NA	3.30	2.14	2.06
22	C	501	CLA	C3B-C4B	3.30	1.50	1.42
22	R	301	CLA	O2A-CGA	3.30	1.41	1.30
22	r	301	CLA	O2A-CGA	3.30	1.41	1.30
22	B	611	CLA	O2A-CGA	3.30	1.41	1.30
22	B	608	CLA	C3B-C4B	3.29	1.50	1.42
22	2	602	CLA	O2A-CGA	3.29	1.41	1.30
22	6	602	CLA	O2A-CGA	3.29	1.41	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	503	CLA	O2A-CGA	3.29	1.41	1.30
22	1	610	CLA	O2A-CGA	3.29	1.41	1.30
22	5	610	CLA	O2A-CGA	3.29	1.41	1.30
22	B	610	CLA	O2A-CGA	3.29	1.41	1.30
22	Y	602	CLA	C4D-ND	-3.29	1.33	1.37
22	y	602	CLA	C4D-ND	-3.29	1.33	1.37
22	S	303	CLA	O2A-CGA	3.29	1.41	1.30
22	s	303	CLA	O2A-CGA	3.29	1.41	1.30
22	c	508	CLA	O2A-CGA	3.29	1.41	1.30
22	b	610	CLA	O2A-CGA	3.29	1.41	1.30
22	c	506	CLA	C4D-ND	-3.29	1.33	1.37
22	a	402	CLA	MG-NA	3.29	2.14	2.06
22	C	509	CLA	MG-NA	3.29	2.14	2.06
22	b	602	CLA	C3B-C4B	3.29	1.50	1.42
22	b	611	CLA	O2A-CGA	3.28	1.41	1.30
22	4	311	CLA	C1B-NB	-3.28	1.33	1.37
22	8	311	CLA	C1B-NB	-3.28	1.33	1.37
22	3	305	CLA	O2A-CGA	3.28	1.41	1.30
22	7	305	CLA	O2A-CGA	3.28	1.41	1.30
22	c	505	CLA	O2A-CGA	3.28	1.41	1.30
22	B	613	CLA	O2A-CGA	3.28	1.41	1.30
22	2	604	CLA	O2A-CGA	3.28	1.41	1.30
22	6	604	CLA	O2A-CGA	3.28	1.41	1.30
22	3	303	CLA	MG-NA	3.28	2.14	2.06
22	7	303	CLA	MG-NA	3.28	2.14	2.06
22	3	313	CLA	C1B-NB	-3.28	1.33	1.37
22	7	313	CLA	C1B-NB	-3.28	1.33	1.37
22	S	301	CLA	MG-NA	3.28	2.14	2.06
24	e	101	HEM	FE-NA	3.28	2.06	1.95
22	b	611	CLA	C3B-C4B	3.28	1.50	1.42
22	3	303	CLA	O2A-CGA	3.28	1.41	1.30
22	7	303	CLA	O2A-CGA	3.28	1.41	1.30
22	S	304	CLA	MG-NA	3.28	2.14	2.06
22	s	304	CLA	MG-NA	3.28	2.14	2.06
22	C	508	CLA	C3B-C4B	3.28	1.50	1.42
22	C	508	CLA	O2A-CGA	3.27	1.41	1.30
22	b	606	CLA	O2A-CGA	3.27	1.41	1.30
22	3	311	CLA	C1B-NB	-3.27	1.33	1.37
22	7	311	CLA	C1B-NB	-3.27	1.33	1.37
22	1	613	CLA	C1B-NB	-3.27	1.33	1.37
22	5	613	CLA	C1B-NB	-3.27	1.33	1.37
22	d	403	CLA	C3B-C4B	3.27	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	613	CLA	O2A-CGA	3.27	1.41	1.30
22	n	613	CLA	O2A-CGA	3.27	1.41	1.30
22	2	612	CLA	MG-NA	3.27	2.14	2.06
22	6	612	CLA	MG-NA	3.27	2.14	2.06
22	b	609	CLA	O2A-CGA	3.27	1.41	1.30
22	Y	613	CLA	O2A-CGA	3.27	1.41	1.30
22	y	613	CLA	O2A-CGA	3.27	1.41	1.30
22	a	403	CLA	MG-NA	3.27	2.14	2.06
22	c	507	CLA	O2A-CGA	3.26	1.41	1.30
22	1	613	CLA	MG-NA	3.26	2.14	2.06
22	5	613	CLA	MG-NA	3.26	2.14	2.06
22	b	613	CLA	O2A-CGA	3.26	1.41	1.30
22	R	302	CLA	MG-NA	3.26	2.14	2.06
22	r	302	CLA	MG-NA	3.26	2.14	2.06
22	1	611	CLA	O2A-CGA	3.26	1.41	1.30
22	5	611	CLA	O2A-CGA	3.26	1.41	1.30
22	3	313	CLA	MG-NA	3.26	2.14	2.06
22	4	301	CLA	MG-NA	3.26	2.14	2.06
22	7	313	CLA	MG-NA	3.26	2.14	2.06
22	8	301	CLA	MG-NA	3.26	2.14	2.06
22	B	604	CLA	O2A-CGA	3.26	1.41	1.30
22	S	304	CLA	O2A-CGA	3.26	1.41	1.30
22	s	304	CLA	O2A-CGA	3.26	1.41	1.30
22	G	603	CLA	MG-NA	3.26	2.14	2.06
22	g	603	CLA	MG-NA	3.26	2.14	2.06
22	1	602	CLA	C1B-NB	-3.26	1.33	1.37
22	5	602	CLA	C1B-NB	-3.26	1.33	1.37
22	R	301	CLA	C4D-ND	-3.26	1.33	1.37
22	r	301	CLA	C4D-ND	-3.26	1.33	1.37
22	C	511	CLA	MG-NA	3.25	2.14	2.06
22	4	301	CLA	O2A-CGA	3.25	1.41	1.30
22	8	301	CLA	O2A-CGA	3.25	1.41	1.30
22	3	314	CLA	C1B-NB	-3.25	1.33	1.37
22	7	314	CLA	C1B-NB	-3.25	1.33	1.37
22	N	604	CLA	O2A-CGA	3.25	1.41	1.30
22	n	604	CLA	O2A-CGA	3.25	1.41	1.30
22	N	614	CLA	C1B-NB	-3.25	1.33	1.37
22	n	614	CLA	C1B-NB	-3.25	1.33	1.37
22	b	608	CLA	C4D-ND	-3.25	1.33	1.37
22	G	614	CLA	MG-NA	3.25	2.14	2.06
22	g	614	CLA	MG-NA	3.25	2.14	2.06
22	C	501	CLA	O2A-CGA	3.25	1.41	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	C3B-C4B	3.25	1.50	1.42
22	c	503	CLA	MG-NA	3.25	2.14	2.06
22	C	506	CLA	C4D-ND	-3.25	1.33	1.37
22	1	604	CLA	MG-NA	3.25	2.14	2.06
22	5	604	CLA	MG-NA	3.25	2.14	2.06
22	b	607	CLA	C3B-C4B	3.25	1.50	1.42
22	N	611	CLA	MG-NA	3.25	2.14	2.06
22	n	611	CLA	MG-NA	3.25	2.14	2.06
22	b	607	CLA	C4D-ND	-3.24	1.33	1.37
22	C	509	CLA	O2A-CGA	3.24	1.41	1.30
22	2	610	CLA	C1B-NB	-3.24	1.33	1.37
22	6	610	CLA	C1B-NB	-3.24	1.33	1.37
22	G	613	CLA	O2A-CGA	3.23	1.41	1.30
22	g	613	CLA	O2A-CGA	3.23	1.41	1.30
22	N	602	CLA	C4D-ND	-3.23	1.33	1.37
22	n	602	CLA	C4D-ND	-3.23	1.33	1.37
22	c	511	CLA	C4D-ND	-3.23	1.33	1.37
22	b	606	CLA	CHD-C4C	3.23	1.46	1.39
22	b	608	CLA	MG-NA	3.23	2.13	2.06
22	B	606	CLA	O2A-CGA	3.23	1.41	1.30
22	C	504	CLA	C4D-ND	-3.23	1.33	1.37
22	1	611	CLA	C1B-NB	-3.22	1.33	1.37
22	5	611	CLA	C1B-NB	-3.22	1.33	1.37
22	A	403	CLA	MG-NA	3.22	2.13	2.06
22	G	604	CLA	C4D-ND	-3.22	1.33	1.37
22	g	604	CLA	C4D-ND	-3.22	1.33	1.37
22	c	501	CLA	O2A-CGA	3.21	1.41	1.30
22	C	510	CLA	C3B-C4B	3.21	1.50	1.42
22	b	613	CLA	C3B-C4B	3.21	1.50	1.42
22	Y	604	CLA	O2A-CGA	3.21	1.41	1.30
22	y	604	CLA	O2A-CGA	3.21	1.41	1.30
22	b	601	CLA	MG-NA	3.21	2.13	2.06
22	N	611	CLA	C4D-ND	-3.21	1.33	1.37
22	n	611	CLA	C4D-ND	-3.21	1.33	1.37
22	R	303	CLA	O2A-CGA	3.21	1.41	1.30
22	r	303	CLA	O2A-CGA	3.21	1.41	1.30
22	S	312	CLA	C3B-C4B	3.21	1.50	1.42
22	s	312	CLA	C3B-C4B	3.21	1.50	1.42
22	C	506	CLA	C3B-C4B	3.21	1.50	1.42
22	G	610	CLA	MG-NA	3.20	2.13	2.06
22	g	610	CLA	MG-NA	3.20	2.13	2.06
22	2	602	CLA	MG-NA	3.20	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	602	CLA	MG-NA	3.20	2.13	2.06
22	B	607	CLA	MG-NA	3.20	2.13	2.06
22	C	501	CLA	C4D-ND	-3.20	1.33	1.37
22	G	614	CLA	C4D-ND	-3.19	1.33	1.37
22	g	614	CLA	C4D-ND	-3.19	1.33	1.37
22	N	612	CLA	MG-NA	3.19	2.13	2.06
22	n	612	CLA	MG-NA	3.19	2.13	2.06
22	Y	604	CLA	MG-NA	3.19	2.13	2.06
22	y	604	CLA	MG-NA	3.19	2.13	2.06
22	c	506	CLA	C3B-C4B	3.19	1.50	1.42
22	2	603	CLA	C1B-NB	-3.19	1.33	1.37
22	6	603	CLA	C1B-NB	-3.19	1.33	1.37
25	3	306	CHL	O2D-CGD	3.19	1.41	1.33
25	7	306	CHL	O2D-CGD	3.19	1.41	1.33
22	B	613	CLA	MG-NA	3.19	2.13	2.06
25	2	605	CHL	O2D-CGD	3.18	1.41	1.33
25	6	605	CHL	O2D-CGD	3.18	1.41	1.33
22	G	602	CLA	C4D-ND	-3.18	1.33	1.37
22	g	602	CLA	C4D-ND	-3.18	1.33	1.37
22	N	610	CLA	O2A-CGA	3.18	1.41	1.30
22	n	610	CLA	O2A-CGA	3.18	1.41	1.30
22	c	504	CLA	C4D-ND	-3.18	1.33	1.37
22	B	604	CLA	MG-NA	3.17	2.13	2.06
22	C	508	CLA	MG-NA	3.17	2.13	2.06
22	B	603	CLA	C4D-ND	-3.17	1.33	1.37
22	G	611	CLA	MG-NA	3.17	2.13	2.06
22	g	611	CLA	MG-NA	3.17	2.13	2.06
25	G	605	CHL	O2D-CGD	3.17	1.40	1.33
25	g	605	CHL	O2D-CGD	3.17	1.40	1.33
22	Y	610	CLA	O2A-CGA	3.16	1.41	1.30
22	y	610	CLA	O2A-CGA	3.16	1.41	1.30
22	d	401	CLA	MG-NA	3.16	2.13	2.06
22	A	405	CLA	MG-NA	3.16	2.13	2.06
22	G	603	CLA	C4D-ND	-3.16	1.33	1.37
22	g	603	CLA	C4D-ND	-3.16	1.33	1.37
22	B	609	CLA	C4D-ND	-3.16	1.33	1.37
22	b	613	CLA	C4D-ND	-3.16	1.33	1.37
22	1	603	CLA	C1B-NB	-3.16	1.33	1.37
22	5	603	CLA	C1B-NB	-3.16	1.33	1.37
22	R	309	CLA	MG-NA	3.16	2.13	2.06
22	r	309	CLA	MG-NA	3.16	2.13	2.06
22	c	509	CLA	O2A-CGA	3.15	1.41	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	505	CLA	C4D-ND	-3.15	1.33	1.37
25	4	307	CHL	O2D-CGD	3.14	1.40	1.33
25	8	307	CHL	O2D-CGD	3.14	1.40	1.33
22	C	502	CLA	C4D-ND	-3.14	1.33	1.37
22	a	405	CLA	C3B-C4B	3.14	1.50	1.42
22	b	609	CLA	MG-NA	3.14	2.13	2.06
22	G	611	CLA	C4D-ND	-3.14	1.33	1.37
22	g	611	CLA	C4D-ND	-3.14	1.33	1.37
22	N	610	CLA	MG-NA	3.14	2.13	2.06
22	n	610	CLA	MG-NA	3.14	2.13	2.06
24	e	101	HEM	CAB-C3B	3.14	1.56	1.47
22	d	404	CLA	MG-NA	3.14	2.13	2.06
22	1	614	CLA	C1B-NB	-3.13	1.33	1.37
22	5	614	CLA	C1B-NB	-3.13	1.33	1.37
22	Y	604	CLA	C3B-C4B	3.13	1.50	1.42
22	y	604	CLA	C3B-C4B	3.13	1.50	1.42
22	b	601	CLA	C4D-ND	-3.13	1.33	1.37
22	S	301	CLA	C4D-ND	-3.13	1.33	1.37
25	4	308	CHL	O2D-CGD	3.13	1.40	1.33
25	8	308	CHL	O2D-CGD	3.13	1.40	1.33
22	Y	611	CLA	MG-NA	3.13	2.13	2.06
22	y	611	CLA	MG-NA	3.13	2.13	2.06
22	4	304	CLA	C1B-NB	-3.12	1.33	1.37
22	8	304	CLA	C1B-NB	-3.12	1.33	1.37
22	B	601	CLA	C4D-ND	-3.12	1.33	1.37
22	b	603	CLA	C4D-ND	-3.12	1.33	1.37
25	1	608	CHL	O2D-CGD	3.12	1.40	1.33
25	5	608	CHL	O2D-CGD	3.12	1.40	1.33
22	G	612	CLA	C4D-ND	-3.12	1.33	1.37
22	g	612	CLA	C4D-ND	-3.12	1.33	1.37
22	R	303	CLA	C4D-ND	-3.11	1.33	1.37
22	r	303	CLA	C4D-ND	-3.11	1.33	1.37
25	4	306	CHL	O2D-CGD	3.11	1.40	1.33
25	8	306	CHL	O2D-CGD	3.11	1.40	1.33
22	c	501	CLA	C3B-C4B	3.11	1.50	1.42
22	b	612	CLA	O2A-CGA	3.10	1.41	1.30
22	b	602	CLA	C4D-ND	-3.10	1.33	1.37
22	3	304	CLA	C1B-NB	-3.10	1.34	1.37
22	7	304	CLA	C1B-NB	-3.10	1.34	1.37
22	D	404	CLA	MG-NA	3.10	2.13	2.06
22	R	308	CLA	C4D-ND	-3.10	1.33	1.37
22	r	308	CLA	C4D-ND	-3.10	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	302	CHL	O2D-CGD	3.10	1.40	1.33
25	7	302	CHL	O2D-CGD	3.10	1.40	1.33
22	4	303	CLA	C1B-C2B	3.09	1.50	1.43
22	8	303	CLA	C1B-C2B	3.09	1.50	1.43
22	b	604	CLA	O2A-CGA	3.09	1.41	1.30
25	R	305	CHL	O2D-CGD	3.09	1.40	1.33
25	r	305	CHL	O2D-CGD	3.09	1.40	1.33
22	d	404	CLA	C4D-ND	-3.09	1.33	1.37
25	4	309	CHL	O2D-CGD	3.09	1.40	1.33
25	8	309	CHL	O2D-CGD	3.09	1.40	1.33
22	D	401	CLA	MG-NA	3.09	2.13	2.06
22	S	305	CLA	C4D-ND	-3.09	1.33	1.37
22	s	305	CLA	C4D-ND	-3.09	1.33	1.37
22	Y	602	CLA	O2A-CGA	3.08	1.41	1.30
22	y	602	CLA	O2A-CGA	3.08	1.41	1.30
25	3	301	CHL	O2D-CGD	3.08	1.40	1.33
25	7	301	CHL	O2D-CGD	3.08	1.40	1.33
22	G	602	CLA	O2A-CGA	3.08	1.41	1.30
22	g	602	CLA	O2A-CGA	3.08	1.41	1.30
25	2	601	CHL	O2D-CGD	3.08	1.40	1.33
25	6	601	CHL	O2D-CGD	3.08	1.40	1.33
22	c	510	CLA	MG-NA	3.08	2.13	2.06
22	C	511	CLA	C4D-ND	-3.08	1.33	1.37
22	C	510	CLA	MG-NA	3.08	2.13	2.06
22	B	612	CLA	O2A-CGA	3.07	1.41	1.30
25	3	309	CHL	O2D-CGD	3.07	1.40	1.33
25	7	309	CHL	O2D-CGD	3.07	1.40	1.33
25	1	601	CHL	O2D-CGD	3.07	1.40	1.33
25	5	601	CHL	O2D-CGD	3.07	1.40	1.33
22	C	509	CLA	C4D-ND	-3.06	1.33	1.37
25	1	609	CHL	O2D-CGD	3.06	1.40	1.33
25	5	609	CHL	O2D-CGD	3.06	1.40	1.33
25	S	306	CHL	O2D-CGD	3.06	1.40	1.33
25	s	306	CHL	O2D-CGD	3.06	1.40	1.33
25	1	605	CHL	O2D-CGD	3.05	1.40	1.33
25	5	605	CHL	O2D-CGD	3.05	1.40	1.33
22	R	309	CLA	C4D-ND	-3.05	1.33	1.37
22	r	309	CLA	C4D-ND	-3.05	1.33	1.37
22	c	504	CLA	MG-NA	3.05	2.13	2.06
22	S	309	CLA	C4D-ND	-3.05	1.33	1.37
22	s	309	CLA	C4D-ND	-3.05	1.33	1.37
22	Y	612	CLA	MG-NA	3.05	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	y	612	CLA	MG-NA	3.05	2.13	2.06
22	R	310	CLA	C4D-ND	-3.05	1.33	1.37
22	r	310	CLA	C4D-ND	-3.05	1.33	1.37
25	1	615	CHL	O2D-CGD	3.04	1.40	1.33
25	5	615	CHL	O2D-CGD	3.04	1.40	1.33
25	2	607	CHL	O2D-CGD	3.04	1.40	1.33
25	6	607	CHL	O2D-CGD	3.04	1.40	1.33
25	1	607	CHL	O2D-CGD	3.04	1.40	1.33
25	5	607	CHL	O2D-CGD	3.04	1.40	1.33
22	1	614	CLA	CHD-C4C	3.04	1.46	1.39
22	5	614	CLA	CHD-C4C	3.04	1.46	1.39
25	3	307	CHL	O2D-CGD	3.04	1.40	1.33
25	7	307	CHL	O2D-CGD	3.04	1.40	1.33
22	B	606	CLA	C4D-ND	-3.04	1.33	1.37
22	N	612	CLA	C4D-ND	-3.04	1.33	1.37
22	n	612	CLA	C4D-ND	-3.04	1.33	1.37
22	S	305	CLA	MG-NA	3.03	2.13	2.06
22	s	305	CLA	MG-NA	3.03	2.13	2.06
22	c	507	CLA	MG-NA	3.03	2.13	2.06
22	R	303	CLA	MG-NA	3.03	2.13	2.06
22	r	303	CLA	MG-NA	3.03	2.13	2.06
25	S	308	CHL	O2D-CGD	3.03	1.40	1.33
25	s	308	CHL	O2D-CGD	3.03	1.40	1.33
22	B	616	CLA	C1B-NB	-3.03	1.34	1.37
22	N	602	CLA	O2A-CGA	3.03	1.40	1.30
22	n	602	CLA	O2A-CGA	3.03	1.40	1.30
22	b	612	CLA	MG-NA	3.02	2.13	2.06
25	1	606	CHL	O2D-CGD	3.02	1.40	1.33
25	5	606	CHL	O2D-CGD	3.02	1.40	1.33
22	R	302	CLA	C4D-ND	-3.02	1.33	1.37
22	r	302	CLA	C4D-ND	-3.02	1.33	1.37
25	2	606	CHL	O2D-CGD	3.02	1.40	1.33
25	6	606	CHL	O2D-CGD	3.02	1.40	1.33
22	a	405	CLA	MG-NA	3.02	2.13	2.06
22	b	605	CLA	C4D-ND	-3.02	1.33	1.37
22	B	612	CLA	C1B-C2B	3.02	1.50	1.43
25	G	609	CHL	O2D-CGD	3.01	1.40	1.33
25	g	609	CHL	O2D-CGD	3.01	1.40	1.33
22	Y	610	CLA	MG-NA	3.01	2.13	2.06
22	y	610	CLA	MG-NA	3.01	2.13	2.06
22	R	307	CLA	C4D-ND	-3.01	1.33	1.37
22	r	307	CLA	C4D-ND	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	607	CLA	MG-NA	3.01	2.13	2.06
22	s	301	CLA	C4D-ND	-3.01	1.33	1.37
25	Y	607	CHL	O2D-CGD	3.01	1.40	1.33
25	y	607	CHL	O2D-CGD	3.01	1.40	1.33
22	d	403	CLA	MG-NA	3.01	2.13	2.06
25	N	607	CHL	O2D-CGD	3.01	1.40	1.33
25	n	607	CHL	O2D-CGD	3.01	1.40	1.33
22	R	307	CLA	MG-NA	3.00	2.13	2.06
22	r	307	CLA	MG-NA	3.00	2.13	2.06
25	G	606	CHL	O2D-CGD	3.00	1.40	1.33
25	g	606	CHL	O2D-CGD	3.00	1.40	1.33
22	Y	603	CLA	MG-NA	3.00	2.13	2.06
22	y	603	CLA	MG-NA	3.00	2.13	2.06
22	b	611	CLA	C1B-C2B	3.00	1.50	1.43
22	3	304	CLA	CHD-C4C	3.00	1.46	1.39
22	7	304	CLA	CHD-C4C	3.00	1.46	1.39
22	R	308	CLA	MG-NA	3.00	2.13	2.06
22	r	308	CLA	MG-NA	3.00	2.13	2.06
22	b	616	CLA	CHD-C4C	2.99	1.46	1.39
22	N	613	CLA	MG-NA	2.99	2.13	2.06
22	n	613	CLA	MG-NA	2.99	2.13	2.06
22	b	613	CLA	MG-NA	2.99	2.13	2.06
24	e	101	HEM	CAC-C3C	2.98	1.55	1.47
22	b	604	CLA	MG-NA	2.98	2.13	2.06
22	C	504	CLA	MG-NA	2.98	2.13	2.06
22	1	604	CLA	C4D-ND	-2.98	1.33	1.37
22	5	604	CLA	C4D-ND	-2.98	1.33	1.37
22	N	614	CLA	CHD-C4C	2.97	1.46	1.39
22	n	614	CLA	CHD-C4C	2.97	1.46	1.39
22	b	610	CLA	C4D-ND	-2.97	1.33	1.37
25	4	302	CHL	O2D-CGD	2.97	1.40	1.33
25	8	302	CHL	O2D-CGD	2.97	1.40	1.33
22	c	510	CLA	C4D-ND	-2.97	1.33	1.37
22	b	611	CLA	MG-NA	2.97	2.13	2.06
22	c	501	CLA	MG-NA	2.97	2.13	2.06
25	S	302	CHL	O2D-CGD	2.96	1.40	1.33
25	s	302	CHL	O2D-CGD	2.96	1.40	1.33
22	b	604	CLA	C4D-ND	-2.96	1.33	1.37
22	Y	614	CLA	MG-NA	2.96	2.13	2.06
22	y	614	CLA	MG-NA	2.96	2.13	2.06
22	S	311	CLA	MG-NA	2.96	2.13	2.06
22	s	311	CLA	MG-NA	2.96	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	603	CLA	CHD-C4C	2.96	1.46	1.39
22	6	603	CLA	CHD-C4C	2.96	1.46	1.39
22	B	610	CLA	C4D-ND	-2.96	1.33	1.37
22	3	305	CLA	CHD-C4C	2.96	1.46	1.39
22	7	305	CLA	CHD-C4C	2.96	1.46	1.39
22	N	602	CLA	MG-NA	2.95	2.13	2.06
22	n	602	CLA	MG-NA	2.95	2.13	2.06
22	B	604	CLA	CHC-C1C	2.95	1.44	1.38
22	N	610	CLA	C4D-ND	-2.95	1.33	1.37
22	n	610	CLA	C4D-ND	-2.95	1.33	1.37
25	N	609	CHL	O2D-CGD	2.95	1.40	1.33
25	n	609	CHL	O2D-CGD	2.95	1.40	1.33
22	B	613	CLA	C4D-ND	-2.95	1.33	1.37
22	G	610	CLA	C4D-ND	-2.95	1.33	1.37
22	g	610	CLA	C4D-ND	-2.95	1.33	1.37
24	F	101	HEM	CAB-C3B	2.94	1.55	1.47
22	B	611	CLA	MG-NA	2.94	2.13	2.06
22	b	615	CLA	C4D-ND	-2.94	1.33	1.37
22	4	301	CLA	C4D-ND	-2.94	1.33	1.37
22	8	301	CLA	C4D-ND	-2.94	1.33	1.37
25	R	306	CHL	O2D-CGD	2.94	1.40	1.33
25	r	306	CHL	O2D-CGD	2.94	1.40	1.33
22	C	511	CLA	CHD-C4C	2.93	1.45	1.39
22	3	314	CLA	CHD-C4C	2.93	1.45	1.39
22	7	314	CLA	CHD-C4C	2.93	1.45	1.39
22	4	305	CLA	C4D-ND	-2.93	1.33	1.37
22	8	305	CLA	C4D-ND	-2.93	1.33	1.37
22	S	314	CLA	MG-NA	2.93	2.13	2.06
22	s	314	CLA	MG-NA	2.93	2.13	2.06
25	R	304	CHL	O2D-CGD	2.93	1.40	1.33
25	r	304	CHL	O2D-CGD	2.93	1.40	1.33
25	G	607	CHL	O2D-CGD	2.92	1.40	1.33
25	g	607	CHL	O2D-CGD	2.92	1.40	1.33
25	N	601	CHL	O2D-CGD	2.92	1.40	1.33
25	n	601	CHL	O2D-CGD	2.92	1.40	1.33
24	F	101	HEM	FE-NB	2.92	2.03	1.94
22	S	304	CLA	C4D-ND	-2.91	1.33	1.37
22	s	304	CLA	C4D-ND	-2.91	1.33	1.37
25	Y	609	CHL	O2D-CGD	2.91	1.40	1.33
25	y	609	CHL	O2D-CGD	2.91	1.40	1.33
22	D	403	CLA	MG-NA	2.91	2.13	2.06
22	R	301	CLA	MG-NA	2.90	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	301	CLA	MG-NA	2.90	2.13	2.06
25	Y	606	CHL	CBA-CGA	2.90	1.57	1.50
25	y	606	CHL	CBA-CGA	2.90	1.57	1.50
24	F	101	HEM	CAC-C3C	2.90	1.55	1.47
25	2	608	CHL	O2D-CGD	2.90	1.40	1.33
25	6	608	CHL	O2D-CGD	2.90	1.40	1.33
22	2	604	CLA	CHD-C4C	2.90	1.45	1.39
22	6	604	CLA	CHD-C4C	2.90	1.45	1.39
22	B	611	CLA	C1B-C2B	2.90	1.50	1.43
22	b	603	CLA	CHD-C4C	2.90	1.45	1.39
25	S	307	CHL	O2D-CGD	2.90	1.40	1.33
25	s	307	CHL	O2D-CGD	2.90	1.40	1.33
22	c	501	CLA	C1B-C2B	2.90	1.50	1.43
22	Y	610	CLA	C4D-ND	-2.90	1.33	1.37
22	y	610	CLA	C4D-ND	-2.90	1.33	1.37
22	1	614	CLA	C1B-C2B	2.89	1.50	1.43
22	5	614	CLA	C1B-C2B	2.89	1.50	1.43
25	3	308	CHL	O2D-CED	-2.89	1.38	1.45
25	7	308	CHL	O2D-CED	-2.89	1.38	1.45
22	1	612	CLA	CHD-C4C	2.89	1.45	1.39
22	5	612	CLA	CHD-C4C	2.89	1.45	1.39
22	C	504	CLA	C1B-C2B	2.88	1.50	1.43
22	4	311	CLA	CHD-C4C	2.88	1.45	1.39
22	8	311	CLA	CHD-C4C	2.88	1.45	1.39
22	c	509	CLA	MG-NA	2.88	2.13	2.06
22	S	312	CLA	MG-NA	2.88	2.13	2.06
22	s	312	CLA	MG-NA	2.88	2.13	2.06
22	1	613	CLA	CHD-C4C	2.88	1.45	1.39
22	5	613	CLA	CHD-C4C	2.88	1.45	1.39
22	S	313	CLA	MG-NA	2.88	2.13	2.06
22	s	313	CLA	MG-NA	2.88	2.13	2.06
22	G	613	CLA	MG-NA	2.88	2.13	2.06
22	g	613	CLA	MG-NA	2.88	2.13	2.06
25	Y	608	CHL	O2D-CGD	2.88	1.40	1.33
25	y	608	CHL	O2D-CGD	2.88	1.40	1.33
22	B	616	CLA	C4D-CHA	2.88	1.48	1.38
25	3	308	CHL	O2D-CGD	2.88	1.40	1.33
25	7	308	CHL	O2D-CGD	2.88	1.40	1.33
23	a	404	PHO	C3B-C4B	2.88	1.44	1.41
22	B	604	CLA	CHD-C4C	2.87	1.45	1.39
22	1	603	CLA	CHD-C4C	2.87	1.45	1.39
22	5	603	CLA	CHD-C4C	2.87	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	614	CLA	C4D-ND	-2.87	1.33	1.37
22	5	614	CLA	C4D-ND	-2.87	1.33	1.37
22	N	603	CLA	MG-NA	2.87	2.13	2.06
22	n	603	CLA	MG-NA	2.87	2.13	2.06
22	4	304	CLA	C1B-C2B	2.87	1.50	1.43
22	8	304	CLA	C1B-C2B	2.87	1.50	1.43
22	3	303	CLA	C4D-ND	-2.87	1.33	1.37
22	7	303	CLA	C4D-ND	-2.87	1.33	1.37
22	2	613	CLA	C1B-C2B	2.87	1.50	1.43
22	6	613	CLA	C1B-C2B	2.87	1.50	1.43
22	N	604	CLA	MG-NA	2.86	2.13	2.06
22	n	604	CLA	MG-NA	2.86	2.13	2.06
22	3	311	CLA	C1B-C2B	2.86	1.50	1.43
22	7	311	CLA	C1B-C2B	2.86	1.50	1.43
22	C	502	CLA	MG-NA	2.86	2.13	2.06
25	Y	606	CHL	O2D-CGD	2.85	1.40	1.33
25	y	606	CHL	O2D-CGD	2.85	1.40	1.33
25	N	606	CHL	O2D-CGD	2.85	1.40	1.33
25	n	606	CHL	O2D-CGD	2.85	1.40	1.33
22	1	602	CLA	C4D-ND	-2.85	1.33	1.37
22	5	602	CLA	C4D-ND	-2.85	1.33	1.37
22	S	304	CLA	C1B-C2B	2.85	1.50	1.43
22	s	304	CLA	C1B-C2B	2.85	1.50	1.43
25	G	608	CHL	O2D-CGD	2.85	1.40	1.33
25	g	608	CHL	O2D-CGD	2.85	1.40	1.33
22	1	603	CLA	C1B-C2B	2.85	1.50	1.43
22	5	603	CLA	C1B-C2B	2.85	1.50	1.43
22	G	602	CLA	MG-NA	2.84	2.13	2.06
22	g	602	CLA	MG-NA	2.84	2.13	2.06
22	R	308	CLA	C1B-C2B	2.84	1.50	1.43
22	r	308	CLA	C1B-C2B	2.84	1.50	1.43
22	Y	613	CLA	MG-NA	2.84	2.13	2.06
22	y	613	CLA	MG-NA	2.84	2.13	2.06
25	G	601	CHL	O2D-CED	-2.84	1.38	1.45
25	g	601	CHL	O2D-CED	-2.84	1.38	1.45
22	2	612	CLA	C4D-ND	-2.84	1.33	1.37
22	6	612	CLA	C4D-ND	-2.84	1.33	1.37
22	N	614	CLA	C1B-C2B	2.84	1.49	1.43
22	n	614	CLA	C1B-C2B	2.84	1.49	1.43
22	1	603	CLA	C4D-ND	-2.84	1.33	1.37
22	5	603	CLA	C4D-ND	-2.84	1.33	1.37
22	S	303	CLA	O2D-CGD	2.84	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	303	CLA	O2D-CGD	2.84	1.40	1.33
22	2	610	CLA	C1B-C2B	2.83	1.49	1.43
22	6	610	CLA	C1B-C2B	2.83	1.49	1.43
22	1	611	CLA	C1B-C2B	2.83	1.49	1.43
22	5	611	CLA	C1B-C2B	2.83	1.49	1.43
22	4	311	CLA	C1B-C2B	2.83	1.49	1.43
22	8	311	CLA	C1B-C2B	2.83	1.49	1.43
22	G	603	CLA	CHD-C4C	2.83	1.45	1.39
22	g	603	CLA	CHD-C4C	2.83	1.45	1.39
22	2	610	CLA	C4D-ND	-2.83	1.33	1.37
22	6	610	CLA	C4D-ND	-2.83	1.33	1.37
22	B	603	CLA	MG-NA	2.83	2.13	2.06
22	D	403	CLA	C1B-C2B	2.83	1.49	1.43
23	D	402	PHO	O2D-CGD	2.83	1.40	1.33
22	2	604	CLA	C4D-ND	-2.82	1.33	1.37
22	6	604	CLA	C4D-ND	-2.82	1.33	1.37
25	Y	605	CHL	O2D-CED	-2.82	1.38	1.45
25	y	605	CHL	O2D-CED	-2.82	1.38	1.45
22	3	312	CLA	C4D-CHA	2.82	1.48	1.38
22	7	312	CLA	C4D-CHA	2.82	1.48	1.38
25	Y	605	CHL	O2D-CGD	2.82	1.40	1.33
25	y	605	CHL	O2D-CGD	2.82	1.40	1.33
22	3	313	CLA	CHD-C4C	2.82	1.45	1.39
22	7	313	CLA	CHD-C4C	2.82	1.45	1.39
22	B	616	CLA	CHD-C4C	2.82	1.45	1.39
22	4	305	CLA	CHD-C4C	2.81	1.45	1.39
22	8	305	CLA	CHD-C4C	2.81	1.45	1.39
22	4	303	CLA	C4D-ND	-2.81	1.33	1.37
22	8	303	CLA	C4D-ND	-2.81	1.33	1.37
22	3	313	CLA	C4D-CHA	2.81	1.48	1.38
22	7	313	CLA	C4D-CHA	2.81	1.48	1.38
25	N	608	CHL	O2D-CGD	2.81	1.40	1.33
25	n	608	CHL	O2D-CGD	2.81	1.40	1.33
22	3	305	CLA	C4D-ND	-2.81	1.33	1.37
22	7	305	CLA	C4D-ND	-2.81	1.33	1.37
22	B	616	CLA	MG-NA	2.81	2.12	2.06
22	R	311	CLA	MG-NA	2.81	2.12	2.06
22	r	311	CLA	MG-NA	2.81	2.12	2.06
22	B	604	CLA	CHC-C4B	2.81	1.45	1.39
22	c	511	CLA	CHD-C4C	2.81	1.45	1.39
22	4	310	CLA	C1B-C2B	2.80	1.49	1.43
22	8	310	CLA	C1B-C2B	2.80	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	304	CLA	C4D-CHA	2.80	1.48	1.38
22	7	304	CLA	C4D-CHA	2.80	1.48	1.38
22	3	313	CLA	C1B-C2B	2.80	1.49	1.43
22	7	313	CLA	C1B-C2B	2.80	1.49	1.43
22	c	512	CLA	MG-NA	2.80	2.12	2.06
22	2	602	CLA	C4D-ND	-2.80	1.33	1.37
22	6	602	CLA	C4D-ND	-2.80	1.33	1.37
22	C	512	CLA	C4D-ND	-2.80	1.33	1.37
22	b	612	CLA	C4D-ND	-2.80	1.33	1.37
22	1	604	CLA	CHD-C4C	2.80	1.45	1.39
22	5	604	CLA	CHD-C4C	2.80	1.45	1.39
22	4	311	CLA	C4D-CHA	2.80	1.48	1.38
22	8	311	CLA	C4D-CHA	2.80	1.48	1.38
22	2	609	CLA	C1B-C2B	2.80	1.49	1.43
22	6	609	CLA	C1B-C2B	2.80	1.49	1.43
23	d	402	PHO	O2D-CGD	2.80	1.40	1.33
22	1	612	CLA	C4D-CHA	2.80	1.48	1.38
22	5	612	CLA	C4D-CHA	2.80	1.48	1.38
22	b	615	CLA	CHD-C4C	2.80	1.45	1.39
22	S	304	CLA	CHD-C4C	2.80	1.45	1.39
22	s	304	CLA	CHD-C4C	2.80	1.45	1.39
22	N	611	CLA	C1B-C2B	2.79	1.49	1.43
22	n	611	CLA	C1B-C2B	2.79	1.49	1.43
25	G	601	CHL	O2D-CGD	2.79	1.40	1.33
25	g	601	CHL	O2D-CGD	2.79	1.40	1.33
22	S	312	CLA	C4D-ND	-2.79	1.33	1.37
22	s	312	CLA	C4D-ND	-2.79	1.33	1.37
22	2	603	CLA	C1B-C2B	2.79	1.49	1.43
22	6	603	CLA	C1B-C2B	2.79	1.49	1.43
22	4	304	CLA	C4D-CHA	2.79	1.48	1.38
22	8	304	CLA	C4D-CHA	2.79	1.48	1.38
22	3	311	CLA	CHD-C4C	2.79	1.45	1.39
22	7	311	CLA	CHD-C4C	2.79	1.45	1.39
22	4	304	CLA	CHD-C4C	2.79	1.45	1.39
22	8	304	CLA	CHD-C4C	2.79	1.45	1.39
25	Y	601	CHL	O2D-CED	-2.79	1.38	1.45
25	y	601	CHL	O2D-CED	-2.79	1.38	1.45
25	N	608	CHL	O2D-CED	-2.78	1.38	1.45
25	n	608	CHL	O2D-CED	-2.78	1.38	1.45
22	1	602	CLA	C1B-C2B	2.78	1.49	1.43
22	5	602	CLA	C1B-C2B	2.78	1.49	1.43
22	2	613	CLA	CHD-C4C	2.78	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	613	CLA	CHD-C4C	2.78	1.45	1.39
22	3	312	CLA	CHD-C4C	2.78	1.45	1.39
22	7	312	CLA	CHD-C4C	2.78	1.45	1.39
22	2	603	CLA	C4D-CHA	2.78	1.48	1.38
22	6	603	CLA	C4D-CHA	2.78	1.48	1.38
22	S	309	CLA	MG-NA	2.78	2.12	2.06
22	s	309	CLA	MG-NA	2.78	2.12	2.06
22	B	604	CLA	C3B-C4B	2.78	1.49	1.42
25	S	307	CHL	O2D-CED	-2.78	1.38	1.45
25	s	307	CHL	O2D-CED	-2.78	1.38	1.45
22	S	309	CLA	C1B-C2B	2.78	1.49	1.43
22	s	309	CLA	C1B-C2B	2.78	1.49	1.43
22	1	614	CLA	C4D-CHA	2.78	1.48	1.38
22	5	614	CLA	C4D-CHA	2.78	1.48	1.38
22	3	303	CLA	CHD-C4C	2.78	1.45	1.39
22	7	303	CLA	CHD-C4C	2.78	1.45	1.39
22	B	605	CLA	MG-NA	2.77	2.12	2.06
22	G	604	CLA	CHD-C4C	2.77	1.45	1.39
22	g	604	CLA	CHD-C4C	2.77	1.45	1.39
22	3	310	CLA	C1B-C2B	2.77	1.49	1.43
22	7	310	CLA	C1B-C2B	2.77	1.49	1.43
22	Y	602	CLA	MG-NA	2.77	2.12	2.06
22	y	602	CLA	MG-NA	2.77	2.12	2.06
25	N	605	CHL	O2D-CGD	2.77	1.40	1.33
25	n	605	CHL	O2D-CGD	2.77	1.40	1.33
22	Y	612	CLA	CHD-C4C	2.77	1.45	1.39
22	y	612	CLA	CHD-C4C	2.77	1.45	1.39
22	B	604	CLA	C1B-C2B	2.77	1.49	1.43
25	G	608	CHL	O2D-CED	-2.77	1.38	1.45
25	g	608	CHL	O2D-CED	-2.77	1.38	1.45
22	2	612	CLA	C4D-CHA	2.77	1.48	1.38
22	6	612	CLA	C4D-CHA	2.77	1.48	1.38
22	1	602	CLA	CHD-C4C	2.76	1.45	1.39
22	5	602	CLA	CHD-C4C	2.76	1.45	1.39
22	d	403	CLA	C1B-C2B	2.76	1.49	1.43
22	3	304	CLA	C1B-C2B	2.76	1.49	1.43
22	7	304	CLA	C1B-C2B	2.76	1.49	1.43
22	1	610	CLA	C1B-C2B	2.76	1.49	1.43
22	5	610	CLA	C1B-C2B	2.76	1.49	1.43
22	B	614	CLA	C4D-ND	-2.76	1.33	1.37
22	S	309	CLA	CHD-C4C	2.76	1.45	1.39
22	s	309	CLA	CHD-C4C	2.76	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	303	CLA	MG-NA	2.76	2.12	2.06
22	8	303	CLA	MG-NA	2.76	2.12	2.06
22	3	304	CLA	C4D-ND	-2.75	1.33	1.37
22	7	304	CLA	C4D-ND	-2.75	1.33	1.37
22	N	603	CLA	CHD-C4C	2.75	1.45	1.39
22	n	603	CLA	CHD-C4C	2.75	1.45	1.39
22	2	611	CLA	C4D-CHA	2.75	1.48	1.38
22	6	611	CLA	C4D-CHA	2.75	1.48	1.38
22	C	512	CLA	CHD-C4C	2.75	1.45	1.39
22	1	611	CLA	CHD-C4C	2.75	1.45	1.39
22	5	611	CLA	CHD-C4C	2.75	1.45	1.39
22	B	609	CLA	CHD-C4C	2.75	1.45	1.39
22	1	611	CLA	C4D-ND	-2.75	1.33	1.37
22	5	611	CLA	C4D-ND	-2.75	1.33	1.37
25	Y	608	CHL	O2D-CED	-2.75	1.38	1.45
25	y	608	CHL	O2D-CED	-2.75	1.38	1.45
22	1	611	CLA	C4D-CHA	2.75	1.48	1.38
22	5	611	CLA	C4D-CHA	2.75	1.48	1.38
22	S	301	CLA	C1B-C2B	2.75	1.49	1.43
22	3	310	CLA	C4D-CHA	2.74	1.48	1.38
22	7	310	CLA	C4D-CHA	2.74	1.48	1.38
25	S	302	CHL	O2D-CED	-2.74	1.38	1.45
25	s	302	CHL	O2D-CED	-2.74	1.38	1.45
22	B	610	CLA	CHD-C4C	2.74	1.45	1.39
22	4	301	CLA	CHD-C4C	2.74	1.45	1.39
22	8	301	CLA	CHD-C4C	2.74	1.45	1.39
22	b	609	CLA	CHD-C4C	2.74	1.45	1.39
25	Y	601	CHL	O2D-CGD	2.74	1.39	1.33
25	y	601	CHL	O2D-CGD	2.74	1.39	1.33
22	2	602	CLA	CHD-C4C	2.74	1.45	1.39
22	6	602	CLA	CHD-C4C	2.74	1.45	1.39
22	R	310	CLA	CHD-C4C	2.74	1.45	1.39
22	r	310	CLA	CHD-C4C	2.74	1.45	1.39
22	C	509	CLA	CHD-C4C	2.73	1.45	1.39
22	R	302	CLA	C4D-CHA	2.73	1.48	1.38
22	r	302	CLA	C4D-CHA	2.73	1.48	1.38
22	2	611	CLA	C1B-C2B	2.73	1.49	1.43
22	6	611	CLA	C1B-C2B	2.73	1.49	1.43
22	2	611	CLA	CHD-C4C	2.73	1.45	1.39
22	6	611	CLA	CHD-C4C	2.73	1.45	1.39
25	1	615	CHL	O2D-CED	-2.73	1.38	1.45
25	5	615	CHL	O2D-CED	-2.73	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	303	CLA	C1B-C2B	2.73	1.49	1.43
22	7	303	CLA	C1B-C2B	2.73	1.49	1.43
22	c	502	CLA	MG-NA	2.73	2.12	2.06
25	N	607	CHL	O2D-CED	-2.73	1.38	1.45
25	n	607	CHL	O2D-CED	-2.73	1.38	1.45
25	G	607	CHL	O2D-CED	-2.73	1.38	1.45
25	g	607	CHL	O2D-CED	-2.73	1.38	1.45
22	3	311	CLA	C4D-CHA	2.73	1.48	1.38
22	7	311	CLA	C4D-CHA	2.73	1.48	1.38
22	C	501	CLA	CHD-C4C	2.73	1.45	1.39
22	3	312	CLA	C1B-C2B	2.73	1.49	1.43
22	7	312	CLA	C1B-C2B	2.73	1.49	1.43
25	N	601	CHL	O2D-CED	-2.73	1.38	1.45
25	n	601	CHL	O2D-CED	-2.73	1.38	1.45
22	R	309	CLA	CHD-C4C	2.73	1.45	1.39
22	r	309	CLA	CHD-C4C	2.73	1.45	1.39
25	Y	609	CHL	CBA-CGA	2.72	1.56	1.50
25	y	609	CHL	CBA-CGA	2.72	1.56	1.50
22	a	402	CLA	CHD-C4C	2.72	1.45	1.39
22	2	610	CLA	CHD-C4C	2.72	1.45	1.39
22	6	610	CLA	CHD-C4C	2.72	1.45	1.39
22	R	307	CLA	C1B-C2B	2.72	1.49	1.43
22	r	307	CLA	C1B-C2B	2.72	1.49	1.43
25	Y	606	CHL	O2D-CED	-2.72	1.38	1.45
25	y	606	CHL	O2D-CED	-2.72	1.38	1.45
22	1	613	CLA	C4D-ND	-2.72	1.34	1.37
22	5	613	CLA	C4D-ND	-2.72	1.34	1.37
22	2	612	CLA	C1B-C2B	2.72	1.49	1.43
22	6	612	CLA	C1B-C2B	2.72	1.49	1.43
22	1	612	CLA	C4D-ND	-2.72	1.34	1.37
22	5	612	CLA	C4D-ND	-2.72	1.34	1.37
22	c	504	CLA	CHD-C4C	2.72	1.45	1.39
22	4	301	CLA	C4D-CHA	2.71	1.48	1.38
22	8	301	CLA	C4D-CHA	2.71	1.48	1.38
22	3	311	CLA	C4D-ND	-2.71	1.34	1.37
22	7	311	CLA	C4D-ND	-2.71	1.34	1.37
22	3	314	CLA	C4D-CHA	2.71	1.48	1.38
22	7	314	CLA	C4D-CHA	2.71	1.48	1.38
22	S	310	CLA	MG-NA	2.71	2.12	2.06
22	s	310	CLA	MG-NA	2.71	2.12	2.06
22	N	614	CLA	C4D-ND	-2.71	1.34	1.37
22	n	614	CLA	C4D-ND	-2.71	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	614	CLA	C4D-CHA	2.71	1.48	1.38
22	n	614	CLA	C4D-CHA	2.71	1.48	1.38
25	2	608	CHL	O2D-CED	-2.71	1.38	1.45
25	6	608	CHL	O2D-CED	-2.71	1.38	1.45
22	C	506	CLA	MG-NA	2.71	2.12	2.06
22	B	616	CLA	C4D-ND	-2.71	1.34	1.37
22	G	610	CLA	C1B-C2B	2.71	1.49	1.43
22	g	610	CLA	C1B-C2B	2.71	1.49	1.43
25	R	304	CHL	O2D-CED	-2.71	1.38	1.45
25	r	304	CHL	O2D-CED	-2.71	1.38	1.45
25	G	609	CHL	CBA-CGA	2.70	1.56	1.50
25	g	609	CHL	CBA-CGA	2.70	1.56	1.50
22	1	603	CLA	C4D-CHA	2.70	1.48	1.38
22	5	603	CLA	C4D-CHA	2.70	1.48	1.38
22	4	303	CLA	C4D-CHA	2.70	1.48	1.38
22	8	303	CLA	C4D-CHA	2.70	1.48	1.38
22	1	613	CLA	C4D-CHA	2.70	1.48	1.38
22	5	613	CLA	C4D-CHA	2.70	1.48	1.38
22	B	608	CLA	C1B-C2B	2.70	1.49	1.43
22	N	603	CLA	C1B-C2B	2.70	1.49	1.43
22	n	603	CLA	C1B-C2B	2.70	1.49	1.43
22	b	607	CLA	C1B-C2B	2.70	1.49	1.43
22	c	512	CLA	C1B-C2B	2.69	1.49	1.43
22	R	310	CLA	C1B-C2B	2.69	1.49	1.43
22	r	310	CLA	C1B-C2B	2.69	1.49	1.43
22	G	614	CLA	CHD-C4C	2.69	1.45	1.39
22	g	614	CLA	CHD-C4C	2.69	1.45	1.39
22	b	608	CLA	CHD-C4C	2.69	1.45	1.39
22	3	313	CLA	C4D-ND	-2.69	1.34	1.37
22	7	313	CLA	C4D-ND	-2.69	1.34	1.37
22	2	610	CLA	C4D-CHA	2.69	1.48	1.38
22	6	610	CLA	C4D-CHA	2.69	1.48	1.38
22	B	608	CLA	MG-NA	2.69	2.12	2.06
22	s	301	CLA	CHD-C4C	2.69	1.45	1.39
22	G	611	CLA	C1B-C2B	2.69	1.49	1.43
22	g	611	CLA	C1B-C2B	2.69	1.49	1.43
23	A	404	PHO	C3B-C4B	2.69	1.44	1.41
22	2	609	CLA	C4D-CHA	2.69	1.48	1.38
22	6	609	CLA	C4D-CHA	2.69	1.48	1.38
22	b	610	CLA	CHD-C4C	2.69	1.45	1.39
22	1	610	CLA	C4D-CHA	2.69	1.48	1.38
22	5	610	CLA	C4D-CHA	2.69	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	305	CHL	CBA-CGA	2.69	1.56	1.50
25	r	305	CHL	CBA-CGA	2.69	1.56	1.50
25	1	605	CHL	O2D-CED	-2.69	1.39	1.45
25	5	605	CHL	O2D-CED	-2.69	1.39	1.45
25	S	308	CHL	O2D-CED	-2.69	1.39	1.45
25	s	308	CHL	O2D-CED	-2.69	1.39	1.45
25	1	607	CHL	O2D-CED	-2.69	1.39	1.45
25	5	607	CHL	O2D-CED	-2.69	1.39	1.45
25	4	302	CHL	CBA-CGA	2.69	1.56	1.50
25	8	302	CHL	CBA-CGA	2.69	1.56	1.50
22	B	614	CLA	C1B-C2B	2.68	1.49	1.43
22	A	402	CLA	MG-NA	2.68	2.12	2.06
22	3	314	CLA	C1B-C2B	2.68	1.49	1.43
22	7	314	CLA	C1B-C2B	2.68	1.49	1.43
22	b	612	CLA	CHD-C4C	2.68	1.45	1.39
22	C	508	CLA	C4D-CHA	2.68	1.47	1.38
22	S	312	CLA	C4D-CHA	2.68	1.47	1.38
22	s	312	CLA	C4D-CHA	2.68	1.47	1.38
25	Y	607	CHL	O2D-CED	-2.68	1.39	1.45
25	y	607	CHL	O2D-CED	-2.68	1.39	1.45
22	N	612	CLA	C1B-C2B	2.68	1.49	1.43
22	n	612	CLA	C1B-C2B	2.68	1.49	1.43
22	d	404	CLA	CHD-C4C	2.68	1.45	1.39
22	S	301	CLA	C4D-CHA	2.68	1.47	1.38
22	2	602	CLA	C1B-C2B	2.68	1.49	1.43
22	6	602	CLA	C1B-C2B	2.68	1.49	1.43
25	4	309	CHL	O2D-CED	-2.68	1.39	1.45
25	8	309	CHL	O2D-CED	-2.68	1.39	1.45
25	1	606	CHL	CBA-CGA	2.68	1.56	1.50
25	5	606	CHL	CBA-CGA	2.68	1.56	1.50
25	N	606	CHL	O2D-CED	-2.68	1.39	1.45
25	n	606	CHL	O2D-CED	-2.68	1.39	1.45
22	b	605	CLA	O2D-CGD	2.68	1.39	1.33
22	C	504	CLA	CHD-C4C	2.67	1.45	1.39
25	4	306	CHL	O2D-CED	-2.67	1.39	1.45
25	8	306	CHL	O2D-CED	-2.67	1.39	1.45
22	G	603	CLA	C1B-C2B	2.67	1.49	1.43
22	g	603	CLA	C1B-C2B	2.67	1.49	1.43
22	d	404	CLA	C1B-C2B	2.67	1.49	1.43
22	b	604	CLA	CHD-C4C	2.67	1.45	1.39
22	2	603	CLA	C4D-ND	-2.67	1.34	1.37
22	6	603	CLA	C4D-ND	-2.67	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	613	CLA	C1B-C2B	2.67	1.49	1.43
22	N	611	CLA	CHD-C4C	2.67	1.45	1.39
22	n	611	CLA	CHD-C4C	2.67	1.45	1.39
25	2	607	CHL	O2D-CED	-2.67	1.39	1.45
25	3	307	CHL	O2D-CED	-2.67	1.39	1.45
25	6	607	CHL	O2D-CED	-2.67	1.39	1.45
25	7	307	CHL	O2D-CED	-2.67	1.39	1.45
22	4	305	CLA	C4D-CHA	2.67	1.47	1.38
22	8	305	CLA	C4D-CHA	2.67	1.47	1.38
25	3	301	CHL	O2D-CED	-2.67	1.39	1.45
25	7	301	CHL	O2D-CED	-2.67	1.39	1.45
22	G	612	CLA	CHD-C4C	2.67	1.45	1.39
22	g	612	CLA	CHD-C4C	2.67	1.45	1.39
25	2	601	CHL	O2D-CED	-2.67	1.39	1.45
25	6	601	CHL	O2D-CED	-2.67	1.39	1.45
22	S	305	CLA	CHD-C4C	2.66	1.45	1.39
22	s	305	CLA	CHD-C4C	2.66	1.45	1.39
22	2	612	CLA	CHD-C4C	2.66	1.45	1.39
22	6	612	CLA	CHD-C4C	2.66	1.45	1.39
22	G	612	CLA	C4D-CHA	2.66	1.47	1.38
22	g	612	CLA	C4D-CHA	2.66	1.47	1.38
25	3	302	CHL	O2D-CED	-2.66	1.39	1.45
25	7	302	CHL	O2D-CED	-2.66	1.39	1.45
22	Y	603	CLA	C1B-C2B	2.66	1.49	1.43
22	y	603	CLA	C1B-C2B	2.66	1.49	1.43
25	1	601	CHL	O2D-CED	-2.66	1.39	1.45
25	5	601	CHL	O2D-CED	-2.66	1.39	1.45
22	c	502	CLA	CHD-C4C	2.66	1.45	1.39
23	D	402	PHO	C3B-C4B	2.66	1.44	1.41
22	B	613	CLA	C4D-CHA	2.66	1.47	1.38
22	Y	612	CLA	C4D-CHA	2.66	1.47	1.38
22	y	612	CLA	C4D-CHA	2.66	1.47	1.38
22	4	304	CLA	C4D-ND	-2.66	1.34	1.37
22	8	304	CLA	C4D-ND	-2.66	1.34	1.37
22	D	404	CLA	CHD-C4C	2.66	1.45	1.39
22	R	303	CLA	CHD-C4C	2.66	1.45	1.39
22	r	303	CLA	CHD-C4C	2.66	1.45	1.39
25	S	306	CHL	O2D-CED	-2.66	1.39	1.45
25	s	306	CHL	O2D-CED	-2.66	1.39	1.45
25	N	609	CHL	CBA-CGA	2.66	1.56	1.50
25	n	609	CHL	CBA-CGA	2.66	1.56	1.50
22	c	501	CLA	CHD-C4C	2.65	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	310	CLA	CHD-C4C	2.65	1.45	1.39
22	s	310	CLA	CHD-C4C	2.65	1.45	1.39
22	A	403	CLA	CHD-C4C	2.65	1.45	1.39
22	G	603	CLA	C4D-CHA	2.65	1.47	1.38
22	g	603	CLA	C4D-CHA	2.65	1.47	1.38
22	2	604	CLA	C4D-CHA	2.65	1.47	1.38
22	6	604	CLA	C4D-CHA	2.65	1.47	1.38
22	B	615	CLA	C1B-C2B	2.65	1.49	1.43
25	R	306	CHL	O2D-CED	-2.65	1.39	1.45
25	N	605	CHL	O2D-CED	-2.65	1.39	1.45
25	r	306	CHL	O2D-CED	-2.65	1.39	1.45
25	n	605	CHL	O2D-CED	-2.65	1.39	1.45
22	4	301	CLA	C1B-C2B	2.65	1.49	1.43
22	8	301	CLA	C1B-C2B	2.65	1.49	1.43
25	2	606	CHL	O2D-CED	-2.65	1.39	1.45
25	6	606	CHL	O2D-CED	-2.65	1.39	1.45
22	1	602	CLA	C4D-CHA	2.65	1.47	1.38
22	5	602	CLA	C4D-CHA	2.65	1.47	1.38
22	B	613	CLA	CHD-C4C	2.65	1.45	1.39
22	c	502	CLA	C4D-CHA	2.64	1.47	1.38
22	D	404	CLA	C1B-C2B	2.64	1.49	1.43
22	3	312	CLA	C4D-ND	-2.64	1.34	1.37
22	7	312	CLA	C4D-ND	-2.64	1.34	1.37
22	c	510	CLA	C4D-CHA	2.64	1.47	1.38
22	b	614	CLA	CHD-C4C	2.64	1.45	1.39
22	1	613	CLA	C1B-C2B	2.64	1.49	1.43
22	5	613	CLA	C1B-C2B	2.64	1.49	1.43
22	B	607	CLA	C1B-C2B	2.64	1.49	1.43
22	S	303	CLA	MG-NA	2.64	2.12	2.06
22	s	303	CLA	MG-NA	2.64	2.12	2.06
22	b	616	CLA	C4D-CHA	2.64	1.47	1.38
22	C	509	CLA	C1B-C2B	2.64	1.49	1.43
22	b	605	CLA	CHD-C4C	2.64	1.45	1.39
22	G	611	CLA	CHD-C4C	2.64	1.45	1.39
22	g	611	CLA	CHD-C4C	2.64	1.45	1.39
22	S	303	CLA	C1B-C2B	2.64	1.49	1.43
22	s	303	CLA	C1B-C2B	2.64	1.49	1.43
22	N	612	CLA	CHD-C4C	2.64	1.45	1.39
22	n	612	CLA	CHD-C4C	2.64	1.45	1.39
22	1	612	CLA	C1B-C2B	2.63	1.49	1.43
22	5	612	CLA	C1B-C2B	2.63	1.49	1.43
25	N	606	CHL	CBA-CGA	2.63	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	606	CHL	CBA-CGA	2.63	1.56	1.50
22	b	613	CLA	C4D-CHA	2.63	1.47	1.38
22	Y	614	CLA	C1B-C2B	2.63	1.49	1.43
22	y	614	CLA	C1B-C2B	2.63	1.49	1.43
22	B	612	CLA	MG-NA	2.63	2.12	2.06
25	4	302	CHL	O2D-CED	-2.63	1.39	1.45
25	8	302	CHL	O2D-CED	-2.63	1.39	1.45
25	G	606	CHL	O2D-CED	-2.63	1.39	1.45
25	g	606	CHL	O2D-CED	-2.63	1.39	1.45
22	2	613	CLA	C4D-CHA	2.63	1.47	1.38
22	6	613	CLA	C4D-CHA	2.63	1.47	1.38
22	B	602	CLA	C4D-CHA	2.63	1.47	1.38
25	1	608	CHL	O2D-CED	-2.63	1.39	1.45
25	5	608	CHL	O2D-CED	-2.63	1.39	1.45
22	3	305	CLA	C4D-CHA	2.63	1.47	1.38
22	7	305	CLA	C4D-CHA	2.63	1.47	1.38
22	2	613	CLA	C4D-ND	-2.63	1.34	1.37
22	6	613	CLA	C4D-ND	-2.63	1.34	1.37
22	b	610	CLA	C4D-CHA	2.63	1.47	1.38
22	Y	610	CLA	C1B-C2B	2.62	1.49	1.43
22	y	610	CLA	C1B-C2B	2.62	1.49	1.43
22	S	312	CLA	CHD-C4C	2.62	1.45	1.39
22	s	312	CLA	CHD-C4C	2.62	1.45	1.39
22	b	604	CLA	C4D-CHA	2.62	1.47	1.38
22	C	503	CLA	CHD-C4C	2.62	1.45	1.39
22	C	507	CLA	C4D-CHA	2.62	1.47	1.38
22	R	301	CLA	C1B-C2B	2.62	1.49	1.43
22	r	301	CLA	C1B-C2B	2.62	1.49	1.43
22	B	603	CLA	CHD-C4C	2.62	1.45	1.39
22	a	403	CLA	O2D-CGD	2.62	1.39	1.33
22	c	508	CLA	C4D-CHA	2.62	1.47	1.38
22	G	611	CLA	C4D-CHA	2.62	1.47	1.38
22	g	611	CLA	C4D-CHA	2.62	1.47	1.38
22	N	611	CLA	C4D-CHA	2.62	1.47	1.38
22	n	611	CLA	C4D-CHA	2.62	1.47	1.38
22	C	501	CLA	C4D-CHA	2.61	1.47	1.38
22	3	303	CLA	C4D-CHA	2.61	1.47	1.38
22	7	303	CLA	C4D-CHA	2.61	1.47	1.38
25	1	606	CHL	O2D-CED	-2.61	1.39	1.45
25	5	606	CHL	O2D-CED	-2.61	1.39	1.45
22	G	614	CLA	C1B-C2B	2.61	1.49	1.43
22	g	614	CLA	C1B-C2B	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	606	CHL	CBA-CGA	2.61	1.56	1.50
25	6	606	CHL	CBA-CGA	2.61	1.56	1.50
22	N	612	CLA	C4D-CHA	2.61	1.47	1.38
22	n	612	CLA	C4D-CHA	2.61	1.47	1.38
22	b	607	CLA	CHD-C4C	2.61	1.45	1.39
22	N	602	CLA	CHD-C4C	2.61	1.45	1.39
22	n	602	CLA	CHD-C4C	2.61	1.45	1.39
22	3	310	CLA	CHD-C4C	2.61	1.45	1.39
22	7	310	CLA	CHD-C4C	2.61	1.45	1.39
22	N	613	CLA	CHD-C4C	2.61	1.45	1.39
22	n	613	CLA	CHD-C4C	2.61	1.45	1.39
25	4	307	CHL	O2D-CED	-2.61	1.39	1.45
25	8	307	CHL	O2D-CED	-2.61	1.39	1.45
22	R	311	CLA	C1B-C2B	2.61	1.49	1.43
22	r	311	CLA	C1B-C2B	2.61	1.49	1.43
22	C	506	CLA	C4D-CHA	2.61	1.47	1.38
22	N	604	CLA	CHD-C4C	2.61	1.45	1.39
22	n	604	CLA	CHD-C4C	2.61	1.45	1.39
22	R	302	CLA	C1B-C2B	2.61	1.49	1.43
22	r	302	CLA	C1B-C2B	2.61	1.49	1.43
22	c	512	CLA	C4D-CHA	2.61	1.47	1.38
25	G	605	CHL	O2D-CED	-2.60	1.39	1.45
25	g	605	CHL	O2D-CED	-2.60	1.39	1.45
22	Y	602	CLA	O2D-CGD	2.60	1.39	1.33
22	y	602	CLA	O2D-CGD	2.60	1.39	1.33
22	c	501	CLA	C4D-CHA	2.60	1.47	1.38
22	R	310	CLA	C4D-CHA	2.60	1.47	1.38
22	r	310	CLA	C4D-CHA	2.60	1.47	1.38
22	R	309	CLA	C1B-C2B	2.60	1.49	1.43
22	r	309	CLA	C1B-C2B	2.60	1.49	1.43
22	N	613	CLA	C1B-C2B	2.60	1.49	1.43
22	n	613	CLA	C1B-C2B	2.60	1.49	1.43
22	B	614	CLA	C4D-CHA	2.60	1.47	1.38
22	2	611	CLA	C4D-ND	-2.60	1.34	1.37
22	6	611	CLA	C4D-ND	-2.60	1.34	1.37
22	B	601	CLA	CHD-C4C	2.60	1.45	1.39
22	2	602	CLA	C4D-CHA	2.60	1.47	1.38
22	6	602	CLA	C4D-CHA	2.60	1.47	1.38
22	C	501	CLA	C1B-C2B	2.60	1.49	1.43
22	B	613	CLA	C1B-C2B	2.60	1.49	1.43
22	B	607	CLA	CHD-C4C	2.59	1.45	1.39
22	R	307	CLA	C4D-CHA	2.59	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	307	CLA	C4D-CHA	2.59	1.47	1.38
22	C	510	CLA	C4D-CHA	2.59	1.47	1.38
23	a	404	PHO	O2D-CGD	2.59	1.39	1.33
22	C	505	CLA	CHD-C4C	2.59	1.45	1.39
22	b	601	CLA	C4D-CHA	2.59	1.47	1.38
25	4	308	CHL	O2D-CED	-2.59	1.39	1.45
25	8	308	CHL	O2D-CED	-2.59	1.39	1.45
22	1	604	CLA	C4D-CHA	2.59	1.47	1.38
22	5	604	CLA	C4D-CHA	2.59	1.47	1.38
22	c	506	CLA	C4D-CHA	2.59	1.47	1.38
22	Y	604	CLA	C1B-C2B	2.59	1.49	1.43
22	y	604	CLA	C1B-C2B	2.59	1.49	1.43
22	B	605	CLA	C1B-C2B	2.59	1.49	1.43
22	b	614	CLA	C1B-C2B	2.59	1.49	1.43
22	c	502	CLA	C1B-C2B	2.59	1.49	1.43
22	C	512	CLA	C4D-CHA	2.58	1.47	1.38
22	b	603	CLA	O2D-CGD	2.58	1.39	1.33
22	N	613	CLA	C4D-CHA	2.58	1.47	1.38
22	n	613	CLA	C4D-CHA	2.58	1.47	1.38
22	C	512	CLA	C1B-C2B	2.58	1.49	1.43
25	3	309	CHL	O2D-CED	-2.58	1.39	1.45
25	7	309	CHL	O2D-CED	-2.58	1.39	1.45
22	R	311	CLA	O2D-CGD	2.58	1.39	1.33
22	r	311	CLA	O2D-CGD	2.58	1.39	1.33
22	1	610	CLA	CHD-C4C	2.58	1.45	1.39
22	5	610	CLA	CHD-C4C	2.58	1.45	1.39
22	4	310	CLA	CHD-C4C	2.58	1.45	1.39
22	8	310	CLA	CHD-C4C	2.58	1.45	1.39
22	A	403	CLA	O2D-CGD	2.58	1.39	1.33
22	B	607	CLA	C4D-CHA	2.58	1.47	1.38
25	R	305	CHL	O2D-CED	-2.58	1.39	1.45
25	r	305	CHL	O2D-CED	-2.58	1.39	1.45
22	b	601	CLA	C1B-C2B	2.58	1.49	1.43
22	b	606	CLA	CHD-C1D	2.57	1.43	1.38
22	3	305	CLA	C1B-C2B	2.57	1.49	1.43
22	7	305	CLA	C1B-C2B	2.57	1.49	1.43
22	G	610	CLA	C4D-CHA	2.57	1.47	1.38
22	g	610	CLA	C4D-CHA	2.57	1.47	1.38
22	B	606	CLA	CHD-C4C	2.57	1.45	1.39
25	3	309	CHL	CBA-CGA	2.57	1.56	1.50
25	7	309	CHL	CBA-CGA	2.57	1.56	1.50
22	D	401	CLA	CHD-C4C	2.57	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	609	CHL	O2D-CED	-2.57	1.39	1.45
25	5	609	CHL	O2D-CED	-2.57	1.39	1.45
22	Y	610	CLA	C4D-CHA	2.57	1.47	1.38
22	y	610	CLA	C4D-CHA	2.57	1.47	1.38
22	1	614	CLA	C4C-C3C	2.57	1.49	1.45
22	5	614	CLA	C4C-C3C	2.57	1.49	1.45
22	B	610	CLA	C1B-C2B	2.57	1.49	1.43
22	B	602	CLA	C1B-C2B	2.57	1.49	1.43
23	A	404	PHO	C3D-C2D	2.57	1.44	1.39
22	c	505	CLA	MG-NA	2.57	2.12	2.06
22	R	303	CLA	C1B-C2B	2.57	1.49	1.43
22	r	303	CLA	C1B-C2B	2.57	1.49	1.43
25	3	301	CHL	CBA-CGA	2.57	1.56	1.50
25	7	301	CHL	CBA-CGA	2.57	1.56	1.50
25	4	306	CHL	CBA-CGA	2.57	1.56	1.50
25	8	306	CHL	CBA-CGA	2.57	1.56	1.50
22	Y	603	CLA	C4D-CHA	2.56	1.47	1.38
22	y	603	CLA	C4D-CHA	2.56	1.47	1.38
22	G	614	CLA	C4D-CHA	2.56	1.47	1.38
22	g	614	CLA	C4D-CHA	2.56	1.47	1.38
22	a	405	CLA	C1B-C2B	2.56	1.49	1.43
22	B	615	CLA	C4D-CHA	2.56	1.47	1.38
22	C	508	CLA	CHD-C4C	2.56	1.45	1.39
22	c	507	CLA	C4D-CHA	2.56	1.47	1.38
23	A	404	PHO	O2D-CGD	2.56	1.39	1.33
25	3	306	CHL	O2D-CED	-2.56	1.39	1.45
25	7	306	CHL	O2D-CED	-2.56	1.39	1.45
22	Y	603	CLA	CHD-C4C	2.56	1.45	1.39
22	y	603	CLA	CHD-C4C	2.56	1.45	1.39
22	2	609	CLA	CHD-C4C	2.56	1.45	1.39
22	6	609	CLA	CHD-C4C	2.56	1.45	1.39
25	1	609	CHL	CBA-CGA	2.56	1.56	1.50
25	5	609	CHL	CBA-CGA	2.56	1.56	1.50
22	c	504	CLA	C1B-C2B	2.56	1.49	1.43
22	c	503	CLA	C4D-CHA	2.56	1.47	1.38
23	d	402	PHO	C3B-C4B	2.55	1.44	1.41
22	S	310	CLA	C1B-C2B	2.55	1.49	1.43
22	s	310	CLA	C1B-C2B	2.55	1.49	1.43
22	1	614	CLA	O2D-CGD	2.55	1.39	1.33
22	5	614	CLA	O2D-CGD	2.55	1.39	1.33
22	N	603	CLA	C4D-CHA	2.55	1.47	1.38
22	n	603	CLA	C4D-CHA	2.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Y	612	CLA	C1B-C2B	2.55	1.49	1.43
22	y	612	CLA	C1B-C2B	2.55	1.49	1.43
22	b	613	CLA	CHD-C4C	2.55	1.45	1.39
22	3	314	CLA	C4D-ND	-2.55	1.34	1.37
22	7	314	CLA	C4D-ND	-2.55	1.34	1.37
22	Y	611	CLA	C1B-C2B	2.55	1.49	1.43
22	y	611	CLA	C1B-C2B	2.55	1.49	1.43
25	1	607	CHL	CBA-CGA	2.55	1.56	1.50
25	5	607	CHL	CBA-CGA	2.55	1.56	1.50
22	R	301	CLA	CHD-C4C	2.55	1.45	1.39
22	r	301	CLA	CHD-C4C	2.55	1.45	1.39
22	b	603	CLA	C1B-C2B	2.55	1.49	1.43
22	S	314	CLA	CHD-C4C	2.55	1.45	1.39
22	s	314	CLA	CHD-C4C	2.55	1.45	1.39
22	B	604	CLA	C4D-CHA	2.55	1.47	1.38
22	B	601	CLA	C1B-C2B	2.55	1.49	1.43
22	G	613	CLA	C1B-C2B	2.54	1.49	1.43
22	g	613	CLA	C1B-C2B	2.54	1.49	1.43
25	2	605	CHL	O2D-CED	-2.54	1.39	1.45
25	6	605	CHL	O2D-CED	-2.54	1.39	1.45
25	Y	609	CHL	O2D-CED	-2.54	1.39	1.45
25	y	609	CHL	O2D-CED	-2.54	1.39	1.45
22	R	309	CLA	C4D-CHA	2.54	1.47	1.38
22	r	309	CLA	C4D-CHA	2.54	1.47	1.38
22	C	502	CLA	CHD-C4C	2.54	1.45	1.39
25	Y	607	CHL	CBA-CGA	2.54	1.56	1.50
25	y	607	CHL	CBA-CGA	2.54	1.56	1.50
22	B	603	CLA	C4D-CHA	2.54	1.47	1.38
22	A	402	CLA	C1B-C2B	2.54	1.49	1.43
25	R	304	CHL	CBA-CGA	2.54	1.56	1.50
25	r	304	CHL	CBA-CGA	2.54	1.56	1.50
22	b	604	CLA	C1B-C2B	2.54	1.49	1.43
22	B	610	CLA	C4D-CHA	2.54	1.47	1.38
22	C	508	CLA	C4C-C3C	2.54	1.49	1.45
22	b	610	CLA	C4C-C3C	2.54	1.49	1.45
22	4	310	CLA	C4D-CHA	2.54	1.47	1.38
22	8	310	CLA	C4D-CHA	2.54	1.47	1.38
22	B	606	CLA	C4D-CHA	2.53	1.47	1.38
22	B	613	CLA	O2D-CGD	2.53	1.39	1.33
22	d	403	CLA	CHD-C4C	2.53	1.45	1.39
22	G	613	CLA	CHD-C4C	2.53	1.45	1.39
22	g	613	CLA	CHD-C4C	2.53	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	613	CLA	C4D-CHA	2.53	1.47	1.38
22	g	613	CLA	C4D-CHA	2.53	1.47	1.38
25	S	307	CHL	CBA-CGA	2.53	1.56	1.50
25	s	307	CHL	CBA-CGA	2.53	1.56	1.50
22	S	304	CLA	C4D-CHA	2.53	1.47	1.38
22	s	304	CLA	C4D-CHA	2.53	1.47	1.38
22	b	615	CLA	C4D-CHA	2.53	1.47	1.38
22	c	510	CLA	C1B-C2B	2.53	1.49	1.43
22	Y	602	CLA	CHD-C4C	2.53	1.45	1.39
22	y	602	CLA	CHD-C4C	2.53	1.45	1.39
22	c	507	CLA	CHD-C4C	2.53	1.45	1.39
22	Y	614	CLA	CHD-C4C	2.53	1.45	1.39
22	y	614	CLA	CHD-C4C	2.53	1.45	1.39
22	Y	613	CLA	CHD-C4C	2.53	1.45	1.39
22	y	613	CLA	CHD-C4C	2.53	1.45	1.39
22	a	405	CLA	C4D-CHA	2.52	1.47	1.38
22	G	612	CLA	C1B-C2B	2.52	1.49	1.43
22	g	612	CLA	C1B-C2B	2.52	1.49	1.43
22	C	509	CLA	C4D-CHA	2.52	1.47	1.38
22	D	401	CLA	C4D-CHA	2.52	1.47	1.38
22	1	604	CLA	C1B-C2B	2.52	1.49	1.43
22	5	604	CLA	C1B-C2B	2.52	1.49	1.43
22	S	313	CLA	CHD-C4C	2.52	1.45	1.39
22	s	313	CLA	CHD-C4C	2.52	1.45	1.39
22	A	405	CLA	C4D-CHA	2.52	1.47	1.38
22	B	612	CLA	C4D-CHA	2.52	1.47	1.38
22	2	609	CLA	O2D-CGD	2.52	1.39	1.33
22	6	609	CLA	O2D-CGD	2.52	1.39	1.33
22	B	609	CLA	C1B-C2B	2.52	1.49	1.43
22	b	606	CLA	C4D-CHA	2.52	1.47	1.38
22	c	510	CLA	CHD-C4C	2.52	1.45	1.39
22	R	308	CLA	CHD-C4C	2.52	1.45	1.39
22	r	308	CLA	CHD-C4C	2.52	1.45	1.39
22	S	303	CLA	CHD-C4C	2.52	1.45	1.39
22	s	303	CLA	CHD-C4C	2.52	1.45	1.39
22	c	505	CLA	CHD-C4C	2.52	1.45	1.39
22	a	403	CLA	C4D-CHA	2.52	1.47	1.38
25	Y	601	CHL	CBA-CGA	2.52	1.56	1.50
25	y	601	CHL	CBA-CGA	2.52	1.56	1.50
25	G	608	CHL	CBA-CGA	2.52	1.56	1.50
25	g	608	CHL	CBA-CGA	2.52	1.56	1.50
22	s	301	CLA	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	510	CLA	CHD-C4C	2.51	1.45	1.39
22	S	313	CLA	C1B-C2B	2.51	1.49	1.43
22	s	313	CLA	C1B-C2B	2.51	1.49	1.43
22	S	314	CLA	C4D-CHA	2.51	1.47	1.38
22	s	314	CLA	C4D-CHA	2.51	1.47	1.38
22	C	511	CLA	C1B-C2B	2.51	1.49	1.43
22	B	605	CLA	CHD-C4C	2.51	1.45	1.39
22	a	402	CLA	C4D-CHA	2.51	1.47	1.38
22	Y	602	CLA	C4D-CHA	2.51	1.47	1.38
22	y	602	CLA	C4D-CHA	2.51	1.47	1.38
22	4	310	CLA	O2D-CGD	2.51	1.39	1.33
22	8	310	CLA	O2D-CGD	2.51	1.39	1.33
22	c	508	CLA	CHD-C4C	2.51	1.45	1.39
22	B	606	CLA	C1B-C2B	2.51	1.49	1.43
22	B	602	CLA	C4D-ND	-2.51	1.34	1.37
22	N	610	CLA	C1B-C2B	2.50	1.49	1.43
22	n	610	CLA	C1B-C2B	2.50	1.49	1.43
22	d	401	CLA	C4D-CHA	2.50	1.47	1.38
22	4	305	CLA	C1B-C2B	2.50	1.49	1.43
22	8	305	CLA	C1B-C2B	2.50	1.49	1.43
22	b	606	CLA	C1B-C2B	2.50	1.49	1.43
25	4	307	CHL	CBA-CGA	2.50	1.56	1.50
25	8	307	CHL	CBA-CGA	2.50	1.56	1.50
22	G	604	CLA	C4D-CHA	2.50	1.47	1.38
22	g	604	CLA	C4D-CHA	2.50	1.47	1.38
22	N	610	CLA	C4D-CHA	2.50	1.47	1.38
22	n	610	CLA	C4D-CHA	2.50	1.47	1.38
22	b	609	CLA	C4D-CHA	2.50	1.47	1.38
22	b	605	CLA	C1B-C2B	2.50	1.49	1.43
22	Y	613	CLA	C1B-C2B	2.50	1.49	1.43
22	y	613	CLA	C1B-C2B	2.50	1.49	1.43
22	b	613	CLA	O2D-CGD	2.50	1.39	1.33
22	4	310	CLA	C4D-ND	-2.50	1.34	1.37
22	8	310	CLA	C4D-ND	-2.50	1.34	1.37
22	b	616	CLA	O2D-CGD	2.50	1.39	1.33
25	G	609	CHL	O2D-CED	-2.49	1.39	1.45
25	g	609	CHL	O2D-CED	-2.49	1.39	1.45
22	S	305	CLA	C1B-C2B	2.49	1.49	1.43
22	s	305	CLA	C1B-C2B	2.49	1.49	1.43
22	b	616	CLA	C4C-C3C	2.49	1.49	1.45
22	c	503	CLA	C1B-C2B	2.49	1.49	1.43
22	B	608	CLA	CHD-C4C	2.49	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	609	CHL	O2D-CED	-2.49	1.39	1.45
25	n	609	CHL	O2D-CED	-2.49	1.39	1.45
22	b	603	CLA	C4D-CHA	2.49	1.47	1.38
22	R	307	CLA	CHD-C4C	2.49	1.44	1.39
22	r	307	CLA	CHD-C4C	2.49	1.44	1.39
22	R	303	CLA	C4D-CHA	2.49	1.47	1.38
22	r	303	CLA	C4D-CHA	2.49	1.47	1.38
22	4	303	CLA	CHD-C4C	2.49	1.44	1.39
22	8	303	CLA	CHD-C4C	2.49	1.44	1.39
22	G	612	CLA	O2D-CGD	2.49	1.39	1.33
22	g	612	CLA	O2D-CGD	2.49	1.39	1.33
25	1	601	CHL	CBA-CGA	2.49	1.56	1.50
25	5	601	CHL	CBA-CGA	2.49	1.56	1.50
22	c	504	CLA	C4D-CHA	2.48	1.47	1.38
22	d	401	CLA	C1B-C2B	2.48	1.49	1.43
22	2	609	CLA	C4D-ND	-2.48	1.34	1.37
22	6	609	CLA	C4D-ND	-2.48	1.34	1.37
22	C	505	CLA	C4D-CHA	2.48	1.47	1.38
22	c	511	CLA	C1B-C2B	2.48	1.49	1.43
22	A	403	CLA	C4D-CHA	2.48	1.47	1.38
22	c	509	CLA	CHD-C4C	2.48	1.44	1.39
22	c	509	CLA	C4D-CHA	2.48	1.47	1.38
22	c	506	CLA	CHD-C4C	2.48	1.44	1.39
22	S	301	CLA	CHD-C4C	2.48	1.44	1.39
22	b	608	CLA	C4D-CHA	2.48	1.47	1.38
22	B	605	CLA	C4D-CHA	2.48	1.47	1.38
25	3	307	CHL	CBA-CGA	2.47	1.56	1.50
25	7	307	CHL	CBA-CGA	2.47	1.56	1.50
22	4	311	CLA	C4D-ND	-2.47	1.34	1.37
22	8	311	CLA	C4D-ND	-2.47	1.34	1.37
22	C	507	CLA	CHD-C4C	2.47	1.44	1.39
22	1	610	CLA	C4D-ND	-2.47	1.34	1.37
22	5	610	CLA	C4D-ND	-2.47	1.34	1.37
22	Y	611	CLA	C4D-CHA	2.47	1.47	1.38
22	y	611	CLA	C4D-CHA	2.47	1.47	1.38
22	2	613	CLA	O2D-CGD	2.47	1.39	1.33
22	6	613	CLA	O2D-CGD	2.47	1.39	1.33
22	b	614	CLA	C4D-CHA	2.47	1.47	1.38
25	3	308	CHL	CBA-CGA	2.47	1.56	1.50
25	7	308	CHL	CBA-CGA	2.47	1.56	1.50
25	S	302	CHL	CBA-CGA	2.47	1.56	1.50
25	s	302	CHL	CBA-CGA	2.47	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	405	CLA	CHD-C4C	2.47	1.44	1.39
22	a	402	CLA	C1B-C2B	2.47	1.49	1.43
22	3	312	CLA	O2D-CGD	2.47	1.39	1.33
22	7	312	CLA	O2D-CGD	2.47	1.39	1.33
22	C	510	CLA	O2D-CGD	2.47	1.39	1.33
22	C	511	CLA	C4D-CHA	2.47	1.47	1.38
25	1	608	CHL	CBA-CGA	2.47	1.56	1.50
25	5	608	CHL	CBA-CGA	2.47	1.56	1.50
22	S	309	CLA	C4D-CHA	2.46	1.47	1.38
22	s	309	CLA	C4D-CHA	2.46	1.47	1.38
22	3	314	CLA	O2D-CGD	2.46	1.39	1.33
22	7	314	CLA	O2D-CGD	2.46	1.39	1.33
22	S	312	CLA	C1B-C2B	2.46	1.49	1.43
22	s	312	CLA	C1B-C2B	2.46	1.49	1.43
22	R	302	CLA	O2D-CGD	2.46	1.39	1.33
22	r	302	CLA	O2D-CGD	2.46	1.39	1.33
22	S	311	CLA	C1B-C2B	2.46	1.49	1.43
22	s	311	CLA	C1B-C2B	2.46	1.49	1.43
22	3	310	CLA	O2D-CGD	2.46	1.39	1.33
22	7	310	CLA	O2D-CGD	2.46	1.39	1.33
22	b	602	CLA	C1B-C2B	2.46	1.49	1.43
22	b	612	CLA	C1B-C2B	2.46	1.49	1.43
22	C	507	CLA	C1B-C2B	2.46	1.49	1.43
25	R	306	CHL	CBA-CGA	2.46	1.56	1.50
25	r	306	CHL	CBA-CGA	2.46	1.56	1.50
22	1	612	CLA	O2D-CGD	2.46	1.39	1.33
22	2	602	CLA	O2D-CGD	2.46	1.39	1.33
22	3	303	CLA	O2D-CGD	2.46	1.39	1.33
22	5	612	CLA	O2D-CGD	2.46	1.39	1.33
22	6	602	CLA	O2D-CGD	2.46	1.39	1.33
22	7	303	CLA	O2D-CGD	2.46	1.39	1.33
22	c	509	CLA	C1B-C2B	2.46	1.49	1.43
22	R	311	CLA	C4D-CHA	2.46	1.47	1.38
22	r	311	CLA	C4D-CHA	2.46	1.47	1.38
22	G	602	CLA	C4D-CHA	2.45	1.47	1.38
22	g	602	CLA	C4D-CHA	2.45	1.47	1.38
22	b	602	CLA	C4D-CHA	2.45	1.47	1.38
22	b	611	CLA	C4D-CHA	2.45	1.47	1.38
22	d	404	CLA	C4D-CHA	2.45	1.47	1.38
23	A	404	PHO	C1D-ND	-2.45	1.34	1.38
22	C	510	CLA	C1B-C2B	2.45	1.49	1.43
22	c	507	CLA	C1B-C2B	2.45	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	608	CHL	CBA-CGA	2.45	1.56	1.50
25	n	608	CHL	CBA-CGA	2.45	1.56	1.50
22	N	602	CLA	C1B-C2B	2.45	1.49	1.43
22	n	602	CLA	C1B-C2B	2.45	1.49	1.43
22	C	508	CLA	O2D-CGD	2.45	1.39	1.33
25	N	601	CHL	CBA-CGA	2.45	1.56	1.50
25	n	601	CHL	CBA-CGA	2.45	1.56	1.50
25	1	615	CHL	CBA-CGA	2.45	1.56	1.50
25	5	615	CHL	CBA-CGA	2.45	1.56	1.50
22	B	609	CLA	C4D-CHA	2.45	1.47	1.38
22	c	508	CLA	O2D-CGD	2.45	1.39	1.33
22	1	613	CLA	O2D-CGD	2.45	1.39	1.33
22	5	613	CLA	O2D-CGD	2.45	1.39	1.33
22	1	610	CLA	O2D-CGD	2.45	1.39	1.33
22	5	610	CLA	O2D-CGD	2.45	1.39	1.33
22	2	603	CLA	O2D-CGD	2.45	1.39	1.33
22	6	603	CLA	O2D-CGD	2.45	1.39	1.33
22	N	612	CLA	O2D-CGD	2.45	1.39	1.33
22	n	612	CLA	O2D-CGD	2.45	1.39	1.33
22	d	401	CLA	CHD-C4C	2.45	1.44	1.39
22	R	301	CLA	C4D-CHA	2.45	1.47	1.38
22	r	301	CLA	C4D-CHA	2.45	1.47	1.38
22	c	503	CLA	CHD-C4C	2.45	1.44	1.39
22	b	607	CLA	O2D-CGD	2.44	1.39	1.33
22	G	602	CLA	CHD-C4C	2.44	1.44	1.39
22	g	602	CLA	CHD-C4C	2.44	1.44	1.39
22	2	604	CLA	C4C-C3C	2.44	1.49	1.45
22	6	604	CLA	C4C-C3C	2.44	1.49	1.45
22	s	301	CLA	C4D-CHA	2.44	1.47	1.38
22	1	602	CLA	O2D-CGD	2.44	1.39	1.33
22	5	602	CLA	O2D-CGD	2.44	1.39	1.33
22	b	612	CLA	C4D-CHA	2.44	1.47	1.38
22	3	305	CLA	C4C-C3C	2.44	1.49	1.45
22	7	305	CLA	C4C-C3C	2.44	1.49	1.45
22	B	615	CLA	MG-NA	2.44	2.12	2.06
22	a	403	CLA	C1B-C2B	2.44	1.49	1.43
22	2	604	CLA	C1B-C2B	2.44	1.49	1.43
22	6	604	CLA	C1B-C2B	2.44	1.49	1.43
22	B	601	CLA	C4D-CHA	2.44	1.47	1.38
22	C	503	CLA	C4D-CHA	2.44	1.47	1.38
22	N	614	CLA	O2D-CGD	2.44	1.39	1.33
22	n	614	CLA	O2D-CGD	2.44	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	305	CLA	O2D-CGD	2.44	1.39	1.33
22	8	305	CLA	O2D-CGD	2.44	1.39	1.33
22	b	601	CLA	CHD-C4C	2.44	1.44	1.39
25	G	606	CHL	CBA-CGA	2.43	1.56	1.50
25	g	606	CHL	CBA-CGA	2.43	1.56	1.50
22	S	305	CLA	C4D-CHA	2.43	1.47	1.38
22	s	305	CLA	C4D-CHA	2.43	1.47	1.38
22	2	604	CLA	O2D-CGD	2.43	1.39	1.33
22	6	604	CLA	O2D-CGD	2.43	1.39	1.33
22	C	511	CLA	O2D-CGD	2.43	1.39	1.33
22	2	610	CLA	O2D-CGD	2.43	1.39	1.33
22	6	610	CLA	O2D-CGD	2.43	1.39	1.33
22	c	511	CLA	C4D-CHA	2.43	1.47	1.38
22	b	610	CLA	C1B-C2B	2.43	1.49	1.43
22	c	512	CLA	CHD-C4C	2.43	1.44	1.39
22	Y	614	CLA	C4D-CHA	2.43	1.47	1.38
22	y	614	CLA	C4D-CHA	2.43	1.47	1.38
22	S	303	CLA	C4D-CHA	2.43	1.47	1.38
22	s	303	CLA	C4D-CHA	2.43	1.47	1.38
22	2	611	CLA	O2D-CGD	2.43	1.39	1.33
22	6	611	CLA	O2D-CGD	2.43	1.39	1.33
25	4	308	CHL	CBA-CGA	2.43	1.56	1.50
25	8	308	CHL	CBA-CGA	2.43	1.56	1.50
25	2	608	CHL	C4D-CHA	2.42	1.47	1.38
25	6	608	CHL	C4D-CHA	2.42	1.47	1.38
22	S	304	CLA	O2D-CGD	2.42	1.39	1.33
22	s	304	CLA	O2D-CGD	2.42	1.39	1.33
22	S	314	CLA	C1B-C2B	2.42	1.49	1.43
22	s	314	CLA	C1B-C2B	2.42	1.49	1.43
22	B	611	CLA	C4D-CHA	2.42	1.47	1.38
22	S	301	CLA	O2D-CGD	2.42	1.39	1.33
22	4	311	CLA	O2D-CGD	2.42	1.39	1.33
22	8	311	CLA	O2D-CGD	2.42	1.39	1.33
23	D	402	PHO	C3D-C2D	2.42	1.43	1.39
22	b	609	CLA	O2D-CGD	2.42	1.39	1.33
22	b	609	CLA	C1B-C2B	2.42	1.48	1.43
25	G	607	CHL	CBA-CGA	2.42	1.56	1.50
25	g	607	CHL	CBA-CGA	2.42	1.56	1.50
22	N	602	CLA	C4D-CHA	2.42	1.47	1.38
22	n	602	CLA	C4D-CHA	2.42	1.47	1.38
25	Y	608	CHL	CBA-CGA	2.42	1.56	1.50
25	y	608	CHL	CBA-CGA	2.42	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	611	CLA	O2D-CGD	2.42	1.39	1.33
22	5	611	CLA	O2D-CGD	2.42	1.39	1.33
22	1	603	CLA	O2D-CGD	2.41	1.39	1.33
22	5	603	CLA	O2D-CGD	2.41	1.39	1.33
22	A	405	CLA	C1B-C2B	2.41	1.48	1.43
22	b	606	CLA	C4D-ND	-2.41	1.34	1.37
22	3	311	CLA	O2D-CGD	2.41	1.39	1.33
22	7	311	CLA	O2D-CGD	2.41	1.39	1.33
22	Y	602	CLA	C1B-C2B	2.41	1.48	1.43
22	y	602	CLA	C1B-C2B	2.41	1.48	1.43
22	Y	603	CLA	O2D-CGD	2.41	1.39	1.33
22	y	603	CLA	O2D-CGD	2.41	1.39	1.33
23	a	404	PHO	C3D-C2D	2.41	1.43	1.39
22	B	616	CLA	O2D-CGD	2.41	1.39	1.33
22	3	304	CLA	O2D-CGD	2.41	1.39	1.33
22	7	304	CLA	O2D-CGD	2.41	1.39	1.33
22	C	504	CLA	C4D-CHA	2.41	1.47	1.38
22	A	402	CLA	C4D-CHA	2.41	1.47	1.38
22	Y	613	CLA	C4D-CHA	2.41	1.47	1.38
22	y	613	CLA	C4D-CHA	2.41	1.47	1.38
22	4	304	CLA	O2D-CGD	2.41	1.39	1.33
22	8	304	CLA	O2D-CGD	2.41	1.39	1.33
25	3	302	CHL	CBA-CGA	2.41	1.56	1.50
25	7	302	CHL	CBA-CGA	2.41	1.56	1.50
22	1	614	CLA	CHD-C1D	2.41	1.43	1.38
22	5	614	CLA	CHD-C1D	2.41	1.43	1.38
22	b	607	CLA	C4D-CHA	2.40	1.46	1.38
22	R	308	CLA	O2D-CGD	2.40	1.39	1.33
22	r	308	CLA	O2D-CGD	2.40	1.39	1.33
25	4	309	CHL	CBA-CGA	2.40	1.56	1.50
25	8	309	CHL	CBA-CGA	2.40	1.56	1.50
22	G	602	CLA	C1B-C2B	2.40	1.48	1.43
22	g	602	CLA	C1B-C2B	2.40	1.48	1.43
22	c	506	CLA	O2D-CGD	2.40	1.39	1.33
22	D	403	CLA	C4D-CHA	2.40	1.46	1.38
22	S	310	CLA	O2D-CGD	2.40	1.39	1.33
22	s	310	CLA	O2D-CGD	2.40	1.39	1.33
22	S	313	CLA	C4D-CHA	2.40	1.46	1.38
22	s	313	CLA	C4D-CHA	2.40	1.46	1.38
25	N	607	CHL	CBA-CGA	2.40	1.56	1.50
25	n	607	CHL	CBA-CGA	2.40	1.56	1.50
22	c	504	CLA	O2D-CGD	2.40	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	312	CLA	O2D-CGD	2.40	1.39	1.33
22	s	312	CLA	O2D-CGD	2.40	1.39	1.33
22	Y	604	CLA	C4D-CHA	2.40	1.46	1.38
22	y	604	CLA	C4D-CHA	2.40	1.46	1.38
22	C	502	CLA	C4D-CHA	2.40	1.46	1.38
22	R	308	CLA	C4D-CHA	2.40	1.46	1.38
22	r	308	CLA	C4D-CHA	2.40	1.46	1.38
22	b	605	CLA	C4D-CHA	2.39	1.46	1.38
22	4	301	CLA	O2D-CGD	2.39	1.39	1.33
22	8	301	CLA	O2D-CGD	2.39	1.39	1.33
22	G	610	CLA	CHD-C4C	2.39	1.44	1.39
22	g	610	CLA	CHD-C4C	2.39	1.44	1.39
25	2	601	CHL	CBA-CGA	2.39	1.56	1.50
25	6	601	CHL	CBA-CGA	2.39	1.56	1.50
22	c	508	CLA	C4C-C3C	2.39	1.49	1.45
22	C	502	CLA	C1B-C2B	2.39	1.48	1.43
22	Y	612	CLA	O2D-CGD	2.39	1.39	1.33
22	y	612	CLA	O2D-CGD	2.39	1.39	1.33
22	B	611	CLA	CHD-C4C	2.39	1.44	1.39
22	c	510	CLA	O2D-CGD	2.39	1.39	1.33
22	R	310	CLA	O2D-CGD	2.39	1.39	1.33
22	r	310	CLA	O2D-CGD	2.39	1.39	1.33
22	1	604	CLA	O2D-CGD	2.39	1.39	1.33
22	5	604	CLA	O2D-CGD	2.39	1.39	1.33
22	3	313	CLA	O2D-CGD	2.38	1.39	1.33
22	7	313	CLA	O2D-CGD	2.38	1.39	1.33
22	N	603	CLA	O2D-CGD	2.38	1.39	1.33
22	n	603	CLA	O2D-CGD	2.38	1.39	1.33
25	2	608	CHL	CBA-CGA	2.38	1.56	1.50
25	6	608	CHL	CBA-CGA	2.38	1.56	1.50
22	B	601	CLA	O2D-CGD	2.38	1.39	1.33
22	A	402	CLA	CHD-C4C	2.37	1.44	1.39
22	S	313	CLA	O2D-CGD	2.37	1.39	1.33
22	S	314	CLA	O2D-CGD	2.37	1.39	1.33
22	s	313	CLA	O2D-CGD	2.37	1.39	1.33
22	s	314	CLA	O2D-CGD	2.37	1.39	1.33
22	a	403	CLA	CHD-C4C	2.37	1.44	1.39
22	C	508	CLA	C1B-C2B	2.37	1.48	1.43
22	G	614	CLA	O2D-CGD	2.37	1.39	1.33
22	g	614	CLA	O2D-CGD	2.37	1.39	1.33
22	N	604	CLA	C4D-CHA	2.37	1.46	1.38
22	n	604	CLA	C4D-CHA	2.37	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	301	CLA	O2D-CGD	2.37	1.39	1.33
22	G	604	CLA	O2D-CGD	2.37	1.39	1.33
22	g	604	CLA	O2D-CGD	2.37	1.39	1.33
22	G	611	CLA	O2D-CGD	2.37	1.39	1.33
22	g	611	CLA	O2D-CGD	2.37	1.39	1.33
22	C	506	CLA	CHD-C4C	2.37	1.44	1.39
22	B	614	CLA	CAA-C2A	2.37	1.58	1.54
22	C	501	CLA	O2D-CGD	2.37	1.39	1.33
22	b	603	CLA	C4C-C3C	2.37	1.49	1.45
22	2	612	CLA	O2D-CGD	2.36	1.39	1.33
22	6	612	CLA	O2D-CGD	2.36	1.39	1.33
22	C	506	CLA	C1B-C2B	2.36	1.48	1.43
22	D	404	CLA	C4D-CHA	2.36	1.46	1.38
22	N	604	CLA	O2D-CGD	2.36	1.39	1.33
22	n	604	CLA	O2D-CGD	2.36	1.39	1.33
25	G	601	CHL	CBA-CGA	2.36	1.56	1.50
25	g	601	CHL	CBA-CGA	2.36	1.56	1.50
22	Y	610	CLA	CHD-C4C	2.36	1.44	1.39
22	y	610	CLA	CHD-C4C	2.36	1.44	1.39
22	B	614	CLA	CHD-C4C	2.36	1.44	1.39
22	S	311	CLA	C4D-CHA	2.36	1.46	1.38
22	s	311	CLA	C4D-CHA	2.36	1.46	1.38
22	N	604	CLA	C1B-C2B	2.36	1.48	1.43
22	n	604	CLA	C1B-C2B	2.36	1.48	1.43
22	B	606	CLA	O2D-CGD	2.36	1.39	1.33
22	3	305	CLA	O2D-CGD	2.36	1.39	1.33
22	7	305	CLA	O2D-CGD	2.36	1.39	1.33
22	c	502	CLA	O2D-CGD	2.36	1.39	1.33
22	d	403	CLA	C4D-CHA	2.36	1.46	1.38
22	a	405	CLA	O2D-CGD	2.35	1.38	1.33
22	b	601	CLA	O2D-CGD	2.35	1.38	1.33
22	B	615	CLA	O2D-CGD	2.35	1.38	1.33
22	N	610	CLA	CHD-C4C	2.35	1.44	1.39
22	n	610	CLA	CHD-C4C	2.35	1.44	1.39
22	D	401	CLA	C1B-C2B	2.35	1.48	1.43
22	3	304	CLA	C4C-C3C	2.35	1.49	1.45
22	7	304	CLA	C4C-C3C	2.35	1.49	1.45
25	3	309	CHL	C4D-CHA	2.35	1.46	1.38
25	7	309	CHL	C4D-CHA	2.35	1.46	1.38
22	R	309	CLA	O2D-CGD	2.35	1.38	1.33
22	r	309	CLA	O2D-CGD	2.35	1.38	1.33
22	S	310	CLA	C4D-CHA	2.35	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	310	CLA	C4D-CHA	2.35	1.46	1.38
22	C	512	CLA	C4C-C3C	2.35	1.49	1.45
22	B	604	CLA	O2D-CGD	2.35	1.38	1.33
22	S	311	CLA	CHD-C4C	2.34	1.44	1.39
22	s	311	CLA	CHD-C4C	2.34	1.44	1.39
22	1	613	CLA	C4C-C3C	2.34	1.49	1.45
22	5	613	CLA	C4C-C3C	2.34	1.49	1.45
22	R	311	CLA	CHD-C4C	2.34	1.44	1.39
22	r	311	CLA	CHD-C4C	2.34	1.44	1.39
22	C	502	CLA	O2D-CGD	2.34	1.38	1.33
22	c	511	CLA	O2D-CGD	2.34	1.38	1.33
22	3	310	CLA	C4D-ND	-2.34	1.34	1.37
22	7	310	CLA	C4D-ND	-2.34	1.34	1.37
22	B	603	CLA	MG-NB	-2.34	2.01	2.05
22	b	614	CLA	CAA-C2A	2.34	1.58	1.54
22	G	603	CLA	O2D-CGD	2.34	1.38	1.33
22	g	603	CLA	O2D-CGD	2.34	1.38	1.33
22	R	301	CLA	O2D-CGD	2.34	1.38	1.33
22	r	301	CLA	O2D-CGD	2.34	1.38	1.33
22	Y	602	CLA	C3D-C2D	2.33	1.45	1.39
22	y	602	CLA	C3D-C2D	2.33	1.45	1.39
22	C	504	CLA	O2D-CGD	2.33	1.38	1.33
25	S	306	CHL	CBA-CGA	2.33	1.56	1.50
25	s	306	CHL	CBA-CGA	2.33	1.56	1.50
22	C	503	CLA	C1B-C2B	2.33	1.48	1.43
22	B	608	CLA	O2D-CGD	2.33	1.38	1.33
22	Y	614	CLA	O2D-CGD	2.33	1.38	1.33
22	y	614	CLA	O2D-CGD	2.33	1.38	1.33
25	2	607	CHL	CBA-CGA	2.33	1.56	1.50
25	6	607	CHL	CBA-CGA	2.33	1.56	1.50
22	d	404	CLA	O2D-CGD	2.33	1.38	1.33
25	3	306	CHL	C4D-CHA	2.33	1.46	1.38
25	7	306	CHL	C4D-CHA	2.33	1.46	1.38
22	R	302	CLA	CHD-C4C	2.33	1.44	1.39
22	r	302	CLA	CHD-C4C	2.33	1.44	1.39
25	2	605	CHL	C4D-CHA	2.33	1.46	1.38
25	6	605	CHL	C4D-CHA	2.33	1.46	1.38
22	b	606	CLA	C4C-C3C	2.33	1.49	1.45
22	B	609	CLA	O2D-CGD	2.33	1.38	1.33
22	1	612	CLA	C3D-C2D	2.32	1.45	1.39
22	5	612	CLA	C3D-C2D	2.32	1.45	1.39
22	Y	604	CLA	CHD-C4C	2.32	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	y	604	CLA	CHD-C4C	2.32	1.44	1.39
22	C	503	CLA	O2D-CGD	2.32	1.38	1.33
22	B	605	CLA	O2D-CGD	2.32	1.38	1.33
22	A	405	CLA	O2D-CGD	2.32	1.38	1.33
22	D	403	CLA	CHD-C4C	2.32	1.44	1.39
22	C	506	CLA	O2D-CGD	2.32	1.38	1.33
22	R	307	CLA	O2D-CGD	2.32	1.38	1.33
22	r	307	CLA	O2D-CGD	2.32	1.38	1.33
22	3	313	CLA	C4C-C3C	2.32	1.49	1.45
22	7	313	CLA	C4C-C3C	2.32	1.49	1.45
22	S	309	CLA	O2D-CGD	2.32	1.38	1.33
22	s	309	CLA	O2D-CGD	2.32	1.38	1.33
22	b	616	CLA	C1B-C2B	2.32	1.48	1.43
22	c	505	CLA	C4D-CHA	2.32	1.46	1.38
22	C	506	CLA	MG-NB	-2.31	2.01	2.05
22	1	604	CLA	C3D-C2D	2.31	1.45	1.39
22	5	604	CLA	C3D-C2D	2.31	1.45	1.39
22	4	304	CLA	C3D-C2D	2.31	1.45	1.39
22	8	304	CLA	C3D-C2D	2.31	1.45	1.39
22	4	303	CLA	O2D-CGD	2.31	1.38	1.33
22	8	303	CLA	O2D-CGD	2.31	1.38	1.33
22	b	614	CLA	O2D-CGD	2.31	1.38	1.33
22	B	608	CLA	C4D-CHA	2.31	1.46	1.38
22	b	615	CLA	O2D-CGD	2.31	1.38	1.33
22	G	613	CLA	O2D-CGD	2.31	1.38	1.33
22	g	613	CLA	O2D-CGD	2.31	1.38	1.33
22	c	505	CLA	C1B-C2B	2.30	1.48	1.43
22	C	511	CLA	C4C-C3C	2.30	1.49	1.45
22	3	313	CLA	C3D-C2D	2.30	1.45	1.39
22	7	313	CLA	C3D-C2D	2.30	1.45	1.39
23	d	402	PHO	C3D-C2D	2.29	1.43	1.39
25	S	308	CHL	CBA-CGA	2.29	1.55	1.50
25	s	308	CHL	CBA-CGA	2.29	1.55	1.50
22	N	602	CLA	O2D-CGD	2.29	1.38	1.33
22	n	602	CLA	O2D-CGD	2.29	1.38	1.33
22	b	604	CLA	O2D-CGD	2.29	1.38	1.33
22	G	604	CLA	C1B-C2B	2.29	1.48	1.43
22	g	604	CLA	C1B-C2B	2.29	1.48	1.43
22	b	611	CLA	CHD-C4C	2.29	1.44	1.39
22	c	506	CLA	C1B-C2B	2.29	1.48	1.43
22	b	602	CLA	CHD-C4C	2.29	1.44	1.39
22	Y	611	CLA	CHD-C4C	2.29	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	y	611	CLA	CHD-C4C	2.29	1.44	1.39
22	C	507	CLA	O2D-CGD	2.29	1.38	1.33
22	B	615	CLA	CHD-C4C	2.29	1.44	1.39
22	3	311	CLA	C4C-C3C	2.29	1.49	1.45
22	7	311	CLA	C4C-C3C	2.29	1.49	1.45
22	Y	613	CLA	O2D-CGD	2.29	1.38	1.33
22	y	613	CLA	O2D-CGD	2.29	1.38	1.33
22	a	405	CLA	MG-NB	-2.29	2.01	2.05
25	3	302	CHL	C4D-CHA	2.29	1.46	1.38
25	7	302	CHL	C4D-CHA	2.29	1.46	1.38
22	1	603	CLA	C4C-C3C	2.29	1.49	1.45
22	4	301	CLA	C4C-C3C	2.29	1.49	1.45
22	5	603	CLA	C4C-C3C	2.29	1.49	1.45
22	8	301	CLA	C4C-C3C	2.29	1.49	1.45
22	1	612	CLA	C4C-C3C	2.28	1.49	1.45
22	5	612	CLA	C4C-C3C	2.28	1.49	1.45
22	3	314	CLA	C4C-C3C	2.28	1.49	1.45
22	4	304	CLA	C4C-C3C	2.28	1.49	1.45
22	4	305	CLA	C4C-C3C	2.28	1.49	1.45
22	7	314	CLA	C4C-C3C	2.28	1.49	1.45
22	8	304	CLA	C4C-C3C	2.28	1.49	1.45
22	8	305	CLA	C4C-C3C	2.28	1.49	1.45
22	a	405	CLA	CHD-C4C	2.28	1.44	1.39
22	2	604	CLA	C3D-C2D	2.28	1.45	1.39
22	6	604	CLA	C3D-C2D	2.28	1.45	1.39
25	2	607	CHL	C4D-CHA	2.28	1.46	1.38
25	6	607	CHL	C4D-CHA	2.28	1.46	1.38
22	3	305	CLA	CAA-C2A	2.28	1.58	1.54
22	7	305	CLA	CAA-C2A	2.28	1.58	1.54
22	C	505	CLA	C1B-C2B	2.28	1.48	1.43
25	G	605	CHL	C4D-CHA	2.28	1.46	1.38
25	g	605	CHL	C4D-CHA	2.28	1.46	1.38
22	G	610	CLA	O2D-CGD	2.28	1.38	1.33
22	g	610	CLA	O2D-CGD	2.28	1.38	1.33
22	R	303	CLA	O2D-CGD	2.28	1.38	1.33
22	r	303	CLA	O2D-CGD	2.28	1.38	1.33
22	G	603	CLA	C4C-C3C	2.28	1.49	1.45
22	g	603	CLA	C4C-C3C	2.28	1.49	1.45
22	N	611	CLA	O2D-CGD	2.28	1.38	1.33
22	n	611	CLA	O2D-CGD	2.28	1.38	1.33
22	2	613	CLA	C4C-C3C	2.28	1.49	1.45
22	6	613	CLA	C4C-C3C	2.28	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	308	CHL	C4D-CHA	2.27	1.46	1.38
25	8	308	CHL	C4D-CHA	2.27	1.46	1.38
22	Y	610	CLA	O2D-CGD	2.27	1.38	1.33
22	y	610	CLA	O2D-CGD	2.27	1.38	1.33
22	3	305	CLA	C3D-C2D	2.27	1.45	1.39
22	7	305	CLA	C3D-C2D	2.27	1.45	1.39
25	3	308	CHL	C4D-CHA	2.27	1.46	1.38
25	7	308	CHL	C4D-CHA	2.27	1.46	1.38
22	B	616	CLA	C4C-C3C	2.27	1.48	1.45
22	1	613	CLA	C3D-C2D	2.27	1.45	1.39
22	5	613	CLA	C3D-C2D	2.27	1.45	1.39
22	3	314	CLA	C3D-C2D	2.27	1.45	1.39
22	7	314	CLA	C3D-C2D	2.27	1.45	1.39
22	G	602	CLA	O2D-CGD	2.27	1.38	1.33
22	g	602	CLA	O2D-CGD	2.27	1.38	1.33
22	b	615	CLA	C1B-C2B	2.27	1.48	1.43
22	3	304	CLA	CHD-C1D	2.27	1.42	1.38
22	7	304	CLA	CHD-C1D	2.27	1.42	1.38
22	B	610	CLA	C4C-C3C	2.26	1.48	1.45
22	A	405	CLA	MG-NB	-2.26	2.01	2.05
22	b	606	CLA	O2D-CGD	2.26	1.38	1.33
22	R	308	CLA	CAA-C2A	2.26	1.58	1.54
22	r	308	CLA	CAA-C2A	2.26	1.58	1.54
22	C	506	CLA	C4C-C3C	2.26	1.48	1.45
22	A	402	CLA	O2D-CGD	2.26	1.38	1.33
22	2	604	CLA	CAA-C2A	2.25	1.58	1.54
22	6	604	CLA	CAA-C2A	2.25	1.58	1.54
22	1	611	CLA	C4C-C3C	2.25	1.48	1.45
22	5	611	CLA	C4C-C3C	2.25	1.48	1.45
22	b	610	CLA	O2D-CGD	2.25	1.38	1.33
22	Y	602	CLA	CAA-C2A	2.25	1.58	1.54
22	y	602	CLA	CAA-C2A	2.25	1.58	1.54
22	c	506	CLA	MG-NB	-2.25	2.01	2.05
22	B	602	CLA	C3D-C2D	2.25	1.45	1.39
22	d	403	CLA	C4C-C3C	2.25	1.48	1.45
22	B	616	CLA	CHB-C1B	2.24	1.44	1.39
22	3	304	CLA	C3D-C2D	2.24	1.45	1.39
22	7	304	CLA	C3D-C2D	2.24	1.45	1.39
22	D	404	CLA	O2D-CGD	2.24	1.38	1.33
22	B	607	CLA	O2D-CGD	2.24	1.38	1.33
22	C	511	CLA	CHD-C1D	2.24	1.42	1.38
22	A	403	CLA	C1B-C2B	2.24	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	311	CLA	C3D-C2D	2.24	1.45	1.39
22	7	311	CLA	C3D-C2D	2.24	1.45	1.39
22	4	311	CLA	C4C-C3C	2.24	1.48	1.45
22	8	311	CLA	C4C-C3C	2.24	1.48	1.45
25	1	608	CHL	C4D-CHA	2.24	1.46	1.38
25	5	608	CHL	C4D-CHA	2.24	1.46	1.38
23	d	402	PHO	C4B-NB	-2.24	1.34	1.38
25	1	609	CHL	C4D-CHA	2.24	1.46	1.38
25	5	609	CHL	C4D-CHA	2.24	1.46	1.38
22	c	506	CLA	C4C-C3C	2.24	1.48	1.45
22	N	602	CLA	CAA-C2A	2.23	1.58	1.54
22	n	602	CLA	CAA-C2A	2.23	1.58	1.54
22	c	501	CLA	O2D-CGD	2.23	1.38	1.33
22	c	508	CLA	MG-NB	-2.23	2.01	2.05
25	1	615	CHL	C4D-CHA	2.22	1.46	1.38
25	5	615	CHL	C4D-CHA	2.22	1.46	1.38
22	S	305	CLA	O2D-CGD	2.22	1.38	1.33
22	s	305	CLA	O2D-CGD	2.22	1.38	1.33
22	c	512	CLA	O2D-CGD	2.22	1.38	1.33
22	1	602	CLA	C4C-C3C	2.22	1.48	1.45
22	5	602	CLA	C4C-C3C	2.22	1.48	1.45
22	Y	611	CLA	O2D-CGD	2.22	1.38	1.33
22	y	611	CLA	O2D-CGD	2.22	1.38	1.33
22	1	604	CLA	C4C-C3C	2.22	1.48	1.45
22	5	604	CLA	C4C-C3C	2.22	1.48	1.45
22	S	312	CLA	CMC-C2C	2.22	1.55	1.50
22	s	312	CLA	CMC-C2C	2.22	1.55	1.50
22	N	614	CLA	C3D-C2D	2.22	1.45	1.39
22	n	614	CLA	C3D-C2D	2.22	1.45	1.39
22	b	607	CLA	C4C-C3C	2.22	1.48	1.45
22	3	312	CLA	C3D-C2D	2.22	1.45	1.39
22	7	312	CLA	C3D-C2D	2.22	1.45	1.39
25	2	606	CHL	C4D-CHA	2.22	1.46	1.38
25	6	606	CHL	C4D-CHA	2.22	1.46	1.38
25	2	601	CHL	C4D-CHA	2.22	1.46	1.38
25	6	601	CHL	C4D-CHA	2.22	1.46	1.38
25	3	307	CHL	C4D-CHA	2.22	1.46	1.38
25	7	307	CHL	C4D-CHA	2.22	1.46	1.38
25	1	605	CHL	C4D-CHA	2.22	1.46	1.38
25	5	605	CHL	C4D-CHA	2.22	1.46	1.38
22	4	303	CLA	C3D-C2D	2.21	1.45	1.39
22	8	303	CLA	C3D-C2D	2.21	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	616	CLA	CHD-C1D	2.21	1.42	1.38
22	B	612	CLA	CHD-C4C	2.21	1.44	1.39
22	N	613	CLA	O2D-CGD	2.21	1.38	1.33
22	n	613	CLA	O2D-CGD	2.21	1.38	1.33
22	4	311	CLA	C3D-C2D	2.21	1.45	1.39
22	8	311	CLA	C3D-C2D	2.21	1.45	1.39
22	N	610	CLA	O2D-CGD	2.21	1.38	1.33
22	n	610	CLA	O2D-CGD	2.21	1.38	1.33
22	4	310	CLA	CAA-C2A	2.21	1.58	1.54
22	8	310	CLA	CAA-C2A	2.21	1.58	1.54
22	1	611	CLA	C3D-C2D	2.21	1.45	1.39
22	5	611	CLA	C3D-C2D	2.21	1.45	1.39
22	G	604	CLA	C4C-C3C	2.21	1.48	1.45
22	g	604	CLA	C4C-C3C	2.21	1.48	1.45
22	N	614	CLA	C4C-C3C	2.21	1.48	1.45
22	n	614	CLA	C4C-C3C	2.21	1.48	1.45
22	B	605	CLA	CAA-C2A	2.20	1.58	1.54
22	Y	604	CLA	O2D-CGD	2.20	1.38	1.33
22	y	604	CLA	O2D-CGD	2.20	1.38	1.33
22	b	608	CLA	C1B-C2B	2.20	1.48	1.43
22	4	305	CLA	C3D-C2D	2.20	1.45	1.39
22	8	305	CLA	C3D-C2D	2.20	1.45	1.39
22	b	612	CLA	O2D-CGD	2.20	1.38	1.33
22	C	512	CLA	CMC-C2C	2.19	1.55	1.50
22	b	610	CLA	C3D-C2D	2.19	1.45	1.39
25	S	307	CHL	C4D-CHA	2.19	1.46	1.38
25	s	307	CHL	C4D-CHA	2.19	1.46	1.38
22	b	608	CLA	C3D-C2D	2.19	1.45	1.39
22	R	302	CLA	C3D-C2D	2.19	1.45	1.39
22	r	302	CLA	C3D-C2D	2.19	1.45	1.39
22	d	401	CLA	O2D-CGD	2.19	1.38	1.33
22	b	612	CLA	C4C-C3C	2.19	1.48	1.45
22	2	610	CLA	C3D-C2D	2.19	1.45	1.39
22	6	610	CLA	C3D-C2D	2.19	1.45	1.39
22	4	303	CLA	CAA-C2A	2.19	1.58	1.54
22	8	303	CLA	CAA-C2A	2.19	1.58	1.54
22	G	604	CLA	C3D-C2D	2.19	1.45	1.39
22	g	604	CLA	C3D-C2D	2.19	1.45	1.39
22	2	612	CLA	C3D-C2D	2.18	1.45	1.39
22	6	612	CLA	C3D-C2D	2.18	1.45	1.39
25	G	607	CHL	C4D-CHA	2.18	1.46	1.38
25	g	607	CHL	C4D-CHA	2.18	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	602	CLA	C3D-C2D	2.18	1.45	1.39
22	5	602	CLA	C3D-C2D	2.18	1.45	1.39
22	2	613	CLA	CAA-C2A	2.18	1.58	1.54
22	6	613	CLA	CAA-C2A	2.18	1.58	1.54
22	s	301	CLA	C4C-C3C	2.18	1.48	1.45
22	2	612	CLA	C4C-C3C	2.18	1.48	1.45
22	6	612	CLA	C4C-C3C	2.18	1.48	1.45
22	b	602	CLA	O2D-CGD	2.18	1.38	1.33
22	4	303	CLA	C4C-C3C	2.18	1.48	1.45
22	8	303	CLA	C4C-C3C	2.18	1.48	1.45
25	4	306	CHL	C4D-CHA	2.18	1.46	1.38
25	8	306	CHL	C4D-CHA	2.18	1.46	1.38
25	Y	605	CHL	C4D-ND	-2.18	1.34	1.37
25	y	605	CHL	C4D-ND	-2.18	1.34	1.37
25	1	607	CHL	C4D-CHA	2.18	1.46	1.38
25	5	607	CHL	C4D-CHA	2.18	1.46	1.38
22	2	611	CLA	C3D-C2D	2.18	1.45	1.39
22	6	611	CLA	C3D-C2D	2.18	1.45	1.39
22	c	506	CLA	C3D-C2D	2.18	1.45	1.39
22	b	616	CLA	C3D-C2D	2.17	1.45	1.39
22	1	612	CLA	CHD-C1D	2.17	1.42	1.38
22	5	612	CLA	CHD-C1D	2.17	1.42	1.38
22	c	503	CLA	O2D-CGD	2.17	1.38	1.33
22	2	602	CLA	C4C-C3C	2.17	1.48	1.45
22	6	602	CLA	C4C-C3C	2.17	1.48	1.45
22	C	505	CLA	O2D-CGD	2.17	1.38	1.33
22	C	511	CLA	CAA-C2A	2.17	1.58	1.54
22	B	604	CLA	CHD-C1D	2.17	1.42	1.38
22	b	615	CLA	C3D-C2D	2.17	1.45	1.39
22	b	608	CLA	O2D-CGD	2.17	1.38	1.33
25	4	307	CHL	C4D-CHA	2.17	1.46	1.38
25	8	307	CHL	C4D-CHA	2.17	1.46	1.38
25	G	609	CHL	C4D-CHA	2.17	1.46	1.38
25	g	609	CHL	C4D-CHA	2.17	1.46	1.38
22	B	609	CLA	C4C-C3C	2.17	1.48	1.45
22	3	314	CLA	CHD-C1D	2.16	1.42	1.38
22	7	314	CLA	CHD-C1D	2.16	1.42	1.38
22	2	603	CLA	C4C-C3C	2.16	1.48	1.45
22	6	603	CLA	C4C-C3C	2.16	1.48	1.45
22	D	401	CLA	C4C-C3C	2.16	1.48	1.45
25	1	606	CHL	C4D-CHA	2.16	1.46	1.38
25	5	606	CHL	C4D-CHA	2.16	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	604	CLA	CHD-C1D	2.16	1.42	1.38
22	6	604	CLA	CHD-C1D	2.16	1.42	1.38
22	3	303	CLA	C4C-C3C	2.16	1.48	1.45
22	7	303	CLA	C4C-C3C	2.16	1.48	1.45
25	1	601	CHL	C4D-CHA	2.16	1.46	1.38
25	5	601	CHL	C4D-CHA	2.16	1.46	1.38
22	1	614	CLA	C3D-C2D	2.16	1.45	1.39
22	5	614	CLA	C3D-C2D	2.16	1.45	1.39
22	3	314	CLA	CAA-C2A	2.16	1.58	1.54
22	7	314	CLA	CAA-C2A	2.16	1.58	1.54
22	b	610	CLA	CMC-C2C	2.16	1.55	1.50
22	C	505	CLA	C3D-C2D	2.15	1.45	1.39
22	Y	612	CLA	C3D-C2D	2.15	1.45	1.39
22	y	612	CLA	C3D-C2D	2.15	1.45	1.39
22	c	504	CLA	C4C-C3C	2.15	1.48	1.45
25	4	309	CHL	C4D-CHA	2.15	1.46	1.38
25	8	309	CHL	C4D-CHA	2.15	1.46	1.38
22	B	602	CLA	O2D-CGD	2.15	1.38	1.33
22	4	311	CLA	CHD-C1D	2.14	1.42	1.38
22	8	311	CLA	CHD-C1D	2.14	1.42	1.38
22	c	508	CLA	C1B-C2B	2.14	1.48	1.43
22	3	312	CLA	C4C-C3C	2.14	1.48	1.45
22	7	312	CLA	C4C-C3C	2.14	1.48	1.45
22	B	613	CLA	C4C-C3C	2.14	1.48	1.45
22	N	614	CLA	CHD-C1D	2.14	1.42	1.38
22	n	614	CLA	CHD-C1D	2.14	1.42	1.38
25	N	609	CHL	C4D-CHA	2.14	1.46	1.38
25	n	609	CHL	C4D-CHA	2.14	1.46	1.38
22	b	611	CLA	O2D-CGD	2.13	1.38	1.33
22	b	609	CLA	C4C-C3C	2.13	1.48	1.45
22	4	311	CLA	CMC-C2C	2.13	1.55	1.50
22	8	311	CLA	CMC-C2C	2.13	1.55	1.50
22	b	604	CLA	CHD-C1D	2.13	1.42	1.38
22	C	509	CLA	CMC-C2C	2.13	1.55	1.50
22	2	611	CLA	CMC-C2C	2.13	1.55	1.50
22	6	611	CLA	CMC-C2C	2.13	1.55	1.50
22	d	404	CLA	C3D-C2D	2.13	1.44	1.39
22	G	602	CLA	MG-NB	-2.13	2.01	2.05
22	g	602	CLA	MG-NB	-2.13	2.01	2.05
22	C	506	CLA	C3D-C2D	2.13	1.44	1.39
23	D	402	PHO	C4B-NB	-2.13	1.34	1.38
22	C	512	CLA	O2D-CGD	2.13	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	311	CLA	CMC-C2C	2.13	1.55	1.50
22	r	311	CLA	CMC-C2C	2.13	1.55	1.50
25	G	606	CHL	C4D-CHA	2.13	1.46	1.38
25	g	606	CHL	C4D-CHA	2.13	1.46	1.38
22	3	305	CLA	CMC-C2C	2.13	1.55	1.50
22	7	305	CLA	CMC-C2C	2.13	1.55	1.50
22	3	303	CLA	C3D-C2D	2.13	1.44	1.39
22	7	303	CLA	C3D-C2D	2.13	1.44	1.39
23	a	404	PHO	C4B-NB	-2.12	1.34	1.38
22	1	602	CLA	CAA-C2A	2.12	1.58	1.54
22	5	602	CLA	CAA-C2A	2.12	1.58	1.54
22	3	313	CLA	CMC-C2C	2.12	1.55	1.50
22	7	313	CLA	CMC-C2C	2.12	1.55	1.50
22	4	305	CLA	CAA-C2A	2.12	1.58	1.54
22	8	305	CLA	CAA-C2A	2.12	1.58	1.54
22	1	613	CLA	CHD-C1D	2.12	1.42	1.38
22	5	613	CLA	CHD-C1D	2.12	1.42	1.38
22	b	606	CLA	C3D-C2D	2.12	1.44	1.39
22	3	311	CLA	CMC-C2C	2.12	1.55	1.50
22	7	311	CLA	CMC-C2C	2.12	1.55	1.50
25	G	608	CHL	C4D-CHA	2.12	1.45	1.38
25	g	608	CHL	C4D-CHA	2.12	1.45	1.38
22	b	603	CLA	CHD-C1D	2.12	1.42	1.38
22	G	602	CLA	CAA-C2A	2.12	1.58	1.54
22	g	602	CLA	CAA-C2A	2.12	1.58	1.54
22	3	304	CLA	CMC-C2C	2.12	1.55	1.50
22	7	304	CLA	CMC-C2C	2.12	1.55	1.50
22	C	501	CLA	CHD-C1D	2.12	1.42	1.38
22	G	603	CLA	C3D-C2D	2.12	1.44	1.39
22	g	603	CLA	C3D-C2D	2.12	1.44	1.39
22	2	603	CLA	C3D-C2D	2.12	1.44	1.39
22	6	603	CLA	C3D-C2D	2.12	1.44	1.39
22	B	602	CLA	CHD-C4C	2.11	1.44	1.39
22	b	610	CLA	CHD-C1D	2.11	1.42	1.38
22	1	603	CLA	C3D-C2D	2.11	1.44	1.39
22	5	603	CLA	C3D-C2D	2.11	1.44	1.39
22	N	614	CLA	CAA-C2A	2.11	1.58	1.54
22	n	614	CLA	CAA-C2A	2.11	1.58	1.54
22	S	309	CLA	C4C-C3C	2.11	1.48	1.45
22	s	309	CLA	C4C-C3C	2.11	1.48	1.45
22	3	305	CLA	CHD-C1D	2.11	1.42	1.38
22	7	305	CLA	CHD-C1D	2.11	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	602	CLA	CAA-C2A	2.11	1.58	1.54
22	6	602	CLA	CAA-C2A	2.11	1.58	1.54
25	R	304	CHL	C4D-CHA	2.11	1.45	1.38
25	r	304	CHL	C4D-CHA	2.11	1.45	1.38
22	Y	613	CLA	CMC-C2C	2.11	1.55	1.50
22	y	613	CLA	CMC-C2C	2.11	1.55	1.50
22	d	404	CLA	C4C-C3C	2.11	1.48	1.45
22	a	402	CLA	O2D-CGD	2.11	1.38	1.33
22	B	603	CLA	O2D-CGD	2.11	1.38	1.33
25	3	301	CHL	C4D-CHA	2.11	1.45	1.38
25	7	301	CHL	C4D-CHA	2.11	1.45	1.38
22	d	401	CLA	C3D-C2D	2.10	1.44	1.39
22	b	613	CLA	C4C-C3C	2.10	1.48	1.45
22	B	607	CLA	C4C-C3C	2.10	1.48	1.45
22	1	614	CLA	CMC-C2C	2.10	1.55	1.50
22	2	602	CLA	CMC-C2C	2.10	1.55	1.50
22	5	614	CLA	CMC-C2C	2.10	1.55	1.50
22	6	602	CLA	CMC-C2C	2.10	1.55	1.50
25	R	306	CHL	C4D-CHA	2.10	1.45	1.38
25	r	306	CHL	C4D-CHA	2.10	1.45	1.38
25	4	302	CHL	C4D-CHA	2.10	1.45	1.38
25	8	302	CHL	C4D-CHA	2.10	1.45	1.38
22	3	311	CLA	CHD-C1D	2.10	1.42	1.38
22	7	311	CLA	CHD-C1D	2.10	1.42	1.38
22	c	511	CLA	C4C-C3C	2.10	1.48	1.45
22	S	312	CLA	C3D-C2D	2.10	1.44	1.39
22	s	312	CLA	C3D-C2D	2.10	1.44	1.39
22	C	511	CLA	C3D-C2D	2.10	1.44	1.39
22	3	303	CLA	CAA-C2A	2.10	1.58	1.54
22	7	303	CLA	CAA-C2A	2.10	1.58	1.54
22	B	611	CLA	O2D-CGD	2.10	1.38	1.33
22	4	301	CLA	CMC-C2C	2.09	1.55	1.50
22	8	301	CLA	CMC-C2C	2.09	1.55	1.50
22	3	310	CLA	C1C-C2C	2.09	1.48	1.44
22	7	310	CLA	C1C-C2C	2.09	1.48	1.44
22	B	610	CLA	O2D-CGD	2.09	1.38	1.33
22	4	305	CLA	CMC-C2C	2.09	1.55	1.50
22	8	305	CLA	CMC-C2C	2.09	1.55	1.50
22	S	311	CLA	O2D-CGD	2.09	1.38	1.33
22	s	311	CLA	O2D-CGD	2.09	1.38	1.33
22	S	310	CLA	CAA-C2A	2.09	1.58	1.54
22	s	310	CLA	CAA-C2A	2.09	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	310	CLA	C3D-C2D	2.09	1.44	1.39
22	8	310	CLA	C3D-C2D	2.09	1.44	1.39
22	A	403	CLA	CAA-C2A	2.09	1.58	1.54
22	2	612	CLA	CMC-C2C	2.09	1.55	1.50
22	6	612	CLA	CMC-C2C	2.09	1.55	1.50
22	G	614	CLA	CAA-C2A	2.09	1.58	1.54
22	g	614	CLA	CAA-C2A	2.09	1.58	1.54
22	S	313	CLA	C3D-C2D	2.09	1.44	1.39
22	s	313	CLA	C3D-C2D	2.09	1.44	1.39
22	b	612	CLA	CMC-C2C	2.09	1.55	1.50
22	3	303	CLA	CMC-C2C	2.09	1.55	1.50
22	7	303	CLA	CMC-C2C	2.09	1.55	1.50
22	s	301	CLA	C3D-C2D	2.09	1.44	1.39
22	c	512	CLA	C4C-C3C	2.09	1.48	1.45
22	2	609	CLA	C1C-C2C	2.09	1.48	1.44
22	6	609	CLA	C1C-C2C	2.09	1.48	1.44
22	1	612	CLA	CMC-C2C	2.08	1.55	1.50
22	5	612	CLA	CMC-C2C	2.08	1.55	1.50
22	2	610	CLA	C4C-C3C	2.08	1.48	1.45
22	6	610	CLA	C4C-C3C	2.08	1.48	1.45
22	B	608	CLA	CAA-C2A	2.08	1.58	1.54
22	4	301	CLA	C3D-C2D	2.08	1.44	1.39
22	8	301	CLA	C3D-C2D	2.08	1.44	1.39
22	c	510	CLA	CMC-C2C	2.08	1.55	1.50
22	c	508	CLA	C3D-C2D	2.08	1.44	1.39
22	A	405	CLA	C4C-C3C	2.08	1.48	1.45
22	1	613	CLA	CMC-C2C	2.08	1.55	1.50
22	5	613	CLA	CMC-C2C	2.08	1.55	1.50
22	b	606	CLA	CAA-C2A	2.08	1.58	1.54
22	R	307	CLA	C4C-C3C	2.08	1.48	1.45
22	r	307	CLA	C4C-C3C	2.08	1.48	1.45
22	c	502	CLA	C3D-C2D	2.08	1.44	1.39
22	1	611	CLA	CMC-C2C	2.08	1.55	1.50
22	5	611	CLA	CMC-C2C	2.08	1.55	1.50
22	1	614	CLA	CAA-C2A	2.08	1.58	1.54
22	5	614	CLA	CAA-C2A	2.08	1.58	1.54
22	N	611	CLA	C3D-C2D	2.08	1.44	1.39
22	n	611	CLA	C3D-C2D	2.08	1.44	1.39
22	B	604	CLA	C4C-C3C	2.08	1.48	1.45
25	S	306	CHL	C4D-CHA	2.07	1.45	1.38
25	s	306	CHL	C4D-CHA	2.07	1.45	1.38
22	c	512	CLA	CMC-C2C	2.07	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	610	CLA	C3D-C2D	2.07	1.44	1.39
22	5	610	CLA	C3D-C2D	2.07	1.44	1.39
22	2	603	CLA	CHD-C1D	2.07	1.42	1.38
22	6	603	CLA	CHD-C1D	2.07	1.42	1.38
22	3	310	CLA	C3D-C2D	2.07	1.44	1.39
22	7	310	CLA	C3D-C2D	2.07	1.44	1.39
25	Y	609	CHL	C4D-CHA	2.07	1.45	1.38
25	y	609	CHL	C4D-CHA	2.07	1.45	1.38
22	c	506	CLA	CMC-C2C	2.07	1.55	1.50
22	3	313	CLA	CHD-C1D	2.07	1.42	1.38
22	7	313	CLA	CHD-C1D	2.07	1.42	1.38
22	2	610	CLA	CMC-C2C	2.07	1.55	1.50
22	4	304	CLA	CMC-C2C	2.07	1.55	1.50
22	6	610	CLA	CMC-C2C	2.07	1.55	1.50
22	8	304	CLA	CMC-C2C	2.07	1.55	1.50
24	e	101	HEM	CMA-C3A	2.07	1.55	1.50
22	B	612	CLA	O2D-CGD	2.07	1.38	1.33
22	1	603	CLA	CMC-C2C	2.07	1.55	1.50
22	5	603	CLA	CMC-C2C	2.07	1.55	1.50
22	1	603	CLA	CHD-C1D	2.07	1.42	1.38
22	5	603	CLA	CHD-C1D	2.07	1.42	1.38
22	3	314	CLA	CMC-C2C	2.07	1.55	1.50
22	7	314	CLA	CMC-C2C	2.07	1.55	1.50
22	B	613	CLA	C3D-C2D	2.07	1.44	1.39
22	N	614	CLA	CMC-C2C	2.07	1.55	1.50
22	n	614	CLA	CMC-C2C	2.07	1.55	1.50
25	R	305	CHL	C4D-CHA	2.07	1.45	1.38
25	r	305	CHL	C4D-CHA	2.07	1.45	1.38
22	d	403	CLA	O2D-CGD	2.07	1.38	1.33
22	R	301	CLA	C3D-C2D	2.06	1.44	1.39
22	r	301	CLA	C3D-C2D	2.06	1.44	1.39
22	4	303	CLA	CHB-C1B	2.06	1.44	1.39
22	8	303	CLA	CHB-C1B	2.06	1.44	1.39
22	G	612	CLA	CMC-C2C	2.06	1.55	1.50
22	g	612	CLA	CMC-C2C	2.06	1.55	1.50
22	a	402	CLA	C4C-C3C	2.06	1.48	1.45
22	b	609	CLA	CMC-C2C	2.06	1.55	1.50
23	a	404	PHO	C1D-ND	-2.06	1.34	1.38
22	C	501	CLA	CMC-C2C	2.06	1.55	1.50
25	Y	608	CHL	C4D-CHA	2.06	1.45	1.38
25	y	608	CHL	C4D-CHA	2.06	1.45	1.38
22	4	310	CLA	CHB-C1B	2.06	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	310	CLA	CHB-C1B	2.06	1.44	1.39
22	4	304	CLA	CHD-C1D	2.06	1.42	1.38
22	8	304	CLA	CHD-C1D	2.06	1.42	1.38
22	N	613	CLA	C4C-C3C	2.06	1.48	1.45
22	n	613	CLA	C4C-C3C	2.06	1.48	1.45
22	b	605	CLA	C3D-C2D	2.06	1.44	1.39
22	b	612	CLA	C3D-C2D	2.06	1.44	1.39
22	c	511	CLA	CAA-C2A	2.06	1.57	1.54
22	c	504	CLA	C3D-C2D	2.06	1.44	1.39
22	s	301	CLA	CMC-C2C	2.05	1.55	1.50
22	2	604	CLA	CMC-C2C	2.05	1.55	1.50
22	2	613	CLA	CMC-C2C	2.05	1.55	1.50
22	6	604	CLA	CMC-C2C	2.05	1.55	1.50
22	6	613	CLA	CMC-C2C	2.05	1.55	1.50
22	D	404	CLA	C4C-C3C	2.05	1.48	1.45
22	B	604	CLA	C3D-C2D	2.05	1.44	1.39
22	2	602	CLA	CHD-C1D	2.05	1.42	1.38
22	6	602	CLA	CHD-C1D	2.05	1.42	1.38
22	2	613	CLA	C3D-C2D	2.05	1.44	1.39
22	6	613	CLA	C3D-C2D	2.05	1.44	1.39
22	b	614	CLA	C3D-C2D	2.05	1.44	1.39
22	D	401	CLA	O2D-CGD	2.05	1.38	1.33
22	G	614	CLA	CMC-C2C	2.05	1.55	1.50
22	g	614	CLA	CMC-C2C	2.05	1.55	1.50
22	C	504	CLA	C4C-C3C	2.05	1.48	1.45
22	S	304	CLA	C3D-C2D	2.05	1.44	1.39
22	s	304	CLA	C3D-C2D	2.05	1.44	1.39
22	G	602	CLA	C3D-C2D	2.05	1.44	1.39
22	g	602	CLA	C3D-C2D	2.05	1.44	1.39
22	C	504	CLA	C3D-C2D	2.05	1.44	1.39
22	G	614	CLA	C3D-C2D	2.04	1.44	1.39
22	g	614	CLA	C3D-C2D	2.04	1.44	1.39
22	c	505	CLA	O2D-CGD	2.04	1.38	1.33
25	S	308	CHL	C4D-CHA	2.04	1.45	1.38
25	s	308	CHL	C4D-CHA	2.04	1.45	1.38
22	C	512	CLA	C3D-C2D	2.04	1.44	1.39
22	b	614	CLA	C4C-C3C	2.04	1.48	1.45
22	c	502	CLA	CAA-C2A	2.04	1.57	1.54
22	C	510	CLA	C4C-C3C	2.04	1.48	1.45
22	b	603	CLA	CMC-C2C	2.04	1.55	1.50
22	B	609	CLA	MG-NB	-2.04	2.01	2.05
22	b	612	CLA	CMA-C3A	-2.04	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	510	CLA	CMC-C2C	2.04	1.55	1.50
22	G	603	CLA	CHD-C1D	2.04	1.42	1.38
22	g	603	CLA	CHD-C1D	2.04	1.42	1.38
22	3	312	CLA	CMC-C2C	2.04	1.55	1.50
22	7	312	CLA	CMC-C2C	2.04	1.55	1.50
22	B	615	CLA	C3D-C2D	2.04	1.44	1.39
22	C	509	CLA	C3D-C2D	2.04	1.44	1.39
22	G	602	CLA	CMC-C2C	2.04	1.55	1.50
22	g	602	CLA	CMC-C2C	2.04	1.55	1.50
25	N	601	CHL	C4D-CHA	2.03	1.45	1.38
25	n	601	CHL	C4D-CHA	2.03	1.45	1.38
22	C	509	CLA	O2D-CGD	2.03	1.38	1.33
22	G	603	CLA	CMC-C2C	2.03	1.55	1.50
22	g	603	CLA	CMC-C2C	2.03	1.55	1.50
22	A	403	CLA	C4C-C3C	2.03	1.48	1.45
22	Y	604	CLA	MG-NB	-2.03	2.01	2.05
22	y	604	CLA	MG-NB	-2.03	2.01	2.05
22	2	603	CLA	CMC-C2C	2.03	1.55	1.50
22	6	603	CLA	CMC-C2C	2.03	1.55	1.50
22	3	312	CLA	CHD-C1D	2.03	1.42	1.38
22	7	312	CLA	CHD-C1D	2.03	1.42	1.38
25	N	606	CHL	C4D-CHA	2.03	1.45	1.38
25	n	606	CHL	C4D-CHA	2.03	1.45	1.38
22	b	608	CLA	C4C-C3C	2.03	1.48	1.45
22	b	605	CLA	C4C-C3C	2.03	1.48	1.45
25	N	605	CHL	C4D-CHA	2.03	1.45	1.38
25	n	605	CHL	C4D-CHA	2.03	1.45	1.38
22	S	305	CLA	C3D-C2D	2.03	1.44	1.39
22	s	305	CLA	C3D-C2D	2.03	1.44	1.39
22	G	604	CLA	CAA-C2A	2.03	1.57	1.54
22	g	604	CLA	CAA-C2A	2.03	1.57	1.54
22	2	602	CLA	C3D-C2D	2.03	1.44	1.39
22	6	602	CLA	C3D-C2D	2.03	1.44	1.39
22	S	301	CLA	C4C-C3C	2.03	1.48	1.45
22	b	615	CLA	CMC-C2C	2.03	1.55	1.50
22	4	303	CLA	CMC-C2C	2.03	1.55	1.50
22	8	303	CLA	CMC-C2C	2.03	1.55	1.50
22	C	508	CLA	C3D-C2D	2.02	1.44	1.39
22	b	601	CLA	C3D-C2D	2.02	1.44	1.39
22	D	404	CLA	C3D-C2D	2.02	1.44	1.39
22	b	615	CLA	CHD-C1D	2.02	1.42	1.38
22	c	512	CLA	C3D-C2D	2.02	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	402	CLA	CMC-C2C	2.02	1.55	1.50
22	1	604	CLA	CHD-C1D	2.02	1.42	1.38
22	5	604	CLA	CHD-C1D	2.02	1.42	1.38
22	C	510	CLA	C3D-C2D	2.02	1.44	1.39
22	C	508	CLA	MG-NB	-2.02	2.01	2.05
25	S	302	CHL	C4D-ND	-2.02	1.34	1.37
25	s	302	CHL	C4D-ND	-2.02	1.34	1.37
22	R	309	CLA	C3D-C2D	2.02	1.44	1.39
22	r	309	CLA	C3D-C2D	2.02	1.44	1.39
25	Y	607	CHL	C4D-CHA	2.02	1.45	1.38
25	y	607	CHL	C4D-CHA	2.02	1.45	1.38
22	c	505	CLA	C3D-C2D	2.02	1.44	1.39
22	N	612	CLA	CMC-C2C	2.02	1.55	1.50
22	n	612	CLA	CMC-C2C	2.02	1.55	1.50
22	R	311	CLA	C3D-C2D	2.01	1.44	1.39
22	r	311	CLA	C3D-C2D	2.01	1.44	1.39
22	A	403	CLA	CMC-C2C	2.01	1.55	1.50
22	c	511	CLA	CHD-C1D	2.01	1.42	1.38
22	1	604	CLA	CMC-C2C	2.01	1.55	1.50
22	5	604	CLA	CMC-C2C	2.01	1.55	1.50
22	b	604	CLA	C3D-C2D	2.01	1.44	1.39
22	R	307	CLA	CAA-C2A	2.01	1.57	1.54
22	r	307	CLA	CAA-C2A	2.01	1.57	1.54
22	4	305	CLA	CHD-C1D	2.01	1.42	1.38
22	8	305	CLA	CHD-C1D	2.01	1.42	1.38
22	1	610	CLA	C4C-C3C	2.01	1.48	1.45
22	5	610	CLA	C4C-C3C	2.01	1.48	1.45
22	b	613	CLA	CMC-C2C	2.01	1.55	1.50
22	1	602	CLA	CHD-C1D	2.01	1.42	1.38
22	5	602	CLA	CHD-C1D	2.01	1.42	1.38
22	B	608	CLA	CMC-C2C	2.01	1.55	1.50
22	B	610	CLA	CMC-C2C	2.01	1.55	1.50
22	B	616	CLA	CMC-C2C	2.01	1.55	1.50
23	A	404	PHO	C4B-NB	-2.01	1.34	1.38
22	1	611	CLA	CHD-C1D	2.01	1.42	1.38
22	5	611	CLA	CHD-C1D	2.01	1.42	1.38
22	c	510	CLA	C3D-C2D	2.01	1.44	1.39
22	2	611	CLA	C4C-C3C	2.01	1.48	1.45
22	6	611	CLA	C4C-C3C	2.01	1.48	1.45
22	c	510	CLA	MG-NB	-2.01	2.01	2.05
22	B	610	CLA	CHD-C1D	2.00	1.42	1.38
22	N	613	CLA	C3D-C2D	2.00	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	n	613	CLA	C3D-C2D	2.00	1.44	1.39
22	C	509	CLA	C4C-C3C	2.00	1.48	1.45
22	R	310	CLA	C4C-C3C	2.00	1.48	1.45
22	r	310	CLA	C4C-C3C	2.00	1.48	1.45
25	4	308	CHL	CBD-CGD	2.00	1.58	1.52
25	8	308	CHL	CBD-CGD	2.00	1.58	1.52
22	C	507	CLA	C3D-C2D	2.00	1.44	1.39
22	R	310	CLA	CMC-C2C	2.00	1.55	1.50
22	r	310	CLA	CMC-C2C	2.00	1.55	1.50

All (7011) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	307	CHL	O2D-CGD-CBD	28.05	161.12	111.27
25	s	307	CHL	O2D-CGD-CBD	28.05	161.12	111.27
25	4	308	CHL	O2D-CGD-CBD	27.92	160.89	111.27
25	8	308	CHL	O2D-CGD-CBD	27.92	160.89	111.27
25	S	307	CHL	O2D-CGD-O1D	-23.93	77.05	123.84
25	s	307	CHL	O2D-CGD-O1D	-23.93	77.05	123.84
25	4	308	CHL	O2D-CGD-O1D	-23.25	78.38	123.84
25	8	308	CHL	O2D-CGD-O1D	-23.25	78.38	123.84
25	4	308	CHL	O1D-CGD-CBD	-20.52	82.50	124.48
25	8	308	CHL	O1D-CGD-CBD	-20.52	82.50	124.48
25	S	307	CHL	O1D-CGD-CBD	-19.75	84.07	124.48
25	s	307	CHL	O1D-CGD-CBD	-19.75	84.07	124.48
23	A	404	PHO	C2D-C1D-ND	12.17	117.93	109.53
25	G	609	CHL	C4A-NA-C1A	10.51	111.43	106.71
25	g	609	CHL	C4A-NA-C1A	10.51	111.43	106.71
25	N	609	CHL	C4A-NA-C1A	10.45	111.41	106.71
25	n	609	CHL	C4A-NA-C1A	10.45	111.41	106.71
25	3	309	CHL	C4A-NA-C1A	10.40	111.38	106.71
25	7	309	CHL	C4A-NA-C1A	10.40	111.38	106.71
22	B	604	CLA	C2C-C1C-NC	10.21	119.54	109.97
25	Y	609	CHL	C4A-NA-C1A	10.18	111.28	106.71
25	y	609	CHL	C4A-NA-C1A	10.18	111.28	106.71
23	a	404	PHO	C2D-C1D-ND	9.95	116.40	109.53
23	D	402	PHO	C2D-C1D-ND	9.62	116.17	109.53
25	1	609	CHL	C4A-NA-C1A	9.60	111.02	106.71
25	5	609	CHL	C4A-NA-C1A	9.60	111.02	106.71
22	C	508	CLA	C2C-C1C-NC	9.57	118.94	109.97
22	C	506	CLA	C2C-C1C-NC	9.53	118.90	109.97
23	d	402	PHO	C2D-C1D-ND	9.48	116.07	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	616	CLA	C2C-C1C-NC	9.25	118.64	109.97
22	c	507	CLA	C2C-C1C-NC	9.19	118.58	109.97
22	c	506	CLA	C2C-C1C-NC	9.19	118.58	109.97
25	2	608	CHL	C4A-NA-C1A	9.10	110.80	106.71
25	6	608	CHL	C4A-NA-C1A	9.10	110.80	106.71
22	b	609	CLA	C2C-C1C-NC	9.08	118.48	109.97
22	C	501	CLA	C2C-C1C-NC	9.05	118.45	109.97
22	c	508	CLA	C2C-C1C-NC	9.04	118.44	109.97
22	C	510	CLA	C2C-C1C-NC	9.04	118.44	109.97
22	c	501	CLA	C2C-C1C-NC	9.04	118.44	109.97
22	B	608	CLA	C2C-C1C-NC	9.03	118.43	109.97
25	N	607	CHL	C4A-NA-C1A	8.94	110.72	106.71
25	n	607	CHL	C4A-NA-C1A	8.94	110.72	106.71
22	Y	613	CLA	C2C-C1C-NC	8.93	118.34	109.97
22	y	613	CLA	C2C-C1C-NC	8.93	118.34	109.97
22	c	512	CLA	C2C-C1C-NC	8.92	118.33	109.97
22	b	616	CLA	C2C-C1C-NC	8.91	118.31	109.97
25	Y	605	CHL	C4A-NA-C1A	8.87	110.69	106.71
25	y	605	CHL	C4A-NA-C1A	8.87	110.69	106.71
22	b	613	CLA	C2C-C1C-NC	8.87	118.28	109.97
22	C	504	CLA	C2C-C1C-NC	8.85	118.26	109.97
22	B	607	CLA	C2C-C1C-NC	8.85	118.26	109.97
22	4	303	CLA	C2C-C1C-NC	8.84	118.25	109.97
22	8	303	CLA	C2C-C1C-NC	8.84	118.25	109.97
22	b	610	CLA	C2C-C1C-NC	8.81	118.22	109.97
22	C	511	CLA	C2C-C1C-NC	8.72	118.14	109.97
25	3	306	CHL	C4A-NA-C1A	8.70	110.62	106.71
25	7	306	CHL	C4A-NA-C1A	8.70	110.62	106.71
22	Y	604	CLA	C2C-C1C-NC	8.69	118.11	109.97
22	y	604	CLA	C2C-C1C-NC	8.69	118.11	109.97
25	N	601	CHL	C4A-NA-C1A	8.67	110.60	106.71
25	n	601	CHL	C4A-NA-C1A	8.67	110.60	106.71
22	S	312	CLA	C2C-C1C-NC	8.66	118.09	109.97
22	s	312	CLA	C2C-C1C-NC	8.66	118.09	109.97
25	G	601	CHL	C4A-NA-C1A	8.63	110.58	106.71
25	g	601	CHL	C4A-NA-C1A	8.63	110.58	106.71
22	b	604	CLA	C2C-C1C-NC	8.61	118.04	109.97
22	a	405	CLA	C2C-C1C-NC	8.60	118.03	109.97
22	1	614	CLA	C2C-C1C-NC	8.60	118.03	109.97
22	5	614	CLA	C2C-C1C-NC	8.60	118.03	109.97
25	2	601	CHL	C4A-NA-C1A	8.59	110.57	106.71
25	6	601	CHL	C4A-NA-C1A	8.59	110.57	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	615	CLA	C2C-C1C-NC	8.58	118.01	109.97
22	C	507	CLA	C2C-C1C-NC	8.57	118.00	109.97
22	D	401	CLA	C2C-C1C-NC	8.57	118.00	109.97
22	S	314	CLA	C2C-C1C-NC	8.56	117.99	109.97
22	s	314	CLA	C2C-C1C-NC	8.56	117.99	109.97
22	d	403	CLA	C2C-C1C-NC	8.51	117.94	109.97
22	N	613	CLA	C2C-C1C-NC	8.51	117.94	109.97
22	n	613	CLA	C2C-C1C-NC	8.51	117.94	109.97
22	G	604	CLA	C2C-C1C-NC	8.51	117.94	109.97
22	g	604	CLA	C2C-C1C-NC	8.51	117.94	109.97
22	B	612	CLA	C2C-C1C-NC	8.49	117.92	109.97
22	N	602	CLA	C2C-C1C-NC	8.46	117.89	109.97
22	n	602	CLA	C2C-C1C-NC	8.46	117.89	109.97
22	b	607	CLA	C2C-C1C-NC	8.45	117.89	109.97
22	S	309	CLA	C2C-C1C-NC	8.45	117.89	109.97
22	s	309	CLA	C2C-C1C-NC	8.45	117.89	109.97
22	G	613	CLA	C2C-C1C-NC	8.45	117.89	109.97
22	g	613	CLA	C2C-C1C-NC	8.45	117.89	109.97
22	B	610	CLA	C2C-C1C-NC	8.43	117.87	109.97
25	2	605	CHL	C4A-NA-C1A	8.43	110.49	106.71
25	6	605	CHL	C4A-NA-C1A	8.43	110.49	106.71
22	2	612	CLA	C2C-C1C-NC	8.42	117.86	109.97
22	6	612	CLA	C2C-C1C-NC	8.42	117.86	109.97
22	S	301	CLA	C2C-C1C-NC	8.40	117.84	109.97
25	N	605	CHL	C4A-NA-C1A	8.39	110.48	106.71
25	n	605	CHL	C4A-NA-C1A	8.39	110.48	106.71
22	Y	602	CLA	C2C-C1C-NC	8.38	117.82	109.97
22	y	602	CLA	C2C-C1C-NC	8.38	117.82	109.97
22	c	510	CLA	C2C-C1C-NC	8.37	117.81	109.97
22	c	502	CLA	C2C-C1C-NC	8.35	117.79	109.97
22	B	609	CLA	C2C-C1C-NC	8.34	117.78	109.97
22	A	405	CLA	C2C-C1C-NC	8.34	117.78	109.97
22	C	505	CLA	C2C-C1C-NC	8.32	117.77	109.97
22	c	503	CLA	C2C-C1C-NC	8.31	117.76	109.97
22	D	403	CLA	C2C-C1C-NC	8.31	117.75	109.97
22	3	313	CLA	C2C-C1C-NC	8.29	117.74	109.97
22	7	313	CLA	C2C-C1C-NC	8.29	117.74	109.97
22	B	605	CLA	C2C-C1C-NC	8.28	117.73	109.97
22	N	611	CLA	C2C-C1C-NC	8.27	117.72	109.97
22	n	611	CLA	C2C-C1C-NC	8.27	117.72	109.97
22	1	611	CLA	C2C-C1C-NC	8.27	117.72	109.97
22	5	611	CLA	C2C-C1C-NC	8.27	117.72	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	603	CLA	C2C-C1C-NC	8.26	117.71	109.97
22	N	612	CLA	C2C-C1C-NC	8.26	117.71	109.97
22	n	612	CLA	C2C-C1C-NC	8.26	117.71	109.97
22	D	404	CLA	C2C-C1C-NC	8.24	117.69	109.97
22	b	603	CLA	C2C-C1C-NC	8.23	117.68	109.97
22	G	602	CLA	C2C-C1C-NC	8.23	117.68	109.97
22	g	602	CLA	C2C-C1C-NC	8.23	117.68	109.97
22	Y	614	CLA	C2C-C1C-NC	8.21	117.66	109.97
22	y	614	CLA	C2C-C1C-NC	8.21	117.66	109.97
22	c	511	CLA	C2C-C1C-NC	8.20	117.65	109.97
22	c	504	CLA	C2C-C1C-NC	8.18	117.64	109.97
25	4	309	CHL	C4A-NA-C1A	8.17	110.38	106.71
25	8	309	CHL	C4A-NA-C1A	8.17	110.38	106.71
22	B	602	CLA	C2C-C1C-NC	8.17	117.63	109.97
22	1	604	CLA	C2C-C1C-NC	8.16	117.62	109.97
22	5	604	CLA	C2C-C1C-NC	8.16	117.62	109.97
22	3	312	CLA	C2C-C1C-NC	8.16	117.62	109.97
22	7	312	CLA	C2C-C1C-NC	8.16	117.62	109.97
25	Y	607	CHL	C4A-NA-C1A	8.15	110.37	106.71
25	y	607	CHL	C4A-NA-C1A	8.15	110.37	106.71
22	1	602	CLA	C2C-C1C-NC	8.15	117.61	109.97
22	5	602	CLA	C2C-C1C-NC	8.15	117.61	109.97
22	R	309	CLA	C2C-C1C-NC	8.14	117.60	109.97
22	r	309	CLA	C2C-C1C-NC	8.14	117.60	109.97
22	G	612	CLA	C2C-C1C-NC	8.14	117.60	109.97
22	g	612	CLA	C2C-C1C-NC	8.14	117.60	109.97
22	G	603	CLA	C2C-C1C-NC	8.14	117.59	109.97
22	g	603	CLA	C2C-C1C-NC	8.14	117.59	109.97
22	1	613	CLA	C2C-C1C-NC	8.13	117.59	109.97
22	5	613	CLA	C2C-C1C-NC	8.13	117.59	109.97
22	R	311	CLA	C2C-C1C-NC	8.13	117.59	109.97
22	r	311	CLA	C2C-C1C-NC	8.13	117.59	109.97
22	1	603	CLA	C2C-C1C-NC	8.12	117.58	109.97
22	5	603	CLA	C2C-C1C-NC	8.12	117.58	109.97
22	Y	611	CLA	C2C-C1C-NC	8.12	117.58	109.97
22	y	611	CLA	C2C-C1C-NC	8.12	117.58	109.97
22	2	602	CLA	C2C-C1C-NC	8.12	117.58	109.97
22	6	602	CLA	C2C-C1C-NC	8.12	117.58	109.97
22	Y	612	CLA	C2C-C1C-NC	8.11	117.57	109.97
22	y	612	CLA	C2C-C1C-NC	8.11	117.57	109.97
22	4	305	CLA	C2C-C1C-NC	8.10	117.56	109.97
22	8	305	CLA	C2C-C1C-NC	8.10	117.56	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	305	CLA	C2C-C1C-NC	8.10	117.56	109.97
22	7	305	CLA	C2C-C1C-NC	8.10	117.56	109.97
22	a	403	CLA	C2C-C1C-NC	8.09	117.56	109.97
22	G	611	CLA	C2C-C1C-NC	8.09	117.55	109.97
22	g	611	CLA	C2C-C1C-NC	8.09	117.55	109.97
22	4	311	CLA	C2C-C1C-NC	8.08	117.54	109.97
22	8	311	CLA	C2C-C1C-NC	8.08	117.54	109.97
25	G	607	CHL	C4A-NA-C1A	8.08	110.34	106.71
25	g	607	CHL	C4A-NA-C1A	8.08	110.34	106.71
22	2	604	CLA	C2C-C1C-NC	8.08	117.54	109.97
22	6	604	CLA	C2C-C1C-NC	8.08	117.54	109.97
22	3	311	CLA	C2C-C1C-NC	8.06	117.52	109.97
22	7	311	CLA	C2C-C1C-NC	8.06	117.52	109.97
22	S	311	CLA	C2C-C1C-NC	8.06	117.52	109.97
22	s	311	CLA	C2C-C1C-NC	8.06	117.52	109.97
22	R	307	CLA	C2C-C1C-NC	8.05	117.52	109.97
22	r	307	CLA	C2C-C1C-NC	8.05	117.52	109.97
22	N	604	CLA	C2C-C1C-NC	8.05	117.52	109.97
22	n	604	CLA	C2C-C1C-NC	8.05	117.52	109.97
22	Y	603	CLA	C2C-C1C-NC	8.05	117.52	109.97
22	y	603	CLA	C2C-C1C-NC	8.05	117.52	109.97
22	4	304	CLA	C2C-C1C-NC	8.05	117.51	109.97
22	8	304	CLA	C2C-C1C-NC	8.05	117.51	109.97
22	S	305	CLA	C2C-C1C-NC	8.04	117.50	109.97
22	s	305	CLA	C2C-C1C-NC	8.04	117.50	109.97
22	C	509	CLA	C2C-C1C-NC	8.03	117.50	109.97
25	G	605	CHL	C4A-NA-C1A	8.03	110.32	106.71
25	g	605	CHL	C4A-NA-C1A	8.03	110.32	106.71
22	N	603	CLA	C2C-C1C-NC	8.03	117.49	109.97
22	n	603	CLA	C2C-C1C-NC	8.03	117.49	109.97
22	R	303	CLA	C2C-C1C-NC	8.02	117.48	109.97
22	r	303	CLA	C2C-C1C-NC	8.02	117.48	109.97
22	D	403	CLA	CAC-C3C-C4C	8.01	135.21	124.81
22	d	401	CLA	C2C-C1C-NC	8.01	117.47	109.97
22	b	602	CLA	C2C-C1C-NC	8.01	117.47	109.97
22	b	614	CLA	C2C-C1C-NC	8.00	117.47	109.97
22	Y	610	CLA	C2C-C1C-NC	8.00	117.46	109.97
22	y	610	CLA	C2C-C1C-NC	8.00	117.46	109.97
22	c	505	CLA	C2C-C1C-NC	7.98	117.45	109.97
22	a	402	CLA	C2C-C1C-NC	7.98	117.45	109.97
25	1	601	CHL	C4A-NA-C1A	7.97	110.29	106.71
25	5	601	CHL	C4A-NA-C1A	7.97	110.29	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	310	CLA	C2C-C1C-NC	7.97	117.44	109.97
22	s	310	CLA	C2C-C1C-NC	7.97	117.44	109.97
22	2	610	CLA	C2C-C1C-NC	7.95	117.42	109.97
22	3	303	CLA	C2C-C1C-NC	7.95	117.42	109.97
22	6	610	CLA	C2C-C1C-NC	7.95	117.42	109.97
22	7	303	CLA	C2C-C1C-NC	7.95	117.42	109.97
22	4	301	CLA	C2C-C1C-NC	7.94	117.41	109.97
22	8	301	CLA	C2C-C1C-NC	7.94	117.41	109.97
22	3	304	CLA	C2C-C1C-NC	7.94	117.41	109.97
22	7	304	CLA	C2C-C1C-NC	7.94	117.41	109.97
22	C	512	CLA	C2C-C1C-NC	7.93	117.40	109.97
22	2	603	CLA	C2C-C1C-NC	7.93	117.40	109.97
22	6	603	CLA	C2C-C1C-NC	7.93	117.40	109.97
22	1	612	CLA	C2C-C1C-NC	7.92	117.39	109.97
22	5	612	CLA	C2C-C1C-NC	7.92	117.39	109.97
22	d	404	CLA	C2C-C1C-NC	7.87	117.34	109.97
22	C	503	CLA	C2C-C1C-NC	7.87	117.34	109.97
22	N	614	CLA	C2C-C1C-NC	7.86	117.33	109.97
22	n	614	CLA	C2C-C1C-NC	7.86	117.33	109.97
22	B	614	CLA	C2C-C1C-NC	7.85	117.33	109.97
25	S	308	CHL	C4A-NA-C1A	7.84	110.23	106.71
25	s	308	CHL	C4A-NA-C1A	7.84	110.23	106.71
22	d	403	CLA	CAC-C3C-C4C	7.82	134.95	124.81
22	A	403	CLA	C2C-C1C-NC	7.81	117.29	109.97
22	R	301	CLA	C2C-C1C-NC	7.80	117.28	109.97
22	r	301	CLA	C2C-C1C-NC	7.80	117.28	109.97
25	1	605	CHL	C4A-NA-C1A	7.80	110.21	106.71
25	5	605	CHL	C4A-NA-C1A	7.80	110.21	106.71
23	A	404	PHO	C4D-ND-C1D	-7.79	100.91	108.83
22	2	613	CLA	C2C-C1C-NC	7.78	117.26	109.97
22	6	613	CLA	C2C-C1C-NC	7.78	117.26	109.97
22	S	303	CLA	C2C-C1C-NC	7.78	117.26	109.97
22	s	303	CLA	C2C-C1C-NC	7.78	117.26	109.97
22	S	313	CLA	C2C-C1C-NC	7.75	117.24	109.97
22	s	313	CLA	C2C-C1C-NC	7.75	117.24	109.97
25	3	302	CHL	C4A-NA-C1A	7.75	110.19	106.71
25	7	302	CHL	C4A-NA-C1A	7.75	110.19	106.71
22	R	310	CLA	C2C-C1C-NC	7.73	117.22	109.97
22	r	310	CLA	C2C-C1C-NC	7.73	117.22	109.97
22	2	611	CLA	C2C-C1C-NC	7.71	117.19	109.97
22	6	611	CLA	C2C-C1C-NC	7.71	117.19	109.97
22	b	611	CLA	C2C-C1C-NC	7.70	117.19	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	614	CLA	C2C-C1C-NC	7.70	117.18	109.97
22	g	614	CLA	C2C-C1C-NC	7.70	117.18	109.97
22	A	402	CLA	C2C-C1C-NC	7.68	117.17	109.97
22	1	610	CLA	C2C-C1C-NC	7.67	117.16	109.97
22	5	610	CLA	C2C-C1C-NC	7.67	117.16	109.97
22	s	301	CLA	C2C-C1C-NC	7.67	117.16	109.97
22	B	613	CLA	C2C-C1C-NC	7.65	117.13	109.97
25	Y	601	CHL	C4A-NA-C1A	7.63	110.14	106.71
25	y	601	CHL	C4A-NA-C1A	7.63	110.14	106.71
22	b	608	CLA	C2C-C1C-NC	7.62	117.11	109.97
25	4	308	CHL	C4A-NA-C1A	7.54	110.09	106.71
25	8	308	CHL	C4A-NA-C1A	7.54	110.09	106.71
22	R	302	CLA	C2C-C1C-NC	7.51	117.01	109.97
22	r	302	CLA	C2C-C1C-NC	7.51	117.01	109.97
25	S	306	CHL	C4A-NA-C1A	7.51	110.08	106.71
25	s	306	CHL	C4A-NA-C1A	7.51	110.08	106.71
22	c	509	CLA	C2C-C1C-NC	7.49	116.99	109.97
25	1	615	CHL	C4A-NA-C1A	7.48	110.07	106.71
25	5	615	CHL	C4A-NA-C1A	7.48	110.07	106.71
22	b	616	CLA	C2B-C1B-NB	7.47	115.24	110.23
25	N	606	CHL	C4A-NA-C1A	7.47	110.06	106.71
25	n	606	CHL	C4A-NA-C1A	7.47	110.06	106.71
22	b	605	CLA	C2C-C1C-NC	7.46	116.96	109.97
22	3	314	CLA	C2C-C1C-NC	7.43	116.93	109.97
22	7	314	CLA	C2C-C1C-NC	7.43	116.93	109.97
22	B	606	CLA	C2C-C1C-NC	7.41	116.92	109.97
25	2	606	CHL	C4A-NA-C1A	7.36	110.02	106.71
25	6	606	CHL	C4A-NA-C1A	7.36	110.02	106.71
22	b	601	CLA	C2C-C1C-NC	7.35	116.86	109.97
25	1	607	CHL	C4A-NA-C1A	7.35	110.01	106.71
25	5	607	CHL	C4A-NA-C1A	7.35	110.01	106.71
25	3	307	CHL	C4A-NA-C1A	7.34	110.01	106.71
25	7	307	CHL	C4A-NA-C1A	7.34	110.01	106.71
25	2	607	CHL	C4A-NA-C1A	7.33	110.00	106.71
25	6	607	CHL	C4A-NA-C1A	7.33	110.00	106.71
22	b	615	CLA	C2C-C1C-NC	7.26	116.77	109.97
22	b	612	CLA	C2B-C1B-NB	7.26	115.10	110.23
22	N	610	CLA	C2C-C1C-NC	7.25	116.77	109.97
22	n	610	CLA	C2C-C1C-NC	7.25	116.77	109.97
22	G	610	CLA	C2C-C1C-NC	7.24	116.75	109.97
22	g	610	CLA	C2C-C1C-NC	7.24	116.75	109.97
22	R	308	CLA	C2C-C1C-NC	7.23	116.74	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r	308	CLA	C2C-C1C-NC	7.23	116.74	109.97
25	3	301	CHL	C4A-NA-C1A	7.19	109.94	106.71
25	7	301	CHL	C4A-NA-C1A	7.19	109.94	106.71
22	3	310	CLA	C2C-C1C-NC	7.18	116.70	109.97
22	7	310	CLA	C2C-C1C-NC	7.18	116.70	109.97
22	B	604	CLA	C1C-C2C-C3C	-7.18	99.41	106.96
22	b	612	CLA	C2C-C1C-NC	7.18	116.70	109.97
22	4	310	CLA	C2C-C1C-NC	7.18	116.70	109.97
22	8	310	CLA	C2C-C1C-NC	7.18	116.70	109.97
23	D	402	PHO	C2B-C1B-NB	7.13	114.45	109.53
22	C	502	CLA	C2C-C1C-NC	7.13	116.65	109.97
22	B	601	CLA	C2C-C1C-NC	7.12	116.64	109.97
25	4	306	CHL	C4A-NA-C1A	7.10	109.90	106.71
25	8	306	CHL	C4A-NA-C1A	7.10	109.90	106.71
22	B	611	CLA	C2C-C1C-NC	7.10	116.62	109.97
22	B	606	CLA	CAC-C3C-C4C	7.05	133.96	124.81
22	2	609	CLA	C2C-C1C-NC	7.05	116.57	109.97
22	6	609	CLA	C2C-C1C-NC	7.05	116.57	109.97
22	S	304	CLA	C2C-C1C-NC	7.04	116.57	109.97
22	s	304	CLA	C2C-C1C-NC	7.04	116.57	109.97
22	c	501	CLA	C1C-C2C-C3C	-7.04	99.56	106.96
22	C	508	CLA	C1D-ND-C4D	7.02	111.33	106.33
25	R	306	CHL	C4A-NA-C1A	6.96	109.83	106.71
25	r	306	CHL	C4A-NA-C1A	6.96	109.83	106.71
23	D	402	PHO	C4D-CHA-CBD	-6.95	105.37	108.52
25	S	307	CHL	C4A-NA-C1A	6.94	109.83	106.71
25	s	307	CHL	C4A-NA-C1A	6.94	109.83	106.71
22	a	405	CLA	CHC-C4B-NB	6.92	131.59	124.26
23	a	404	PHO	C4D-ND-C1D	-6.92	101.79	108.83
22	b	606	CLA	C2B-C1B-NB	6.89	114.85	110.23
22	b	614	CLA	CAC-C3C-C4C	6.89	133.75	124.81
25	1	606	CHL	C4A-NA-C1A	6.88	109.80	106.71
25	5	606	CHL	C4A-NA-C1A	6.88	109.80	106.71
23	a	404	PHO	C2B-C1B-NB	6.87	114.27	109.53
25	3	308	CHL	C4A-NA-C1A	6.86	109.79	106.71
25	7	308	CHL	C4A-NA-C1A	6.86	109.79	106.71
22	c	505	CLA	C2B-C1B-NB	6.86	114.83	110.23
25	4	307	CHL	C4A-NA-C1A	6.86	109.79	106.71
25	8	307	CHL	C4A-NA-C1A	6.86	109.79	106.71
22	R	307	CLA	CAC-C3C-C4C	6.85	133.70	124.81
22	r	307	CLA	CAC-C3C-C4C	6.85	133.70	124.81
25	R	305	CHL	C4A-NA-C1A	6.79	109.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	305	CHL	C4A-NA-C1A	6.79	109.76	106.71
22	S	313	CLA	CAC-C3C-C4C	6.79	133.62	124.81
22	s	313	CLA	CAC-C3C-C4C	6.79	133.62	124.81
22	b	616	CLA	C4A-NA-C1A	-6.78	103.66	106.71
23	d	402	PHO	C4D-ND-C1D	-6.77	101.94	108.83
22	b	609	CLA	C1C-C2C-C3C	-6.75	99.86	106.96
22	1	614	CLA	CAC-C3C-C4C	6.74	133.55	124.81
22	5	614	CLA	CAC-C3C-C4C	6.74	133.55	124.81
22	b	604	CLA	C1C-C2C-C3C	-6.74	99.88	106.96
22	b	602	CLA	CHC-C4B-NB	6.72	131.37	124.26
22	c	506	CLA	CHC-C4B-NB	6.71	131.36	124.26
22	C	510	CLA	CHC-C4B-NB	6.66	131.31	124.26
22	b	616	CLA	C1D-ND-C4D	6.64	111.05	106.33
22	B	605	CLA	CAC-C3C-C4C	6.64	133.43	124.81
25	4	302	CHL	C4A-NA-C1A	6.63	109.69	106.71
25	8	302	CHL	C4A-NA-C1A	6.63	109.69	106.71
22	B	604	CLA	CHC-C4B-NB	6.62	131.27	124.26
22	B	615	CLA	CAC-C3C-C4C	6.62	133.41	124.81
22	S	312	CLA	C1C-C2C-C3C	-6.62	99.99	106.96
22	s	312	CLA	C1C-C2C-C3C	-6.62	99.99	106.96
22	b	615	CLA	C2B-C1B-NB	6.62	114.67	110.23
22	B	616	CLA	C1C-C2C-C3C	-6.61	100.00	106.96
22	b	606	CLA	C2C-C1C-NC	6.61	116.16	109.97
25	R	304	CHL	C4A-NA-C1A	6.61	109.68	106.71
25	r	304	CHL	C4A-NA-C1A	6.61	109.68	106.71
23	D	402	PHO	C4D-ND-C1D	-6.60	102.11	108.83
25	1	608	CHL	C4A-NA-C1A	6.60	109.67	106.71
25	5	608	CHL	C4A-NA-C1A	6.60	109.67	106.71
22	Y	604	CLA	CHC-C4B-NB	6.60	131.24	124.26
22	y	604	CLA	CHC-C4B-NB	6.60	131.24	124.26
22	B	608	CLA	C1C-C2C-C3C	-6.60	100.02	106.96
23	d	402	PHO	C2B-C1B-NB	6.59	114.08	109.53
22	c	506	CLA	CAC-C3C-C4C	6.58	133.35	124.81
23	A	404	PHO	C1C-C2C-C3C	-6.56	103.16	108.61
22	Y	613	CLA	C1C-C2C-C3C	-6.56	100.06	106.96
22	y	613	CLA	C1C-C2C-C3C	-6.56	100.06	106.96
22	A	402	CLA	CAC-C3C-C4C	6.55	133.31	124.81
22	b	613	CLA	CHC-C4B-NB	6.54	131.18	124.26
22	c	508	CLA	C1D-ND-C4D	6.54	110.98	106.33
22	C	501	CLA	C1C-C2C-C3C	-6.53	100.09	106.96
22	c	505	CLA	CAC-C3C-C4C	6.53	133.28	124.81
22	C	504	CLA	C1C-C2C-C3C	-6.52	100.10	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	607	CLA	CAC-C3C-C4C	6.49	133.23	124.81
22	c	501	CLA	CHC-C4B-NB	6.48	131.12	124.26
22	C	504	CLA	CHC-C4B-NB	6.46	131.10	124.26
22	C	508	CLA	CAC-C3C-C4C	6.46	133.19	124.81
22	c	508	CLA	CAC-C3C-C4C	6.46	133.19	124.81
25	Y	606	CHL	C4A-NA-C1A	6.45	109.61	106.71
25	y	606	CHL	C4A-NA-C1A	6.45	109.61	106.71
22	C	510	CLA	C1C-C2C-C3C	-6.45	100.17	106.96
25	Y	608	CHL	C4A-NA-C1A	6.45	109.61	106.71
25	y	608	CHL	C4A-NA-C1A	6.45	109.61	106.71
22	c	506	CLA	C1C-C2C-C3C	-6.43	100.19	106.96
22	c	507	CLA	C1C-C2C-C3C	-6.43	100.19	106.96
22	b	611	CLA	CAC-C3C-C4C	6.43	133.16	124.81
22	C	505	CLA	CAC-C3C-C4C	6.43	133.15	124.81
22	B	606	CLA	C2B-C1B-NB	6.41	114.53	110.23
25	G	606	CHL	C4A-NA-C1A	6.41	109.59	106.71
25	g	606	CHL	C4A-NA-C1A	6.41	109.59	106.71
22	B	609	CLA	CHC-C4B-NB	6.40	131.03	124.26
22	C	506	CLA	C1C-C2C-C3C	-6.39	100.24	106.96
22	Y	604	CLA	C1C-C2C-C3C	-6.38	100.25	106.96
22	y	604	CLA	C1C-C2C-C3C	-6.38	100.25	106.96
23	d	402	PHO	C4D-CHA-CBD	-6.37	105.63	108.52
22	N	612	CLA	C1C-C2C-C3C	-6.37	100.26	106.96
22	n	612	CLA	C1C-C2C-C3C	-6.37	100.26	106.96
22	b	613	CLA	C1C-C2C-C3C	-6.37	100.26	106.96
22	B	615	CLA	CHC-C4B-NB	6.35	130.98	124.26
22	C	507	CLA	CHC-C4B-NB	6.35	130.98	124.26
22	1	614	CLA	C1D-ND-C4D	6.34	110.84	106.33
22	5	614	CLA	C1D-ND-C4D	6.34	110.84	106.33
22	B	611	CLA	CAC-C3C-C4C	6.34	133.04	124.81
22	b	609	CLA	CHC-C4B-NB	6.34	130.97	124.26
22	b	607	CLA	CHC-C4B-NB	6.34	130.97	124.26
22	C	506	CLA	CAC-C3C-C4C	6.34	133.03	124.81
22	b	616	CLA	CAC-C3C-C4C	6.33	133.02	124.81
22	A	405	CLA	CHC-C4B-NB	6.33	130.96	124.26
22	G	602	CLA	C1C-C2C-C3C	-6.31	100.32	106.96
22	g	602	CLA	C1C-C2C-C3C	-6.31	100.32	106.96
22	S	304	CLA	CAC-C3C-C4C	6.31	133.00	124.81
22	G	603	CLA	CAC-C3C-C4C	6.31	133.00	124.81
22	s	304	CLA	CAC-C3C-C4C	6.31	133.00	124.81
22	g	603	CLA	CAC-C3C-C4C	6.31	133.00	124.81
25	N	608	CHL	C4A-NA-C1A	6.29	109.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	n	608	CHL	C4A-NA-C1A	6.29	109.53	106.71
22	1	614	CLA	C1C-C2C-C3C	-6.29	100.35	106.96
22	5	614	CLA	C1C-C2C-C3C	-6.29	100.35	106.96
23	A	404	PHO	C4D-CHA-CBD	-6.28	105.67	108.52
22	B	609	CLA	CAC-C3C-C4C	6.28	132.96	124.81
22	B	608	CLA	CHC-C4B-NB	6.28	130.91	124.26
22	Y	612	CLA	C1D-ND-C4D	6.28	110.79	106.33
22	y	612	CLA	C1D-ND-C4D	6.28	110.79	106.33
22	N	603	CLA	CAC-C3C-C4C	6.28	132.95	124.81
22	n	603	CLA	CAC-C3C-C4C	6.28	132.95	124.81
22	b	616	CLA	C1C-C2C-C3C	-6.27	100.36	106.96
22	N	602	CLA	C1C-C2C-C3C	-6.27	100.36	106.96
22	n	602	CLA	C1C-C2C-C3C	-6.27	100.36	106.96
22	c	510	CLA	C1C-C2C-C3C	-6.27	100.36	106.96
22	G	612	CLA	C1C-C2C-C3C	-6.27	100.36	106.96
22	g	612	CLA	C1C-C2C-C3C	-6.27	100.36	106.96
22	N	611	CLA	C1C-C2C-C3C	-6.26	100.37	106.96
22	n	611	CLA	C1C-C2C-C3C	-6.26	100.37	106.96
22	Y	612	CLA	C1C-C2C-C3C	-6.26	100.38	106.96
22	y	612	CLA	C1C-C2C-C3C	-6.26	100.38	106.96
22	A	405	CLA	CAC-C3C-C4C	6.25	132.92	124.81
22	B	606	CLA	CHC-C4B-NB	6.25	130.87	124.26
22	C	509	CLA	C1C-C2C-C3C	-6.25	100.39	106.96
22	b	603	CLA	C1C-C2C-C3C	-6.22	100.42	106.96
22	4	310	CLA	CAC-C3C-C4C	6.22	132.87	124.81
22	8	310	CLA	CAC-C3C-C4C	6.22	132.87	124.81
22	A	403	CLA	C2B-C1B-NB	6.21	114.40	110.23
22	Y	603	CLA	C1C-C2C-C3C	-6.21	100.42	106.96
22	y	603	CLA	C1C-C2C-C3C	-6.21	100.42	106.96
22	C	511	CLA	C1C-C2C-C3C	-6.21	100.42	106.96
22	S	312	CLA	CHC-C4B-NB	6.21	130.83	124.26
22	s	312	CLA	CHC-C4B-NB	6.21	130.83	124.26
22	S	314	CLA	C1C-C2C-C3C	-6.20	100.43	106.96
22	s	314	CLA	C1C-C2C-C3C	-6.20	100.43	106.96
22	C	508	CLA	C1C-C2C-C3C	-6.19	100.44	106.96
22	c	512	CLA	C1C-C2C-C3C	-6.19	100.44	106.96
22	C	504	CLA	CAC-C3C-C4C	6.19	132.84	124.81
22	B	604	CLA	C1D-ND-C4D	6.19	110.73	106.33
22	a	405	CLA	CAC-C3C-C4C	6.19	132.84	124.81
23	a	404	PHO	C4D-CHA-CBD	-6.18	105.72	108.52
22	G	604	CLA	C1C-C2C-C3C	-6.17	100.47	106.96
22	g	604	CLA	C1C-C2C-C3C	-6.17	100.47	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	511	CLA	C1C-C2C-C3C	-6.17	100.47	106.96
22	N	602	CLA	CHC-C4B-NB	6.17	130.79	124.26
22	n	602	CLA	CHC-C4B-NB	6.17	130.79	124.26
22	Y	611	CLA	C1C-C2C-C3C	-6.17	100.47	106.96
22	y	611	CLA	C1C-C2C-C3C	-6.17	100.47	106.96
22	3	304	CLA	CAC-C3C-C4C	6.16	132.81	124.81
22	7	304	CLA	CAC-C3C-C4C	6.16	132.81	124.81
22	4	303	CLA	C1C-C2C-C3C	-6.16	100.48	106.96
22	8	303	CLA	C1C-C2C-C3C	-6.16	100.48	106.96
22	B	603	CLA	CAC-C3C-C4C	6.16	132.81	124.81
22	c	503	CLA	CAC-C3C-C4C	6.16	132.80	124.81
23	A	404	PHO	C2B-C1B-NB	6.16	113.78	109.53
22	S	305	CLA	C1C-C2C-C3C	-6.16	100.48	106.96
22	s	305	CLA	C1C-C2C-C3C	-6.16	100.48	106.96
22	C	506	CLA	C1D-ND-C4D	6.15	110.71	106.33
22	B	607	CLA	CHC-C4B-NB	6.15	130.76	124.26
22	Y	614	CLA	C1C-C2C-C3C	-6.15	100.50	106.96
22	y	614	CLA	C1C-C2C-C3C	-6.15	100.50	106.96
25	G	608	CHL	C4A-NA-C1A	6.15	109.47	106.71
25	g	608	CHL	C4A-NA-C1A	6.15	109.47	106.71
22	b	604	CLA	O2D-CGD-CBD	6.14	122.18	111.27
22	b	606	CLA	C1D-ND-C4D	6.14	110.70	106.33
22	R	311	CLA	C1C-C2C-C3C	-6.14	100.50	106.96
22	r	311	CLA	C1C-C2C-C3C	-6.14	100.50	106.96
22	c	503	CLA	CHC-C4B-NB	6.13	130.75	124.26
22	R	311	CLA	CAC-C3C-C4C	6.13	132.77	124.81
22	r	311	CLA	CAC-C3C-C4C	6.13	132.77	124.81
22	c	502	CLA	C1C-C2C-C3C	-6.13	100.51	106.96
22	G	613	CLA	C1C-C2C-C3C	-6.12	100.52	106.96
22	g	613	CLA	C1C-C2C-C3C	-6.12	100.52	106.96
22	Y	602	CLA	C1C-C2C-C3C	-6.12	100.52	106.96
22	y	602	CLA	C1C-C2C-C3C	-6.12	100.52	106.96
22	G	611	CLA	C1C-C2C-C3C	-6.12	100.52	106.96
22	g	611	CLA	C1C-C2C-C3C	-6.12	100.52	106.96
22	Y	614	CLA	CHC-C4B-NB	6.11	130.73	124.26
22	y	614	CLA	CHC-C4B-NB	6.11	130.73	124.26
22	N	603	CLA	C1C-C2C-C3C	-6.10	100.54	106.96
22	n	603	CLA	C1C-C2C-C3C	-6.10	100.54	106.96
22	B	602	CLA	CHC-C4B-NB	6.10	130.72	124.26
22	c	508	CLA	C1C-C2C-C3C	-6.10	100.54	106.96
22	N	610	CLA	CAC-C3C-C4C	6.09	132.72	124.81
22	n	610	CLA	CAC-C3C-C4C	6.09	132.72	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	504	CLA	CAC-C3C-C4C	6.09	132.71	124.81
22	b	603	CLA	CAC-C3C-C4C	6.09	132.71	124.81
22	b	606	CLA	CAC-C3C-C4C	6.09	132.71	124.81
22	c	506	CLA	C1D-ND-C4D	6.08	110.66	106.33
22	b	610	CLA	CHC-C4B-NB	6.08	130.70	124.26
22	2	612	CLA	C1C-C2C-C3C	-6.08	100.56	106.96
22	6	612	CLA	C1C-C2C-C3C	-6.08	100.56	106.96
25	S	302	CHL	C4A-NA-C1A	6.08	109.44	106.71
25	s	302	CHL	C4A-NA-C1A	6.08	109.44	106.71
22	s	301	CLA	CAC-C3C-C4C	6.08	132.69	124.81
22	R	309	CLA	C1C-C2C-C3C	-6.08	100.57	106.96
22	r	309	CLA	C1C-C2C-C3C	-6.08	100.57	106.96
22	B	603	CLA	C1C-C2C-C3C	-6.07	100.57	106.96
22	b	607	CLA	C1C-C2C-C3C	-6.07	100.57	106.96
22	C	506	CLA	CHC-C4B-NB	6.07	130.68	124.26
22	Y	602	CLA	CHC-C4B-NB	6.07	130.68	124.26
22	y	602	CLA	CHC-C4B-NB	6.07	130.68	124.26
22	B	612	CLA	CAC-C3C-C4C	6.07	132.68	124.81
22	d	403	CLA	C1C-C2C-C3C	-6.07	100.58	106.96
22	N	614	CLA	C1C-C2C-C3C	-6.07	100.58	106.96
22	n	614	CLA	C1C-C2C-C3C	-6.07	100.58	106.96
22	B	614	CLA	CHC-C4B-NB	6.06	130.68	124.26
22	G	603	CLA	C1C-C2C-C3C	-6.06	100.58	106.96
22	g	603	CLA	C1C-C2C-C3C	-6.06	100.58	106.96
22	S	309	CLA	C1C-C2C-C3C	-6.06	100.59	106.96
22	s	309	CLA	C1C-C2C-C3C	-6.06	100.59	106.96
22	S	311	CLA	C1C-C2C-C3C	-6.06	100.59	106.96
22	s	311	CLA	C1C-C2C-C3C	-6.06	100.59	106.96
22	C	501	CLA	CHC-C4B-NB	6.06	130.67	124.26
22	B	610	CLA	C1C-C2C-C3C	-6.06	100.59	106.96
22	N	613	CLA	C1C-C2C-C3C	-6.06	100.59	106.96
22	n	613	CLA	C1C-C2C-C3C	-6.06	100.59	106.96
22	Y	613	CLA	CHC-C4B-NB	6.05	130.67	124.26
22	y	613	CLA	CHC-C4B-NB	6.05	130.67	124.26
22	S	310	CLA	C1C-C2C-C3C	-6.05	100.60	106.96
22	s	310	CLA	C1C-C2C-C3C	-6.05	100.60	106.96
22	1	603	CLA	CAC-C3C-C4C	6.05	132.66	124.81
22	5	603	CLA	CAC-C3C-C4C	6.05	132.66	124.81
22	N	612	CLA	CHC-C4B-NB	6.04	130.65	124.26
22	n	612	CLA	CHC-C4B-NB	6.04	130.65	124.26
22	2	604	CLA	CAC-C3C-C4C	6.04	132.65	124.81
22	6	604	CLA	CAC-C3C-C4C	6.04	132.65	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	613	CLA	CHC-C4B-NB	6.04	130.65	124.26
22	n	613	CLA	CHC-C4B-NB	6.04	130.65	124.26
22	B	607	CLA	C1C-C2C-C3C	-6.04	100.61	106.96
22	R	303	CLA	O2D-CGD-CBD	6.04	122.00	111.27
22	r	303	CLA	O2D-CGD-CBD	6.04	122.00	111.27
22	3	304	CLA	C2B-C1B-NB	6.03	114.28	110.23
22	7	304	CLA	C2B-C1B-NB	6.03	114.28	110.23
22	b	611	CLA	CHC-C4B-NB	6.03	130.64	124.26
22	b	608	CLA	C2B-C1B-NB	6.03	114.28	110.23
22	1	604	CLA	C1C-C2C-C3C	-6.03	100.62	106.96
22	5	604	CLA	C1C-C2C-C3C	-6.03	100.62	106.96
22	S	301	CLA	C1C-C2C-C3C	-6.03	100.62	106.96
22	3	313	CLA	C1C-C2C-C3C	-6.02	100.62	106.96
22	7	313	CLA	C1C-C2C-C3C	-6.02	100.62	106.96
22	S	301	CLA	CAC-C3C-C4C	6.02	132.62	124.81
22	4	303	CLA	CAC-C3C-C4C	6.02	132.62	124.81
22	8	303	CLA	CAC-C3C-C4C	6.02	132.62	124.81
22	N	604	CLA	C1C-C2C-C3C	-6.02	100.63	106.96
22	n	604	CLA	C1C-C2C-C3C	-6.02	100.63	106.96
22	A	402	CLA	CHC-C4B-NB	6.02	130.63	124.26
22	b	605	CLA	CAC-C3C-C4C	6.01	132.61	124.81
22	S	314	CLA	CHC-C4B-NB	6.01	130.62	124.26
22	s	314	CLA	CHC-C4B-NB	6.01	130.62	124.26
22	1	613	CLA	C1C-C2C-C3C	-6.01	100.64	106.96
22	5	613	CLA	C1C-C2C-C3C	-6.01	100.64	106.96
22	c	509	CLA	C1C-C2C-C3C	-6.01	100.64	106.96
22	Y	610	CLA	CHC-C4B-NB	6.00	130.61	124.26
22	y	610	CLA	CHC-C4B-NB	6.00	130.61	124.26
22	D	404	CLA	C1C-C2C-C3C	-6.00	100.65	106.96
22	R	303	CLA	C1C-C2C-C3C	-6.00	100.65	106.96
22	r	303	CLA	C1C-C2C-C3C	-6.00	100.65	106.96
22	A	405	CLA	C1D-ND-C4D	6.00	110.59	106.33
22	b	602	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
22	C	507	CLA	C1C-C2C-C3C	-5.99	100.66	106.96
22	3	304	CLA	C1C-C2C-C3C	-5.98	100.67	106.96
22	7	304	CLA	C1C-C2C-C3C	-5.98	100.67	106.96
22	G	604	CLA	CAC-C3C-C4C	5.98	132.57	124.81
22	g	604	CLA	CAC-C3C-C4C	5.98	132.57	124.81
22	S	314	CLA	CAC-C3C-C4C	5.98	132.57	124.81
22	s	314	CLA	CAC-C3C-C4C	5.98	132.57	124.81
22	G	610	CLA	CAC-C3C-C4C	5.98	132.57	124.81
22	g	610	CLA	CAC-C3C-C4C	5.98	132.57	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	311	CLA	C2B-C1B-NB	5.98	114.24	110.23
22	s	311	CLA	C2B-C1B-NB	5.98	114.24	110.23
22	d	403	CLA	CHC-C4B-NB	5.98	130.59	124.26
22	1	611	CLA	C1C-C2C-C3C	-5.98	100.67	106.96
22	5	611	CLA	C1C-C2C-C3C	-5.98	100.67	106.96
22	2	602	CLA	C1C-C2C-C3C	-5.97	100.68	106.96
22	6	602	CLA	C1C-C2C-C3C	-5.97	100.68	106.96
22	S	310	CLA	CHC-C4B-NB	5.97	130.58	124.26
22	s	310	CLA	CHC-C4B-NB	5.97	130.58	124.26
22	G	604	CLA	CHC-C4B-NB	5.97	130.57	124.26
22	g	604	CLA	CHC-C4B-NB	5.97	130.57	124.26
22	B	610	CLA	CHC-C4B-NB	5.96	130.57	124.26
22	b	614	CLA	C1C-C2C-C3C	-5.96	100.69	106.96
22	4	311	CLA	C1C-C2C-C3C	-5.96	100.69	106.96
22	8	311	CLA	C1C-C2C-C3C	-5.96	100.69	106.96
22	B	609	CLA	C1C-C2C-C3C	-5.96	100.69	106.96
22	D	403	CLA	CHC-C4B-NB	5.95	130.56	124.26
22	R	308	CLA	CHC-C4B-NB	5.95	130.56	124.26
22	r	308	CLA	CHC-C4B-NB	5.95	130.56	124.26
22	B	613	CLA	CAC-C3C-C4C	5.95	132.53	124.81
22	3	305	CLA	CAC-C3C-C4C	5.95	132.53	124.81
22	7	305	CLA	CAC-C3C-C4C	5.95	132.53	124.81
22	1	603	CLA	C1C-C2C-C3C	-5.95	100.70	106.96
22	5	603	CLA	C1C-C2C-C3C	-5.95	100.70	106.96
22	b	608	CLA	CAC-C3C-C4C	5.95	132.53	124.81
22	4	305	CLA	C1C-C2C-C3C	-5.95	100.70	106.96
22	8	305	CLA	C1C-C2C-C3C	-5.95	100.70	106.96
22	1	602	CLA	CAC-C3C-C4C	5.95	132.53	124.81
22	5	602	CLA	CAC-C3C-C4C	5.95	132.53	124.81
22	b	614	CLA	CHC-C4B-NB	5.94	130.55	124.26
22	Y	612	CLA	CHC-C4B-NB	5.94	130.55	124.26
22	y	612	CLA	CHC-C4B-NB	5.94	130.55	124.26
22	G	602	CLA	CHC-C4B-NB	5.94	130.54	124.26
22	g	602	CLA	CHC-C4B-NB	5.94	130.54	124.26
22	2	603	CLA	CAC-C3C-C4C	5.94	132.51	124.81
22	6	603	CLA	CAC-C3C-C4C	5.94	132.51	124.81
22	c	509	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
22	Y	610	CLA	C1C-C2C-C3C	-5.93	100.72	106.96
22	y	610	CLA	C1C-C2C-C3C	-5.93	100.72	106.96
22	3	305	CLA	C1C-C2C-C3C	-5.93	100.72	106.96
22	7	305	CLA	C1C-C2C-C3C	-5.93	100.72	106.96
22	c	501	CLA	C1D-ND-C4D	5.93	110.55	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Y	604	CLA	CAC-C3C-C4C	5.93	132.50	124.81
22	y	604	CLA	CAC-C3C-C4C	5.93	132.50	124.81
22	3	303	CLA	C1C-C2C-C3C	-5.93	100.72	106.96
22	7	303	CLA	C1C-C2C-C3C	-5.93	100.72	106.96
22	A	405	CLA	C1C-C2C-C3C	-5.93	100.73	106.96
23	D	402	PHO	C1C-C2C-C3C	-5.93	103.68	108.61
22	R	311	CLA	CHC-C4B-NB	5.92	130.53	124.26
22	r	311	CLA	CHC-C4B-NB	5.92	130.53	124.26
22	4	304	CLA	C1C-C2C-C3C	-5.92	100.73	106.96
22	8	304	CLA	C1C-C2C-C3C	-5.92	100.73	106.96
22	b	615	CLA	C1C-C2C-C3C	-5.92	100.73	106.96
22	C	508	CLA	CHC-C4B-NB	5.91	130.52	124.26
22	R	310	CLA	C1C-C2C-C3C	-5.91	100.74	106.96
22	r	310	CLA	C1C-C2C-C3C	-5.91	100.74	106.96
22	3	311	CLA	C1C-C2C-C3C	-5.91	100.74	106.96
22	7	311	CLA	C1C-C2C-C3C	-5.91	100.74	106.96
23	a	404	PHO	C1C-C2C-C3C	-5.91	103.69	108.61
22	2	603	CLA	C1C-C2C-C3C	-5.91	100.74	106.96
22	6	603	CLA	C1C-C2C-C3C	-5.91	100.74	106.96
22	D	403	CLA	C1C-C2C-C3C	-5.91	100.74	106.96
22	G	614	CLA	C1C-C2C-C3C	-5.91	100.74	106.96
22	g	614	CLA	C1C-C2C-C3C	-5.91	100.74	106.96
22	a	405	CLA	C1C-C2C-C3C	-5.91	100.75	106.96
22	G	603	CLA	C1D-ND-C4D	5.91	110.53	106.33
22	g	603	CLA	C1D-ND-C4D	5.91	110.53	106.33
22	2	604	CLA	C1C-C2C-C3C	-5.91	100.75	106.96
22	6	604	CLA	C1C-C2C-C3C	-5.91	100.75	106.96
22	s	301	CLA	C1C-C2C-C3C	-5.90	100.75	106.96
22	C	503	CLA	CAC-C3C-C4C	5.90	132.47	124.81
22	4	305	CLA	CAC-C3C-C4C	5.90	132.47	124.81
22	8	305	CLA	CAC-C3C-C4C	5.90	132.47	124.81
22	3	310	CLA	CAC-C3C-C4C	5.90	132.47	124.81
22	7	310	CLA	CAC-C3C-C4C	5.90	132.47	124.81
22	C	511	CLA	C2B-C1B-NB	5.90	114.19	110.23
22	3	312	CLA	C1C-C2C-C3C	-5.90	100.76	106.96
22	7	312	CLA	C1C-C2C-C3C	-5.90	100.76	106.96
22	N	604	CLA	CAC-C3C-C4C	5.89	132.46	124.81
22	n	604	CLA	CAC-C3C-C4C	5.89	132.46	124.81
22	2	609	CLA	CAC-C3C-C4C	5.89	132.46	124.81
22	6	609	CLA	CAC-C3C-C4C	5.89	132.46	124.81
22	B	612	CLA	C2B-C1B-NB	5.89	114.18	110.23
22	1	612	CLA	C1C-C2C-C3C	-5.89	100.77	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	612	CLA	C1C-C2C-C3C	-5.89	100.77	106.96
22	Y	610	CLA	CAC-C3C-C4C	5.88	132.44	124.81
22	y	610	CLA	CAC-C3C-C4C	5.88	132.44	124.81
22	2	602	CLA	CAC-C3C-C4C	5.88	132.44	124.81
22	6	602	CLA	CAC-C3C-C4C	5.88	132.44	124.81
22	c	503	CLA	C1C-C2C-C3C	-5.88	100.78	106.96
22	1	610	CLA	CAC-C3C-C4C	5.88	132.43	124.81
22	5	610	CLA	CAC-C3C-C4C	5.88	132.43	124.81
22	b	610	CLA	C1C-C2C-C3C	-5.88	100.78	106.96
22	S	303	CLA	C1C-C2C-C3C	-5.88	100.78	106.96
22	s	303	CLA	C1C-C2C-C3C	-5.88	100.78	106.96
22	N	604	CLA	C2B-C1B-NB	5.87	114.17	110.23
22	n	604	CLA	C2B-C1B-NB	5.87	114.17	110.23
22	1	602	CLA	C1C-C2C-C3C	-5.87	100.78	106.96
22	5	602	CLA	C1C-C2C-C3C	-5.87	100.78	106.96
22	1	611	CLA	CAC-C3C-C4C	5.87	132.43	124.81
22	5	611	CLA	CAC-C3C-C4C	5.87	132.43	124.81
22	d	404	CLA	C1C-C2C-C3C	-5.86	100.79	106.96
22	2	611	CLA	C1C-C2C-C3C	-5.86	100.79	106.96
22	6	611	CLA	C1C-C2C-C3C	-5.86	100.79	106.96
22	D	404	CLA	CAC-C3C-C4C	5.85	132.40	124.81
22	S	305	CLA	C2B-C1B-NB	5.85	114.15	110.23
22	s	305	CLA	C2B-C1B-NB	5.85	114.15	110.23
22	B	616	CLA	CAC-C3C-C4C	5.85	132.40	124.81
22	N	613	CLA	CAC-C3C-C4C	5.85	132.40	124.81
22	n	613	CLA	CAC-C3C-C4C	5.85	132.40	124.81
22	C	505	CLA	CHC-C4B-NB	5.85	130.45	124.26
22	b	603	CLA	C1D-ND-C4D	5.84	110.49	106.33
22	S	305	CLA	O2D-CGD-CBD	5.84	121.65	111.27
22	s	305	CLA	O2D-CGD-CBD	5.84	121.65	111.27
22	1	604	CLA	CAC-C3C-C4C	5.84	132.39	124.81
22	5	604	CLA	CAC-C3C-C4C	5.84	132.39	124.81
22	A	402	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
22	Y	614	CLA	CAC-C3C-C4C	5.84	132.38	124.81
22	y	614	CLA	CAC-C3C-C4C	5.84	132.38	124.81
22	B	614	CLA	CAC-C3C-C4C	5.84	132.38	124.81
22	4	301	CLA	C1C-C2C-C3C	-5.84	100.82	106.96
22	8	301	CLA	C1C-C2C-C3C	-5.84	100.82	106.96
22	c	508	CLA	CHC-C4B-NB	5.83	130.43	124.26
22	B	615	CLA	C1C-C2C-C3C	-5.83	100.82	106.96
22	3	313	CLA	CAC-C3C-C4C	5.83	132.38	124.81
22	7	313	CLA	CAC-C3C-C4C	5.83	132.38	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	311	CLA	CAC-C3C-C4C	5.83	132.37	124.81
22	7	311	CLA	CAC-C3C-C4C	5.83	132.37	124.81
22	2	610	CLA	C1C-C2C-C3C	-5.83	100.83	106.96
22	6	610	CLA	C1C-C2C-C3C	-5.83	100.83	106.96
22	b	602	CLA	C1C-C2C-C3C	-5.82	100.83	106.96
22	Y	612	CLA	C2B-C1B-NB	5.82	114.14	110.23
22	y	612	CLA	C2B-C1B-NB	5.82	114.14	110.23
22	B	612	CLA	C1C-C2C-C3C	-5.82	100.84	106.96
22	C	512	CLA	C1C-C2C-C3C	-5.82	100.84	106.96
22	b	603	CLA	CHC-C4B-NB	5.81	130.41	124.26
23	d	402	PHO	C1C-C2C-C3C	-5.81	103.78	108.61
22	B	601	CLA	C1C-C2C-C3C	-5.81	100.84	106.96
22	C	511	CLA	CAC-C3C-C4C	5.81	132.35	124.81
22	C	503	CLA	C1C-C2C-C3C	-5.81	100.85	106.96
22	c	504	CLA	C1C-C2C-C3C	-5.81	100.85	106.96
22	R	308	CLA	CAC-C3C-C4C	5.81	132.35	124.81
22	r	308	CLA	CAC-C3C-C4C	5.81	132.35	124.81
22	4	304	CLA	CAC-C3C-C4C	5.81	132.34	124.81
22	8	304	CLA	CAC-C3C-C4C	5.81	132.34	124.81
22	S	305	CLA	CHC-C4B-NB	5.81	130.40	124.26
22	s	305	CLA	CHC-C4B-NB	5.81	130.40	124.26
22	b	613	CLA	CAC-C3C-C4C	5.81	132.34	124.81
22	S	303	CLA	CAC-C3C-C4C	5.80	132.34	124.81
22	s	303	CLA	CAC-C3C-C4C	5.80	132.34	124.81
22	a	402	CLA	C2B-C1B-NB	5.80	114.12	110.23
22	C	505	CLA	C1C-C2C-C3C	-5.80	100.86	106.96
22	2	612	CLA	CAC-C3C-C4C	5.79	132.32	124.81
22	6	612	CLA	CAC-C3C-C4C	5.79	132.32	124.81
22	Y	611	CLA	C2B-C1B-NB	5.79	114.11	110.23
22	y	611	CLA	C2B-C1B-NB	5.79	114.11	110.23
22	S	301	CLA	CHC-C4B-NB	5.78	130.38	124.26
22	3	314	CLA	C1C-C2C-C3C	-5.78	100.88	106.96
22	7	314	CLA	C1C-C2C-C3C	-5.78	100.88	106.96
22	4	301	CLA	CAC-C3C-C4C	5.77	132.30	124.81
22	8	301	CLA	CAC-C3C-C4C	5.77	132.30	124.81
22	D	404	CLA	CHC-C4B-NB	5.77	130.37	124.26
22	C	510	CLA	CAC-C3C-C4C	5.77	132.30	124.81
22	C	512	CLA	C2B-C1B-NB	5.77	114.10	110.23
22	D	401	CLA	C1D-ND-C4D	5.77	110.43	106.33
22	2	613	CLA	C1C-C2C-C3C	-5.76	100.90	106.96
22	6	613	CLA	C1C-C2C-C3C	-5.76	100.90	106.96
22	b	608	CLA	C1C-C2C-C3C	-5.76	100.90	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	d	401	CLA	CAC-C3C-C4C	5.76	132.28	124.81
22	S	313	CLA	C2B-C1B-NB	5.76	114.09	110.23
22	s	313	CLA	C2B-C1B-NB	5.76	114.09	110.23
22	3	303	CLA	CAC-C3C-C4C	5.75	132.28	124.81
22	7	303	CLA	CAC-C3C-C4C	5.75	132.28	124.81
22	R	309	CLA	CAC-C3C-C4C	5.74	132.26	124.81
22	r	309	CLA	CAC-C3C-C4C	5.74	132.26	124.81
22	b	601	CLA	C1C-C2C-C3C	-5.74	100.92	106.96
22	C	505	CLA	C2B-C1B-NB	5.74	114.08	110.23
22	G	613	CLA	CHC-C4B-NB	5.74	130.33	124.26
22	g	613	CLA	CHC-C4B-NB	5.74	130.33	124.26
22	C	502	CLA	C1C-C2C-C3C	-5.74	100.92	106.96
22	1	613	CLA	CAC-C3C-C4C	5.74	132.25	124.81
22	5	613	CLA	CAC-C3C-C4C	5.74	132.25	124.81
22	d	401	CLA	CHC-C4B-NB	5.73	130.33	124.26
22	a	402	CLA	C1C-C2C-C3C	-5.73	100.93	106.96
22	C	503	CLA	CHC-C4B-NB	5.73	130.32	124.26
23	A	404	PHO	C3D-C4D-ND	5.73	115.53	107.72
22	3	314	CLA	CAC-C3C-C4C	5.73	132.24	124.81
22	7	314	CLA	CAC-C3C-C4C	5.73	132.24	124.81
22	2	613	CLA	CAC-C3C-C4C	5.73	132.24	124.81
22	6	613	CLA	CAC-C3C-C4C	5.73	132.24	124.81
22	R	302	CLA	C1C-C2C-C3C	-5.72	100.94	106.96
22	r	302	CLA	C1C-C2C-C3C	-5.72	100.94	106.96
22	4	303	CLA	CHC-C4B-NB	5.72	130.31	124.26
22	8	303	CLA	CHC-C4B-NB	5.72	130.31	124.26
22	c	511	CLA	C2B-C1B-NB	5.72	114.07	110.23
22	1	611	CLA	CHC-C4B-NB	5.72	130.31	124.26
22	5	611	CLA	CHC-C4B-NB	5.72	130.31	124.26
22	a	403	CLA	C1C-C2C-C3C	-5.72	100.94	106.96
22	N	613	CLA	C1D-ND-C4D	5.71	110.39	106.33
22	n	613	CLA	C1D-ND-C4D	5.71	110.39	106.33
22	B	614	CLA	O2D-CGD-CBD	5.71	121.42	111.27
22	N	610	CLA	CHC-C4B-NB	5.71	130.30	124.26
22	n	610	CLA	CHC-C4B-NB	5.71	130.30	124.26
22	Y	611	CLA	CAC-C3C-C4C	5.71	132.22	124.81
22	y	611	CLA	CAC-C3C-C4C	5.71	132.22	124.81
22	G	611	CLA	C2B-C1B-NB	5.70	114.06	110.23
22	g	611	CLA	C2B-C1B-NB	5.70	114.06	110.23
22	1	614	CLA	C2B-C1B-NB	5.70	114.05	110.23
22	5	614	CLA	C2B-C1B-NB	5.70	114.05	110.23
22	3	303	CLA	CHC-C4B-NB	5.70	130.29	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	303	CLA	CHC-C4B-NB	5.70	130.29	124.26
22	B	613	CLA	C1D-ND-C4D	5.69	110.38	106.33
22	B	613	CLA	C1C-C2C-C3C	-5.69	100.97	106.96
22	B	605	CLA	CHC-C4B-NB	5.69	130.28	124.26
22	c	510	CLA	CHC-C4B-NB	5.69	130.28	124.26
22	b	610	CLA	C1D-ND-C4D	5.69	110.38	106.33
22	N	611	CLA	CHC-C4B-NB	5.69	130.28	124.26
22	n	611	CLA	CHC-C4B-NB	5.69	130.28	124.26
22	d	404	CLA	CAC-C3C-C4C	5.68	132.19	124.81
22	R	301	CLA	CAC-C3C-C4C	5.68	132.18	124.81
22	r	301	CLA	CAC-C3C-C4C	5.68	132.18	124.81
22	C	510	CLA	C1D-ND-C4D	5.68	110.37	106.33
22	1	613	CLA	CHC-C4B-NB	5.68	130.27	124.26
22	5	613	CLA	CHC-C4B-NB	5.68	130.27	124.26
22	G	612	CLA	CHC-C4B-NB	5.67	130.26	124.26
22	g	612	CLA	CHC-C4B-NB	5.67	130.26	124.26
22	1	604	CLA	CHC-C4B-NB	5.67	130.26	124.26
22	5	604	CLA	CHC-C4B-NB	5.67	130.26	124.26
22	4	305	CLA	CHC-C4B-NB	5.67	130.26	124.26
22	8	305	CLA	CHC-C4B-NB	5.67	130.26	124.26
22	B	610	CLA	CAC-C3C-C4C	5.67	132.17	124.81
22	B	602	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
22	D	401	CLA	CAC-C3C-C4C	5.67	132.16	124.81
22	B	614	CLA	C1C-C2C-C3C	-5.66	101.00	106.96
22	N	602	CLA	CAC-C3C-C4C	5.66	132.15	124.81
22	n	602	CLA	CAC-C3C-C4C	5.66	132.15	124.81
22	2	612	CLA	CHC-C4B-NB	5.66	130.25	124.26
22	6	612	CLA	CHC-C4B-NB	5.66	130.25	124.26
22	b	614	CLA	C2B-C1B-NB	5.66	114.03	110.23
22	R	301	CLA	C1C-C2C-C3C	-5.66	101.01	106.96
22	r	301	CLA	C1C-C2C-C3C	-5.66	101.01	106.96
22	C	512	CLA	CAC-C3C-C4C	5.65	132.15	124.81
22	b	615	CLA	C1D-ND-C4D	5.65	110.35	106.33
22	1	610	CLA	CHC-C4B-NB	5.65	130.24	124.26
22	5	610	CLA	CHC-C4B-NB	5.65	130.24	124.26
22	b	601	CLA	CHC-C4B-NB	5.65	130.24	124.26
22	1	612	CLA	C2B-C1B-NB	5.65	114.02	110.23
22	5	612	CLA	C2B-C1B-NB	5.65	114.02	110.23
22	1	610	CLA	C1C-C2C-C3C	-5.65	101.02	106.96
22	5	610	CLA	C1C-C2C-C3C	-5.65	101.02	106.96
22	B	607	CLA	CAC-C3C-C4C	5.64	132.13	124.81
22	G	611	CLA	CAC-C3C-C4C	5.64	132.13	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	611	CLA	CAC-C3C-C4C	5.64	132.13	124.81
22	B	613	CLA	CHC-C4B-NB	5.64	130.23	124.26
22	2	602	CLA	CHC-C4B-NB	5.64	130.23	124.26
22	6	602	CLA	CHC-C4B-NB	5.64	130.23	124.26
22	b	611	CLA	O2D-CGD-CBD	5.64	121.29	111.27
22	B	605	CLA	C1C-C2C-C3C	-5.64	101.03	106.96
22	G	610	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
22	g	610	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
22	2	610	CLA	CAC-C3C-C4C	5.64	132.13	124.81
22	6	610	CLA	CAC-C3C-C4C	5.64	132.13	124.81
22	R	302	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
22	r	302	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
22	c	512	CLA	CHC-C4B-NB	5.64	130.23	124.26
22	b	612	CLA	C1C-C2C-C3C	-5.64	101.03	106.96
22	c	505	CLA	C1C-C2C-C3C	-5.64	101.03	106.96
22	S	313	CLA	C1C-C2C-C3C	-5.63	101.03	106.96
22	s	313	CLA	C1C-C2C-C3C	-5.63	101.03	106.96
22	A	403	CLA	C1C-C2C-C3C	-5.63	101.04	106.96
22	G	614	CLA	CAC-C3C-C4C	5.63	132.11	124.81
22	g	614	CLA	CAC-C3C-C4C	5.63	132.11	124.81
22	4	310	CLA	CHC-C4B-NB	5.62	130.21	124.26
22	8	310	CLA	CHC-C4B-NB	5.62	130.21	124.26
22	b	612	CLA	CAC-C3C-C4C	5.62	132.10	124.81
22	D	401	CLA	C2B-C1B-NB	5.62	114.00	110.23
22	c	512	CLA	C2B-C1B-NB	5.62	114.00	110.23
22	b	609	CLA	CAC-C3C-C4C	5.62	132.10	124.81
22	Y	603	CLA	CAC-C3C-C4C	5.62	132.10	124.81
22	y	603	CLA	CAC-C3C-C4C	5.62	132.10	124.81
22	s	301	CLA	CHC-C4B-NB	5.62	130.20	124.26
22	B	608	CLA	CAC-C3C-C4C	5.61	132.09	124.81
22	R	307	CLA	C1C-C2C-C3C	-5.61	101.06	106.96
22	r	307	CLA	C1C-C2C-C3C	-5.61	101.06	106.96
22	Y	603	CLA	CHC-C4B-NB	5.61	130.20	124.26
22	y	603	CLA	CHC-C4B-NB	5.61	130.20	124.26
22	R	308	CLA	C2D-C1D-ND	5.61	114.24	110.10
22	r	308	CLA	C2D-C1D-ND	5.61	114.24	110.10
22	N	610	CLA	C2D-C1D-ND	5.61	114.24	110.10
22	n	610	CLA	C2D-C1D-ND	5.61	114.24	110.10
22	3	304	CLA	C1D-ND-C4D	5.61	110.32	106.33
22	7	304	CLA	C1D-ND-C4D	5.61	110.32	106.33
22	B	601	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
22	R	303	CLA	CHC-C4B-NB	5.61	130.19	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r	303	CLA	CHC-C4B-NB	5.61	130.19	124.26
22	A	403	CLA	CAC-C3C-C4C	5.60	132.08	124.81
22	c	504	CLA	CHC-C4B-NB	5.60	130.19	124.26
22	G	602	CLA	CAC-C3C-C4C	5.60	132.08	124.81
22	g	602	CLA	CAC-C3C-C4C	5.60	132.08	124.81
22	3	312	CLA	CAC-C3C-C4C	5.60	132.08	124.81
22	7	312	CLA	CAC-C3C-C4C	5.60	132.08	124.81
22	c	507	CLA	CHC-C4B-NB	5.60	130.19	124.26
22	S	304	CLA	C1C-C2C-C3C	-5.60	101.07	106.96
22	s	304	CLA	C1C-C2C-C3C	-5.60	101.07	106.96
22	b	603	CLA	C2B-C1B-NB	5.60	113.99	110.23
22	c	502	CLA	CHC-C4B-NB	5.60	130.19	124.26
22	R	302	CLA	CHC-C4B-NB	5.60	130.19	124.26
22	r	302	CLA	CHC-C4B-NB	5.60	130.19	124.26
22	N	611	CLA	CAC-C3C-C4C	5.59	132.07	124.81
22	n	611	CLA	CAC-C3C-C4C	5.59	132.07	124.81
22	b	605	CLA	C4A-NA-C1A	-5.59	104.19	106.71
22	2	609	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
22	6	609	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
22	a	402	CLA	CAC-C3C-C4C	5.59	132.06	124.81
22	G	610	CLA	CHC-C4B-NB	5.59	130.17	124.26
22	g	610	CLA	CHC-C4B-NB	5.59	130.17	124.26
22	1	612	CLA	CHC-C4B-NB	5.59	130.17	124.26
22	5	612	CLA	CHC-C4B-NB	5.59	130.17	124.26
22	c	502	CLA	C1D-ND-C4D	5.58	110.30	106.33
22	N	614	CLA	CAC-C3C-C4C	5.58	132.05	124.81
22	n	614	CLA	CAC-C3C-C4C	5.58	132.05	124.81
22	3	310	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
22	7	310	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
22	c	511	CLA	CAC-C3C-C4C	5.58	132.05	124.81
22	N	611	CLA	C2B-C1B-NB	5.58	113.97	110.23
22	n	611	CLA	C2B-C1B-NB	5.58	113.97	110.23
22	D	401	CLA	CHC-C4B-NB	5.58	130.16	124.26
22	b	616	CLA	CHC-C4B-NB	5.58	130.16	124.26
22	N	610	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
22	n	610	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
22	G	614	CLA	C2B-C1B-NB	5.58	113.97	110.23
22	g	614	CLA	C2B-C1B-NB	5.58	113.97	110.23
22	1	612	CLA	CAC-C3C-C4C	5.57	132.04	124.81
22	5	612	CLA	CAC-C3C-C4C	5.57	132.04	124.81
22	N	604	CLA	CHC-C4B-NB	5.57	130.16	124.26
22	n	604	CLA	CHC-C4B-NB	5.57	130.16	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	611	CLA	CHC-C4B-NB	5.57	130.15	124.26
22	S	310	CLA	CAC-C3C-C4C	5.57	132.03	124.81
22	s	310	CLA	CAC-C3C-C4C	5.57	132.03	124.81
22	S	305	CLA	CAC-C3C-C4C	5.57	132.03	124.81
22	s	305	CLA	CAC-C3C-C4C	5.57	132.03	124.81
22	S	301	CLA	C1D-ND-C4D	5.57	110.29	106.33
22	1	602	CLA	CHC-C4B-NB	5.57	130.15	124.26
22	5	602	CLA	CHC-C4B-NB	5.57	130.15	124.26
22	3	312	CLA	CHC-C4B-NB	5.56	130.15	124.26
22	7	312	CLA	CHC-C4B-NB	5.56	130.15	124.26
22	B	602	CLA	CAC-C3C-C4C	5.56	132.02	124.81
22	B	616	CLA	CHC-C4B-NB	5.56	130.14	124.26
22	2	611	CLA	CHC-C4B-NB	5.56	130.14	124.26
22	6	611	CLA	CHC-C4B-NB	5.56	130.14	124.26
22	Y	613	CLA	C1D-ND-C4D	5.56	110.28	106.33
22	y	613	CLA	C1D-ND-C4D	5.56	110.28	106.33
22	G	613	CLA	C1D-ND-C4D	5.56	110.28	106.33
22	g	613	CLA	C1D-ND-C4D	5.56	110.28	106.33
22	b	610	CLA	CAC-C3C-C4C	5.55	132.02	124.81
22	N	614	CLA	C2B-C1B-NB	5.55	113.95	110.23
22	n	614	CLA	C2B-C1B-NB	5.55	113.95	110.23
22	c	505	CLA	CHC-C4B-NB	5.55	130.13	124.26
22	c	510	CLA	CAC-C3C-C4C	5.55	132.01	124.81
22	D	401	CLA	C1C-C2C-C3C	-5.55	101.13	106.96
22	G	611	CLA	CHC-C4B-NB	5.54	130.13	124.26
22	g	611	CLA	CHC-C4B-NB	5.54	130.13	124.26
22	G	610	CLA	C2D-C1D-ND	5.54	114.19	110.10
22	g	610	CLA	C2D-C1D-ND	5.54	114.19	110.10
22	B	612	CLA	C1D-ND-C4D	5.54	110.27	106.33
22	R	309	CLA	C2B-C1B-NB	5.54	113.94	110.23
22	r	309	CLA	C2B-C1B-NB	5.54	113.94	110.23
22	1	614	CLA	CHC-C4B-NB	5.53	130.12	124.26
22	5	614	CLA	CHC-C4B-NB	5.53	130.12	124.26
22	C	511	CLA	CHC-C4B-NB	5.53	130.11	124.26
22	d	404	CLA	CHC-C4B-NB	5.53	130.11	124.26
22	N	603	CLA	C1D-ND-C4D	5.52	110.26	106.33
22	n	603	CLA	C1D-ND-C4D	5.52	110.26	106.33
23	a	404	PHO	C3D-C4D-ND	5.52	115.25	107.72
22	B	601	CLA	C2D-C1D-ND	5.52	114.17	110.10
22	a	402	CLA	CHC-C4B-NB	5.52	130.10	124.26
22	1	612	CLA	C1D-ND-C4D	5.52	110.25	106.33
22	5	612	CLA	C1D-ND-C4D	5.52	110.25	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	403	CLA	CAC-C3C-C4C	5.50	131.95	124.81
22	a	405	CLA	C1D-ND-C4D	5.50	110.24	106.33
22	b	604	CLA	CHC-C4B-NB	5.49	130.07	124.26
22	3	311	CLA	CHC-C4B-NB	5.49	130.07	124.26
22	7	311	CLA	CHC-C4B-NB	5.49	130.07	124.26
22	G	613	CLA	CAC-C3C-C4C	5.49	131.94	124.81
22	g	613	CLA	CAC-C3C-C4C	5.49	131.94	124.81
22	b	605	CLA	C1C-C2C-C3C	-5.49	101.18	106.96
22	B	601	CLA	CHC-C4B-NB	5.49	130.07	124.26
22	d	401	CLA	C1C-C2C-C3C	-5.49	101.18	106.96
22	4	301	CLA	C2B-C1B-NB	5.48	113.91	110.23
22	8	301	CLA	C2B-C1B-NB	5.48	113.91	110.23
22	R	301	CLA	CHC-C4B-NB	5.48	130.06	124.26
22	r	301	CLA	CHC-C4B-NB	5.48	130.06	124.26
22	B	607	CLA	C1D-ND-C4D	5.48	110.23	106.33
22	Y	602	CLA	CAC-C3C-C4C	5.48	131.92	124.81
22	y	602	CLA	CAC-C3C-C4C	5.48	131.92	124.81
22	C	501	CLA	C2B-C1B-NB	5.47	113.90	110.23
22	S	303	CLA	CHC-C4B-NB	5.47	130.05	124.26
22	s	303	CLA	CHC-C4B-NB	5.47	130.05	124.26
22	S	311	CLA	CHC-C4B-NB	5.47	130.05	124.26
22	s	311	CLA	CHC-C4B-NB	5.47	130.05	124.26
22	2	604	CLA	CHC-C4B-NB	5.47	130.04	124.26
22	6	604	CLA	CHC-C4B-NB	5.47	130.04	124.26
22	1	614	CLA	O2D-CGD-CBD	5.46	120.98	111.27
22	5	614	CLA	O2D-CGD-CBD	5.46	120.98	111.27
22	S	313	CLA	C1D-ND-C4D	5.46	110.22	106.33
22	s	313	CLA	C1D-ND-C4D	5.46	110.22	106.33
22	3	305	CLA	CHC-C4B-NB	5.46	130.04	124.26
22	7	305	CLA	CHC-C4B-NB	5.46	130.04	124.26
22	S	312	CLA	CAC-C3C-C4C	5.46	131.90	124.81
22	s	312	CLA	CAC-C3C-C4C	5.46	131.90	124.81
23	d	402	PHO	C3D-C4D-ND	5.46	115.17	107.72
22	b	601	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
22	3	310	CLA	C1C-C2C-C3C	-5.45	101.23	106.96
22	7	310	CLA	C1C-C2C-C3C	-5.45	101.23	106.96
22	a	403	CLA	CHC-C4B-NB	5.45	130.03	124.26
22	B	615	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
22	Y	613	CLA	CAC-C3C-C4C	5.44	131.86	124.81
22	y	613	CLA	CAC-C3C-C4C	5.44	131.86	124.81
22	Y	612	CLA	CAC-C3C-C4C	5.43	131.86	124.81
22	y	612	CLA	CAC-C3C-C4C	5.43	131.86	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	311	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
22	s	311	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
22	2	612	CLA	C1D-ND-C4D	5.43	110.19	106.33
22	6	612	CLA	C1D-ND-C4D	5.43	110.19	106.33
22	b	606	CLA	C1C-C2C-C3C	-5.43	101.25	106.96
22	R	303	CLA	CAC-C3C-C4C	5.42	131.85	124.81
22	r	303	CLA	CAC-C3C-C4C	5.42	131.85	124.81
22	3	314	CLA	C2B-C1B-NB	5.42	113.87	110.23
22	7	314	CLA	C2B-C1B-NB	5.42	113.87	110.23
22	c	512	CLA	C1D-ND-C4D	5.42	110.18	106.33
22	B	602	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
22	R	308	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
22	r	308	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
22	2	609	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
22	6	609	CLA	C1C-C2C-C3C	-5.41	101.27	106.96
22	2	610	CLA	C2B-C1B-NB	5.41	113.86	110.23
22	6	610	CLA	C2B-C1B-NB	5.41	113.86	110.23
22	C	511	CLA	C1D-ND-C4D	5.41	110.17	106.33
22	3	313	CLA	CHC-C4B-NB	5.40	129.97	124.26
22	7	313	CLA	CHC-C4B-NB	5.40	129.97	124.26
22	G	612	CLA	CAC-C3C-C4C	5.40	131.81	124.81
22	g	612	CLA	CAC-C3C-C4C	5.40	131.81	124.81
22	B	614	CLA	CHD-C4C-C3C	-5.39	116.91	124.84
22	S	309	CLA	C2B-C1B-NB	5.39	113.84	110.23
22	s	309	CLA	C2B-C1B-NB	5.39	113.84	110.23
22	c	503	CLA	C1D-ND-C4D	5.39	110.16	106.33
22	B	602	CLA	C1D-ND-C4D	5.39	110.16	106.33
22	c	512	CLA	CAC-C3C-C4C	5.38	131.80	124.81
22	R	309	CLA	CHC-C4B-NB	5.38	129.95	124.26
22	r	309	CLA	CHC-C4B-NB	5.38	129.95	124.26
22	G	610	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
22	g	610	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
22	c	511	CLA	CHC-C4B-NB	5.38	129.95	124.26
22	B	613	CLA	CHA-C4D-ND	5.38	143.75	132.50
22	A	405	CLA	CHA-C4D-ND	5.37	143.74	132.50
22	2	609	CLA	C2D-C1D-ND	5.36	114.06	110.10
22	6	609	CLA	C2D-C1D-ND	5.36	114.06	110.10
22	R	311	CLA	C1D-ND-C4D	5.36	110.14	106.33
22	r	311	CLA	C1D-ND-C4D	5.36	110.14	106.33
22	N	614	CLA	CHC-C4B-NB	5.36	129.93	124.26
22	n	614	CLA	CHC-C4B-NB	5.36	129.93	124.26
22	B	610	CLA	C1D-ND-C4D	5.36	110.14	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	615	CLA	CAC-C3C-C4C	5.36	131.76	124.81
22	B	615	CLA	O2D-CGD-CBD	5.36	120.78	111.27
22	N	603	CLA	CHC-C4B-NB	5.35	129.93	124.26
22	n	603	CLA	CHC-C4B-NB	5.35	129.93	124.26
22	c	510	CLA	C1D-ND-C4D	5.35	110.13	106.33
22	Y	614	CLA	C2B-C1B-NB	5.35	113.82	110.23
22	y	614	CLA	C2B-C1B-NB	5.35	113.82	110.23
22	Y	610	CLA	CHD-C4C-C3C	-5.34	116.98	124.84
22	y	610	CLA	CHD-C4C-C3C	-5.34	116.98	124.84
23	D	402	PHO	C3D-C4D-ND	5.34	115.00	107.72
22	B	603	CLA	CHC-C4B-NB	5.34	129.91	124.26
22	1	610	CLA	C2D-C1D-ND	5.34	114.04	110.10
22	5	610	CLA	C2D-C1D-ND	5.34	114.04	110.10
22	A	403	CLA	C1D-ND-C4D	5.34	110.13	106.33
25	Y	605	CHL	CAA-C2A-C3A	-5.33	103.66	116.10
25	y	605	CHL	CAA-C2A-C3A	-5.33	103.66	116.10
22	R	307	CLA	C2B-C1B-NB	5.33	113.81	110.23
22	r	307	CLA	C2B-C1B-NB	5.33	113.81	110.23
22	C	506	CLA	CHA-C4D-ND	5.33	143.65	132.50
22	4	310	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
22	8	310	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
22	C	502	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
22	b	610	CLA	C2B-C1B-NB	5.33	113.80	110.23
22	1	610	CLA	CHD-C4C-C3C	-5.32	117.01	124.84
22	5	610	CLA	CHD-C4C-C3C	-5.32	117.01	124.84
22	b	612	CLA	CHA-C4D-ND	5.32	143.63	132.50
22	R	310	CLA	CAC-C3C-C4C	5.32	131.71	124.81
22	r	310	CLA	CAC-C3C-C4C	5.32	131.71	124.81
22	a	403	CLA	C1D-ND-C4D	5.32	110.11	106.33
22	R	308	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
22	r	308	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
22	N	610	CLA	C1C-C2C-C3C	-5.31	101.38	106.96
22	n	610	CLA	C1C-C2C-C3C	-5.31	101.38	106.96
22	G	603	CLA	CHC-C4B-NB	5.31	129.87	124.26
22	g	603	CLA	CHC-C4B-NB	5.31	129.87	124.26
23	D	402	PHO	O2D-CGD-CBD	5.31	117.72	111.00
22	Y	611	CLA	CHD-C4C-C3C	-5.30	117.04	124.84
22	y	611	CLA	CHD-C4C-C3C	-5.30	117.04	124.84
22	c	504	CLA	C2B-C1B-NB	5.30	113.79	110.23
22	1	603	CLA	CHC-C4B-NB	5.30	129.87	124.26
22	5	603	CLA	CHC-C4B-NB	5.30	129.87	124.26
22	c	502	CLA	CAC-C3C-C4C	5.30	131.69	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	613	CLA	C1D-ND-C4D	5.29	110.09	106.33
22	5	613	CLA	C1D-ND-C4D	5.29	110.09	106.33
22	a	405	CLA	CHA-C4D-ND	5.29	143.56	132.50
22	C	508	CLA	CHA-C4D-ND	5.29	143.56	132.50
22	4	304	CLA	CHC-C4B-NB	5.28	129.85	124.26
22	8	304	CLA	CHC-C4B-NB	5.28	129.85	124.26
22	G	612	CLA	C2B-C1B-NB	5.28	113.77	110.23
22	g	612	CLA	C2B-C1B-NB	5.28	113.77	110.23
22	C	509	CLA	CHC-C4B-NB	5.28	129.85	124.26
22	3	310	CLA	CHC-C4B-NB	5.28	129.85	124.26
22	7	310	CLA	CHC-C4B-NB	5.28	129.85	124.26
22	G	613	CLA	C2B-C1B-NB	5.27	113.77	110.23
22	g	613	CLA	C2B-C1B-NB	5.27	113.77	110.23
22	2	610	CLA	CHC-C4B-NB	5.27	129.84	124.26
22	6	610	CLA	CHC-C4B-NB	5.27	129.84	124.26
22	S	309	CLA	CHC-C4B-NB	5.27	129.83	124.26
22	s	309	CLA	CHC-C4B-NB	5.27	129.83	124.26
25	4	306	CHL	CBA-CAA-C2A	5.26	129.40	113.86
25	8	306	CHL	CBA-CAA-C2A	5.26	129.40	113.86
22	C	512	CLA	CHA-C4D-ND	5.26	143.51	132.50
22	B	604	CLA	CHA-C4D-ND	5.26	143.51	132.50
22	C	502	CLA	CHC-C4B-NB	5.26	129.83	124.26
22	a	402	CLA	C1D-ND-C4D	5.26	110.07	106.33
22	S	301	CLA	CHA-C4D-ND	5.26	143.50	132.50
22	B	608	CLA	C2B-C1B-NB	5.26	113.76	110.23
22	C	501	CLA	C1D-ND-C4D	5.26	110.07	106.33
22	3	310	CLA	C2D-C1D-ND	5.26	113.98	110.10
22	7	310	CLA	C2D-C1D-ND	5.26	113.98	110.10
22	4	311	CLA	C1D-ND-C4D	5.25	110.07	106.33
22	8	311	CLA	C1D-ND-C4D	5.25	110.07	106.33
22	B	610	CLA	C2B-C1B-NB	5.25	113.75	110.23
22	3	311	CLA	C2B-C1B-NB	5.25	113.75	110.23
22	7	311	CLA	C2B-C1B-NB	5.25	113.75	110.23
22	B	616	CLA	C2D-C1D-ND	5.25	113.97	110.10
22	C	507	CLA	CAC-C3C-C4C	5.25	131.62	124.81
22	a	403	CLA	C2B-C1B-NB	5.25	113.75	110.23
22	d	403	CLA	C1D-ND-C4D	5.25	110.06	106.33
22	S	304	CLA	C2B-C1B-NB	5.25	113.75	110.23
22	s	304	CLA	C2B-C1B-NB	5.25	113.75	110.23
22	Y	611	CLA	CHC-C4B-NB	5.25	129.81	124.26
22	y	611	CLA	CHC-C4B-NB	5.25	129.81	124.26
22	a	403	CLA	CHD-C4C-C3C	-5.24	117.13	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	503	CLA	CHA-C4D-ND	5.24	143.47	132.50
22	R	301	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
22	r	301	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
22	B	605	CLA	C1D-ND-C4D	5.23	110.05	106.33
22	4	310	CLA	C2D-C1D-ND	5.23	113.96	110.10
22	8	310	CLA	C2D-C1D-ND	5.23	113.96	110.10
22	R	307	CLA	CHC-C4B-NB	5.23	129.79	124.26
22	r	307	CLA	CHC-C4B-NB	5.23	129.79	124.26
22	c	510	CLA	CHA-C4D-ND	5.23	143.44	132.50
22	b	615	CLA	C4A-NA-C1A	-5.23	104.36	106.71
22	B	601	CLA	C2B-C1B-NB	5.23	113.74	110.23
22	Y	604	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
22	y	604	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
22	c	508	CLA	CHA-C4D-ND	5.22	143.43	132.50
22	Y	603	CLA	C1D-ND-C4D	5.22	110.05	106.33
22	y	603	CLA	C1D-ND-C4D	5.22	110.05	106.33
22	2	609	CLA	CHC-C4B-NB	5.22	129.78	124.26
22	6	609	CLA	CHC-C4B-NB	5.22	129.78	124.26
22	4	310	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
22	8	310	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
22	Y	604	CLA	C1D-ND-C4D	5.21	110.04	106.33
22	y	604	CLA	C1D-ND-C4D	5.21	110.04	106.33
22	C	501	CLA	CHA-C4D-ND	5.21	143.40	132.50
22	b	614	CLA	C1D-ND-C4D	5.20	110.03	106.33
22	N	603	CLA	C2B-C1B-NB	5.20	113.72	110.23
22	n	603	CLA	C2B-C1B-NB	5.20	113.72	110.23
22	d	401	CLA	C1D-ND-C4D	5.20	110.03	106.33
22	3	313	CLA	C1D-ND-C4D	5.20	110.03	106.33
22	7	313	CLA	C1D-ND-C4D	5.20	110.03	106.33
22	B	616	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
22	G	603	CLA	C2B-C1B-NB	5.19	113.71	110.23
22	g	603	CLA	C2B-C1B-NB	5.19	113.71	110.23
22	d	403	CLA	C2B-C1B-NB	5.19	113.71	110.23
22	B	610	CLA	CHA-C4D-ND	5.19	143.35	132.50
22	R	311	CLA	CHD-C4C-C3C	-5.19	117.22	124.84
22	r	311	CLA	CHD-C4C-C3C	-5.19	117.22	124.84
22	b	611	CLA	CHA-C4D-ND	5.19	143.35	132.50
22	d	401	CLA	C2B-C1B-NB	5.18	113.70	110.23
22	c	512	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
22	c	507	CLA	C2B-C1B-NB	5.17	113.70	110.23
22	S	312	CLA	C2B-C1B-NB	5.17	113.70	110.23
22	s	312	CLA	C2B-C1B-NB	5.17	113.70	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	507	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
22	B	611	CLA	C2B-C1B-NB	5.17	113.70	110.23
22	N	612	CLA	C2D-C1D-ND	5.17	113.91	110.10
22	n	612	CLA	C2D-C1D-ND	5.17	113.91	110.10
22	R	301	CLA	O2D-CGD-CBD	5.17	120.45	111.27
22	r	301	CLA	O2D-CGD-CBD	5.17	120.45	111.27
22	b	608	CLA	C1D-ND-C4D	5.16	110.00	106.33
22	c	506	CLA	CHA-C4D-ND	5.16	143.30	132.50
22	N	614	CLA	C1D-ND-C4D	5.16	110.00	106.33
22	n	614	CLA	C1D-ND-C4D	5.16	110.00	106.33
22	a	403	CLA	CHA-C4D-ND	5.15	143.28	132.50
22	b	604	CLA	C1D-ND-C4D	5.15	109.99	106.33
22	b	606	CLA	CHA-C4D-ND	5.15	143.27	132.50
22	b	611	CLA	C1C-C2C-C3C	-5.15	101.55	106.96
22	C	502	CLA	C2B-C1B-NB	5.15	113.68	110.23
22	d	403	CLA	CHA-C4D-ND	5.15	143.26	132.50
22	2	613	CLA	CHC-C4B-NB	5.15	129.70	124.26
22	6	613	CLA	CHC-C4B-NB	5.15	129.70	124.26
22	C	509	CLA	C2B-C1B-NB	5.14	113.68	110.23
22	b	613	CLA	C1D-ND-C4D	5.14	109.99	106.33
22	b	602	CLA	C2D-C1D-ND	5.14	113.89	110.10
22	B	606	CLA	CHA-C4D-ND	5.14	143.25	132.50
22	b	613	CLA	CHA-C4D-ND	5.14	143.25	132.50
22	B	612	CLA	CHC-C4B-NB	5.14	129.70	124.26
22	4	301	CLA	C1D-ND-C4D	5.14	109.98	106.33
22	8	301	CLA	C1D-ND-C4D	5.14	109.98	106.33
22	c	505	CLA	CMA-C3A-C4A	-5.14	97.97	111.77
22	c	503	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
22	c	501	CLA	CHA-C4D-ND	5.13	143.23	132.50
22	4	311	CLA	CHC-C4B-NB	5.13	129.68	124.26
22	8	311	CLA	CHC-C4B-NB	5.13	129.68	124.26
22	C	509	CLA	CHA-C4D-ND	5.12	143.22	132.50
22	G	614	CLA	CHC-C4B-NB	5.12	129.68	124.26
22	g	614	CLA	CHC-C4B-NB	5.12	129.68	124.26
22	B	611	CLA	O2D-CGD-CBD	5.12	120.37	111.27
22	b	615	CLA	CHA-C4D-ND	5.12	143.21	132.50
22	N	603	CLA	CHA-C4D-ND	5.12	143.21	132.50
22	n	603	CLA	CHA-C4D-ND	5.12	143.21	132.50
22	S	314	CLA	C1D-ND-C4D	5.12	109.97	106.33
22	s	314	CLA	C1D-ND-C4D	5.12	109.97	106.33
22	S	303	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
22	s	303	CLA	CHD-C4C-C3C	-5.12	117.31	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	603	CLA	CHA-C4D-ND	5.12	143.21	132.50
22	2	611	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
22	6	611	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
22	S	303	CLA	C2B-C1B-NB	5.11	113.66	110.23
22	s	303	CLA	C2B-C1B-NB	5.11	113.66	110.23
22	c	512	CLA	CHA-C4D-ND	5.11	143.19	132.50
22	S	313	CLA	CHC-C4B-NB	5.11	129.67	124.26
22	s	313	CLA	CHC-C4B-NB	5.11	129.67	124.26
22	4	311	CLA	CAC-C3C-C4C	5.11	131.44	124.81
22	8	311	CLA	CAC-C3C-C4C	5.11	131.44	124.81
22	c	511	CLA	CHA-C4D-ND	5.11	143.18	132.50
22	B	606	CLA	C1C-C2C-C3C	-5.10	101.59	106.96
22	S	312	CLA	CHA-C4D-ND	5.10	143.17	132.50
22	s	312	CLA	CHA-C4D-ND	5.10	143.17	132.50
22	B	612	CLA	CHA-C4D-ND	5.10	143.17	132.50
22	c	509	CLA	C2B-C1B-NB	5.10	113.65	110.23
22	S	311	CLA	CAC-C3C-C4C	5.10	131.43	124.81
22	s	311	CLA	CAC-C3C-C4C	5.10	131.43	124.81
22	B	603	CLA	CHA-C4D-ND	5.10	143.16	132.50
22	S	313	CLA	CHA-C4D-ND	5.10	143.16	132.50
22	s	313	CLA	CHA-C4D-ND	5.10	143.16	132.50
22	1	611	CLA	C2B-C1B-NB	5.10	113.65	110.23
22	5	611	CLA	C2B-C1B-NB	5.10	113.65	110.23
22	c	509	CLA	CHC-C4B-NB	5.09	129.65	124.26
22	B	605	CLA	C2B-C1B-NB	5.09	113.64	110.23
22	b	605	CLA	C2B-C1B-NB	5.09	113.64	110.23
22	1	614	CLA	CHA-C4D-ND	5.09	143.15	132.50
22	5	614	CLA	CHA-C4D-ND	5.09	143.15	132.50
22	s	301	CLA	C1D-ND-C4D	5.09	109.95	106.33
22	c	502	CLA	C2B-C1B-NB	5.09	113.64	110.23
22	Y	602	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
22	y	602	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
22	C	505	CLA	C1D-ND-C4D	5.08	109.95	106.33
22	A	403	CLA	CHA-C4D-ND	5.08	143.13	132.50
22	A	402	CLA	C2B-C1B-NB	5.08	113.64	110.23
22	G	614	CLA	C1D-ND-C4D	5.08	109.94	106.33
22	g	614	CLA	C1D-ND-C4D	5.08	109.94	106.33
22	G	613	CLA	CHA-C4D-ND	5.08	143.12	132.50
22	g	613	CLA	CHA-C4D-ND	5.08	143.12	132.50
22	C	510	CLA	CHA-C4D-ND	5.08	143.12	132.50
22	G	603	CLA	CHA-C4D-ND	5.08	143.12	132.50
22	g	603	CLA	CHA-C4D-ND	5.08	143.12	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	301	CLA	CHC-C4B-NB	5.08	129.63	124.26
22	8	301	CLA	CHC-C4B-NB	5.08	129.63	124.26
22	3	303	CLA	C2B-C1B-NB	5.08	113.64	110.23
22	7	303	CLA	C2B-C1B-NB	5.08	113.64	110.23
22	c	505	CLA	O2D-CGD-CBD	5.07	120.29	111.27
22	Y	603	CLA	C2B-C1B-NB	5.07	113.63	110.23
22	y	603	CLA	C2B-C1B-NB	5.07	113.63	110.23
22	a	402	CLA	CHA-C4D-ND	5.07	143.10	132.50
22	b	614	CLA	CHA-C4D-ND	5.07	143.10	132.50
22	s	301	CLA	CHA-C4D-ND	5.06	143.09	132.50
22	C	509	CLA	C1D-ND-C4D	5.06	109.93	106.33
22	B	607	CLA	C2B-C1B-NB	5.06	113.62	110.23
22	4	305	CLA	C1D-ND-C4D	5.06	109.93	106.33
22	8	305	CLA	C1D-ND-C4D	5.06	109.93	106.33
22	b	605	CLA	CHC-C4B-NB	5.06	129.61	124.26
22	C	501	CLA	CAC-C3C-C4C	5.06	131.37	124.81
22	B	614	CLA	CHA-C4D-ND	5.05	143.07	132.50
22	b	616	CLA	CHA-C4D-ND	5.05	143.06	132.50
22	2	603	CLA	C1D-ND-C4D	5.05	109.92	106.33
22	6	603	CLA	C1D-ND-C4D	5.05	109.92	106.33
22	1	603	CLA	C2B-C1B-NB	5.05	113.62	110.23
22	5	603	CLA	C2B-C1B-NB	5.05	113.62	110.23
22	3	304	CLA	CHC-C4B-NB	5.05	129.60	124.26
22	7	304	CLA	CHC-C4B-NB	5.05	129.60	124.26
22	1	604	CLA	C2B-C1B-NB	5.05	113.62	110.23
22	5	604	CLA	C2B-C1B-NB	5.05	113.62	110.23
22	C	511	CLA	CHA-C4D-ND	5.05	143.06	132.50
22	C	512	CLA	C1D-ND-C4D	5.05	109.92	106.33
22	b	607	CLA	CHA-C4D-ND	5.04	143.05	132.50
22	B	607	CLA	CHA-C4D-ND	5.04	143.05	132.50
22	B	611	CLA	CHA-C4D-ND	5.04	143.05	132.50
22	N	613	CLA	CHA-C4D-ND	5.04	143.05	132.50
22	n	613	CLA	CHA-C4D-ND	5.04	143.05	132.50
22	2	603	CLA	CHC-C4B-NB	5.04	129.59	124.26
22	6	603	CLA	CHC-C4B-NB	5.04	129.59	124.26
22	b	608	CLA	CHC-C4B-NB	5.04	129.59	124.26
22	D	401	CLA	CHA-C4D-ND	5.04	143.04	132.50
22	2	609	CLA	CHA-C4D-ND	5.04	143.03	132.50
22	6	609	CLA	CHA-C4D-ND	5.04	143.03	132.50
22	S	303	CLA	O2D-CGD-CBD	5.03	120.22	111.27
22	s	303	CLA	O2D-CGD-CBD	5.03	120.22	111.27
22	b	610	CLA	CHA-C4D-ND	5.03	143.02	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	505	CLA	O2D-CGD-CBD	5.03	120.20	111.27
22	S	301	CLA	CHD-C4C-C3C	-5.03	117.45	124.84
22	2	611	CLA	C2B-C1B-NB	5.03	113.60	110.23
22	4	311	CLA	C2B-C1B-NB	5.03	113.60	110.23
22	6	611	CLA	C2B-C1B-NB	5.03	113.60	110.23
22	8	311	CLA	C2B-C1B-NB	5.03	113.60	110.23
22	Y	603	CLA	CHD-C4C-C3C	-5.02	117.46	124.84
22	y	603	CLA	CHD-C4C-C3C	-5.02	117.46	124.84
22	4	305	CLA	C2B-C1B-NB	5.02	113.60	110.23
22	8	305	CLA	C2B-C1B-NB	5.02	113.60	110.23
22	4	311	CLA	CHA-C4D-ND	5.02	143.00	132.50
22	8	311	CLA	CHA-C4D-ND	5.02	143.00	132.50
22	2	604	CLA	C1D-ND-C4D	5.02	109.90	106.33
22	6	604	CLA	C1D-ND-C4D	5.02	109.90	106.33
22	B	615	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
22	G	610	CLA	CHA-C4D-ND	5.02	142.99	132.50
22	g	610	CLA	CHA-C4D-ND	5.02	142.99	132.50
22	S	310	CLA	CHA-C4D-ND	5.01	142.99	132.50
22	Y	604	CLA	CHA-C4D-ND	5.01	142.99	132.50
22	s	310	CLA	CHA-C4D-ND	5.01	142.99	132.50
22	y	604	CLA	CHA-C4D-ND	5.01	142.99	132.50
22	d	404	CLA	C1D-ND-C4D	5.01	109.90	106.33
22	G	610	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
22	g	610	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
22	3	312	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
22	7	312	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
22	N	610	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
22	n	610	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
22	b	601	CLA	CAC-C3C-C4C	5.01	131.31	124.81
25	4	309	CHL	CAA-C2A-C3A	-5.01	99.06	112.78
25	8	309	CHL	CAA-C2A-C3A	-5.01	99.06	112.78
22	C	505	CLA	CHA-C4D-ND	5.01	142.97	132.50
22	3	314	CLA	C1D-ND-C4D	5.01	109.89	106.33
22	7	314	CLA	C1D-ND-C4D	5.01	109.89	106.33
22	Y	603	CLA	CHA-C4D-ND	5.01	142.97	132.50
22	y	603	CLA	CHA-C4D-ND	5.01	142.97	132.50
22	G	614	CLA	CHA-C4D-ND	5.01	142.97	132.50
22	g	614	CLA	CHA-C4D-ND	5.01	142.97	132.50
22	R	303	CLA	CHA-C4D-ND	5.00	142.97	132.50
22	r	303	CLA	CHA-C4D-ND	5.00	142.97	132.50
22	N	611	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	n	611	CLA	O2D-CGD-CBD	5.00	120.16	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	405	CLA	CHD-C4C-C3C	-5.00	117.49	124.84
22	R	308	CLA	CHA-C4D-ND	5.00	142.96	132.50
22	Y	610	CLA	CHA-C4D-ND	5.00	142.96	132.50
22	r	308	CLA	CHA-C4D-ND	5.00	142.96	132.50
22	y	610	CLA	CHA-C4D-ND	5.00	142.96	132.50
22	R	310	CLA	CHA-C4D-ND	5.00	142.96	132.50
22	r	310	CLA	CHA-C4D-ND	5.00	142.96	132.50
22	N	610	CLA	CHA-C4D-ND	5.00	142.96	132.50
22	n	610	CLA	CHA-C4D-ND	5.00	142.96	132.50
22	2	603	CLA	C2B-C1B-NB	5.00	113.58	110.23
22	6	603	CLA	C2B-C1B-NB	5.00	113.58	110.23
25	Y	606	CHL	CBA-CAA-C2A	5.00	128.61	113.86
25	y	606	CHL	CBA-CAA-C2A	5.00	128.61	113.86
22	C	503	CLA	CHA-C4D-ND	4.99	142.95	132.50
22	N	612	CLA	CAC-C3C-C4C	4.99	131.29	124.81
22	n	612	CLA	CAC-C3C-C4C	4.99	131.29	124.81
22	D	404	CLA	C2B-C1B-NB	4.99	113.58	110.23
22	D	404	CLA	O2D-CGD-CBD	4.99	120.14	111.27
22	4	303	CLA	CHD-C4C-C3C	-4.99	117.50	124.84
22	8	303	CLA	CHD-C4C-C3C	-4.99	117.50	124.84
22	b	607	CLA	C1D-ND-C4D	4.99	109.88	106.33
22	Y	612	CLA	CHA-C4D-ND	4.99	142.94	132.50
22	y	612	CLA	CHA-C4D-ND	4.99	142.94	132.50
22	C	507	CLA	C1D-ND-C4D	4.99	109.88	106.33
22	b	612	CLA	C1D-ND-C4D	4.99	109.88	106.33
22	b	608	CLA	CHA-C4D-ND	4.99	142.93	132.50
22	Y	602	CLA	C2D-C1D-ND	4.99	113.78	110.10
22	y	602	CLA	C2D-C1D-ND	4.99	113.78	110.10
22	c	505	CLA	CHA-C4D-ND	4.99	142.93	132.50
22	B	601	CLA	CAC-C3C-C4C	4.99	131.28	124.81
22	Y	614	CLA	C1D-ND-C4D	4.98	109.88	106.33
22	y	614	CLA	C1D-ND-C4D	4.98	109.88	106.33
22	Y	611	CLA	O2D-CGD-CBD	4.98	120.12	111.27
22	y	611	CLA	O2D-CGD-CBD	4.98	120.12	111.27
22	C	510	CLA	CHD-C4C-C3C	-4.98	117.51	124.84
22	c	509	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
22	2	613	CLA	CHA-C4D-ND	4.98	142.92	132.50
22	6	613	CLA	CHA-C4D-ND	4.98	142.92	132.50
22	D	403	CLA	CHA-C4D-ND	4.98	142.92	132.50
22	S	314	CLA	C2B-C1B-NB	4.98	113.57	110.23
22	s	314	CLA	C2B-C1B-NB	4.98	113.57	110.23
22	Y	614	CLA	CHA-C4D-ND	4.98	142.91	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	y	614	CLA	CHA-C4D-ND	4.98	142.91	132.50
22	3	314	CLA	CHA-C4D-ND	4.98	142.91	132.50
22	7	314	CLA	CHA-C4D-ND	4.98	142.91	132.50
22	C	509	CLA	CAC-C3C-C4C	4.98	131.27	124.81
22	B	605	CLA	CHA-C4D-ND	4.98	142.91	132.50
22	C	507	CLA	CHA-C4D-ND	4.97	142.91	132.50
22	c	510	CLA	CHD-C4C-C3C	-4.97	117.53	124.84
22	A	402	CLA	CHA-C4D-ND	4.97	142.90	132.50
22	2	612	CLA	CHA-C4D-ND	4.97	142.90	132.50
22	6	612	CLA	CHA-C4D-ND	4.97	142.90	132.50
22	Y	610	CLA	C2D-C1D-ND	4.97	113.77	110.10
22	y	610	CLA	C2D-C1D-ND	4.97	113.77	110.10
22	G	602	CLA	CHD-C4C-C3C	-4.97	117.54	124.84
22	g	602	CLA	CHD-C4C-C3C	-4.97	117.54	124.84
22	B	611	CLA	C1C-C2C-C3C	-4.97	101.73	106.96
22	2	604	CLA	C2B-C1B-NB	4.97	113.56	110.23
22	6	604	CLA	C2B-C1B-NB	4.97	113.56	110.23
22	c	502	CLA	CHD-C4C-C3C	-4.96	117.54	124.84
22	b	613	CLA	C2B-C1B-NB	4.96	113.56	110.23
22	b	602	CLA	CHA-C4D-ND	4.96	142.88	132.50
22	b	609	CLA	CHA-C4D-ND	4.96	142.88	132.50
22	C	510	CLA	C2B-C1B-NB	4.96	113.56	110.23
22	b	601	CLA	C2B-C1B-NB	4.96	113.56	110.23
22	A	402	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
22	4	304	CLA	C1D-ND-C4D	4.96	109.86	106.33
22	8	304	CLA	C1D-ND-C4D	4.96	109.86	106.33
22	2	603	CLA	CHA-C4D-ND	4.96	142.87	132.50
22	6	603	CLA	CHA-C4D-ND	4.96	142.87	132.50
22	B	609	CLA	CHA-C4D-ND	4.96	142.87	132.50
22	d	401	CLA	CHA-C4D-ND	4.96	142.87	132.50
22	G	612	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
22	g	612	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
22	b	609	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
22	b	605	CLA	CHA-C4D-ND	4.95	142.86	132.50
22	3	314	CLA	CHC-C4B-NB	4.95	129.49	124.26
22	7	314	CLA	CHC-C4B-NB	4.95	129.49	124.26
22	c	509	CLA	CHA-C4D-ND	4.95	142.85	132.50
22	A	403	CLA	CHC-C4B-NB	4.94	129.49	124.26
22	C	503	CLA	C1D-ND-C4D	4.94	109.85	106.33
22	Y	613	CLA	CHA-C4D-ND	4.94	142.84	132.50
22	y	613	CLA	CHA-C4D-ND	4.94	142.84	132.50
22	4	301	CLA	CHA-C4D-ND	4.94	142.84	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	301	CLA	CHA-C4D-ND	4.94	142.84	132.50
22	S	304	CLA	CHA-C4D-ND	4.94	142.84	132.50
22	s	304	CLA	CHA-C4D-ND	4.94	142.84	132.50
22	N	612	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
22	n	612	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
22	d	404	CLA	CHA-C4D-ND	4.94	142.84	132.50
22	c	507	CLA	CHD-C4C-C3C	-4.94	117.58	124.84
22	G	604	CLA	C1D-ND-C4D	4.94	109.84	106.33
22	g	604	CLA	C1D-ND-C4D	4.94	109.84	106.33
22	b	601	CLA	CHA-C4D-ND	4.94	142.83	132.50
22	C	504	CLA	C1D-ND-C4D	4.93	109.84	106.33
22	A	402	CLA	C2D-C1D-ND	4.93	113.74	110.10
22	S	314	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
22	s	314	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
22	3	304	CLA	CHA-C4D-ND	4.93	142.81	132.50
22	7	304	CLA	CHA-C4D-ND	4.93	142.81	132.50
25	S	306	CHL	CBA-CAA-C2A	4.93	128.41	113.86
25	s	306	CHL	CBA-CAA-C2A	4.93	128.41	113.86
22	d	404	CLA	C2B-C1B-NB	4.93	113.53	110.23
22	c	504	CLA	C1D-ND-C4D	4.93	109.83	106.33
22	N	612	CLA	CHD-C4C-C3C	-4.92	117.60	124.84
22	n	612	CLA	CHD-C4C-C3C	-4.92	117.60	124.84
22	3	310	CLA	CHA-C4D-ND	4.92	142.80	132.50
22	7	310	CLA	CHA-C4D-ND	4.92	142.80	132.50
22	b	604	CLA	CHA-C4D-ND	4.92	142.80	132.50
22	a	403	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
22	G	612	CLA	C2D-C1D-ND	4.92	113.73	110.10
22	g	612	CLA	C2D-C1D-ND	4.92	113.73	110.10
22	C	504	CLA	CHA-C4D-ND	4.92	142.79	132.50
22	c	502	CLA	CHA-C4D-ND	4.92	142.79	132.50
22	G	611	CLA	CHA-C4D-ND	4.92	142.79	132.50
22	g	611	CLA	CHA-C4D-ND	4.92	142.79	132.50
22	d	401	CLA	CHD-C4C-C3C	-4.92	117.61	124.84
22	S	314	CLA	CHA-C4D-ND	4.92	142.79	132.50
22	s	314	CLA	CHA-C4D-ND	4.92	142.79	132.50
22	R	302	CLA	C2D-C1D-ND	4.92	113.73	110.10
22	r	302	CLA	C2D-C1D-ND	4.92	113.73	110.10
22	4	303	CLA	O2D-CGD-CBD	4.92	120.00	111.27
22	8	303	CLA	O2D-CGD-CBD	4.92	120.00	111.27
22	3	311	CLA	CHA-C4D-ND	4.92	142.78	132.50
22	7	311	CLA	CHA-C4D-ND	4.92	142.78	132.50
22	c	504	CLA	CHA-C4D-ND	4.91	142.78	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	305	CLA	C1D-ND-C4D	4.91	109.82	106.33
22	7	305	CLA	C1D-ND-C4D	4.91	109.82	106.33
25	R	305	CHL	CBA-CAA-C2A	4.91	128.35	113.86
25	r	305	CHL	CBA-CAA-C2A	4.91	128.35	113.86
22	2	609	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
22	6	609	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
22	S	311	CLA	CHA-C4D-ND	4.91	142.76	132.50
22	s	311	CLA	CHA-C4D-ND	4.91	142.76	132.50
22	c	512	CLA	C3D-C2D-C1D	-4.91	99.14	105.83
22	R	310	CLA	CHC-C4B-NB	4.90	129.45	124.26
22	r	310	CLA	CHC-C4B-NB	4.90	129.45	124.26
22	c	505	CLA	C3B-C2B-C1B	-4.90	101.24	107.16
22	N	602	CLA	CHA-C4D-ND	4.90	142.76	132.50
22	n	602	CLA	CHA-C4D-ND	4.90	142.76	132.50
22	2	602	CLA	CHA-C4D-ND	4.90	142.76	132.50
22	6	602	CLA	CHA-C4D-ND	4.90	142.76	132.50
22	G	611	CLA	O2D-CGD-CBD	4.90	119.98	111.27
22	g	611	CLA	O2D-CGD-CBD	4.90	119.98	111.27
22	2	611	CLA	CAC-C3C-C4C	4.90	131.17	124.81
22	6	611	CLA	CAC-C3C-C4C	4.90	131.17	124.81
22	R	308	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
22	r	308	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
22	S	311	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
22	s	311	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
22	b	615	CLA	O2D-CGD-CBD	4.90	119.98	111.27
22	R	307	CLA	CHA-C4D-ND	4.90	142.74	132.50
22	r	307	CLA	CHA-C4D-ND	4.90	142.74	132.50
22	1	610	CLA	CHA-C4D-ND	4.90	142.74	132.50
22	5	610	CLA	CHA-C4D-ND	4.90	142.74	132.50
22	1	603	CLA	CHA-C4D-ND	4.90	142.74	132.50
22	5	603	CLA	CHA-C4D-ND	4.90	142.74	132.50
22	4	303	CLA	CHA-C4D-ND	4.89	142.74	132.50
22	8	303	CLA	CHA-C4D-ND	4.89	142.74	132.50
22	S	313	CLA	O2D-CGD-CBD	4.89	119.96	111.27
22	s	313	CLA	O2D-CGD-CBD	4.89	119.96	111.27
22	b	603	CLA	O2D-CGD-CBD	4.89	119.95	111.27
22	1	612	CLA	CHA-C4D-ND	4.89	142.72	132.50
22	5	612	CLA	CHA-C4D-ND	4.89	142.72	132.50
22	B	606	CLA	C1D-ND-C4D	4.89	109.81	106.33
22	b	612	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
22	N	611	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
22	n	611	CLA	C3D-C2D-C1D	-4.89	99.16	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	405	CLA	C2B-C1B-NB	4.89	113.51	110.23
22	S	305	CLA	CHA-C4D-ND	4.88	142.72	132.50
22	s	305	CLA	CHA-C4D-ND	4.88	142.72	132.50
22	3	313	CLA	CHA-C4D-ND	4.88	142.72	132.50
22	7	313	CLA	CHA-C4D-ND	4.88	142.72	132.50
22	G	611	CLA	CHD-C4C-C3C	-4.88	117.66	124.84
22	g	611	CLA	CHD-C4C-C3C	-4.88	117.66	124.84
22	G	602	CLA	CHA-C4D-ND	4.88	142.71	132.50
22	g	602	CLA	CHA-C4D-ND	4.88	142.71	132.50
22	3	305	CLA	C2B-C1B-NB	4.88	113.50	110.23
22	7	305	CLA	C2B-C1B-NB	4.88	113.50	110.23
22	N	611	CLA	CHA-C4D-ND	4.88	142.71	132.50
22	n	611	CLA	CHA-C4D-ND	4.88	142.71	132.50
22	Y	611	CLA	C2D-C1D-ND	4.88	113.70	110.10
22	y	611	CLA	C2D-C1D-ND	4.88	113.70	110.10
22	B	612	CLA	CHD-C4C-C3C	-4.88	117.67	124.84
22	S	304	CLA	C1D-ND-C4D	4.87	109.80	106.33
22	s	304	CLA	C1D-ND-C4D	4.87	109.80	106.33
22	2	610	CLA	CHA-C4D-ND	4.87	142.69	132.50
22	6	610	CLA	CHA-C4D-ND	4.87	142.69	132.50
22	2	611	CLA	CHA-C4D-ND	4.87	142.69	132.50
22	6	611	CLA	CHA-C4D-ND	4.87	142.69	132.50
22	D	403	CLA	CAC-C3C-C2C	-4.87	119.20	127.53
22	b	611	CLA	CHD-C4C-C3C	-4.87	117.68	124.84
22	b	611	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
22	G	612	CLA	CHA-C4D-ND	4.87	142.69	132.50
22	g	612	CLA	CHA-C4D-ND	4.87	142.69	132.50
22	R	309	CLA	CHA-C4D-ND	4.87	142.68	132.50
22	r	309	CLA	CHA-C4D-ND	4.87	142.68	132.50
22	C	507	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
22	Y	602	CLA	C1D-ND-C4D	4.86	109.79	106.33
22	y	602	CLA	C1D-ND-C4D	4.86	109.79	106.33
22	4	304	CLA	CHA-C4D-ND	4.86	142.67	132.50
22	8	304	CLA	CHA-C4D-ND	4.86	142.67	132.50
22	c	507	CLA	CHA-C4D-ND	4.86	142.67	132.50
22	2	611	CLA	C2D-C1D-ND	4.86	113.69	110.10
22	6	611	CLA	C2D-C1D-ND	4.86	113.69	110.10
22	R	302	CLA	CHA-C4D-ND	4.86	142.67	132.50
22	r	302	CLA	CHA-C4D-ND	4.86	142.67	132.50
22	C	503	CLA	CHD-C4C-C3C	-4.86	117.69	124.84
22	B	601	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
22	R	303	CLA	C2B-C1B-NB	4.86	113.49	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r	303	CLA	C2B-C1B-NB	4.86	113.49	110.23
22	2	612	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
22	6	612	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
22	4	305	CLA	CHA-C4D-ND	4.85	142.65	132.50
22	8	305	CLA	CHA-C4D-ND	4.85	142.65	132.50
22	S	310	CLA	CHD-C4C-C3C	-4.85	117.71	124.84
22	s	310	CLA	CHD-C4C-C3C	-4.85	117.71	124.84
22	1	613	CLA	CHA-C4D-ND	4.85	142.65	132.50
22	5	613	CLA	CHA-C4D-ND	4.85	142.65	132.50
22	c	507	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
22	G	604	CLA	C2B-C1B-NB	4.85	113.48	110.23
22	g	604	CLA	C2B-C1B-NB	4.85	113.48	110.23
22	C	509	CLA	CHD-C4C-C3C	-4.85	117.72	124.84
22	A	402	CLA	C1C-C2C-C3C	-4.85	101.86	106.96
22	N	611	CLA	CHD-C4C-C3C	-4.84	117.72	124.84
22	n	611	CLA	CHD-C4C-C3C	-4.84	117.72	124.84
22	N	614	CLA	CHA-C4D-ND	4.84	142.63	132.50
22	n	614	CLA	CHA-C4D-ND	4.84	142.63	132.50
22	1	602	CLA	CHA-C4D-ND	4.84	142.63	132.50
22	5	602	CLA	CHA-C4D-ND	4.84	142.63	132.50
22	B	615	CLA	CHA-C4D-ND	4.84	142.63	132.50
22	R	310	CLA	CHD-C4C-C3C	-4.84	117.72	124.84
22	r	310	CLA	CHD-C4C-C3C	-4.84	117.72	124.84
22	R	301	CLA	CHA-C4D-ND	4.84	142.63	132.50
22	r	301	CLA	CHA-C4D-ND	4.84	142.63	132.50
22	Y	611	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
22	y	611	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
22	B	615	CLA	C1D-ND-C4D	4.84	109.77	106.33
22	B	608	CLA	O2D-CGD-CBD	4.84	119.87	111.27
22	S	312	CLA	C1D-ND-C4D	4.84	109.77	106.33
22	s	312	CLA	C1D-ND-C4D	4.84	109.77	106.33
22	c	501	CLA	C2B-C1B-NB	4.84	113.47	110.23
22	1	613	CLA	C2B-C1B-NB	4.84	113.47	110.23
22	5	613	CLA	C2B-C1B-NB	4.84	113.47	110.23
22	N	612	CLA	CHA-C4D-ND	4.84	142.62	132.50
22	n	612	CLA	CHA-C4D-ND	4.84	142.62	132.50
22	Y	613	CLA	CHD-C4C-C3C	-4.83	117.73	124.84
22	y	613	CLA	CHD-C4C-C3C	-4.83	117.73	124.84
22	b	609	CLA	C2D-C1D-ND	4.83	113.67	110.10
22	b	609	CLA	C2B-C1B-NB	4.83	113.47	110.23
22	B	611	CLA	CHD-C4C-C3C	-4.83	117.74	124.84
22	1	610	CLA	C3D-C2D-C1D	-4.83	99.24	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	610	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
22	3	305	CLA	O2D-CGD-CBD	4.83	119.85	111.27
22	7	305	CLA	O2D-CGD-CBD	4.83	119.85	111.27
22	3	303	CLA	CHD-C4C-C3C	-4.83	117.74	124.84
22	7	303	CLA	CHD-C4C-C3C	-4.83	117.74	124.84
22	C	501	CLA	C4A-NA-C1A	-4.83	104.54	106.71
22	3	312	CLA	C2B-C1B-NB	4.82	113.47	110.23
22	7	312	CLA	C2B-C1B-NB	4.82	113.47	110.23
22	Y	602	CLA	O2D-CGD-CBD	4.82	119.84	111.27
22	y	602	CLA	O2D-CGD-CBD	4.82	119.84	111.27
22	Y	603	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
22	y	603	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
22	R	307	CLA	C1D-ND-C4D	4.82	109.76	106.33
22	r	307	CLA	C1D-ND-C4D	4.82	109.76	106.33
22	2	610	CLA	CHD-C4C-C3C	-4.82	117.76	124.84
22	6	610	CLA	CHD-C4C-C3C	-4.82	117.76	124.84
22	b	613	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
22	N	613	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
22	n	613	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
22	b	611	CLA	C2B-C1B-NB	4.82	113.46	110.23
22	c	509	CLA	C2D-C1D-ND	4.81	113.65	110.10
22	b	613	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
22	C	503	CLA	C2B-C1B-NB	4.81	113.46	110.23
22	R	310	CLA	O2D-CGD-CBD	4.81	119.82	111.27
22	r	310	CLA	O2D-CGD-CBD	4.81	119.82	111.27
22	b	601	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
22	D	403	CLA	C1D-ND-C4D	4.81	109.75	106.33
22	Y	614	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
22	y	614	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
22	3	311	CLA	C1D-ND-C4D	4.81	109.75	106.33
22	7	311	CLA	C1D-ND-C4D	4.81	109.75	106.33
22	D	404	CLA	CHA-C4D-ND	4.81	142.55	132.50
22	S	314	CLA	CHD-C4C-C3C	-4.81	117.78	124.84
22	s	314	CLA	CHD-C4C-C3C	-4.81	117.78	124.84
22	G	611	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
22	g	611	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
22	3	305	CLA	CHA-C4D-ND	4.80	142.54	132.50
22	7	305	CLA	CHA-C4D-ND	4.80	142.54	132.50
22	b	604	CLA	C2B-C1B-NB	4.80	113.45	110.23
22	G	602	CLA	C1D-ND-C4D	4.80	109.74	106.33
22	g	602	CLA	C1D-ND-C4D	4.80	109.74	106.33
22	2	604	CLA	CHA-C4D-ND	4.80	142.54	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	604	CLA	CHA-C4D-ND	4.80	142.54	132.50
22	3	312	CLA	CHA-C4D-ND	4.80	142.54	132.50
22	7	312	CLA	CHA-C4D-ND	4.80	142.54	132.50
22	4	310	CLA	CHA-C4D-ND	4.80	142.53	132.50
22	8	310	CLA	CHA-C4D-ND	4.80	142.53	132.50
22	a	405	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
22	3	303	CLA	CHA-C4D-ND	4.79	142.53	132.50
22	7	303	CLA	CHA-C4D-ND	4.79	142.53	132.50
22	b	615	CLA	CHC-C4B-NB	4.79	129.33	124.26
22	B	608	CLA	CHD-C4C-C3C	-4.79	117.80	124.84
22	C	502	CLA	CHA-C4D-ND	4.79	142.52	132.50
22	b	609	CLA	CHD-C4C-C3C	-4.79	117.80	124.84
22	b	601	CLA	C2D-C1D-ND	4.79	113.63	110.10
22	s	301	CLA	C2B-C1B-NB	4.79	113.44	110.23
22	R	302	CLA	C1D-ND-C4D	4.79	109.74	106.33
22	r	302	CLA	C1D-ND-C4D	4.79	109.74	106.33
22	2	611	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
22	6	611	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
22	B	603	CLA	C2B-C1B-NB	4.78	113.44	110.23
22	C	511	CLA	O2D-CGD-CBD	4.78	119.77	111.27
22	B	608	CLA	CHA-C4D-ND	4.78	142.50	132.50
22	Y	611	CLA	CHA-C4D-ND	4.78	142.50	132.50
22	y	611	CLA	CHA-C4D-ND	4.78	142.50	132.50
22	Y	613	CLA	C2B-C1B-NB	4.78	113.44	110.23
22	y	613	CLA	C2B-C1B-NB	4.78	113.44	110.23
22	S	303	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
22	s	303	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
22	1	611	CLA	CHA-C4D-ND	4.78	142.49	132.50
22	5	611	CLA	CHA-C4D-ND	4.78	142.49	132.50
22	S	312	CLA	O2D-CGD-CBD	4.77	119.75	111.27
22	s	312	CLA	O2D-CGD-CBD	4.77	119.75	111.27
22	G	604	CLA	CHA-C4D-ND	4.77	142.48	132.50
22	g	604	CLA	CHA-C4D-ND	4.77	142.48	132.50
22	2	604	CLA	O2D-CGD-CBD	4.77	119.75	111.27
22	6	604	CLA	O2D-CGD-CBD	4.77	119.75	111.27
22	a	402	CLA	CHD-C4C-C3C	-4.77	117.83	124.84
22	3	310	CLA	C2B-C1B-NB	4.77	113.43	110.23
22	7	310	CLA	C2B-C1B-NB	4.77	113.43	110.23
22	G	613	CLA	CHD-C4C-C3C	-4.77	117.83	124.84
22	g	613	CLA	CHD-C4C-C3C	-4.77	117.83	124.84
22	a	402	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
22	1	603	CLA	C1D-ND-C4D	4.77	109.72	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	603	CLA	C1D-ND-C4D	4.77	109.72	106.33
22	R	309	CLA	CHD-C4C-C3C	-4.77	117.83	124.84
22	r	309	CLA	CHD-C4C-C3C	-4.77	117.83	124.84
22	c	501	CLA	CAC-C3C-C4C	4.77	130.99	124.81
22	1	604	CLA	C1D-ND-C4D	4.76	109.72	106.33
22	5	604	CLA	C1D-ND-C4D	4.76	109.72	106.33
22	3	310	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
22	7	310	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
22	N	613	CLA	CHD-C4C-C3C	-4.76	117.84	124.84
22	n	613	CLA	CHD-C4C-C3C	-4.76	117.84	124.84
22	S	309	CLA	CAC-C3C-C4C	4.76	130.98	124.81
22	s	309	CLA	CAC-C3C-C4C	4.76	130.98	124.81
22	c	507	CLA	C1D-ND-C4D	4.76	109.71	106.33
22	3	303	CLA	O2D-CGD-CBD	4.75	119.71	111.27
22	7	303	CLA	O2D-CGD-CBD	4.75	119.71	111.27
22	d	403	CLA	CAC-C3C-C2C	-4.74	119.42	127.53
22	Y	602	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
22	y	602	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
22	N	610	CLA	C2B-C1B-NB	4.74	113.41	110.23
22	n	610	CLA	C2B-C1B-NB	4.74	113.41	110.23
22	G	614	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
22	g	614	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
22	1	602	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
22	5	602	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
22	c	509	CLA	C1D-ND-C4D	4.74	109.70	106.33
22	G	612	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
22	g	612	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
22	B	609	CLA	CHD-C4C-C3C	-4.74	117.88	124.84
22	B	602	CLA	CHA-C4D-ND	4.73	142.40	132.50
22	C	509	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
22	R	301	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
22	r	301	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
22	S	311	CLA	C2D-C1D-ND	4.73	113.59	110.10
22	s	311	CLA	C2D-C1D-ND	4.73	113.59	110.10
22	3	312	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
22	7	312	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
22	A	403	CLA	CHD-C4C-C3C	-4.72	117.89	124.84
22	Y	602	CLA	CHA-C4D-ND	4.72	142.38	132.50
22	y	602	CLA	CHA-C4D-ND	4.72	142.38	132.50
22	Y	610	CLA	C2B-C1B-NB	4.72	113.40	110.23
22	y	610	CLA	C2B-C1B-NB	4.72	113.40	110.23
22	Y	612	CLA	C3D-C2D-C1D	-4.72	99.39	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	y	612	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
22	R	311	CLA	CHA-C4D-ND	4.72	142.38	132.50
22	r	311	CLA	CHA-C4D-ND	4.72	142.38	132.50
22	S	310	CLA	C2B-C1B-NB	4.72	113.40	110.23
22	s	310	CLA	C2B-C1B-NB	4.72	113.40	110.23
22	S	309	CLA	CHA-C4D-ND	4.72	142.37	132.50
22	s	309	CLA	CHA-C4D-ND	4.72	142.37	132.50
22	3	313	CLA	C2B-C1B-NB	4.72	113.39	110.23
22	7	313	CLA	C2B-C1B-NB	4.72	113.39	110.23
22	N	602	CLA	C1D-ND-C4D	4.72	109.69	106.33
22	n	602	CLA	C1D-ND-C4D	4.72	109.69	106.33
22	2	610	CLA	C3D-C2D-C1D	-4.72	99.40	105.83
22	6	610	CLA	C3D-C2D-C1D	-4.72	99.40	105.83
22	b	611	CLA	C2D-C1D-ND	4.72	113.58	110.10
25	3	306	CHL	CAA-C2A-C3A	-4.72	105.10	116.10
25	7	306	CHL	CAA-C2A-C3A	-4.72	105.10	116.10
22	Y	610	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
22	y	610	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
22	R	310	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
22	r	310	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
22	N	602	CLA	CHD-C4C-C3C	-4.71	117.91	124.84
22	n	602	CLA	CHD-C4C-C3C	-4.71	117.91	124.84
22	A	405	CLA	CHD-C4C-C3C	-4.71	117.92	124.84
22	1	611	CLA	C1D-ND-C4D	4.71	109.68	106.33
22	5	611	CLA	C1D-ND-C4D	4.71	109.68	106.33
22	b	606	CLA	CHC-C4B-NB	4.71	129.24	124.26
22	c	511	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
22	B	603	CLA	C1D-ND-C4D	4.71	109.68	106.33
22	S	309	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
22	s	309	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
22	N	613	CLA	C2B-C1B-NB	4.71	113.39	110.23
22	n	613	CLA	C2B-C1B-NB	4.71	113.39	110.23
25	N	605	CHL	CAA-C2A-C3A	-4.71	105.12	116.10
25	n	605	CHL	CAA-C2A-C3A	-4.71	105.12	116.10
22	C	506	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
22	B	608	CLA	CBC-CAC-C3C	-4.70	99.47	112.43
22	C	502	CLA	C2D-C1D-ND	4.70	113.57	110.10
22	S	303	CLA	CHA-C4D-ND	4.70	142.33	132.50
22	s	303	CLA	CHA-C4D-ND	4.70	142.33	132.50
22	S	301	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
22	A	405	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
22	B	615	CLA	C2D-C1D-ND	4.70	113.56	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	C3D-C2D-C1D	-4.69	99.42	105.83
22	B	611	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
22	C	510	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
22	4	301	CLA	CHD-C4C-C3C	-4.69	117.94	124.84
22	8	301	CLA	CHD-C4C-C3C	-4.69	117.94	124.84
22	b	602	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
22	B	611	CLA	C2D-C1D-ND	4.69	113.56	110.10
22	D	403	CLA	C2B-C1B-NB	4.69	113.37	110.23
22	N	603	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
22	n	603	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
25	2	605	CHL	CAA-C2A-C3A	-4.69	105.16	116.10
25	6	605	CHL	CAA-C2A-C3A	-4.69	105.16	116.10
22	S	305	CLA	CHD-C4C-C3C	-4.69	117.95	124.84
22	s	305	CLA	CHD-C4C-C3C	-4.69	117.95	124.84
22	R	301	CLA	C2B-C1B-NB	4.69	113.37	110.23
22	r	301	CLA	C2B-C1B-NB	4.69	113.37	110.23
22	1	604	CLA	CHA-C4D-ND	4.68	142.29	132.50
22	5	604	CLA	CHA-C4D-ND	4.68	142.29	132.50
22	b	606	CLA	O2D-CGD-CBD	4.68	119.58	111.27
22	c	505	CLA	C1D-ND-C4D	4.67	109.65	106.33
25	1	605	CHL	CAA-C2A-C3A	-4.67	105.21	116.10
25	5	605	CHL	CAA-C2A-C3A	-4.67	105.21	116.10
22	N	612	CLA	C2B-C1B-NB	4.67	113.36	110.23
22	n	612	CLA	C2B-C1B-NB	4.67	113.36	110.23
22	Y	613	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
22	y	613	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
22	4	303	CLA	C1D-ND-C4D	4.67	109.65	106.33
22	8	303	CLA	C1D-ND-C4D	4.67	109.65	106.33
22	G	614	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
22	g	614	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
22	b	614	CLA	CHD-C4C-C3C	-4.66	117.99	124.84
22	B	601	CLA	CHA-C4D-ND	4.66	142.25	132.50
22	R	309	CLA	C1D-ND-C4D	4.66	109.64	106.33
22	Y	611	CLA	C1D-ND-C4D	4.66	109.64	106.33
22	r	309	CLA	C1D-ND-C4D	4.66	109.64	106.33
22	y	611	CLA	C1D-ND-C4D	4.66	109.64	106.33
22	R	303	CLA	C1D-ND-C4D	4.66	109.64	106.33
22	r	303	CLA	C1D-ND-C4D	4.66	109.64	106.33
22	G	602	CLA	C2B-C1B-NB	4.66	113.35	110.23
22	g	602	CLA	C2B-C1B-NB	4.66	113.35	110.23
22	G	603	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
22	g	603	CLA	C3D-C2D-C1D	-4.65	99.48	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	613	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
22	g	613	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
22	S	312	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
22	s	312	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
22	B	613	CLA	C2B-C1B-NB	4.65	113.35	110.23
22	1	602	CLA	C1D-ND-C4D	4.65	109.64	106.33
22	5	602	CLA	C1D-ND-C4D	4.65	109.64	106.33
25	R	304	CHL	CBA-CAA-C2A	4.65	127.59	113.86
25	r	304	CHL	CBA-CAA-C2A	4.65	127.59	113.86
22	3	313	CLA	CHD-C4C-C3C	-4.65	118.01	124.84
22	7	313	CLA	CHD-C4C-C3C	-4.65	118.01	124.84
22	C	512	CLA	CHC-C4B-NB	4.65	129.18	124.26
22	b	610	CLA	CHD-C4C-C3C	-4.65	118.01	124.84
22	2	602	CLA	CHD-C4C-C3C	-4.65	118.01	124.84
22	6	602	CLA	CHD-C4C-C3C	-4.65	118.01	124.84
22	B	616	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
22	Y	604	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
22	y	604	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
22	2	613	CLA	C2B-C1B-NB	4.64	113.34	110.23
22	6	613	CLA	C2B-C1B-NB	4.64	113.34	110.23
25	G	606	CHL	C2B-C1B-NB	-4.64	107.12	110.23
25	g	606	CHL	C2B-C1B-NB	-4.64	107.12	110.23
22	b	608	CLA	O2D-CGD-CBD	4.64	119.51	111.27
22	R	302	CLA	CAC-C3C-C4C	4.64	130.83	124.81
22	r	302	CLA	CAC-C3C-C4C	4.64	130.83	124.81
22	S	311	CLA	C1D-ND-C4D	4.64	109.63	106.33
22	s	311	CLA	C1D-ND-C4D	4.64	109.63	106.33
22	B	616	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
22	D	404	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
22	4	304	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
22	8	304	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
22	c	511	CLA	C1D-ND-C4D	4.64	109.63	106.33
22	R	309	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
22	r	309	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
22	1	611	CLA	CHD-C4C-C3C	-4.63	118.03	124.84
22	5	611	CLA	CHD-C4C-C3C	-4.63	118.03	124.84
22	c	508	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
22	R	302	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
22	r	302	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
22	B	610	CLA	CHD-C4C-C3C	-4.63	118.04	124.84
22	S	303	CLA	C2D-C1D-ND	4.63	113.51	110.10
22	s	303	CLA	C2D-C1D-ND	4.63	113.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	606	CHL	CBA-CAA-C2A	4.63	127.52	113.86
25	n	606	CHL	CBA-CAA-C2A	4.63	127.52	113.86
22	D	401	CLA	CHD-C4C-C3C	-4.62	118.04	124.84
22	C	505	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
22	G	610	CLA	C2B-C1B-NB	4.62	113.33	110.23
22	g	610	CLA	C2B-C1B-NB	4.62	113.33	110.23
22	R	310	CLA	C2B-C1B-NB	4.62	113.33	110.23
22	r	310	CLA	C2B-C1B-NB	4.62	113.33	110.23
22	C	508	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
22	N	611	CLA	C1D-ND-C4D	4.61	109.61	106.33
22	n	611	CLA	C1D-ND-C4D	4.61	109.61	106.33
22	2	602	CLA	C1D-ND-C4D	4.61	109.61	106.33
22	6	602	CLA	C1D-ND-C4D	4.61	109.61	106.33
22	B	613	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
22	D	401	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
22	G	611	CLA	C1D-ND-C4D	4.60	109.60	106.33
22	g	611	CLA	C1D-ND-C4D	4.60	109.60	106.33
22	b	605	CLA	C2D-C1D-ND	4.60	113.49	110.10
22	Y	611	CLA	CBC-CAC-C3C	-4.60	99.75	112.43
22	y	611	CLA	CBC-CAC-C3C	-4.60	99.75	112.43
22	1	602	CLA	C2B-C1B-NB	4.60	113.31	110.23
22	5	602	CLA	C2B-C1B-NB	4.60	113.31	110.23
22	b	612	CLA	CMA-C3A-C4A	-4.60	99.42	111.77
25	2	606	CHL	CBA-CAA-C2A	4.60	127.43	113.86
25	6	606	CHL	CBA-CAA-C2A	4.60	127.43	113.86
22	N	604	CLA	CHA-C4D-ND	4.60	142.11	132.50
22	n	604	CLA	CHA-C4D-ND	4.60	142.11	132.50
22	R	302	CLA	C2B-C1B-NB	4.60	113.31	110.23
22	r	302	CLA	C2B-C1B-NB	4.60	113.31	110.23
22	S	309	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
22	s	309	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
22	Y	614	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
22	y	614	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
22	1	603	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
22	5	603	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
22	B	606	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
22	3	311	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
22	7	311	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
22	R	303	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
22	r	303	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
22	b	615	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
22	4	310	CLA	C3D-C2D-C1D	-4.58	99.58	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	310	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
22	3	311	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
22	7	311	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
22	2	612	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
22	6	612	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
22	S	305	CLA	C1D-ND-C4D	4.58	109.59	106.33
22	s	305	CLA	C1D-ND-C4D	4.58	109.59	106.33
22	1	611	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
22	5	611	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
22	R	310	CLA	C1D-ND-C4D	4.58	109.59	106.33
22	r	310	CLA	C1D-ND-C4D	4.58	109.59	106.33
22	G	614	CLA	O2D-CGD-CBD	4.57	119.40	111.27
22	g	614	CLA	O2D-CGD-CBD	4.57	119.40	111.27
22	B	602	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
22	R	308	CLA	C2B-C1B-NB	4.57	113.30	110.23
22	r	308	CLA	C2B-C1B-NB	4.57	113.30	110.23
22	N	611	CLA	C2D-C1D-ND	4.57	113.47	110.10
22	n	611	CLA	C2D-C1D-ND	4.57	113.47	110.10
22	S	310	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
22	s	310	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
22	R	307	CLA	CHD-C4C-C3C	-4.57	118.12	124.84
22	r	307	CLA	CHD-C4C-C3C	-4.57	118.12	124.84
22	c	502	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
22	b	615	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
22	S	313	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
22	s	313	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
22	c	504	CLA	CHD-C4C-C3C	-4.56	118.13	124.84
22	3	310	CLA	O2D-CGD-CBD	4.56	119.38	111.27
22	7	310	CLA	O2D-CGD-CBD	4.56	119.38	111.27
22	B	608	CLA	C2D-C1D-ND	4.56	113.47	110.10
22	c	506	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
22	3	312	CLA	C2D-C1D-ND	4.56	113.47	110.10
22	7	312	CLA	C2D-C1D-ND	4.56	113.47	110.10
22	N	602	CLA	O2D-CGD-CBD	4.56	119.37	111.27
22	n	602	CLA	O2D-CGD-CBD	4.56	119.37	111.27
22	c	510	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
22	d	401	CLA	O2D-CGD-CBD	4.56	119.37	111.27
25	Y	609	CHL	CBA-CAA-C2A	4.56	127.31	113.86
25	y	609	CHL	CBA-CAA-C2A	4.56	127.31	113.86
22	4	301	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
22	8	301	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
22	B	616	CLA	CHA-C4D-ND	4.55	142.03	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	503	CLA	C2B-C1B-NB	4.55	113.28	110.23
22	B	609	CLA	C1D-ND-C4D	4.55	109.57	106.33
22	4	311	CLA	CHD-C4C-C3C	-4.55	118.15	124.84
22	8	311	CLA	CHD-C4C-C3C	-4.55	118.15	124.84
22	b	611	CLA	C1D-ND-C4D	4.55	109.57	106.33
22	2	613	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
22	6	613	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
22	3	303	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
22	7	303	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
22	Y	604	CLA	C2B-C1B-NB	4.55	113.28	110.23
22	y	604	CLA	C2B-C1B-NB	4.55	113.28	110.23
25	3	309	CHL	CAA-C2A-C3A	-4.55	100.33	112.78
25	7	309	CHL	CAA-C2A-C3A	-4.55	100.33	112.78
22	2	602	CLA	O2D-CGD-CBD	4.55	119.34	111.27
22	6	602	CLA	O2D-CGD-CBD	4.55	119.34	111.27
22	N	603	CLA	CHD-C4C-C3C	-4.54	118.16	124.84
22	n	603	CLA	CHD-C4C-C3C	-4.54	118.16	124.84
22	4	305	CLA	CHD-C4C-C3C	-4.54	118.16	124.84
22	8	305	CLA	CHD-C4C-C3C	-4.54	118.16	124.84
22	2	610	CLA	C2D-C1D-ND	4.54	113.45	110.10
22	6	610	CLA	C2D-C1D-ND	4.54	113.45	110.10
22	c	501	CLA	CBC-CAC-C3C	-4.54	99.91	112.43
22	2	610	CLA	O2D-CGD-CBD	4.54	119.33	111.27
22	6	610	CLA	O2D-CGD-CBD	4.54	119.33	111.27
22	B	614	CLA	C1D-ND-C4D	4.54	109.56	106.33
22	1	612	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
22	5	612	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
22	C	502	CLA	CAC-C3C-C4C	4.54	130.70	124.81
22	3	313	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
22	7	313	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
22	B	608	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
22	3	311	CLA	O2D-CGD-CBD	4.53	119.32	111.27
22	7	311	CLA	O2D-CGD-CBD	4.53	119.32	111.27
22	c	503	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
22	B	607	CLA	CHD-C4C-C3C	-4.53	118.18	124.84
22	R	301	CLA	C2D-C1D-ND	4.53	113.44	110.10
22	r	301	CLA	C2D-C1D-ND	4.53	113.44	110.10
22	1	610	CLA	O2D-CGD-CBD	4.53	119.31	111.27
22	5	610	CLA	O2D-CGD-CBD	4.53	119.31	111.27
22	Y	602	CLA	C2B-C1B-NB	4.53	113.27	110.23
22	y	602	CLA	C2B-C1B-NB	4.53	113.27	110.23
22	Y	614	CLA	O2D-CGD-CBD	4.53	119.31	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	y	614	CLA	O2D-CGD-CBD	4.53	119.31	111.27
22	B	604	CLA	O2D-CGD-CBD	4.52	119.31	111.27
22	C	502	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
22	2	603	CLA	CHD-C4C-C3C	-4.52	118.19	124.84
22	6	603	CLA	CHD-C4C-C3C	-4.52	118.19	124.84
22	B	609	CLA	O2D-CGD-CBD	4.52	119.30	111.27
22	C	508	CLA	O2D-CGD-CBD	4.52	119.30	111.27
22	b	601	CLA	C1D-ND-C4D	4.52	109.55	106.33
22	B	604	CLA	C1D-CHD-C4C	-4.52	116.31	126.06
22	4	303	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
22	8	303	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
22	c	504	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
22	N	602	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
22	n	602	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
22	1	611	CLA	O2D-CGD-CBD	4.51	119.29	111.27
22	5	611	CLA	O2D-CGD-CBD	4.51	119.29	111.27
22	2	602	CLA	C2B-C1B-NB	4.51	113.26	110.23
22	6	602	CLA	C2B-C1B-NB	4.51	113.26	110.23
22	B	607	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
22	S	311	CLA	C3B-C2B-C1B	-4.51	101.71	107.16
22	s	311	CLA	C3B-C2B-C1B	-4.51	101.71	107.16
22	2	603	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
22	6	603	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
22	2	610	CLA	C1D-ND-C4D	4.51	109.54	106.33
22	6	610	CLA	C1D-ND-C4D	4.51	109.54	106.33
22	b	610	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
22	C	512	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
22	R	303	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
22	r	303	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
22	b	602	CLA	CAC-C3C-C4C	4.50	130.65	124.81
22	N	604	CLA	CHD-C4C-C3C	-4.50	118.22	124.84
22	n	604	CLA	CHD-C4C-C3C	-4.50	118.22	124.84
22	1	613	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	5	613	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	1	603	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	5	603	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	C	504	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	4	301	CLA	O2D-CGD-CBD	4.50	119.26	111.27
22	8	301	CLA	O2D-CGD-CBD	4.50	119.26	111.27
22	3	312	CLA	C1D-ND-C4D	4.49	109.53	106.33
22	7	312	CLA	C1D-ND-C4D	4.49	109.53	106.33
22	2	613	CLA	C2D-C1D-ND	4.49	113.42	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	613	CLA	C2D-C1D-ND	4.49	113.42	110.10
22	b	616	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
22	c	501	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
22	A	402	CLA	C1D-CHD-C4C	-4.49	116.37	126.06
22	c	511	CLA	CHD-C4C-C3C	-4.49	118.24	124.84
22	b	605	CLA	CHD-C4C-C3C	-4.49	118.25	124.84
22	c	507	CLA	C2D-C1D-ND	4.49	113.41	110.10
22	B	603	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
22	2	613	CLA	CHD-C4C-C3C	-4.48	118.25	124.84
22	6	613	CLA	CHD-C4C-C3C	-4.48	118.25	124.84
22	G	602	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
22	g	602	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
22	D	404	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
22	S	313	CLA	CHD-C4C-C3C	-4.48	118.25	124.84
22	s	313	CLA	CHD-C4C-C3C	-4.48	118.25	124.84
25	G	605	CHL	CAA-C2A-C3A	-4.48	105.64	116.10
25	g	605	CHL	CAA-C2A-C3A	-4.48	105.64	116.10
22	b	605	CLA	CED-O2D-CGD	4.48	126.07	115.94
22	1	610	CLA	C2B-C1B-NB	4.48	113.23	110.23
22	5	610	CLA	C2B-C1B-NB	4.48	113.23	110.23
22	D	404	CLA	C1D-ND-C4D	4.47	109.51	106.33
22	1	602	CLA	O2D-CGD-CBD	4.47	119.21	111.27
22	5	602	CLA	O2D-CGD-CBD	4.47	119.21	111.27
25	3	307	CHL	CBA-CAA-C2A	4.47	127.05	113.86
25	7	307	CHL	CBA-CAA-C2A	4.47	127.05	113.86
22	2	612	CLA	C2B-C1B-NB	4.47	113.23	110.23
22	6	612	CLA	C2B-C1B-NB	4.47	113.23	110.23
22	C	503	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
22	R	311	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
22	r	311	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
22	c	506	CLA	CHD-C4C-C3C	-4.46	118.28	124.84
22	1	602	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
22	5	602	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
22	B	609	CLA	C2D-C1D-ND	4.46	113.39	110.10
25	1	609	CHL	CBA-CAA-C2A	4.46	127.03	113.86
25	5	609	CHL	CBA-CAA-C2A	4.46	127.03	113.86
22	B	603	CLA	CHD-C4C-C3C	-4.46	118.28	124.84
22	d	403	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
22	b	614	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
23	d	402	PHO	O2D-CGD-CBD	4.46	116.65	111.00
22	4	311	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
22	8	311	CLA	C3D-C2D-C1D	-4.46	99.75	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	304	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
22	8	304	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
22	B	612	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
22	S	304	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
22	s	304	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
22	4	305	CLA	O2D-CGD-CBD	4.45	119.18	111.27
22	8	305	CLA	O2D-CGD-CBD	4.45	119.18	111.27
22	C	504	CLA	CHD-C4C-C3C	-4.45	118.30	124.84
22	B	613	CLA	O2D-CGD-CBD	4.45	119.18	111.27
22	B	611	CLA	C3B-C2B-C1B	-4.45	101.79	107.16
22	D	403	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
22	b	613	CLA	O2D-CGD-CBD	4.45	119.17	111.27
22	3	314	CLA	O2D-CGD-CBD	4.44	119.17	111.27
22	7	314	CLA	O2D-CGD-CBD	4.44	119.17	111.27
22	c	505	CLA	CHD-C4C-C3C	-4.44	118.31	124.84
22	Y	603	CLA	O2D-CGD-CBD	4.44	119.16	111.27
22	y	603	CLA	O2D-CGD-CBD	4.44	119.16	111.27
22	N	604	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
22	n	604	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
22	B	615	CLA	C1D-CHD-C4C	-4.44	116.48	126.06
22	B	609	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
22	S	304	CLA	CHD-C4C-C3C	-4.44	118.32	124.84
22	s	304	CLA	CHD-C4C-C3C	-4.44	118.32	124.84
22	1	613	CLA	CHD-C4C-C3C	-4.44	118.32	124.84
22	5	613	CLA	CHD-C4C-C3C	-4.44	118.32	124.84
22	S	314	CLA	O2D-CGD-CBD	4.43	119.15	111.27
22	s	314	CLA	O2D-CGD-CBD	4.43	119.15	111.27
22	d	404	CLA	O2D-CGD-CBD	4.43	119.14	111.27
22	d	404	CLA	CHD-C4C-C3C	-4.43	118.33	124.84
22	b	607	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
22	A	403	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
22	d	401	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
22	1	612	CLA	CHD-C4C-C3C	-4.43	118.33	124.84
22	5	612	CLA	CHD-C4C-C3C	-4.43	118.33	124.84
22	s	301	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
22	B	606	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
22	B	605	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
22	S	309	CLA	C2D-C1D-ND	4.42	113.36	110.10
22	s	309	CLA	C2D-C1D-ND	4.42	113.36	110.10
22	1	613	CLA	O2D-CGD-CBD	4.42	119.12	111.27
22	5	613	CLA	O2D-CGD-CBD	4.42	119.12	111.27
22	B	602	CLA	C3C-C4C-NC	4.42	115.53	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	612	CLA	C1D-ND-C4D	4.42	109.47	106.33
22	g	612	CLA	C1D-ND-C4D	4.42	109.47	106.33
22	B	604	CLA	CHC-C1C-C2C	-4.42	114.47	126.73
22	B	614	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
22	G	611	CLA	C2D-C1D-ND	4.42	113.36	110.10
22	g	611	CLA	C2D-C1D-ND	4.42	113.36	110.10
22	C	501	CLA	C3B-C2B-C1B	-4.41	101.83	107.16
22	c	501	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
22	2	604	CLA	CHD-C4C-C3C	-4.41	118.35	124.84
22	6	604	CLA	CHD-C4C-C3C	-4.41	118.35	124.84
22	Y	611	CLA	C1D-CHD-C4C	-4.41	116.54	126.06
22	y	611	CLA	C1D-CHD-C4C	-4.41	116.54	126.06
22	G	604	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
22	g	604	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
22	d	403	CLA	O2D-CGD-CBD	4.41	119.10	111.27
22	c	511	CLA	O2D-CGD-CBD	4.41	119.10	111.27
22	C	512	CLA	CHD-C4C-C3C	-4.40	118.37	124.84
22	S	305	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
22	s	305	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
25	3	309	CHL	CBA-CAA-C2A	4.40	126.85	113.86
25	7	309	CHL	CBA-CAA-C2A	4.40	126.85	113.86
22	N	604	CLA	C1D-ND-C4D	4.40	109.46	106.33
22	n	604	CLA	C1D-ND-C4D	4.40	109.46	106.33
22	2	609	CLA	C2B-C1B-NB	4.40	113.18	110.23
22	6	609	CLA	C2B-C1B-NB	4.40	113.18	110.23
22	b	603	CLA	C4A-NA-C1A	-4.40	104.73	106.71
22	S	311	CLA	C1D-CHD-C4C	-4.40	116.58	126.06
22	s	311	CLA	C1D-CHD-C4C	-4.40	116.58	126.06
22	D	401	CLA	C3B-C2B-C1B	-4.40	101.86	107.16
22	3	304	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
22	7	304	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
22	2	613	CLA	O2D-CGD-CBD	4.40	119.08	111.27
22	6	613	CLA	O2D-CGD-CBD	4.40	119.08	111.27
22	C	507	CLA	C2B-C1B-NB	4.39	113.18	110.23
22	1	611	CLA	C2D-C1D-ND	4.39	113.34	110.10
22	5	611	CLA	C2D-C1D-ND	4.39	113.34	110.10
22	d	403	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
22	G	604	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
22	g	604	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
22	b	607	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
22	Y	610	CLA	O2D-CGD-CBD	4.39	119.06	111.27
22	y	610	CLA	O2D-CGD-CBD	4.39	119.06	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	505	CLA	C3B-C2B-C1B	-4.39	101.87	107.16
25	3	302	CHL	CBA-CAA-C2A	4.38	126.80	113.86
25	7	302	CHL	CBA-CAA-C2A	4.38	126.80	113.86
22	3	305	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
22	7	305	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
22	B	604	CLA	C2B-C1B-NB	4.38	113.17	110.23
22	b	608	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
22	C	505	CLA	CHD-C4C-C3C	-4.38	118.40	124.84
22	b	616	CLA	O2D-CGD-CBD	4.38	119.05	111.27
22	4	304	CLA	C2B-C1B-NB	4.38	113.17	110.23
22	8	304	CLA	C2B-C1B-NB	4.38	113.17	110.23
22	4	303	CLA	C2D-C1D-ND	4.38	113.33	110.10
22	8	303	CLA	C2D-C1D-ND	4.38	113.33	110.10
22	A	402	CLA	O2D-CGD-CBD	4.38	119.05	111.27
22	A	403	CLA	O2D-CGD-CBD	4.38	119.05	111.27
22	1	604	CLA	CHD-C4C-C3C	-4.38	118.41	124.84
22	5	604	CLA	CHD-C4C-C3C	-4.38	118.41	124.84
22	N	614	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
22	n	614	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
22	R	302	CLA	C1D-CHD-C4C	-4.38	116.62	126.06
22	r	302	CLA	C1D-CHD-C4C	-4.38	116.62	126.06
22	B	614	CLA	C2D-C1D-ND	4.38	113.33	110.10
22	2	604	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
22	6	604	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
22	C	501	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
22	R	302	CLA	O2D-CGD-CBD	4.37	119.04	111.27
22	r	302	CLA	O2D-CGD-CBD	4.37	119.04	111.27
22	1	604	CLA	O2D-CGD-CBD	4.37	119.04	111.27
22	5	604	CLA	O2D-CGD-CBD	4.37	119.04	111.27
22	R	307	CLA	C2D-C1D-ND	4.37	113.33	110.10
22	r	307	CLA	C2D-C1D-ND	4.37	113.33	110.10
22	2	602	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
22	6	602	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
22	s	301	CLA	O2D-CGD-CBD	4.37	119.03	111.27
22	N	614	CLA	CHD-C4C-C3C	-4.37	118.42	124.84
22	n	614	CLA	CHD-C4C-C3C	-4.37	118.42	124.84
22	N	610	CLA	O2D-CGD-CBD	4.36	119.02	111.27
22	n	610	CLA	O2D-CGD-CBD	4.36	119.02	111.27
22	C	507	CLA	C2D-C1D-ND	4.36	113.32	110.10
22	4	305	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
22	8	305	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
22	B	610	CLA	C3D-C2D-C1D	-4.36	99.88	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	403	CLA	C2D-C1D-ND	4.36	113.32	110.10
22	B	605	CLA	CHD-C4C-C3C	-4.36	118.44	124.84
22	a	403	CLA	O2D-CGD-CBD	4.35	119.00	111.27
22	C	506	CLA	CHD-C4C-C3C	-4.35	118.44	124.84
25	S	307	CHL	CBA-CAA-C2A	4.35	126.70	113.86
25	s	307	CHL	CBA-CAA-C2A	4.35	126.70	113.86
22	S	309	CLA	O2D-CGD-CBD	4.35	119.00	111.27
22	s	309	CLA	O2D-CGD-CBD	4.35	119.00	111.27
25	1	606	CHL	CBA-CAA-C2A	4.35	126.70	113.86
25	5	606	CHL	CBA-CAA-C2A	4.35	126.70	113.86
22	Y	614	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
22	y	614	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
22	b	604	CLA	O2D-CGD-O1D	-4.34	115.35	123.84
22	2	609	CLA	O2D-CGD-CBD	4.34	118.98	111.27
22	6	609	CLA	O2D-CGD-CBD	4.34	118.98	111.27
22	S	314	CLA	C2D-C1D-ND	4.34	113.30	110.10
22	s	314	CLA	C2D-C1D-ND	4.34	113.30	110.10
22	S	310	CLA	O2D-CGD-CBD	4.34	118.97	111.27
22	s	310	CLA	O2D-CGD-CBD	4.34	118.97	111.27
22	3	314	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
22	7	314	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
22	b	607	CLA	C2B-C1B-NB	4.33	113.14	110.23
22	B	607	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
22	c	508	CLA	O2D-CGD-CBD	4.33	118.96	111.27
22	R	310	CLA	C2D-C1D-ND	4.33	113.29	110.10
22	r	310	CLA	C2D-C1D-ND	4.33	113.29	110.10
22	1	604	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
22	5	604	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
22	S	305	CLA	O2D-CGD-O1D	-4.32	115.38	123.84
22	s	305	CLA	O2D-CGD-O1D	-4.32	115.38	123.84
22	G	611	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
22	g	611	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
22	N	604	CLA	C2D-C1D-ND	4.32	113.29	110.10
22	n	604	CLA	C2D-C1D-ND	4.32	113.29	110.10
22	b	605	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
22	B	606	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
22	b	616	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
22	s	301	CLA	CHD-C4C-C3C	-4.31	118.50	124.84
22	3	303	CLA	C2D-C1D-ND	4.31	113.28	110.10
22	7	303	CLA	C2D-C1D-ND	4.31	113.28	110.10
22	N	604	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
22	n	604	CLA	C3B-C2B-C1B	-4.31	101.96	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	305	CLA	CHD-C4C-C3C	-4.31	118.50	124.84
22	7	305	CLA	CHD-C4C-C3C	-4.31	118.50	124.84
22	R	309	CLA	O2D-CGD-CBD	4.31	118.93	111.27
22	r	309	CLA	O2D-CGD-CBD	4.31	118.93	111.27
22	a	402	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
22	b	608	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
25	N	606	CHL	C2B-C1B-NB	-4.30	107.35	110.23
25	n	606	CHL	C2B-C1B-NB	-4.30	107.35	110.23
22	S	310	CLA	CBC-CAC-C3C	-4.30	100.56	112.43
22	s	310	CLA	CBC-CAC-C3C	-4.30	100.56	112.43
22	B	616	CLA	C2B-C1B-NB	4.30	113.12	110.23
22	d	404	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
22	3	304	CLA	O2D-CGD-CBD	4.30	118.91	111.27
22	7	304	CLA	O2D-CGD-CBD	4.30	118.91	111.27
22	3	312	CLA	O2D-CGD-CBD	4.30	118.91	111.27
22	7	312	CLA	O2D-CGD-CBD	4.30	118.91	111.27
22	2	603	CLA	O2D-CGD-CBD	4.30	118.91	111.27
22	6	603	CLA	O2D-CGD-CBD	4.30	118.91	111.27
22	b	613	CLA	C2D-C1D-ND	4.30	113.27	110.10
22	G	610	CLA	O2D-CGD-CBD	4.30	118.91	111.27
22	g	610	CLA	O2D-CGD-CBD	4.30	118.91	111.27
22	Y	604	CLA	C1D-CHD-C4C	-4.30	116.78	126.06
22	y	604	CLA	C1D-CHD-C4C	-4.30	116.78	126.06
22	c	503	CLA	C1D-CHD-C4C	-4.30	116.79	126.06
25	G	606	CHL	CBA-CAA-C2A	4.30	126.54	113.86
25	g	606	CHL	CBA-CAA-C2A	4.30	126.54	113.86
22	b	611	CLA	C1D-CHD-C4C	-4.29	116.79	126.06
22	C	511	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
22	Y	612	CLA	O2D-CGD-CBD	4.29	118.90	111.27
22	y	612	CLA	O2D-CGD-CBD	4.29	118.90	111.27
22	B	612	CLA	C1D-CHD-C4C	-4.29	116.80	126.06
22	b	602	CLA	C1D-CHD-C4C	-4.29	116.80	126.06
22	b	606	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
22	b	603	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
22	R	301	CLA	C1D-ND-C4D	4.29	109.38	106.33
22	r	301	CLA	C1D-ND-C4D	4.29	109.38	106.33
22	D	403	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
22	A	403	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
22	R	307	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
22	r	307	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
25	1	607	CHL	CBA-CAA-C2A	4.29	126.52	113.86
25	5	607	CHL	CBA-CAA-C2A	4.29	126.52	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Y	613	CLA	O2D-CGD-CBD	4.29	118.88	111.27
22	y	613	CLA	O2D-CGD-CBD	4.29	118.88	111.27
22	D	403	CLA	CHD-C4C-C3C	-4.28	118.54	124.84
22	N	602	CLA	C2B-C1B-NB	4.28	113.10	110.23
22	n	602	CLA	C2B-C1B-NB	4.28	113.10	110.23
22	Y	614	CLA	C1D-CHD-C4C	-4.28	116.83	126.06
22	y	614	CLA	C1D-CHD-C4C	-4.28	116.83	126.06
22	G	602	CLA	C2D-C1D-ND	4.28	113.26	110.10
22	g	602	CLA	C2D-C1D-ND	4.28	113.26	110.10
22	3	303	CLA	C1D-ND-C4D	4.28	109.37	106.33
22	7	303	CLA	C1D-ND-C4D	4.28	109.37	106.33
22	b	608	CLA	CHD-C4C-C3C	-4.27	118.56	124.84
22	Y	603	CLA	C2D-C1D-ND	4.27	113.25	110.10
22	y	603	CLA	C2D-C1D-ND	4.27	113.25	110.10
25	4	307	CHL	CBA-CAA-C2A	4.27	126.47	113.86
25	8	307	CHL	CBA-CAA-C2A	4.27	126.47	113.86
22	R	309	CLA	C2D-C1D-ND	4.27	113.25	110.10
22	r	309	CLA	C2D-C1D-ND	4.27	113.25	110.10
22	S	305	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
22	s	305	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
22	R	311	CLA	O2D-CGD-CBD	4.27	118.85	111.27
22	r	311	CLA	O2D-CGD-CBD	4.27	118.85	111.27
22	4	304	CLA	O2D-CGD-CBD	4.26	118.84	111.27
22	8	304	CLA	O2D-CGD-CBD	4.26	118.84	111.27
22	N	611	CLA	CBC-CAC-C3C	-4.26	100.68	112.43
22	n	611	CLA	CBC-CAC-C3C	-4.26	100.68	112.43
22	C	502	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
22	b	615	CLA	CHD-C4C-C3C	-4.26	118.57	124.84
22	C	505	CLA	C2D-C1D-ND	4.26	113.25	110.10
22	b	605	CLA	O2D-CGD-CBD	4.26	118.84	111.27
22	S	312	CLA	C2D-C1D-ND	4.26	113.24	110.10
22	s	312	CLA	C2D-C1D-ND	4.26	113.24	110.10
22	S	310	CLA	C2D-C1D-ND	4.26	113.24	110.10
22	s	310	CLA	C2D-C1D-ND	4.26	113.24	110.10
22	B	616	CLA	C1D-CHD-C4C	-4.26	116.88	126.06
22	B	611	CLA	C1D-ND-C4D	4.25	109.36	106.33
22	A	405	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
22	Y	612	CLA	CHD-C4C-C3C	-4.25	118.59	124.84
22	y	612	CLA	CHD-C4C-C3C	-4.25	118.59	124.84
22	N	611	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
22	n	611	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
22	A	402	CLA	C1D-ND-C4D	4.25	109.35	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	603	CLA	CHD-C4C-C3C	-4.25	118.60	124.84
22	g	603	CLA	CHD-C4C-C3C	-4.25	118.60	124.84
22	B	604	CLA	CMB-C2B-C1B	4.25	131.84	125.37
22	Y	612	CLA	C3B-C2B-C1B	-4.25	102.04	107.16
22	y	612	CLA	C3B-C2B-C1B	-4.25	102.04	107.16
22	b	609	CLA	C1D-ND-C4D	4.25	109.35	106.33
22	a	403	CLA	C3B-C2B-C1B	-4.24	102.04	107.16
22	B	612	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
22	S	313	CLA	C3B-C2B-C1B	-4.24	102.05	107.16
22	s	313	CLA	C3B-C2B-C1B	-4.24	102.05	107.16
22	B	611	CLA	C1D-CHD-C4C	-4.24	116.92	126.06
22	N	614	CLA	O2D-CGD-CBD	4.23	118.79	111.27
22	n	614	CLA	O2D-CGD-CBD	4.23	118.79	111.27
22	B	615	CLA	C2B-C1B-NB	4.23	113.07	110.23
22	3	303	CLA	C3B-C2B-C1B	-4.23	102.05	107.16
22	7	303	CLA	C3B-C2B-C1B	-4.23	102.05	107.16
22	S	303	CLA	C1D-CHD-C4C	-4.23	116.93	126.06
22	s	303	CLA	C1D-CHD-C4C	-4.23	116.93	126.06
22	B	613	CLA	CHD-C4C-C3C	-4.23	118.62	124.84
22	2	613	CLA	C1D-ND-C4D	4.23	109.34	106.33
22	6	613	CLA	C1D-ND-C4D	4.23	109.34	106.33
22	C	509	CLA	C2D-C1D-ND	4.23	113.22	110.10
22	3	304	CLA	CHD-C4C-C3C	-4.23	118.63	124.84
22	7	304	CLA	CHD-C4C-C3C	-4.23	118.63	124.84
22	B	601	CLA	O2D-CGD-CBD	4.23	118.78	111.27
22	c	510	CLA	C2B-C1B-NB	4.23	113.06	110.23
22	3	314	CLA	C3B-C2B-C1B	-4.23	102.06	107.16
22	7	314	CLA	C3B-C2B-C1B	-4.23	102.06	107.16
22	R	303	CLA	O2D-CGD-O1D	-4.22	115.58	123.84
22	r	303	CLA	O2D-CGD-O1D	-4.22	115.58	123.84
22	Y	611	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
22	y	611	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
22	S	301	CLA	C2B-C1B-NB	4.22	113.06	110.23
22	b	611	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
22	a	403	CLA	C1D-CHD-C4C	-4.22	116.97	126.06
22	b	612	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
22	b	602	CLA	C2B-C1B-NB	4.21	113.06	110.23
22	Y	604	CLA	C2D-C1D-ND	4.21	113.21	110.10
22	y	604	CLA	C2D-C1D-ND	4.21	113.21	110.10
22	2	611	CLA	C1D-ND-C4D	4.21	109.33	106.33
22	6	611	CLA	C1D-ND-C4D	4.21	109.33	106.33
25	G	609	CHL	CBA-CAA-C2A	4.21	126.29	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	g	609	CHL	CBA-CAA-C2A	4.21	126.29	113.86
25	2	608	CHL	CBA-CAA-C2A	4.21	126.29	113.86
25	6	608	CHL	CBA-CAA-C2A	4.21	126.29	113.86
22	2	611	CLA	O2D-CGD-CBD	4.21	118.74	111.27
22	6	611	CLA	O2D-CGD-CBD	4.21	118.74	111.27
22	c	505	CLA	C3D-C2D-C1D	-4.20	100.09	105.83
22	D	404	CLA	C2D-C1D-ND	4.20	113.20	110.10
22	S	310	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
22	s	310	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
22	G	611	CLA	CBC-CAC-C3C	-4.20	100.85	112.43
22	g	611	CLA	CBC-CAC-C3C	-4.20	100.85	112.43
22	N	612	CLA	O2D-CGD-CBD	4.20	118.73	111.27
22	n	612	CLA	O2D-CGD-CBD	4.20	118.73	111.27
22	a	405	CLA	C2D-C1D-ND	4.20	113.20	110.10
22	B	601	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
22	Y	613	CLA	C1D-CHD-C4C	-4.20	117.00	126.06
22	y	613	CLA	C1D-CHD-C4C	-4.20	117.00	126.06
22	a	403	CLA	C2D-C1D-ND	4.19	113.19	110.10
22	3	311	CLA	C2D-C1D-ND	4.19	113.19	110.10
22	7	311	CLA	C2D-C1D-ND	4.19	113.19	110.10
22	b	611	CLA	CGD-CBD-CAD	-4.19	97.16	110.73
22	G	602	CLA	O2D-CGD-CBD	4.19	118.72	111.27
22	g	602	CLA	O2D-CGD-CBD	4.19	118.72	111.27
22	A	402	CLA	C3B-C2B-C1B	-4.19	102.10	107.16
22	B	605	CLA	C3B-C2B-C1B	-4.19	102.10	107.16
22	S	310	CLA	C1D-ND-C4D	4.19	109.31	106.33
22	s	310	CLA	C1D-ND-C4D	4.19	109.31	106.33
22	c	511	CLA	C3B-C2B-C1B	-4.19	102.10	107.16
25	Y	609	CHL	CAA-C2A-C3A	-4.19	101.31	112.78
25	y	609	CHL	CAA-C2A-C3A	-4.19	101.31	112.78
22	C	511	CLA	C3B-C2B-C1B	-4.19	102.11	107.16
22	d	401	CLA	C3B-C2B-C1B	-4.19	102.11	107.16
22	1	612	CLA	O2D-CGD-CBD	4.18	118.70	111.27
22	5	612	CLA	O2D-CGD-CBD	4.18	118.70	111.27
22	D	401	CLA	C1D-CHD-C4C	-4.18	117.03	126.06
25	2	601	CHL	CBA-CAA-C2A	4.18	126.20	113.86
25	6	601	CHL	CBA-CAA-C2A	4.18	126.20	113.86
22	G	614	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
22	g	614	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
22	Y	603	CLA	C1D-CHD-C4C	-4.18	117.05	126.06
22	y	603	CLA	C1D-CHD-C4C	-4.18	117.05	126.06
22	1	612	CLA	C3B-C2B-C1B	-4.17	102.12	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	612	CLA	C3B-C2B-C1B	-4.17	102.12	107.16
22	S	303	CLA	C1D-ND-C4D	4.17	109.30	106.33
22	s	303	CLA	C1D-ND-C4D	4.17	109.30	106.33
22	R	311	CLA	C2B-C1B-NB	4.17	113.03	110.23
22	r	311	CLA	C2B-C1B-NB	4.17	113.03	110.23
22	b	601	CLA	O2D-CGD-CBD	4.17	118.67	111.27
25	3	301	CHL	CBA-CAA-C2A	4.17	126.16	113.86
25	7	301	CHL	CBA-CAA-C2A	4.17	126.16	113.86
22	3	313	CLA	O2D-CGD-CBD	4.17	118.67	111.27
22	7	313	CLA	O2D-CGD-CBD	4.17	118.67	111.27
25	1	601	CHL	CBA-CAA-C2A	4.17	126.16	113.86
25	5	601	CHL	CBA-CAA-C2A	4.17	126.16	113.86
22	c	502	CLA	CBC-CAC-C3C	-4.16	100.95	112.43
22	G	612	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
22	g	612	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
22	c	512	CLA	C2D-C1D-ND	4.16	113.17	110.10
22	S	311	CLA	O2D-CGD-CBD	4.16	118.66	111.27
22	s	311	CLA	O2D-CGD-CBD	4.16	118.66	111.27
22	G	613	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
22	g	613	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
22	c	512	CLA	C1D-CHD-C4C	-4.15	117.09	126.06
25	1	615	CHL	CBA-CAA-C2A	4.15	126.12	113.86
25	5	615	CHL	CBA-CAA-C2A	4.15	126.12	113.86
22	B	604	CLA	CMC-C2C-C3C	4.15	137.39	126.12
22	R	308	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
22	Y	610	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
22	r	308	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
22	y	610	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
22	S	304	CLA	C2D-C1D-ND	4.15	113.16	110.10
22	s	304	CLA	C2D-C1D-ND	4.15	113.16	110.10
22	N	614	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
22	n	614	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
22	c	501	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
22	G	613	CLA	O2D-CGD-CBD	4.15	118.64	111.27
22	g	613	CLA	O2D-CGD-CBD	4.15	118.64	111.27
25	N	607	CHL	CBA-CAA-C2A	4.14	126.09	113.86
25	n	607	CHL	CBA-CAA-C2A	4.14	126.09	113.86
22	1	614	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
22	5	614	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
22	4	310	CLA	O2D-CGD-CBD	4.14	118.63	111.27
22	8	310	CLA	O2D-CGD-CBD	4.14	118.63	111.27
22	C	512	CLA	C3B-C2B-C1B	-4.14	102.16	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	605	CLA	C1D-CHD-C4C	-4.14	117.12	126.06
22	C	511	CLA	CHD-C4C-C3C	-4.14	118.75	124.84
22	c	509	CLA	C1D-CHD-C4C	-4.14	117.13	126.06
22	B	606	CLA	O2D-CGD-CBD	4.14	118.62	111.27
22	B	613	CLA	C3B-C2B-C1B	-4.14	102.17	107.16
22	b	612	CLA	CHD-C4C-C3C	-4.14	118.76	124.84
22	S	312	CLA	CHD-C4C-C3C	-4.14	118.76	124.84
22	s	312	CLA	CHD-C4C-C3C	-4.14	118.76	124.84
22	d	401	CLA	C1D-CHD-C4C	-4.13	117.14	126.06
25	S	308	CHL	CAA-C2A-C3A	-4.13	101.46	112.78
25	s	308	CHL	CAA-C2A-C3A	-4.13	101.46	112.78
22	R	307	CLA	C3B-C2B-C1B	-4.13	102.17	107.16
22	r	307	CLA	C3B-C2B-C1B	-4.13	102.17	107.16
22	b	605	CLA	C3B-C2B-C1B	-4.13	102.18	107.16
22	1	604	CLA	C2D-C1D-ND	4.13	113.14	110.10
22	5	604	CLA	C2D-C1D-ND	4.13	113.14	110.10
22	B	610	CLA	C3B-C2B-C1B	-4.12	102.18	107.16
22	G	602	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
22	g	602	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
22	c	507	CLA	CAC-C3C-C4C	4.12	130.16	124.81
22	R	307	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
22	r	307	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
22	a	405	CLA	C2B-C1B-NB	4.12	112.99	110.23
22	S	305	CLA	C2D-C1D-ND	4.12	113.14	110.10
22	s	305	CLA	C2D-C1D-ND	4.12	113.14	110.10
22	B	601	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
22	c	511	CLA	C2D-C1D-ND	4.12	113.14	110.10
22	c	502	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
22	b	610	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
22	Y	603	CLA	CBC-CAC-C3C	-4.12	101.08	112.43
22	y	603	CLA	CBC-CAC-C3C	-4.12	101.08	112.43
22	2	611	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
22	6	611	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
22	4	310	CLA	C1D-CHD-C4C	-4.11	117.20	126.06
22	8	310	CLA	C1D-CHD-C4C	-4.11	117.20	126.06
25	Y	607	CHL	CBA-CAA-C2A	4.10	125.98	113.86
25	y	607	CHL	CBA-CAA-C2A	4.10	125.98	113.86
22	b	604	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
22	R	302	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
22	r	302	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
25	S	306	CHL	CAA-C2A-C3A	-4.10	101.54	112.78
25	s	306	CHL	CAA-C2A-C3A	-4.10	101.54	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	503	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
22	4	303	CLA	CMA-C3A-C4A	-4.10	100.75	111.77
22	8	303	CLA	CMA-C3A-C4A	-4.10	100.75	111.77
22	c	504	CLA	O2D-CGD-CBD	4.10	118.55	111.27
22	3	310	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
22	7	310	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
25	G	607	CHL	CBA-CAA-C2A	4.10	125.96	113.86
25	g	607	CHL	CBA-CAA-C2A	4.10	125.96	113.86
22	a	402	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
22	S	314	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
22	s	314	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
22	3	311	CLA	C3B-C2B-C1B	-4.09	102.22	107.16
22	7	311	CLA	C3B-C2B-C1B	-4.09	102.22	107.16
22	C	510	CLA	O2D-CGD-CBD	4.09	118.53	111.27
22	B	604	CLA	CAC-C3C-C4C	4.09	130.12	124.81
23	A	404	PHO	CAC-C3C-C2C	4.09	134.52	127.53
22	C	502	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
22	a	405	CLA	CGD-CBD-CAD	-4.08	97.51	110.73
22	b	612	CLA	CHC-C4B-NB	4.08	128.58	124.26
22	R	301	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
22	r	301	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
22	S	312	CLA	C3B-C2B-C1B	-4.08	102.23	107.16
22	s	312	CLA	C3B-C2B-C1B	-4.08	102.23	107.16
22	Y	604	CLA	C3B-C2B-C1B	-4.08	102.24	107.16
22	y	604	CLA	C3B-C2B-C1B	-4.08	102.24	107.16
22	N	604	CLA	O2D-CGD-CBD	4.08	118.51	111.27
22	n	604	CLA	O2D-CGD-CBD	4.08	118.51	111.27
22	d	404	CLA	C3B-C2B-C1B	-4.08	102.24	107.16
22	b	616	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
25	G	609	CHL	CAA-C2A-C3A	-4.08	101.62	112.78
25	g	609	CHL	CAA-C2A-C3A	-4.08	101.62	112.78
22	b	605	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
22	B	608	CLA	C3B-C2B-C1B	-4.07	102.24	107.16
22	S	301	CLA	C2D-C1D-ND	4.07	113.11	110.10
22	1	614	CLA	CAC-C3C-C2C	-4.07	120.56	127.53
22	5	614	CLA	CAC-C3C-C2C	-4.07	120.56	127.53
22	b	609	CLA	O2D-CGD-CBD	4.07	118.50	111.27
22	R	311	CLA	C2D-C1D-ND	4.07	113.10	110.10
22	r	311	CLA	C2D-C1D-ND	4.07	113.10	110.10
22	A	402	CLA	C3C-C4C-NC	4.07	115.14	110.57
22	Y	610	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
22	y	610	CLA	C1D-CHD-C4C	-4.07	117.28	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	R	303	CLA	C2D-C1D-ND	4.07	113.10	110.10
22	r	303	CLA	C2D-C1D-ND	4.07	113.10	110.10
22	R	311	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
22	r	311	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
22	G	604	CLA	O2D-CGD-CBD	4.07	118.49	111.27
22	g	604	CLA	O2D-CGD-CBD	4.07	118.49	111.27
22	2	612	CLA	O2D-CGD-CBD	4.07	118.49	111.27
22	6	612	CLA	O2D-CGD-CBD	4.07	118.49	111.27
22	3	314	CLA	CHD-C4C-C3C	-4.06	118.87	124.84
22	7	314	CLA	CHD-C4C-C3C	-4.06	118.87	124.84
22	2	610	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
22	6	610	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
22	c	503	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
22	D	403	CLA	O2D-CGD-CBD	4.06	118.48	111.27
22	c	504	CLA	C3B-C2B-C1B	-4.06	102.27	107.16
22	G	613	CLA	C1D-CHD-C4C	-4.05	117.31	126.06
22	g	613	CLA	C1D-CHD-C4C	-4.05	117.31	126.06
22	S	309	CLA	C1D-ND-C4D	4.05	109.21	106.33
22	s	309	CLA	C1D-ND-C4D	4.05	109.21	106.33
22	b	602	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
22	1	603	CLA	O2D-CGD-CBD	4.05	118.47	111.27
22	5	603	CLA	O2D-CGD-CBD	4.05	118.47	111.27
22	N	610	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
22	n	610	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
22	Y	610	CLA	C1D-ND-C4D	4.05	109.21	106.33
22	y	610	CLA	C1D-ND-C4D	4.05	109.21	106.33
22	N	602	CLA	C2D-C1D-ND	4.05	113.09	110.10
22	n	602	CLA	C2D-C1D-ND	4.05	113.09	110.10
22	G	610	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
22	g	610	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
22	G	614	CLA	C2D-C1D-ND	4.05	113.09	110.10
22	g	614	CLA	C2D-C1D-ND	4.05	113.09	110.10
22	b	614	CLA	C3B-C2B-C1B	-4.05	102.28	107.16
22	S	314	CLA	C3B-C2B-C1B	-4.05	102.28	107.16
22	s	314	CLA	C3B-C2B-C1B	-4.05	102.28	107.16
22	N	612	CLA	CBC-CAC-C3C	-4.05	101.28	112.43
22	n	612	CLA	CBC-CAC-C3C	-4.05	101.28	112.43
22	c	502	CLA	C1D-CHD-C4C	-4.05	117.33	126.06
22	c	512	CLA	C3B-C2B-C1B	-4.05	102.28	107.16
22	N	603	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
22	n	603	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
22	c	509	CLA	O2D-CGD-CBD	4.04	118.45	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	308	CHL	CBA-CAA-C2A	4.04	125.79	113.86
25	7	308	CHL	CBA-CAA-C2A	4.04	125.79	113.86
22	G	602	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
22	g	602	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
22	N	613	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
22	n	613	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
22	4	311	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
22	8	311	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
22	N	613	CLA	O2D-CGD-CBD	4.03	118.43	111.27
22	n	613	CLA	O2D-CGD-CBD	4.03	118.43	111.27
22	a	402	CLA	C2D-C1D-ND	4.03	113.08	110.10
22	1	611	CLA	C3B-C2B-C1B	-4.03	102.30	107.16
22	5	611	CLA	C3B-C2B-C1B	-4.03	102.30	107.16
22	G	612	CLA	O2D-CGD-CBD	4.03	118.43	111.27
22	g	612	CLA	O2D-CGD-CBD	4.03	118.43	111.27
22	b	602	CLA	C3C-C4C-NC	4.03	115.09	110.57
22	4	304	CLA	C2D-C1D-ND	4.03	113.07	110.10
22	8	304	CLA	C2D-C1D-ND	4.03	113.07	110.10
22	G	603	CLA	O2D-CGD-CBD	4.03	118.43	111.27
22	g	603	CLA	O2D-CGD-CBD	4.03	118.43	111.27
22	c	506	CLA	O2D-CGD-CBD	4.03	118.42	111.27
22	B	603	CLA	C2D-C1D-ND	4.02	113.07	110.10
22	Y	614	CLA	CBC-CAC-C3C	-4.02	101.34	112.43
22	y	614	CLA	CBC-CAC-C3C	-4.02	101.34	112.43
22	b	604	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
22	N	603	CLA	O2D-CGD-CBD	4.02	118.42	111.27
22	n	603	CLA	O2D-CGD-CBD	4.02	118.42	111.27
22	C	510	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
22	C	504	CLA	C2D-C1D-ND	4.02	113.07	110.10
22	S	303	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
22	G	610	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
22	s	303	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
22	g	610	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
25	G	609	CHL	O2D-CGD-CBD	4.02	118.41	111.27
25	g	609	CHL	O2D-CGD-CBD	4.02	118.41	111.27
22	1	603	CLA	C2D-C1D-ND	4.02	113.06	110.10
22	5	603	CLA	C2D-C1D-ND	4.02	113.06	110.10
22	C	503	CLA	C1D-CHD-C4C	-4.02	117.40	126.06
22	B	606	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
22	b	614	CLA	CAC-C3C-C2C	-4.01	120.67	127.53
22	B	605	CLA	CBC-CAC-C3C	-4.01	101.39	112.43
22	Y	613	CLA	C3B-C2B-C1B	-4.00	102.33	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	y	613	CLA	C3B-C2B-C1B	-4.00	102.33	107.16
22	S	304	CLA	CBC-CAC-C3C	-4.00	101.40	112.43
22	s	304	CLA	CBC-CAC-C3C	-4.00	101.40	112.43
22	c	508	CLA	CHD-C4C-C3C	-4.00	118.96	124.84
22	C	506	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
22	N	612	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
22	n	612	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
22	N	612	CLA	C1D-ND-C4D	3.99	109.17	106.33
22	n	612	CLA	C1D-ND-C4D	3.99	109.17	106.33
22	Y	602	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
22	y	602	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
22	a	405	CLA	C1D-CHD-C4C	-3.99	117.44	126.06
22	N	603	CLA	CBC-CAC-C3C	-3.99	101.42	112.43
22	n	603	CLA	CBC-CAC-C3C	-3.99	101.42	112.43
22	3	313	CLA	C2D-C1D-ND	3.99	113.05	110.10
22	7	313	CLA	C2D-C1D-ND	3.99	113.05	110.10
22	R	301	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
22	r	301	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
22	4	301	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
22	8	301	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
22	c	504	CLA	C2D-C1D-ND	3.99	113.05	110.10
22	2	613	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
22	6	613	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
22	b	607	CLA	C3B-C2B-C1B	-3.99	102.35	107.16
22	C	510	CLA	C1D-CHD-C4C	-3.99	117.46	126.06
22	B	614	CLA	C3B-C2B-C1B	-3.99	102.35	107.16
22	B	608	CLA	C1D-ND-C4D	3.98	109.17	106.33
22	b	613	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
22	1	602	CLA	C2D-C1D-ND	3.98	113.04	110.10
22	5	602	CLA	C2D-C1D-ND	3.98	113.04	110.10
22	b	614	CLA	O2D-CGD-CBD	3.98	118.34	111.27
22	3	304	CLA	C3B-C2B-C1B	-3.98	102.36	107.16
22	7	304	CLA	C3B-C2B-C1B	-3.98	102.36	107.16
22	b	607	CLA	CMB-C2B-C1B	3.97	131.42	125.37
22	2	609	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
22	6	609	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
22	a	405	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
22	B	609	CLA	C1D-CHD-C4C	-3.97	117.49	126.06
23	a	404	PHO	O2D-CGD-CBD	3.97	116.03	111.00
22	4	301	CLA	C2D-C1D-ND	3.97	113.03	110.10
22	8	301	CLA	C2D-C1D-ND	3.97	113.03	110.10
22	4	301	CLA	C1D-CHD-C4C	-3.97	117.49	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	301	CLA	C1D-CHD-C4C	-3.97	117.49	126.06
22	s	301	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
22	N	603	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
22	N	612	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
22	n	603	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
22	n	612	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
22	S	313	CLA	C2D-C1D-ND	3.97	113.03	110.10
22	s	313	CLA	C2D-C1D-ND	3.97	113.03	110.10
22	G	612	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
22	g	612	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
22	C	504	CLA	O2D-CGD-CBD	3.97	118.32	111.27
22	S	310	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
22	G	614	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
22	s	310	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
22	g	614	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
22	4	303	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
22	8	303	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
22	D	404	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
22	C	507	CLA	O2D-CGD-CBD	3.96	118.31	111.27
22	B	611	CLA	CGD-CBD-CAD	-3.96	97.91	110.73
22	A	403	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
22	4	311	CLA	O2D-CGD-CBD	3.96	118.31	111.27
22	8	311	CLA	O2D-CGD-CBD	3.96	118.31	111.27
22	1	614	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
22	5	614	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
22	b	604	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
22	b	601	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
22	N	613	CLA	C2D-C1D-ND	3.96	113.02	110.10
22	n	613	CLA	C2D-C1D-ND	3.96	113.02	110.10
22	R	309	CLA	C3B-C2B-C1B	-3.96	102.39	107.16
22	N	613	CLA	C3B-C2B-C1B	-3.96	102.39	107.16
22	r	309	CLA	C3B-C2B-C1B	-3.96	102.39	107.16
22	n	613	CLA	C3B-C2B-C1B	-3.96	102.39	107.16
22	D	403	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
22	S	312	CLA	CBC-CAC-C3C	-3.95	101.53	112.43
22	s	312	CLA	CBC-CAC-C3C	-3.95	101.53	112.43
25	N	601	CHL	CBA-CAA-C2A	3.95	125.53	113.86
25	n	601	CHL	CBA-CAA-C2A	3.95	125.53	113.86
22	c	510	CLA	O2D-CGD-CBD	3.95	118.29	111.27
22	1	610	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
22	3	313	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
22	5	610	CLA	C3B-C2B-C1B	-3.95	102.39	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	313	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
25	1	609	CHL	CAA-C2A-C3A	-3.95	101.96	112.78
25	5	609	CHL	CAA-C2A-C3A	-3.95	101.96	112.78
22	b	607	CLA	O2D-CGD-CBD	3.95	118.29	111.27
22	N	611	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
22	n	611	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
22	2	609	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
22	6	609	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
25	2	607	CHL	CBA-CAA-C2A	3.95	125.52	113.86
25	6	607	CHL	CBA-CAA-C2A	3.95	125.52	113.86
22	c	510	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
22	2	602	CLA	C2D-C1D-ND	3.94	113.01	110.10
22	6	602	CLA	C2D-C1D-ND	3.94	113.01	110.10
22	G	611	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
22	g	611	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
22	Y	614	CLA	C2D-C1D-ND	3.94	113.01	110.10
22	y	614	CLA	C2D-C1D-ND	3.94	113.01	110.10
22	c	512	CLA	O2D-CGD-CBD	3.94	118.27	111.27
22	N	604	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
22	n	604	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
22	b	603	CLA	C3B-C2B-C1B	-3.94	102.41	107.16
22	B	607	CLA	C1D-CHD-C4C	-3.94	117.57	126.06
22	b	606	CLA	C4A-NA-C1A	-3.93	104.94	106.71
22	B	602	CLA	C2D-C1D-ND	3.93	113.00	110.10
22	c	505	CLA	C2D-C1D-ND	3.93	113.00	110.10
22	B	606	CLA	C2D-C1D-ND	3.93	113.00	110.10
22	R	307	CLA	O2D-CGD-CBD	3.93	118.25	111.27
22	r	307	CLA	O2D-CGD-CBD	3.93	118.25	111.27
22	B	602	CLA	C3B-C2B-C1B	-3.93	102.42	107.16
22	3	312	CLA	C3B-C2B-C1B	-3.92	102.42	107.16
22	7	312	CLA	C3B-C2B-C1B	-3.92	102.42	107.16
22	C	504	CLA	C2B-C1B-NB	3.92	112.86	110.23
22	1	602	CLA	C3B-C2B-C1B	-3.92	102.43	107.16
22	5	602	CLA	C3B-C2B-C1B	-3.92	102.43	107.16
22	2	603	CLA	C2D-C1D-ND	3.92	112.99	110.10
22	6	603	CLA	C2D-C1D-ND	3.92	112.99	110.10
22	c	505	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
22	Y	604	CLA	CBC-CAC-C3C	-3.92	101.63	112.43
22	y	604	CLA	CBC-CAC-C3C	-3.92	101.63	112.43
22	C	505	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
22	b	613	CLA	CBC-CAC-C3C	-3.92	101.63	112.43
22	1	610	CLA	C1D-CHD-C4C	-3.92	117.61	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	610	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
22	c	510	CLA	C2D-C1D-ND	3.91	112.99	110.10
22	C	509	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
22	C	509	CLA	O2D-CGD-CBD	3.91	118.22	111.27
22	4	303	CLA	CMB-C2B-C1B	3.91	131.33	125.37
22	8	303	CLA	CMB-C2B-C1B	3.91	131.33	125.37
22	C	508	CLA	CHC-C1C-C2C	-3.91	115.87	126.73
22	C	508	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
22	2	612	CLA	C2D-C1D-ND	3.91	112.99	110.10
22	6	612	CLA	C2D-C1D-ND	3.91	112.99	110.10
22	C	503	CLA	O2D-CGD-CBD	3.91	118.22	111.27
22	Y	603	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
22	y	603	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
22	C	506	CLA	CHC-C1C-C2C	-3.91	115.87	126.73
22	R	303	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
22	r	303	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
22	3	310	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
22	7	310	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
25	S	302	CHL	CBA-CAA-C2A	3.91	125.39	113.86
25	s	302	CHL	CBA-CAA-C2A	3.91	125.39	113.86
22	d	401	CLA	C2D-C1D-ND	3.91	112.98	110.10
22	B	608	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
22	s	301	CLA	C2D-C1D-ND	3.90	112.98	110.10
22	N	602	CLA	C3B-C2B-C1B	-3.90	102.45	107.16
22	n	602	CLA	C3B-C2B-C1B	-3.90	102.45	107.16
22	G	604	CLA	C2D-C1D-ND	3.90	112.98	110.10
22	g	604	CLA	C2D-C1D-ND	3.90	112.98	110.10
22	b	611	CLA	O2D-CGD-O1D	-3.90	116.22	123.84
22	b	605	CLA	CBC-CAC-C3C	-3.89	101.70	112.43
22	Y	613	CLA	CBC-CAC-C3C	-3.89	101.71	112.43
22	y	613	CLA	CBC-CAC-C3C	-3.89	101.71	112.43
22	2	612	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
22	6	612	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
22	R	308	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
22	r	308	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
22	2	610	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
22	6	610	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
25	N	609	CHL	CBA-CAA-C2A	3.89	125.34	113.86
25	n	609	CHL	CBA-CAA-C2A	3.89	125.34	113.86
22	b	612	CLA	O2D-CGD-CBD	3.89	118.17	111.27
22	Y	613	CLA	C2D-C1D-ND	3.88	112.97	110.10
22	y	613	CLA	C2D-C1D-ND	3.88	112.97	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	309	CHL	CBA-CAA-C2A	3.88	125.32	113.86
25	8	309	CHL	CBA-CAA-C2A	3.88	125.32	113.86
22	B	612	CLA	C2D-C1D-ND	3.88	112.97	110.10
22	1	612	CLA	C2D-C1D-ND	3.88	112.96	110.10
22	5	612	CLA	C2D-C1D-ND	3.88	112.96	110.10
22	b	612	CLA	C2D-C1D-ND	3.88	112.96	110.10
22	R	309	CLA	CBC-CAC-C3C	-3.88	101.74	112.43
22	r	309	CLA	CBC-CAC-C3C	-3.88	101.74	112.43
22	b	607	CLA	C2D-C1D-ND	3.88	112.96	110.10
22	C	508	CLA	CHD-C4C-C3C	-3.88	119.14	124.84
22	R	303	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
22	S	313	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
22	r	303	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
22	s	313	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
22	C	501	CLA	O2D-CGD-CBD	3.87	118.15	111.27
22	b	613	CLA	C3B-C2B-C1B	-3.87	102.49	107.16
22	S	309	CLA	C3B-C2B-C1B	-3.87	102.49	107.16
22	s	309	CLA	C3B-C2B-C1B	-3.87	102.49	107.16
22	1	614	CLA	CHD-C4C-C3C	-3.87	119.15	124.84
22	5	614	CLA	CHD-C4C-C3C	-3.87	119.15	124.84
22	C	501	CLA	CHD-C4C-C3C	-3.87	119.15	124.84
22	S	301	CLA	O2D-CGD-CBD	3.87	118.14	111.27
22	4	305	CLA	C3B-C2B-C1B	-3.87	102.49	107.16
22	8	305	CLA	C3B-C2B-C1B	-3.87	102.49	107.16
22	B	613	CLA	CMA-C3A-C2A	-3.87	98.23	113.83
22	C	502	CLA	CBC-CAC-C3C	-3.87	101.77	112.43
22	N	602	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
22	n	602	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
22	B	605	CLA	O2D-CGD-CBD	3.86	118.13	111.27
22	S	304	CLA	CAC-C3C-C2C	-3.86	120.93	127.53
22	s	304	CLA	CAC-C3C-C2C	-3.86	120.93	127.53
22	2	611	CLA	C1D-CHD-C4C	-3.85	117.74	126.06
22	6	611	CLA	C1D-CHD-C4C	-3.85	117.74	126.06
22	C	502	CLA	C1D-ND-C4D	3.85	109.07	106.33
22	B	604	CLA	CHD-C4C-C3C	-3.85	119.17	124.84
22	b	610	CLA	C3C-C4C-NC	3.85	114.89	110.57
22	Y	612	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
22	y	612	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
22	C	506	CLA	C2D-C1D-ND	3.85	112.94	110.10
22	Y	602	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
22	y	602	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
22	A	405	CLA	C1D-CHD-C4C	-3.85	117.75	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	608	CLA	C2D-C1D-ND	3.85	112.94	110.10
22	1	613	CLA	C2D-C1D-ND	3.85	112.94	110.10
22	5	613	CLA	C2D-C1D-ND	3.85	112.94	110.10
22	B	614	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
22	2	612	CLA	C3B-C2B-C1B	-3.85	102.52	107.16
22	6	612	CLA	C3B-C2B-C1B	-3.85	102.52	107.16
22	c	502	CLA	O2D-CGD-CBD	3.84	118.10	111.27
22	C	507	CLA	C3B-C2B-C1B	-3.84	102.52	107.16
22	d	403	CLA	C2D-C1D-ND	3.84	112.93	110.10
22	d	403	CLA	CHD-C4C-C3C	-3.84	119.20	124.84
22	c	507	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
22	G	603	CLA	C3B-C2B-C1B	-3.84	102.53	107.16
22	g	603	CLA	C3B-C2B-C1B	-3.84	102.53	107.16
22	R	309	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
22	r	309	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
22	G	613	CLA	C2D-C1D-ND	3.84	112.93	110.10
22	g	613	CLA	C2D-C1D-ND	3.84	112.93	110.10
22	C	501	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
22	4	305	CLA	C2D-C1D-ND	3.84	112.93	110.10
22	4	311	CLA	C2D-C1D-ND	3.84	112.93	110.10
22	8	305	CLA	C2D-C1D-ND	3.84	112.93	110.10
22	8	311	CLA	C2D-C1D-ND	3.84	112.93	110.10
22	D	404	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
22	4	305	CLA	C1D-CHD-C4C	-3.83	117.78	126.06
22	8	305	CLA	C1D-CHD-C4C	-3.83	117.78	126.06
22	B	615	CLA	CBC-CAC-C3C	-3.83	101.86	112.43
22	c	509	CLA	C3B-C2B-C1B	-3.83	102.54	107.16
22	B	612	CLA	C3C-C4C-NC	3.83	114.86	110.57
22	B	613	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
22	S	301	CLA	C3B-C2B-C1B	-3.83	102.54	107.16
22	2	602	CLA	C3B-C2B-C1B	-3.83	102.54	107.16
22	6	602	CLA	C3B-C2B-C1B	-3.83	102.54	107.16
25	G	601	CHL	CBA-CAA-C2A	3.82	125.15	113.86
25	g	601	CHL	CBA-CAA-C2A	3.82	125.15	113.86
22	2	603	CLA	CBC-CAC-C3C	-3.82	101.89	112.43
22	6	603	CLA	CBC-CAC-C3C	-3.82	101.89	112.43
22	R	302	CLA	CBC-CAC-C3C	-3.82	101.90	112.43
22	r	302	CLA	CBC-CAC-C3C	-3.82	101.90	112.43
22	3	305	CLA	C2D-C1D-ND	3.82	112.92	110.10
22	7	305	CLA	C2D-C1D-ND	3.82	112.92	110.10
22	B	603	CLA	O2D-CGD-CBD	3.82	118.05	111.27
22	c	510	CLA	C3B-C2B-C1B	-3.82	102.56	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	312	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
22	7	312	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
22	R	308	CLA	O2D-CGD-CBD	3.81	118.04	111.27
22	r	308	CLA	O2D-CGD-CBD	3.81	118.04	111.27
22	b	603	CLA	CHD-C4C-C3C	-3.81	119.24	124.84
22	N	610	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
22	n	610	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
25	G	608	CHL	CBA-CAA-C2A	3.81	125.11	113.86
25	g	608	CHL	CBA-CAA-C2A	3.81	125.11	113.86
22	1	604	CLA	C3B-C2B-C1B	-3.81	102.56	107.16
22	1	613	CLA	C3B-C2B-C1B	-3.81	102.56	107.16
22	5	604	CLA	C3B-C2B-C1B	-3.81	102.56	107.16
22	5	613	CLA	C3B-C2B-C1B	-3.81	102.56	107.16
22	B	606	CLA	C4A-NA-C1A	-3.81	105.00	106.71
22	B	607	CLA	O2D-CGD-CBD	3.80	118.03	111.27
22	N	604	CLA	CAA-C2A-C3A	-3.80	102.36	112.78
22	n	604	CLA	CAA-C2A-C3A	-3.80	102.36	112.78
22	G	612	CLA	CBC-CAC-C3C	-3.80	101.95	112.43
22	g	612	CLA	CBC-CAC-C3C	-3.80	101.95	112.43
22	B	612	CLA	CMD-C2D-C3D	3.80	136.36	127.61
25	1	607	CHL	O2D-CGD-CBD	3.80	118.02	111.27
25	5	607	CHL	O2D-CGD-CBD	3.80	118.02	111.27
22	S	311	CLA	CBC-CAC-C3C	-3.80	101.96	112.43
22	s	311	CLA	CBC-CAC-C3C	-3.80	101.96	112.43
22	C	501	CLA	CBC-CAC-C3C	-3.80	101.96	112.43
22	b	601	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
22	4	304	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
22	8	304	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
22	C	512	CLA	C2D-C1D-ND	3.80	112.90	110.10
22	2	613	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
22	6	613	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
22	C	510	CLA	C2D-C1D-ND	3.79	112.90	110.10
25	2	608	CHL	CAA-C2A-C3A	-3.79	102.40	112.78
25	6	608	CHL	CAA-C2A-C3A	-3.79	102.40	112.78
22	B	606	CLA	CAC-C3C-C2C	-3.79	121.05	127.53
22	1	602	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
22	5	602	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
22	c	503	CLA	O2D-CGD-CBD	3.79	118.00	111.27
25	3	302	CHL	CAA-C2A-C3A	-3.79	102.41	112.78
25	7	302	CHL	CAA-C2A-C3A	-3.79	102.41	112.78
22	R	310	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
22	r	310	CLA	C1D-CHD-C4C	-3.78	117.90	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	614	CLA	C3C-C4C-NC	3.78	114.81	110.57
22	B	602	CLA	C2B-C1B-NB	3.78	112.77	110.23
22	3	303	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
22	7	303	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
22	2	604	CLA	C2D-C1D-ND	3.78	112.89	110.10
22	6	604	CLA	C2D-C1D-ND	3.78	112.89	110.10
22	3	311	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
22	7	311	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
22	G	603	CLA	CBC-CAC-C3C	-3.78	102.01	112.43
22	g	603	CLA	CBC-CAC-C3C	-3.78	102.01	112.43
22	C	503	CLA	C2D-C1D-ND	3.78	112.89	110.10
22	C	508	CLA	C2B-C1B-NB	3.77	112.76	110.23
25	Y	608	CHL	CAA-C2A-C3A	-3.77	102.45	112.78
25	y	608	CHL	CAA-C2A-C3A	-3.77	102.45	112.78
25	R	305	CHL	CAA-C2A-C3A	-3.77	102.45	112.78
25	r	305	CHL	CAA-C2A-C3A	-3.77	102.45	112.78
22	3	313	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
22	7	313	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
25	4	306	CHL	CAA-C2A-C3A	-3.77	102.46	112.78
25	8	306	CHL	CAA-C2A-C3A	-3.77	102.46	112.78
22	B	614	CLA	C2B-C1B-NB	3.77	112.76	110.23
22	b	614	CLA	C2D-C1D-ND	3.77	112.88	110.10
22	N	614	CLA	C2D-C1D-ND	3.77	112.88	110.10
22	n	614	CLA	C2D-C1D-ND	3.77	112.88	110.10
22	c	501	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
22	c	508	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
22	S	301	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
22	3	314	CLA	C2D-C1D-ND	3.77	112.88	110.10
22	7	314	CLA	C2D-C1D-ND	3.77	112.88	110.10
22	Y	612	CLA	CBC-CAC-C3C	-3.76	102.06	112.43
22	y	612	CLA	CBC-CAC-C3C	-3.76	102.06	112.43
22	S	305	CLA	CBC-CAC-C3C	-3.76	102.06	112.43
22	s	305	CLA	CBC-CAC-C3C	-3.76	102.06	112.43
22	R	302	CLA	CMD-C2D-C3D	3.76	136.26	127.61
22	r	302	CLA	CMD-C2D-C3D	3.76	136.26	127.61
22	C	510	CLA	CBC-CAC-C3C	-3.76	102.07	112.43
22	C	507	CLA	CBC-CAC-C3C	-3.76	102.07	112.43
22	b	602	CLA	O2D-CGD-CBD	3.76	117.94	111.27
22	c	511	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
22	A	405	CLA	CGD-CBD-CAD	-3.76	98.57	110.73
22	S	313	CLA	CAC-C3C-C2C	-3.75	121.11	127.53
22	s	313	CLA	CAC-C3C-C2C	-3.75	121.11	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	306	CHL	CBA-CAA-C2A	3.75	124.94	113.86
25	r	306	CHL	CBA-CAA-C2A	3.75	124.94	113.86
22	1	611	CLA	C1D-CHD-C4C	-3.75	117.96	126.06
22	5	611	CLA	C1D-CHD-C4C	-3.75	117.96	126.06
22	1	603	CLA	C3B-C2B-C1B	-3.75	102.64	107.16
22	2	603	CLA	C3B-C2B-C1B	-3.75	102.64	107.16
22	5	603	CLA	C3B-C2B-C1B	-3.75	102.64	107.16
22	6	603	CLA	C3B-C2B-C1B	-3.75	102.64	107.16
22	G	604	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
22	g	604	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
22	2	602	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
22	6	602	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
22	B	602	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
22	S	309	CLA	CGD-CBD-CAD	-3.74	98.63	110.73
22	s	309	CLA	CGD-CBD-CAD	-3.74	98.63	110.73
22	a	405	CLA	O2D-CGD-CBD	3.73	117.91	111.27
22	C	502	CLA	O2D-CGD-CBD	3.73	117.90	111.27
22	B	607	CLA	C2D-C1D-ND	3.73	112.85	110.10
22	c	501	CLA	O2D-CGD-CBD	3.73	117.89	111.27
22	C	509	CLA	C3B-C2B-C1B	-3.73	102.66	107.16
22	c	512	CLA	C3C-C4C-NC	3.72	114.75	110.57
22	d	404	CLA	C2D-C1D-ND	3.72	112.85	110.10
22	B	603	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
22	R	303	CLA	CBC-CAC-C3C	-3.72	102.17	112.43
22	r	303	CLA	CBC-CAC-C3C	-3.72	102.17	112.43
22	4	304	CLA	C3B-C2B-C1B	-3.72	102.67	107.16
22	8	304	CLA	C3B-C2B-C1B	-3.72	102.67	107.16
22	1	604	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
22	5	604	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
22	C	507	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
25	N	609	CHL	O2D-CGD-CBD	3.72	117.88	111.27
25	n	609	CHL	O2D-CGD-CBD	3.72	117.88	111.27
22	1	603	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
22	5	603	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
22	C	504	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
22	S	313	CLA	CBC-CAC-C3C	-3.71	102.19	112.43
22	s	313	CLA	CBC-CAC-C3C	-3.71	102.19	112.43
22	a	405	CLA	C3C-C4C-NC	3.71	114.74	110.57
22	C	507	CLA	C3C-C4C-NC	3.71	114.73	110.57
22	A	405	CLA	C2D-C1D-ND	3.71	112.84	110.10
22	S	309	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
22	s	309	CLA	C1D-CHD-C4C	-3.71	118.05	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	603	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
22	6	603	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
22	c	511	CLA	C4A-NA-C1A	-3.71	105.04	106.71
22	b	602	CLA	C1D-ND-C4D	3.71	108.97	106.33
22	R	311	CLA	C3B-C2B-C1B	-3.70	102.69	107.16
22	r	311	CLA	C3B-C2B-C1B	-3.70	102.69	107.16
22	G	603	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
22	g	603	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
22	c	507	CLA	C3B-C2B-C1B	-3.70	102.70	107.16
22	b	606	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
22	S	312	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
22	s	312	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
22	2	609	CLA	CBC-CAC-C3C	-3.70	102.24	112.43
22	6	609	CLA	CBC-CAC-C3C	-3.70	102.24	112.43
22	c	504	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
22	B	609	CLA	CMA-C3A-C4A	-3.69	101.85	111.77
22	b	606	CLA	CMA-C3A-C4A	-3.69	101.86	111.77
22	B	615	CLA	O2D-CGD-O1D	-3.69	116.63	123.84
22	N	614	CLA	CBC-CAC-C3C	-3.69	102.26	112.43
22	n	614	CLA	CBC-CAC-C3C	-3.69	102.26	112.43
25	1	608	CHL	CBA-CAA-C2A	3.69	124.75	113.86
25	5	608	CHL	CBA-CAA-C2A	3.69	124.75	113.86
22	B	615	CLA	C3C-C4C-NC	3.69	114.70	110.57
22	C	512	CLA	C1D-CHD-C4C	-3.69	118.11	126.06
22	c	508	CLA	CBC-CAC-C3C	-3.68	102.28	112.43
22	B	613	CLA	C2D-C1D-ND	3.68	112.82	110.10
22	B	602	CLA	O2D-CGD-CBD	3.68	117.81	111.27
22	a	403	CLA	C3C-C4C-NC	3.68	114.69	110.57
22	S	301	CLA	C3C-C4C-NC	3.68	114.69	110.57
22	B	609	CLA	CBC-CAC-C3C	-3.68	102.30	112.43
22	B	615	CLA	C3B-C2B-C1B	-3.68	102.72	107.16
22	N	603	CLA	CAC-C3C-C2C	-3.67	121.25	127.53
22	n	603	CLA	CAC-C3C-C2C	-3.67	121.25	127.53
22	N	610	CLA	C3C-C4C-NC	3.67	114.69	110.57
22	n	610	CLA	C3C-C4C-NC	3.67	114.69	110.57
22	B	604	CLA	C3B-C2B-C1B	-3.67	102.73	107.16
22	b	609	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
22	C	503	CLA	CBC-CAC-C3C	-3.67	102.31	112.43
25	3	309	CHL	O2D-CGD-CBD	3.67	117.79	111.27
25	7	309	CHL	O2D-CGD-CBD	3.67	117.79	111.27
22	R	310	CLA	C3B-C2B-C1B	-3.67	102.73	107.16
22	r	310	CLA	C3B-C2B-C1B	-3.67	102.73	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	R	307	CLA	CAC-C3C-C2C	-3.67	121.26	127.53
22	r	307	CLA	CAC-C3C-C2C	-3.67	121.26	127.53
22	b	607	CLA	C1D-CHD-C4C	-3.67	118.15	126.06
22	b	610	CLA	C2D-C1D-ND	3.66	112.80	110.10
22	b	616	CLA	CHD-C4C-C3C	-3.66	119.46	124.84
22	C	506	CLA	O2D-CGD-CBD	3.66	117.77	111.27
22	B	610	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
22	C	507	CLA	CGD-CBD-CAD	-3.65	98.90	110.73
22	N	603	CLA	C2D-C1D-ND	3.65	112.80	110.10
22	n	603	CLA	C2D-C1D-ND	3.65	112.80	110.10
22	d	404	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
22	c	509	CLA	CBC-CAC-C3C	-3.65	102.37	112.43
22	1	613	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
22	5	613	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
22	C	511	CLA	C1D-CHD-C4C	-3.64	118.19	126.06
22	c	506	CLA	C2D-C1D-ND	3.64	112.79	110.10
22	b	609	CLA	C3B-C2B-C1B	-3.64	102.76	107.16
22	b	605	CLA	C1D-ND-C4D	3.64	108.92	106.33
22	S	314	CLA	CBC-CAC-C3C	-3.64	102.40	112.43
22	s	314	CLA	CBC-CAC-C3C	-3.64	102.40	112.43
22	G	604	CLA	C3B-C2B-C1B	-3.64	102.77	107.16
22	g	604	CLA	C3B-C2B-C1B	-3.64	102.77	107.16
25	2	606	CHL	C2B-C1B-NB	-3.63	107.80	110.23
25	6	606	CHL	C2B-C1B-NB	-3.63	107.80	110.23
22	c	506	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
22	N	613	CLA	CBC-CAC-C3C	-3.63	102.43	112.43
22	n	613	CLA	CBC-CAC-C3C	-3.63	102.43	112.43
22	d	403	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
22	3	305	CLA	C1D-CHD-C4C	-3.63	118.24	126.06
22	7	305	CLA	C1D-CHD-C4C	-3.63	118.24	126.06
22	c	506	CLA	CAC-C3C-C2C	-3.62	121.33	127.53
22	c	507	CLA	CHC-C1C-C2C	-3.62	116.67	126.73
22	G	603	CLA	CAC-C3C-C2C	-3.62	121.34	127.53
22	g	603	CLA	CAC-C3C-C2C	-3.62	121.34	127.53
22	S	304	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
22	s	304	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
22	3	304	CLA	CBC-CAC-C3C	-3.61	102.47	112.43
22	7	304	CLA	CBC-CAC-C3C	-3.61	102.47	112.43
22	2	604	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
22	6	604	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
22	c	503	CLA	C2D-C1D-ND	3.61	112.76	110.10
22	b	608	CLA	CBC-CAC-C3C	-3.61	102.49	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	614	CLA	C1D-CHD-C4C	-3.60	118.28	126.06
22	n	614	CLA	C1D-CHD-C4C	-3.60	118.28	126.06
23	A	404	PHO	CMB-C2B-C3B	3.60	131.42	124.68
22	B	605	CLA	CAC-C3C-C2C	-3.60	121.36	127.53
22	c	502	CLA	C2D-C1D-ND	3.60	112.76	110.10
22	R	310	CLA	CBC-CAC-C3C	-3.60	102.50	112.43
22	r	310	CLA	CBC-CAC-C3C	-3.60	102.50	112.43
22	b	603	CLA	CGD-CBD-CAD	-3.60	99.09	110.73
22	R	308	CLA	C4D-CHA-C1A	-3.59	116.88	121.25
22	r	308	CLA	C4D-CHA-C1A	-3.59	116.88	121.25
22	4	311	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
22	8	311	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
22	c	503	CLA	CBC-CAC-C3C	-3.59	102.53	112.43
22	1	612	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
22	5	612	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
22	b	616	CLA	CAC-C3C-C2C	-3.59	121.39	127.53
22	C	504	CLA	C3B-C2B-C1B	-3.59	102.83	107.16
22	4	303	CLA	C3C-C4C-NC	3.59	114.59	110.57
22	8	303	CLA	C3C-C4C-NC	3.59	114.59	110.57
22	1	614	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
22	5	614	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
22	R	311	CLA	C3C-C4C-NC	3.58	114.59	110.57
22	r	311	CLA	C3C-C4C-NC	3.58	114.59	110.57
22	C	512	CLA	O2D-CGD-CBD	3.58	117.64	111.27
22	b	610	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
22	2	604	CLA	C3B-C2B-C1B	-3.58	102.84	107.16
22	6	604	CLA	C3B-C2B-C1B	-3.58	102.84	107.16
22	G	613	CLA	CBC-CAC-C3C	-3.58	102.56	112.43
22	g	613	CLA	CBC-CAC-C3C	-3.58	102.56	112.43
22	b	608	CLA	C4A-NA-C1A	-3.58	105.10	106.71
22	B	603	CLA	CBC-CAC-C3C	-3.58	102.57	112.43
22	c	509	CLA	CAC-C3C-C4C	3.58	129.45	124.81
22	G	614	CLA	CBC-CAC-C3C	-3.58	102.58	112.43
22	g	614	CLA	CBC-CAC-C3C	-3.58	102.58	112.43
22	b	615	CLA	CBC-CAC-C3C	-3.57	102.58	112.43
22	C	504	CLA	CAC-C3C-C2C	-3.57	121.42	127.53
22	3	305	CLA	C3B-C2B-C1B	-3.57	102.85	107.16
22	7	305	CLA	C3B-C2B-C1B	-3.57	102.85	107.16
22	S	305	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
22	s	305	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
25	4	302	CHL	CBA-CAA-C2A	3.57	124.39	113.86
25	8	302	CHL	CBA-CAA-C2A	3.57	124.39	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	614	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
22	B	609	CLA	C2B-C1B-NB	3.56	112.62	110.23
22	b	604	CLA	CHD-C4C-C3C	-3.56	119.60	124.84
22	4	303	CLA	C3B-C2B-C1B	-3.56	102.86	107.16
22	8	303	CLA	C3B-C2B-C1B	-3.56	102.86	107.16
22	R	308	CLA	OBD-CAD-C3D	-3.56	119.94	128.52
22	r	308	CLA	OBD-CAD-C3D	-3.56	119.94	128.52
22	b	612	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
25	R	304	CHL	O2D-CGD-CBD	3.56	117.60	111.27
25	r	304	CHL	O2D-CGD-CBD	3.56	117.60	111.27
22	G	603	CLA	C2D-C1D-ND	3.56	112.73	110.10
22	g	603	CLA	C2D-C1D-ND	3.56	112.73	110.10
22	G	610	CLA	C1D-ND-C4D	3.56	108.86	106.33
22	g	610	CLA	C1D-ND-C4D	3.56	108.86	106.33
22	G	602	CLA	CBC-CAC-C3C	-3.56	102.62	112.43
22	g	602	CLA	CBC-CAC-C3C	-3.56	102.62	112.43
22	C	508	CLA	CBC-CAC-C3C	-3.56	102.63	112.43
22	b	608	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
22	3	304	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
22	7	304	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
22	Y	612	CLA	C2D-C1D-ND	3.55	112.72	110.10
22	y	612	CLA	C2D-C1D-ND	3.55	112.72	110.10
22	C	509	CLA	CBC-CAC-C3C	-3.55	102.65	112.43
22	G	610	CLA	C3C-C4C-NC	3.55	114.55	110.57
22	g	610	CLA	C3C-C4C-NC	3.55	114.55	110.57
22	c	508	CLA	C2B-C1B-NB	3.54	112.61	110.23
22	S	304	CLA	O2D-CGD-CBD	3.54	117.55	111.27
22	s	304	CLA	O2D-CGD-CBD	3.54	117.55	111.27
22	b	614	CLA	CMC-C2C-C1C	3.53	130.42	125.04
22	N	602	CLA	CBC-CAC-C3C	-3.53	102.69	112.43
22	n	602	CLA	CBC-CAC-C3C	-3.53	102.69	112.43
22	A	405	CLA	O2D-CGD-CBD	3.53	117.54	111.27
22	R	302	CLA	C3C-C4C-NC	3.53	114.53	110.57
22	r	302	CLA	C3C-C4C-NC	3.53	114.53	110.57
22	S	304	CLA	CHC-C4B-NB	3.53	127.99	124.26
22	s	304	CLA	CHC-C4B-NB	3.53	127.99	124.26
22	3	304	CLA	C2D-C1D-ND	3.52	112.70	110.10
22	7	304	CLA	C2D-C1D-ND	3.52	112.70	110.10
22	1	603	CLA	CBC-CAC-C3C	-3.52	102.72	112.43
22	5	603	CLA	CBC-CAC-C3C	-3.52	102.72	112.43
22	b	616	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
22	B	609	CLA	C3B-C2B-C1B	-3.52	102.92	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	310	CLA	C1D-ND-C4D	3.51	108.83	106.33
22	7	310	CLA	C1D-ND-C4D	3.51	108.83	106.33
22	b	615	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
22	b	607	CLA	CAC-C3C-C2C	-3.51	121.52	127.53
25	N	608	CHL	O2A-CGA-CBA	3.51	125.31	114.03
25	n	608	CHL	O2A-CGA-CBA	3.51	125.31	114.03
22	3	314	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
22	7	314	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
22	B	615	CLA	CAC-C3C-C2C	-3.51	121.53	127.53
22	3	310	CLA	CBC-CAC-C3C	-3.51	102.77	112.43
22	7	310	CLA	CBC-CAC-C3C	-3.51	102.77	112.43
22	R	301	CLA	CBC-CAC-C3C	-3.50	102.77	112.43
22	r	301	CLA	CBC-CAC-C3C	-3.50	102.77	112.43
25	3	301	CHL	O2D-CGD-CBD	3.50	117.49	111.27
25	7	301	CHL	O2D-CGD-CBD	3.50	117.49	111.27
22	b	604	CLA	CBC-CAC-C3C	-3.50	102.77	112.43
22	3	310	CLA	CMC-C2C-C1C	3.50	130.37	125.04
22	7	310	CLA	CMC-C2C-C1C	3.50	130.37	125.04
22	3	304	CLA	CAC-C3C-C2C	-3.50	121.55	127.53
22	7	304	CLA	CAC-C3C-C2C	-3.50	121.55	127.53
22	b	604	CLA	CMC-C2C-C3C	3.49	135.60	126.12
22	b	612	CLA	C4D-CHA-C1A	-3.49	117.00	121.25
22	b	615	CLA	C2D-C1D-ND	3.49	112.67	110.10
22	Y	604	CLA	CMD-C2D-C3D	3.49	135.64	127.61
22	y	604	CLA	CMD-C2D-C3D	3.49	135.64	127.61
22	A	405	CLA	C3C-C4C-NC	3.49	114.48	110.57
22	B	610	CLA	O2D-CGD-CBD	3.49	117.46	111.27
22	B	612	CLA	O2D-CGD-CBD	3.49	117.46	111.27
22	A	405	CLA	CBC-CAC-C3C	-3.48	102.82	112.43
22	c	509	CLA	C3C-C4C-NC	3.48	114.48	110.57
22	b	614	CLA	CBC-CAC-C3C	-3.48	102.83	112.43
22	1	610	CLA	C3C-C4C-NC	3.48	114.47	110.57
22	5	610	CLA	C3C-C4C-NC	3.48	114.47	110.57
22	4	310	CLA	C2B-C1B-NB	3.48	112.56	110.23
22	8	310	CLA	C2B-C1B-NB	3.48	112.56	110.23
22	1	610	CLA	C1D-ND-C4D	3.48	108.81	106.33
22	5	610	CLA	C1D-ND-C4D	3.48	108.81	106.33
22	S	303	CLA	CBC-CAC-C3C	-3.48	102.84	112.43
22	s	303	CLA	CBC-CAC-C3C	-3.48	102.84	112.43
22	B	605	CLA	C2D-C1D-ND	3.48	112.67	110.10
25	4	308	CHL	CBA-CAA-C2A	3.48	124.13	113.86
25	8	308	CHL	CBA-CAA-C2A	3.48	124.13	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	510	CLA	C3C-C4C-NC	3.48	114.47	110.57
22	B	611	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
22	b	601	CLA	CBC-CAC-C3C	-3.48	102.85	112.43
22	N	610	CLA	C1D-ND-C4D	3.47	108.80	106.33
22	n	610	CLA	C1D-ND-C4D	3.47	108.80	106.33
22	3	310	CLA	C3C-C4C-NC	3.47	114.47	110.57
22	7	310	CLA	C3C-C4C-NC	3.47	114.47	110.57
25	Y	606	CHL	O2A-CGA-CBA	3.47	125.17	114.03
25	y	606	CHL	O2A-CGA-CBA	3.47	125.17	114.03
22	R	303	CLA	C4D-CHA-C1A	-3.47	117.03	121.25
22	r	303	CLA	C4D-CHA-C1A	-3.47	117.03	121.25
22	b	609	CLA	CBC-CAC-C3C	-3.46	102.88	112.43
22	a	403	CLA	OBD-CAD-C3D	-3.46	120.19	128.52
22	A	403	CLA	C4A-NA-C1A	-3.46	105.15	106.71
25	N	607	CHL	O2D-CGD-CBD	3.46	117.42	111.27
25	n	607	CHL	O2D-CGD-CBD	3.46	117.42	111.27
22	B	616	CLA	CAC-C3C-C2C	-3.46	121.61	127.53
22	R	303	CLA	CAA-C2A-C3A	-3.46	103.30	112.78
22	r	303	CLA	CAA-C2A-C3A	-3.46	103.30	112.78
22	C	503	CLA	C4A-NA-C1A	-3.46	105.15	106.71
22	N	604	CLA	CBC-CAC-C3C	-3.46	102.90	112.43
22	n	604	CLA	CBC-CAC-C3C	-3.46	102.90	112.43
22	B	613	CLA	CAA-C2A-C3A	-3.46	103.31	112.78
22	b	602	CLA	CBC-CAC-C3C	-3.46	102.90	112.43
22	3	305	CLA	C4A-NA-C1A	-3.46	105.15	106.71
22	7	305	CLA	C4A-NA-C1A	-3.46	105.15	106.71
22	b	604	CLA	CHC-C1C-C2C	-3.46	117.13	126.73
22	c	508	CLA	CHC-C1C-C2C	-3.46	117.13	126.73
22	c	510	CLA	CBC-CAC-C3C	-3.45	102.91	112.43
22	1	614	CLA	CBC-CAC-C3C	-3.45	102.91	112.43
22	5	614	CLA	CBC-CAC-C3C	-3.45	102.91	112.43
22	Y	604	CLA	C3C-C4C-NC	3.45	114.44	110.57
22	y	604	CLA	C3C-C4C-NC	3.45	114.44	110.57
22	A	403	CLA	CED-O2D-CGD	3.45	123.73	115.94
22	2	609	CLA	CMC-C2C-C1C	3.44	130.28	125.04
22	6	609	CLA	CMC-C2C-C1C	3.44	130.28	125.04
22	c	508	CLA	C2D-C1D-ND	3.44	112.64	110.10
22	b	606	CLA	C3D-C2D-C1D	-3.44	101.13	105.83
22	B	616	CLA	O2D-CGD-CBD	3.44	117.38	111.27
22	1	611	CLA	CBC-CAC-C3C	-3.44	102.94	112.43
22	5	611	CLA	CBC-CAC-C3C	-3.44	102.94	112.43
22	b	616	CLA	CBC-CAC-C3C	-3.44	102.95	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	609	CHL	O2D-CGD-CBD	3.44	117.38	111.27
25	y	609	CHL	O2D-CGD-CBD	3.44	117.38	111.27
22	R	303	CLA	OBD-CAD-C3D	-3.44	120.24	128.52
22	r	303	CLA	OBD-CAD-C3D	-3.44	120.24	128.52
22	R	307	CLA	CMD-C2D-C3D	3.44	135.52	127.61
22	r	307	CLA	CMD-C2D-C3D	3.44	135.52	127.61
22	b	606	CLA	CAC-C3C-C2C	-3.44	121.65	127.53
22	G	604	CLA	CAA-C2A-C3A	-3.44	103.37	112.78
22	g	604	CLA	CAA-C2A-C3A	-3.44	103.37	112.78
22	c	503	CLA	C3C-C4C-NC	3.44	114.42	110.57
22	1	613	CLA	CBC-CAC-C3C	-3.44	102.96	112.43
22	5	613	CLA	CBC-CAC-C3C	-3.44	102.96	112.43
22	1	604	CLA	CAA-C2A-C3A	-3.44	103.37	112.78
22	5	604	CLA	CAA-C2A-C3A	-3.44	103.37	112.78
22	D	401	CLA	C2D-C1D-ND	3.43	112.64	110.10
22	C	505	CLA	C4A-NA-C1A	-3.43	105.16	106.71
22	c	506	CLA	C3C-C4C-NC	3.43	114.42	110.57
25	G	601	CHL	CAA-C2A-C3A	-3.43	103.38	112.78
25	g	601	CHL	CAA-C2A-C3A	-3.43	103.38	112.78
25	Y	606	CHL	CAA-CBA-CGA	3.43	121.61	112.51
25	y	606	CHL	CAA-CBA-CGA	3.43	121.61	112.51
22	Y	611	CLA	CMD-C2D-C3D	3.43	135.50	127.61
22	y	611	CLA	CMD-C2D-C3D	3.43	135.50	127.61
22	2	611	CLA	CBC-CAC-C3C	-3.43	102.98	112.43
22	6	611	CLA	CBC-CAC-C3C	-3.43	102.98	112.43
22	2	612	CLA	C3C-C4C-NC	3.43	114.41	110.57
22	6	612	CLA	C3C-C4C-NC	3.43	114.41	110.57
22	B	603	CLA	CAC-C3C-C2C	-3.42	121.68	127.53
22	4	303	CLA	C2B-C1B-NB	3.42	112.53	110.23
22	8	303	CLA	C2B-C1B-NB	3.42	112.53	110.23
22	b	613	CLA	CMA-C3A-C2A	-3.42	100.03	113.83
22	2	612	CLA	CBC-CAC-C3C	-3.42	103.00	112.43
22	6	612	CLA	CBC-CAC-C3C	-3.42	103.00	112.43
22	2	609	CLA	C3C-C4C-NC	3.42	114.41	110.57
22	6	609	CLA	C3C-C4C-NC	3.42	114.41	110.57
22	c	508	CLA	CMD-C2D-C3D	3.42	135.47	127.61
22	c	511	CLA	CBC-CAC-C3C	-3.41	103.02	112.43
22	C	505	CLA	CAC-C3C-C2C	-3.41	121.70	127.53
22	C	505	CLA	CBC-CAC-C3C	-3.41	103.04	112.43
22	S	301	CLA	CGD-CBD-CAD	-3.41	99.70	110.73
22	3	311	CLA	CBC-CAC-C3C	-3.40	103.04	112.43
22	7	311	CLA	CBC-CAC-C3C	-3.40	103.04	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Y	602	CLA	CBC-CAC-C3C	-3.40	103.05	112.43
22	y	602	CLA	CBC-CAC-C3C	-3.40	103.05	112.43
22	B	609	CLA	CMD-C2D-C3D	3.40	135.44	127.61
22	b	606	CLA	C4D-CHA-C1A	-3.40	117.11	121.25
25	Y	601	CHL	CBA-CAA-C2A	3.40	123.90	113.86
25	y	601	CHL	CBA-CAA-C2A	3.40	123.90	113.86
22	B	613	CLA	CBC-CAC-C3C	-3.40	103.06	112.43
22	S	311	CLA	C3C-C4C-NC	3.40	114.38	110.57
22	s	311	CLA	C3C-C4C-NC	3.40	114.38	110.57
22	c	505	CLA	CAC-C3C-C2C	-3.39	121.73	127.53
22	2	604	CLA	C4A-NA-C1A	-3.39	105.18	106.71
22	6	604	CLA	C4A-NA-C1A	-3.39	105.18	106.71
22	b	603	CLA	CAC-C3C-C2C	-3.39	121.73	127.53
22	R	303	CLA	CAA-CBA-CGA	3.39	121.50	112.51
22	r	303	CLA	CAA-CBA-CGA	3.39	121.50	112.51
22	c	507	CLA	O2D-CGD-CBD	3.39	117.29	111.27
22	1	604	CLA	CBC-CAC-C3C	-3.39	103.09	112.43
22	5	604	CLA	CBC-CAC-C3C	-3.39	103.09	112.43
22	B	615	CLA	CAA-C2A-C3A	-3.39	103.50	112.78
22	C	501	CLA	C2D-C1D-ND	3.39	112.60	110.10
22	b	604	CLA	C2D-C1D-ND	3.38	112.60	110.10
22	s	301	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
22	2	610	CLA	CBC-CAC-C3C	-3.38	103.12	112.43
22	6	610	CLA	CBC-CAC-C3C	-3.38	103.12	112.43
22	b	606	CLA	CBC-CAC-C3C	-3.37	103.13	112.43
22	4	304	CLA	CBC-CAC-C3C	-3.37	103.13	112.43
22	8	304	CLA	CBC-CAC-C3C	-3.37	103.13	112.43
22	G	604	CLA	CBC-CAC-C3C	-3.37	103.14	112.43
22	g	604	CLA	CBC-CAC-C3C	-3.37	103.14	112.43
22	4	303	CLA	CMD-C2D-C3D	3.37	135.36	127.61
22	8	303	CLA	CMD-C2D-C3D	3.37	135.36	127.61
22	a	405	CLA	CBC-CAC-C3C	-3.37	103.15	112.43
25	Y	608	CHL	CBA-CAA-C2A	3.37	123.80	113.86
25	y	608	CHL	CBA-CAA-C2A	3.37	123.80	113.86
22	b	613	CLA	C3C-C4C-NC	3.36	114.34	110.57
25	N	601	CHL	CAA-C2A-C3A	-3.36	103.58	112.78
25	n	601	CHL	CAA-C2A-C3A	-3.36	103.58	112.78
22	R	301	CLA	C3C-C4C-NC	3.36	114.34	110.57
22	r	301	CLA	C3C-C4C-NC	3.36	114.34	110.57
22	B	615	CLA	CGD-CBD-CAD	-3.36	99.86	110.73
25	2	608	CHL	O2D-CGD-CBD	3.36	117.23	111.27
25	6	608	CHL	O2D-CGD-CBD	3.36	117.23	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	607	CLA	CHC-C1C-C2C	-3.36	117.40	126.73
22	N	610	CLA	C4D-CHA-C1A	-3.36	117.16	121.25
22	n	610	CLA	C4D-CHA-C1A	-3.36	117.16	121.25
22	B	609	CLA	CAC-C3C-C2C	-3.36	121.79	127.53
22	b	616	CLA	CHC-C1C-C2C	-3.36	117.41	126.73
22	C	506	CLA	CAC-C3C-C2C	-3.35	121.79	127.53
23	d	402	PHO	CMB-C2B-C3B	3.35	130.95	124.68
22	b	610	CLA	O2D-CGD-CBD	3.35	117.22	111.27
24	F	101	HEM	C3B-C2B-C1B	3.34	108.97	106.49
22	3	314	CLA	CBC-CAC-C3C	-3.34	103.22	112.43
22	7	314	CLA	CBC-CAC-C3C	-3.34	103.22	112.43
22	3	313	CLA	CBC-CAC-C3C	-3.34	103.23	112.43
22	7	313	CLA	CBC-CAC-C3C	-3.34	103.23	112.43
22	C	506	CLA	CMD-C2D-C3D	3.33	135.28	127.61
22	R	308	CLA	C3C-C4C-NC	3.33	114.30	110.57
22	r	308	CLA	C3C-C4C-NC	3.33	114.30	110.57
22	b	601	CLA	C3C-C4C-NC	3.33	114.30	110.57
22	1	603	CLA	CAC-C3C-C2C	-3.33	121.84	127.53
22	5	603	CLA	CAC-C3C-C2C	-3.33	121.84	127.53
22	Y	610	CLA	C3C-C4C-NC	3.33	114.30	110.57
22	y	610	CLA	C3C-C4C-NC	3.33	114.30	110.57
23	a	404	PHO	CMB-C2B-C3B	3.32	130.90	124.68
22	B	601	CLA	CMC-C2C-C1C	3.32	130.10	125.04
22	R	309	CLA	CGD-CBD-CAD	-3.32	99.97	110.73
22	r	309	CLA	CGD-CBD-CAD	-3.32	99.97	110.73
22	B	616	CLA	CHC-C1C-C2C	-3.32	117.50	126.73
22	1	602	CLA	C3C-C4C-NC	3.32	114.30	110.57
22	5	602	CLA	C3C-C4C-NC	3.32	114.30	110.57
22	R	308	CLA	C1D-ND-C4D	3.32	108.69	106.33
22	r	308	CLA	C1D-ND-C4D	3.32	108.69	106.33
25	2	601	CHL	CAA-C2A-C3A	-3.32	103.69	112.78
25	6	601	CHL	CAA-C2A-C3A	-3.32	103.69	112.78
22	B	601	CLA	CHD-C4C-NC	3.32	129.43	124.20
22	D	404	CLA	CBC-CAC-C3C	-3.32	103.28	112.43
22	C	508	CLA	CAC-C3C-C2C	-3.32	121.85	127.53
22	1	612	CLA	CBC-CAC-C3C	-3.32	103.28	112.43
22	5	612	CLA	CBC-CAC-C3C	-3.32	103.28	112.43
25	R	304	CHL	C2B-C1B-NB	-3.32	108.01	110.23
25	r	304	CHL	C2B-C1B-NB	-3.32	108.01	110.23
22	R	311	CLA	CBC-CAC-C3C	-3.32	103.29	112.43
22	r	311	CLA	CBC-CAC-C3C	-3.32	103.29	112.43
22	4	305	CLA	CBC-CAC-C3C	-3.32	103.29	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	305	CLA	CBC-CAC-C3C	-3.32	103.29	112.43
22	S	313	CLA	CMD-C2D-C3D	3.32	135.24	127.61
22	s	313	CLA	CMD-C2D-C3D	3.32	135.24	127.61
22	c	501	CLA	C2D-C1D-ND	3.32	112.55	110.10
22	4	310	CLA	C3C-C4C-NC	3.31	114.28	110.57
22	8	310	CLA	C3C-C4C-NC	3.31	114.28	110.57
22	C	506	CLA	C3C-C4C-NC	3.31	114.28	110.57
25	G	606	CHL	CHC-C4B-NB	3.31	127.76	124.26
25	g	606	CHL	CHC-C4B-NB	3.31	127.76	124.26
22	c	508	CLA	CAC-C3C-C2C	-3.31	121.87	127.53
22	b	616	CLA	C3B-C4B-NB	3.31	113.58	110.52
22	1	610	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
22	5	610	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
22	3	312	CLA	CBC-CAC-C3C	-3.30	103.32	112.43
22	7	312	CLA	CBC-CAC-C3C	-3.30	103.32	112.43
22	c	506	CLA	CBC-CAC-C3C	-3.30	103.33	112.43
22	c	509	CLA	CHD-C4C-NC	3.30	129.40	124.20
22	2	609	CLA	C1D-ND-C4D	3.30	108.68	106.33
22	6	609	CLA	C1D-ND-C4D	3.30	108.68	106.33
22	c	512	CLA	CBC-CAC-C3C	-3.30	103.33	112.43
22	c	507	CLA	C3C-C4C-NC	3.30	114.27	110.57
22	c	506	CLA	CHC-C1C-C2C	-3.30	117.58	126.73
22	C	506	CLA	CBC-CAC-C3C	-3.29	103.35	112.43
22	B	610	CLA	C2D-C1D-ND	3.29	112.53	110.10
22	3	312	CLA	C3C-C4C-NC	3.29	114.26	110.57
22	7	312	CLA	C3C-C4C-NC	3.29	114.26	110.57
22	4	303	CLA	CBC-CAC-C3C	-3.29	103.37	112.43
22	8	303	CLA	CBC-CAC-C3C	-3.29	103.37	112.43
22	Y	614	CLA	CAC-C3C-C2C	-3.28	121.91	127.53
22	y	614	CLA	CAC-C3C-C2C	-3.28	121.91	127.53
22	D	401	CLA	C3C-C4C-NC	3.28	114.25	110.57
22	c	507	CLA	CBC-CAC-C3C	-3.27	103.40	112.43
22	D	401	CLA	CHC-C1C-C2C	-3.27	117.64	126.73
22	Y	602	CLA	CMD-C2D-C3D	3.27	135.15	127.61
22	y	602	CLA	CMD-C2D-C3D	3.27	135.15	127.61
22	S	309	CLA	CHC-C1C-C2C	-3.27	117.64	126.73
22	s	309	CLA	CHC-C1C-C2C	-3.27	117.64	126.73
22	S	312	CLA	CHC-C1C-C2C	-3.27	117.64	126.73
22	s	312	CLA	CHC-C1C-C2C	-3.27	117.64	126.73
22	R	311	CLA	CMD-C2D-C3D	3.27	135.14	127.61
22	r	311	CLA	CMD-C2D-C3D	3.27	135.14	127.61
22	B	604	CLA	C2D-C1D-ND	3.27	112.52	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	306	CHL	O2D-CGD-CBD	3.27	117.08	111.27
25	r	306	CHL	O2D-CGD-CBD	3.27	117.08	111.27
22	2	603	CLA	CAC-C3C-C2C	-3.27	121.94	127.53
22	6	603	CLA	CAC-C3C-C2C	-3.27	121.94	127.53
24	e	101	HEM	C4D-ND-C1D	3.27	108.45	105.07
22	R	311	CLA	CAC-C3C-C2C	-3.27	121.94	127.53
22	r	311	CLA	CAC-C3C-C2C	-3.27	121.94	127.53
22	B	608	CLA	C4D-CHA-C1A	-3.26	117.28	121.25
22	4	311	CLA	CBC-CAC-C3C	-3.26	103.44	112.43
22	8	311	CLA	CBC-CAC-C3C	-3.26	103.44	112.43
22	4	303	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
22	8	303	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
25	G	608	CHL	O2A-CGA-CBA	3.26	124.50	114.03
25	g	608	CHL	O2A-CGA-CBA	3.26	124.50	114.03
22	B	610	CLA	C3C-C4C-NC	3.26	114.23	110.57
25	4	308	CHL	CAA-C2A-C3A	-3.26	103.86	112.78
25	8	308	CHL	CAA-C2A-C3A	-3.26	103.86	112.78
22	c	510	CLA	C3C-C4C-NC	3.26	114.22	110.57
22	4	310	CLA	C3B-C2B-C1B	-3.25	103.23	107.16
22	8	310	CLA	C3B-C2B-C1B	-3.25	103.23	107.16
22	d	403	CLA	CHC-C1C-C2C	-3.25	117.71	126.73
22	A	403	CLA	C2D-C1D-ND	3.25	112.50	110.10
22	B	607	CLA	C3C-C4C-NC	3.25	114.21	110.57
22	C	511	CLA	CHC-C1C-C2C	-3.25	117.71	126.73
22	Y	604	CLA	O2D-CGD-CBD	3.25	117.04	111.27
22	y	604	CLA	O2D-CGD-CBD	3.25	117.04	111.27
22	s	301	CLA	CAC-C3C-C2C	-3.25	121.98	127.53
22	d	401	CLA	C3C-C4C-NC	3.24	114.21	110.57
22	3	310	CLA	C4D-CHA-C1A	-3.24	117.31	121.25
22	7	310	CLA	C4D-CHA-C1A	-3.24	117.31	121.25
22	3	310	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
22	7	310	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
22	B	608	CLA	C3C-C4C-NC	3.24	114.20	110.57
25	N	606	CHL	O2A-CGA-CBA	3.24	124.43	114.03
25	n	606	CHL	O2A-CGA-CBA	3.24	124.43	114.03
25	Y	609	CHL	CAA-CBA-CGA	3.23	121.09	112.51
25	y	609	CHL	CAA-CBA-CGA	3.23	121.09	112.51
22	D	401	CLA	C4A-NA-C1A	-3.23	105.25	106.71
22	2	609	CLA	C4D-CHA-C1A	-3.23	117.31	121.25
22	6	609	CLA	C4D-CHA-C1A	-3.23	117.31	121.25
22	D	401	CLA	O2D-CGD-CBD	3.23	117.01	111.27
22	d	401	CLA	CAA-C2A-C3A	-3.23	103.93	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	d	401	CLA	CBC-CAC-C3C	-3.23	103.52	112.43
22	Y	612	CLA	CHC-C1C-C2C	-3.23	117.76	126.73
22	y	612	CLA	CHC-C1C-C2C	-3.23	117.76	126.73
22	2	602	CLA	C3C-C4C-NC	3.23	114.19	110.57
22	6	602	CLA	C3C-C4C-NC	3.23	114.19	110.57
24	e	101	HEM	C3B-C2B-C1B	3.23	108.88	106.49
25	G	607	CHL	O2D-CGD-CBD	3.23	117.01	111.27
25	g	607	CHL	O2D-CGD-CBD	3.23	117.01	111.27
22	2	604	CLA	CAC-C3C-C2C	-3.23	122.01	127.53
22	6	604	CLA	CAC-C3C-C2C	-3.23	122.01	127.53
22	c	506	CLA	CMD-C2D-C3D	3.23	135.03	127.61
22	b	611	CLA	CBC-CAC-C3C	-3.22	103.54	112.43
22	G	604	CLA	CAC-C3C-C2C	-3.22	122.02	127.53
22	g	604	CLA	CAC-C3C-C2C	-3.22	122.02	127.53
25	4	302	CHL	O2D-CGD-CBD	3.22	117.00	111.27
25	8	302	CHL	O2D-CGD-CBD	3.22	117.00	111.27
22	c	503	CLA	CAC-C3C-C2C	-3.22	122.02	127.53
22	2	609	CLA	OBD-CAD-C3D	-3.22	120.77	128.52
22	6	609	CLA	OBD-CAD-C3D	-3.22	120.77	128.52
22	c	507	CLA	CMC-C2C-C3C	3.22	134.86	126.12
25	G	606	CHL	O2A-CGA-CBA	3.22	124.37	114.03
25	g	606	CHL	O2A-CGA-CBA	3.22	124.37	114.03
22	B	611	CLA	CBC-CAC-C3C	-3.22	103.56	112.43
23	A	404	PHO	CMD-C2D-C3D	3.22	130.70	124.68
22	Y	612	CLA	C4A-NA-C1A	-3.22	105.26	106.71
22	y	612	CLA	C4A-NA-C1A	-3.22	105.26	106.71
22	Y	613	CLA	C3C-C4C-NC	3.22	114.18	110.57
22	y	613	CLA	C3C-C4C-NC	3.22	114.18	110.57
22	3	305	CLA	CAC-C3C-C2C	-3.21	122.03	127.53
22	7	305	CLA	CAC-C3C-C2C	-3.21	122.03	127.53
22	C	505	CLA	CHC-C1C-C2C	-3.21	117.81	126.73
22	3	303	CLA	C3C-C4C-NC	3.21	114.17	110.57
22	7	303	CLA	C3C-C4C-NC	3.21	114.17	110.57
25	1	607	CHL	O1D-CGD-CBD	-3.21	117.91	124.48
25	5	607	CHL	O1D-CGD-CBD	-3.21	117.91	124.48
22	B	608	CLA	CHC-C1C-C2C	-3.21	117.81	126.73
22	b	609	CLA	CAC-C3C-C2C	-3.21	122.04	127.53
25	Y	601	CHL	O2A-CGA-CBA	3.21	124.33	114.03
25	y	601	CHL	O2A-CGA-CBA	3.21	124.33	114.03
22	b	604	CLA	CMD-C2D-C3D	3.21	134.99	127.61
22	b	613	CLA	CMA-C3A-C4A	-3.21	103.15	111.77
22	3	313	CLA	C3C-C4C-NC	3.21	114.17	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	313	CLA	C3C-C4C-NC	3.21	114.17	110.57
22	S	314	CLA	CAC-C3C-C2C	-3.21	122.05	127.53
22	s	314	CLA	CAC-C3C-C2C	-3.21	122.05	127.53
22	a	403	CLA	CED-O2D-CGD	3.21	123.19	115.94
22	B	610	CLA	CBC-CAC-C3C	-3.20	103.60	112.43
22	B	609	CLA	C3C-C4C-NC	3.20	114.16	110.57
25	N	609	CHL	CAA-C2A-C3A	-3.20	104.00	112.78
25	n	609	CHL	CAA-C2A-C3A	-3.20	104.00	112.78
25	3	307	CHL	O2A-CGA-CBA	3.20	124.32	114.03
25	7	307	CHL	O2A-CGA-CBA	3.20	124.32	114.03
22	B	606	CLA	C4D-CHA-C1A	-3.20	117.35	121.25
22	Y	604	CLA	CAC-C3C-C2C	-3.20	122.05	127.53
22	y	604	CLA	CAC-C3C-C2C	-3.20	122.05	127.53
22	R	310	CLA	CGD-CBD-CAD	-3.20	100.37	110.73
22	r	310	CLA	CGD-CBD-CAD	-3.20	100.37	110.73
25	2	606	CHL	O2A-CGA-CBA	3.20	124.30	114.03
25	6	606	CHL	O2A-CGA-CBA	3.20	124.30	114.03
22	1	614	CLA	CHC-C1C-C2C	-3.20	117.85	126.73
22	5	614	CLA	CHC-C1C-C2C	-3.20	117.85	126.73
22	c	501	CLA	CHC-C1C-C2C	-3.20	117.85	126.73
22	C	502	CLA	CHD-C4C-NC	3.20	129.24	124.20
22	C	504	CLA	CHC-C1C-C2C	-3.20	117.86	126.73
22	d	403	CLA	CGD-CBD-CAD	-3.20	100.39	110.73
22	B	609	CLA	CMB-C2B-C1B	3.19	130.24	125.37
22	1	602	CLA	CBC-CAC-C3C	-3.19	103.62	112.43
22	4	301	CLA	CBC-CAC-C3C	-3.19	103.62	112.43
22	5	602	CLA	CBC-CAC-C3C	-3.19	103.62	112.43
22	8	301	CLA	CBC-CAC-C3C	-3.19	103.62	112.43
22	B	603	CLA	C3B-C2B-C1B	-3.19	103.31	107.16
22	c	502	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
22	B	605	CLA	CHC-C1C-C2C	-3.19	117.88	126.73
22	b	603	CLA	C2D-C1D-ND	3.19	112.45	110.10
22	3	305	CLA	CBC-CAC-C3C	-3.19	103.65	112.43
22	7	305	CLA	CBC-CAC-C3C	-3.19	103.65	112.43
22	A	403	CLA	C3C-C4C-NC	3.19	114.14	110.57
22	C	505	CLA	CMD-C2D-C3D	3.19	134.94	127.61
22	1	604	CLA	CMD-C2D-C3D	3.18	134.94	127.61
22	5	604	CLA	CMD-C2D-C3D	3.18	134.94	127.61
22	B	607	CLA	CBC-CAC-C3C	-3.18	103.65	112.43
22	b	603	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
25	1	615	CHL	CAA-C2A-C3A	-3.18	104.06	112.78
25	5	615	CHL	CAA-C2A-C3A	-3.18	104.06	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	611	CLA	CMD-C2D-C3D	3.18	134.93	127.61
25	Y	607	CHL	O2D-CGD-CBD	3.18	116.92	111.27
25	y	607	CHL	O2D-CGD-CBD	3.18	116.92	111.27
22	b	609	CLA	C3C-C4C-NC	3.18	114.14	110.57
22	2	613	CLA	CBC-CAC-C3C	-3.18	103.67	112.43
22	6	613	CLA	CBC-CAC-C3C	-3.18	103.67	112.43
22	D	403	CLA	CHC-C1C-C2C	-3.18	117.90	126.73
25	Y	605	CHL	C2B-C1B-NB	-3.18	108.10	110.23
25	y	605	CHL	C2B-C1B-NB	-3.18	108.10	110.23
25	N	608	CHL	CBA-CAA-C2A	3.18	123.24	113.86
25	n	608	CHL	CBA-CAA-C2A	3.18	123.24	113.86
22	G	604	CLA	CAA-CBA-CGA	3.18	120.94	112.51
22	g	604	CLA	CAA-CBA-CGA	3.18	120.94	112.51
22	a	402	CLA	C4A-NA-C1A	-3.17	105.28	106.71
25	G	605	CHL	O2D-CGD-CBD	3.17	116.91	111.27
25	g	605	CHL	O2D-CGD-CBD	3.17	116.91	111.27
22	D	401	CLA	OBD-CAD-C3D	-3.17	120.88	128.52
23	A	404	PHO	CMA-C3A-C4A	-3.17	107.43	114.38
22	R	308	CLA	CMD-C2D-C3D	3.17	134.91	127.61
22	r	308	CLA	CMD-C2D-C3D	3.17	134.91	127.61
25	Y	608	CHL	O2A-CGA-CBA	3.17	124.22	114.03
25	y	608	CHL	O2A-CGA-CBA	3.17	124.22	114.03
25	4	302	CHL	O2A-CGA-CBA	3.17	124.21	114.03
25	8	302	CHL	O2A-CGA-CBA	3.17	124.21	114.03
25	R	304	CHL	CAA-C2A-C3A	-3.17	104.10	112.78
25	r	304	CHL	CAA-C2A-C3A	-3.17	104.10	112.78
22	C	512	CLA	C4A-NA-C1A	-3.17	105.28	106.71
22	c	512	CLA	CHC-C1C-C2C	-3.17	117.94	126.73
22	A	405	CLA	CAC-C3C-C2C	-3.16	122.12	127.53
25	Y	609	CHL	CHC-C4B-NB	3.16	127.60	124.26
25	y	609	CHL	CHC-C4B-NB	3.16	127.60	124.26
22	A	403	CLA	CBC-CAC-C3C	-3.16	103.72	112.43
22	N	610	CLA	OBD-CAD-C3D	-3.16	120.91	128.52
22	n	610	CLA	OBD-CAD-C3D	-3.16	120.91	128.52
22	B	606	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
22	a	402	CLA	CBC-CAC-C3C	-3.16	103.73	112.43
22	4	301	CLA	C3C-C4C-NC	3.16	114.11	110.57
22	8	301	CLA	C3C-C4C-NC	3.16	114.11	110.57
22	a	402	CLA	C3C-C4C-NC	3.15	114.11	110.57
22	Y	604	CLA	C4A-NA-C1A	-3.15	105.29	106.71
22	y	604	CLA	C4A-NA-C1A	-3.15	105.29	106.71
22	Y	603	CLA	CAC-C3C-C2C	-3.15	122.15	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	y	603	CLA	CAC-C3C-C2C	-3.15	122.15	127.53
22	1	611	CLA	C3C-C4C-NC	3.14	114.09	110.57
22	5	611	CLA	C3C-C4C-NC	3.14	114.09	110.57
22	C	508	CLA	CMC-C2C-C3C	3.14	134.65	126.12
25	1	606	CHL	O2A-CGA-CBA	3.14	124.12	114.03
25	5	606	CHL	O2A-CGA-CBA	3.14	124.12	114.03
22	c	505	CLA	CHC-C1C-C2C	-3.14	118.00	126.73
22	4	310	CLA	C1D-ND-C4D	3.14	108.57	106.33
22	8	310	CLA	C1D-ND-C4D	3.14	108.57	106.33
22	4	310	CLA	CAC-C3C-C2C	-3.14	122.16	127.53
22	8	310	CLA	CAC-C3C-C2C	-3.14	122.16	127.53
22	C	501	CLA	CHC-C1C-C2C	-3.14	118.01	126.73
23	d	402	PHO	CMA-C3A-C4A	-3.14	107.50	114.38
22	a	403	CLA	CBC-CAC-C3C	-3.14	103.78	112.43
22	C	511	CLA	C2D-C1D-ND	3.14	112.42	110.10
22	d	404	CLA	CBC-CAC-C3C	-3.14	103.79	112.43
22	B	601	CLA	C1D-ND-C4D	3.13	108.56	106.33
22	N	604	CLA	CAC-C3C-C2C	-3.13	122.17	127.53
22	n	604	CLA	CAC-C3C-C2C	-3.13	122.17	127.53
22	D	403	CLA	CAA-C2A-C3A	-3.13	104.20	112.78
22	B	611	CLA	CAC-C3C-C2C	-3.13	122.17	127.53
22	N	602	CLA	CAC-C3C-C2C	-3.13	122.18	127.53
22	n	602	CLA	CAC-C3C-C2C	-3.13	122.18	127.53
22	C	504	CLA	CBC-CAC-C3C	-3.13	103.81	112.43
22	C	503	CLA	C3C-C4C-NC	3.13	114.08	110.57
22	2	610	CLA	C3C-C4C-NC	3.13	114.08	110.57
22	6	610	CLA	C3C-C4C-NC	3.13	114.08	110.57
22	2	604	CLA	CBC-CAC-C3C	-3.13	103.81	112.43
22	6	604	CLA	CBC-CAC-C3C	-3.13	103.81	112.43
22	4	305	CLA	CAC-C3C-C2C	-3.13	122.18	127.53
22	8	305	CLA	CAC-C3C-C2C	-3.13	122.18	127.53
22	B	615	CLA	CHC-C1C-C2C	-3.12	118.06	126.73
25	1	609	CHL	O2D-CGD-CBD	3.12	116.81	111.27
25	5	609	CHL	O2D-CGD-CBD	3.12	116.81	111.27
22	Y	611	CLA	C3C-C4C-NC	3.12	114.07	110.57
22	y	611	CLA	C3C-C4C-NC	3.12	114.07	110.57
22	b	611	CLA	CAC-C3C-C2C	-3.12	122.19	127.53
22	B	604	CLA	C3B-C4B-NB	3.12	113.41	110.52
25	S	308	CHL	CBA-CAA-C2A	3.12	123.07	113.86
25	s	308	CHL	CBA-CAA-C2A	3.12	123.07	113.86
22	B	611	CLA	CAA-C2A-C3A	-3.12	104.24	112.78
22	B	616	CLA	C1D-ND-C4D	3.12	108.55	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	402	CLA	O2D-CGD-CBD	3.12	116.81	111.27
22	D	403	CLA	CMD-C2D-C3D	3.12	134.78	127.61
22	b	613	CLA	CHC-C1C-C2C	-3.11	118.08	126.73
22	Y	610	CLA	C4D-CHA-C1A	-3.11	117.46	121.25
22	y	610	CLA	C4D-CHA-C1A	-3.11	117.46	121.25
22	S	303	CLA	CAC-C3C-C2C	-3.11	122.20	127.53
22	s	303	CLA	CAC-C3C-C2C	-3.11	122.20	127.53
22	S	312	CLA	CAC-C3C-C2C	-3.11	122.20	127.53
22	s	312	CLA	CAC-C3C-C2C	-3.11	122.20	127.53
22	b	611	CLA	C3C-C4C-NC	3.11	114.06	110.57
22	s	301	CLA	CBC-CAC-C3C	-3.11	103.85	112.43
25	1	608	CHL	O2A-CGA-CBA	3.11	124.03	114.03
25	5	608	CHL	O2A-CGA-CBA	3.11	124.03	114.03
22	S	301	CLA	CBC-CAC-C3C	-3.11	103.86	112.43
22	C	508	CLA	C3B-C2B-C1B	-3.11	103.41	107.16
22	3	314	CLA	CAC-C3C-C2C	-3.11	122.21	127.53
22	7	314	CLA	CAC-C3C-C2C	-3.11	122.21	127.53
22	C	510	CLA	CHC-C1C-C2C	-3.11	118.10	126.73
22	G	610	CLA	OBD-CAD-C3D	-3.11	121.05	128.52
22	g	610	CLA	OBD-CAD-C3D	-3.11	121.05	128.52
22	2	611	CLA	C3C-C4C-NC	3.10	114.05	110.57
22	6	611	CLA	C3C-C4C-NC	3.10	114.05	110.57
22	G	603	CLA	CHC-C1C-C2C	-3.10	118.11	126.73
22	g	603	CLA	CHC-C1C-C2C	-3.10	118.11	126.73
22	Y	603	CLA	CMD-C2D-C3D	3.10	134.75	127.61
22	y	603	CLA	CMD-C2D-C3D	3.10	134.75	127.61
23	D	402	PHO	CMA-C3A-C4A	-3.10	107.59	114.38
22	c	508	CLA	C3C-C4C-NC	3.10	114.05	110.57
22	A	402	CLA	CMD-C2D-C3D	3.10	134.74	127.61
22	S	314	CLA	C3C-C4C-NC	3.10	114.05	110.57
22	s	314	CLA	C3C-C4C-NC	3.10	114.05	110.57
25	R	306	CHL	O2A-CGA-CBA	3.10	123.98	114.03
25	r	306	CHL	O2A-CGA-CBA	3.10	123.98	114.03
25	1	608	CHL	CAA-C2A-C3A	-3.10	104.30	112.78
25	5	608	CHL	CAA-C2A-C3A	-3.10	104.30	112.78
22	1	612	CLA	CMD-C2D-C3D	3.10	134.74	127.61
22	5	612	CLA	CMD-C2D-C3D	3.10	134.74	127.61
22	2	602	CLA	CAC-C3C-C2C	-3.10	122.23	127.53
22	6	602	CLA	CAC-C3C-C2C	-3.10	122.23	127.53
22	3	303	CLA	CBC-CAC-C3C	-3.10	103.89	112.43
22	7	303	CLA	CBC-CAC-C3C	-3.10	103.89	112.43
22	b	613	CLA	CAC-C3C-C2C	-3.10	122.23	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	608	CHL	O2D-CGD-CBD	3.10	116.77	111.27
25	g	608	CHL	O2D-CGD-CBD	3.10	116.77	111.27
22	R	307	CLA	C3C-C4C-NC	3.10	114.04	110.57
22	r	307	CLA	C3C-C4C-NC	3.10	114.04	110.57
22	b	608	CLA	CAC-C3C-C2C	-3.10	122.23	127.53
22	Y	611	CLA	CAC-C3C-C2C	-3.10	122.23	127.53
22	y	611	CLA	CAC-C3C-C2C	-3.10	122.23	127.53
22	1	604	CLA	CAC-C3C-C2C	-3.09	122.24	127.53
22	5	604	CLA	CAC-C3C-C2C	-3.09	122.24	127.53
22	B	613	CLA	CAC-C3C-C2C	-3.09	122.24	127.53
22	R	309	CLA	CAC-C3C-C2C	-3.09	122.24	127.53
22	G	602	CLA	CAC-C3C-C2C	-3.09	122.24	127.53
22	r	309	CLA	CAC-C3C-C2C	-3.09	122.24	127.53
22	g	602	CLA	CAC-C3C-C2C	-3.09	122.24	127.53
22	1	611	CLA	CMD-C2D-C3D	3.09	134.73	127.61
22	5	611	CLA	CMD-C2D-C3D	3.09	134.73	127.61
25	1	601	CHL	C2B-C1B-NB	-3.09	108.16	110.23
25	5	601	CHL	C2B-C1B-NB	-3.09	108.16	110.23
22	C	511	CLA	CAC-C3C-C2C	-3.09	122.24	127.53
22	b	613	CLA	OBD-CAD-C3D	-3.09	121.08	128.52
22	N	611	CLA	CAC-C3C-C2C	-3.09	122.24	127.53
22	n	611	CLA	CAC-C3C-C2C	-3.09	122.24	127.53
22	1	614	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
22	5	614	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
22	G	610	CLA	C4D-CHA-C1A	-3.09	117.49	121.25
22	g	610	CLA	C4D-CHA-C1A	-3.09	117.49	121.25
25	4	309	CHL	O2A-CGA-CBA	3.09	123.96	114.03
25	8	309	CHL	O2A-CGA-CBA	3.09	123.96	114.03
23	a	404	PHO	CMA-C3A-C4A	-3.09	107.61	114.38
22	Y	602	CLA	C3C-C4C-NC	3.09	114.03	110.57
22	y	602	CLA	C3C-C4C-NC	3.09	114.03	110.57
22	2	602	CLA	CBC-CAC-C3C	-3.09	103.92	112.43
22	6	602	CLA	CBC-CAC-C3C	-3.09	103.92	112.43
22	1	610	CLA	C4D-CHA-C1A	-3.09	117.49	121.25
22	5	610	CLA	C4D-CHA-C1A	-3.09	117.49	121.25
22	S	304	CLA	C3B-C2B-C1B	-3.09	103.44	107.16
22	s	304	CLA	C3B-C2B-C1B	-3.09	103.44	107.16
22	C	503	CLA	CAC-C3C-C2C	-3.09	122.25	127.53
22	b	607	CLA	C3C-C4C-NC	3.08	114.03	110.57
22	N	603	CLA	CHC-C1C-C2C	-3.08	118.16	126.73
22	n	603	CLA	CHC-C1C-C2C	-3.08	118.16	126.73
25	R	304	CHL	O2A-CGA-CBA	3.08	123.94	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	304	CHL	O2A-CGA-CBA	3.08	123.94	114.03
22	d	403	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
25	4	307	CHL	CAA-C2A-C3A	-3.08	104.34	112.78
25	8	307	CHL	CAA-C2A-C3A	-3.08	104.34	112.78
25	Y	608	CHL	CHB-C1B-NB	3.08	127.52	124.26
25	y	608	CHL	CHB-C1B-NB	3.08	127.52	124.26
22	c	504	CLA	CAC-C3C-C2C	-3.08	122.26	127.53
22	G	613	CLA	C3C-C4C-NC	3.08	114.03	110.57
22	g	613	CLA	C3C-C4C-NC	3.08	114.03	110.57
22	D	404	CLA	C3C-C4C-NC	3.08	114.03	110.57
22	1	614	CLA	CED-O2D-CGD	3.08	122.90	115.94
22	5	614	CLA	CED-O2D-CGD	3.08	122.90	115.94
22	a	405	CLA	CAC-C3C-C2C	-3.08	122.26	127.53
22	N	613	CLA	CAC-C3C-C2C	-3.08	122.26	127.53
22	n	613	CLA	CAC-C3C-C2C	-3.08	122.26	127.53
22	b	611	CLA	CMD-C2D-C3D	3.08	134.69	127.61
22	N	604	CLA	CMD-C2D-C3D	3.08	134.69	127.61
22	n	604	CLA	CMD-C2D-C3D	3.08	134.69	127.61
22	S	301	CLA	CAC-C3C-C2C	-3.08	122.27	127.53
22	a	403	CLA	CMD-C2D-C3D	3.08	134.69	127.61
25	Y	607	CHL	CAA-C2A-C3A	-3.08	104.35	112.78
25	y	607	CHL	CAA-C2A-C3A	-3.08	104.35	112.78
22	S	309	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
22	s	309	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
22	B	606	CLA	C3C-C4C-NC	3.08	114.02	110.57
22	1	610	CLA	CBC-CAC-C3C	-3.07	103.95	112.43
22	5	610	CLA	CBC-CAC-C3C	-3.07	103.95	112.43
22	N	614	CLA	CAC-C3C-C2C	-3.07	122.27	127.53
22	n	614	CLA	CAC-C3C-C2C	-3.07	122.27	127.53
22	1	611	CLA	CAC-C3C-C2C	-3.07	122.27	127.53
22	5	611	CLA	CAC-C3C-C2C	-3.07	122.27	127.53
22	c	507	CLA	CGD-CBD-CAD	-3.07	100.78	110.73
25	1	615	CHL	O2A-CGA-CBA	3.07	123.90	114.03
25	5	615	CHL	O2A-CGA-CBA	3.07	123.90	114.03
22	b	611	CLA	CHC-C1C-C2C	-3.07	118.20	126.73
22	1	602	CLA	CAC-C3C-C2C	-3.07	122.28	127.53
22	5	602	CLA	CAC-C3C-C2C	-3.07	122.28	127.53
22	b	604	CLA	CAC-C3C-C4C	3.07	128.79	124.81
22	4	304	CLA	C3C-C4C-NC	3.07	114.01	110.57
22	8	304	CLA	C3C-C4C-NC	3.07	114.01	110.57
22	R	308	CLA	CMC-C2C-C1C	3.07	129.71	125.04
22	r	308	CLA	CMC-C2C-C1C	3.07	129.71	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	509	CLA	C3C-C4C-NC	3.07	114.01	110.57
25	S	307	CHL	O2A-CGA-CBA	3.07	123.89	114.03
25	s	307	CHL	O2A-CGA-CBA	3.07	123.89	114.03
22	b	602	CLA	C4A-NA-C1A	-3.07	105.33	106.71
25	2	608	CHL	C2A-C1A-CHA	3.07	129.22	123.86
25	6	608	CHL	C2A-C1A-CHA	3.07	129.22	123.86
22	3	311	CLA	CAC-C3C-C2C	-3.07	122.28	127.53
22	7	311	CLA	CAC-C3C-C2C	-3.07	122.28	127.53
22	Y	604	CLA	CAA-C2A-C3A	-3.07	104.38	112.78
22	y	604	CLA	CAA-C2A-C3A	-3.07	104.38	112.78
22	G	611	CLA	CAC-C3C-C2C	-3.06	122.29	127.53
22	g	611	CLA	CAC-C3C-C2C	-3.06	122.29	127.53
22	b	614	CLA	C3C-C4C-NC	3.06	114.01	110.57
25	1	601	CHL	O2A-CGA-CBA	3.06	123.87	114.03
25	5	601	CHL	O2A-CGA-CBA	3.06	123.87	114.03
22	N	613	CLA	C3C-C4C-NC	3.06	114.00	110.57
22	n	613	CLA	C3C-C4C-NC	3.06	114.00	110.57
22	B	612	CLA	CHC-C1C-C2C	-3.06	118.23	126.73
22	c	505	CLA	CBC-CAC-C3C	-3.06	104.00	112.43
22	Y	610	CLA	CAC-C3C-C2C	-3.06	122.30	127.53
22	y	610	CLA	CAC-C3C-C2C	-3.06	122.30	127.53
22	1	613	CLA	CAC-C3C-C2C	-3.06	122.30	127.53
22	5	613	CLA	CAC-C3C-C2C	-3.06	122.30	127.53
22	B	612	CLA	CBC-CAC-C3C	-3.06	104.00	112.43
22	B	601	CLA	CMD-C2D-C3D	3.06	134.65	127.61
22	B	603	CLA	C3C-C4C-NC	3.06	114.00	110.57
22	4	303	CLA	CAC-C3C-C2C	-3.06	122.30	127.53
22	8	303	CLA	CAC-C3C-C2C	-3.06	122.30	127.53
22	A	402	CLA	CBC-CAC-C3C	-3.06	104.00	112.43
22	3	311	CLA	C3C-C4C-NC	3.06	114.00	110.57
22	7	311	CLA	C3C-C4C-NC	3.06	114.00	110.57
22	G	602	CLA	C3C-C4C-NC	3.05	114.00	110.57
22	g	602	CLA	C3C-C4C-NC	3.05	114.00	110.57
22	C	510	CLA	CAC-C3C-C2C	-3.05	122.30	127.53
22	b	609	CLA	CHC-C1C-C2C	-3.05	118.25	126.73
22	b	603	CLA	CBC-CAC-C3C	-3.05	104.02	112.43
22	N	613	CLA	CMD-C2D-C3D	3.05	134.63	127.61
22	n	613	CLA	CMD-C2D-C3D	3.05	134.63	127.61
22	Y	613	CLA	CMD-C2D-C3D	3.05	134.63	127.61
22	y	613	CLA	CMD-C2D-C3D	3.05	134.63	127.61
25	Y	601	CHL	C2B-C1B-NB	-3.05	108.19	110.23
25	y	601	CHL	C2B-C1B-NB	-3.05	108.19	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	610	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
22	n	610	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
22	C	508	CLA	C3C-C4C-NC	3.05	113.99	110.57
22	C	502	CLA	CMD-C2D-C3D	3.05	134.62	127.61
22	4	311	CLA	C3C-C4C-NC	3.04	113.98	110.57
22	8	311	CLA	C3C-C4C-NC	3.04	113.98	110.57
25	3	308	CHL	O2A-CGA-CBA	3.04	123.80	114.03
25	7	308	CHL	O2A-CGA-CBA	3.04	123.80	114.03
22	Y	612	CLA	CAC-C3C-C2C	-3.04	122.33	127.53
22	y	612	CLA	CAC-C3C-C2C	-3.04	122.33	127.53
22	S	311	CLA	CMD-C2D-C3D	3.04	134.61	127.61
22	s	311	CLA	CMD-C2D-C3D	3.04	134.61	127.61
22	G	604	CLA	CMD-C2D-C3D	3.04	134.61	127.61
22	g	604	CLA	CMD-C2D-C3D	3.04	134.61	127.61
22	b	606	CLA	CHD-C4C-C3C	-3.04	120.37	124.84
22	S	303	CLA	CED-O2D-CGD	3.04	122.81	115.94
22	s	303	CLA	CED-O2D-CGD	3.04	122.81	115.94
22	4	304	CLA	CAC-C3C-C2C	-3.04	122.33	127.53
22	8	304	CLA	CAC-C3C-C2C	-3.04	122.33	127.53
23	A	404	PHO	O2D-CGD-CBD	3.04	114.85	111.00
22	3	313	CLA	CAC-C3C-C2C	-3.04	122.33	127.53
22	7	313	CLA	CAC-C3C-C2C	-3.04	122.33	127.53
22	b	612	CLA	CMD-C2D-C3D	3.04	134.60	127.61
22	c	508	CLA	C4A-NA-C1A	-3.04	105.34	106.71
22	B	608	CLA	CAC-C3C-C2C	-3.04	122.34	127.53
25	2	601	CHL	O2A-CGA-CBA	3.03	123.78	114.03
25	6	601	CHL	O2A-CGA-CBA	3.03	123.78	114.03
22	Y	613	CLA	CHC-C1C-C2C	-3.03	118.30	126.73
22	y	613	CLA	CHC-C1C-C2C	-3.03	118.30	126.73
25	N	608	CHL	O2D-CGD-CBD	3.03	116.66	111.27
25	n	608	CHL	O2D-CGD-CBD	3.03	116.66	111.27
22	c	504	CLA	CHC-C1C-C2C	-3.03	118.31	126.73
22	b	602	CLA	CMD-C2D-C3D	3.03	134.59	127.61
22	2	609	CLA	CAC-C3C-C2C	-3.03	122.35	127.53
22	6	609	CLA	CAC-C3C-C2C	-3.03	122.35	127.53
22	3	310	CLA	CAC-C3C-C2C	-3.03	122.35	127.53
22	7	310	CLA	CAC-C3C-C2C	-3.03	122.35	127.53
22	B	601	CLA	C3C-C4C-NC	3.03	113.97	110.57
25	1	607	CHL	O2A-CGA-CBA	3.03	123.76	114.03
25	5	607	CHL	O2A-CGA-CBA	3.03	123.76	114.03
22	S	304	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
22	s	304	CLA	CHC-C1C-C2C	-3.03	118.32	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	609	CLA	CHD-C4C-NC	3.03	128.97	124.20
22	6	609	CLA	CHD-C4C-NC	3.03	128.97	124.20
22	D	404	CLA	CAC-C3C-C2C	-3.03	122.35	127.53
22	S	304	CLA	CHD-C4C-NC	3.03	128.97	124.20
22	s	304	CLA	CHD-C4C-NC	3.03	128.97	124.20
25	G	601	CHL	O2A-CGA-CBA	3.02	123.75	114.03
25	g	601	CHL	O2A-CGA-CBA	3.02	123.75	114.03
25	N	608	CHL	CAA-C2A-C3A	-3.02	104.50	112.78
25	n	608	CHL	CAA-C2A-C3A	-3.02	104.50	112.78
25	1	615	CHL	O2D-CGD-CBD	3.02	116.64	111.27
25	5	615	CHL	O2D-CGD-CBD	3.02	116.64	111.27
22	G	613	CLA	CHC-C1C-C2C	-3.02	118.34	126.73
22	g	613	CLA	CHC-C1C-C2C	-3.02	118.34	126.73
22	N	610	CLA	CMD-C2D-C3D	3.02	134.56	127.61
22	n	610	CLA	CMD-C2D-C3D	3.02	134.56	127.61
22	S	305	CLA	CGD-CBD-CAD	-3.02	100.95	110.73
22	s	305	CLA	CGD-CBD-CAD	-3.02	100.95	110.73
22	Y	614	CLA	CHC-C1C-C2C	-3.02	118.34	126.73
22	y	614	CLA	CHC-C1C-C2C	-3.02	118.34	126.73
25	G	609	CHL	C2A-C1A-CHA	3.02	129.14	123.86
25	g	609	CHL	C2A-C1A-CHA	3.02	129.14	123.86
22	d	401	CLA	CMD-C2D-C3D	3.02	134.56	127.61
22	c	511	CLA	CAC-C3C-C2C	-3.02	122.36	127.53
25	R	305	CHL	O2A-CGA-CBA	3.02	123.73	114.03
25	r	305	CHL	O2A-CGA-CBA	3.02	123.73	114.03
22	c	510	CLA	CHC-C1C-C2C	-3.02	118.35	126.73
22	B	606	CLA	CBC-CAC-C3C	-3.02	104.11	112.43
22	N	613	CLA	OBD-CAD-C3D	-3.01	121.27	128.52
22	n	613	CLA	OBD-CAD-C3D	-3.01	121.27	128.52
22	b	604	CLA	CMB-C2B-C1B	3.01	129.96	125.37
22	B	614	CLA	CBC-CAC-C3C	-3.01	104.13	112.43
25	G	607	CHL	O2A-CGA-CBA	3.01	123.70	114.03
25	g	607	CHL	O2A-CGA-CBA	3.01	123.70	114.03
22	b	605	CLA	CAC-C3C-C2C	-3.01	122.38	127.53
22	4	304	CLA	CMD-C2D-C3D	3.01	134.53	127.61
22	8	304	CLA	CMD-C2D-C3D	3.01	134.53	127.61
25	S	302	CHL	CAA-C2A-C3A	-3.01	104.54	112.78
25	s	302	CHL	CAA-C2A-C3A	-3.01	104.54	112.78
22	2	612	CLA	OBD-CAD-C3D	-3.01	121.28	128.52
22	6	612	CLA	OBD-CAD-C3D	-3.01	121.28	128.52
22	c	505	CLA	CMD-C2D-C3D	3.01	134.53	127.61
22	N	612	CLA	CHC-C1C-C2C	-3.01	118.38	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	n	612	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
22	c	504	CLA	C3C-C4C-NC	3.00	113.94	110.57
25	N	601	CHL	O2A-CGA-CBA	3.00	123.68	114.03
25	n	601	CHL	O2A-CGA-CBA	3.00	123.68	114.03
22	b	608	CLA	CMD-C2D-C3D	3.00	134.52	127.61
22	G	614	CLA	CAC-C3C-C2C	-3.00	122.39	127.53
22	g	614	CLA	CAC-C3C-C2C	-3.00	122.39	127.53
22	2	612	CLA	CAC-C3C-C2C	-3.00	122.39	127.53
22	6	612	CLA	CAC-C3C-C2C	-3.00	122.39	127.53
22	c	504	CLA	CBC-CAC-C3C	-3.00	104.16	112.43
22	b	605	CLA	CMD-C2D-C3D	3.00	134.52	127.61
22	4	305	CLA	C3C-C4C-NC	3.00	113.94	110.57
22	8	305	CLA	C3C-C4C-NC	3.00	113.94	110.57
22	C	512	CLA	C3C-C4C-NC	3.00	113.94	110.57
22	Y	604	CLA	CMC-C2C-C1C	3.00	129.61	125.04
22	y	604	CLA	CMC-C2C-C1C	3.00	129.61	125.04
25	4	306	CHL	O2A-CGA-CBA	3.00	123.67	114.03
25	8	306	CHL	O2A-CGA-CBA	3.00	123.67	114.03
22	c	509	CLA	CMD-C2D-C3D	3.00	134.51	127.61
22	3	303	CLA	CAC-C3C-C2C	-3.00	122.40	127.53
22	7	303	CLA	CAC-C3C-C2C	-3.00	122.40	127.53
23	D	402	PHO	CMB-C2B-C3B	3.00	130.29	124.68
25	2	607	CHL	CAA-C2A-C3A	-3.00	104.57	112.78
25	6	607	CHL	CAA-C2A-C3A	-3.00	104.57	112.78
25	4	308	CHL	O2A-CGA-CBA	2.99	123.65	114.03
25	8	308	CHL	O2A-CGA-CBA	2.99	123.65	114.03
25	Y	608	CHL	O2D-CGD-CBD	2.99	116.59	111.27
25	y	608	CHL	O2D-CGD-CBD	2.99	116.59	111.27
22	R	302	CLA	CHD-C4C-NC	2.99	128.92	124.20
22	r	302	CLA	CHD-C4C-NC	2.99	128.92	124.20
25	3	301	CHL	O2A-CGA-CBA	2.99	123.65	114.03
25	7	301	CHL	O2A-CGA-CBA	2.99	123.65	114.03
22	G	604	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
22	g	604	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
25	4	307	CHL	O2A-CGA-CBA	2.99	123.64	114.03
25	8	307	CHL	O2A-CGA-CBA	2.99	123.64	114.03
22	C	511	CLA	CBC-CAC-C3C	-2.99	104.20	112.43
22	N	613	CLA	CHC-C1C-C2C	-2.99	118.44	126.73
22	n	613	CLA	CHC-C1C-C2C	-2.99	118.44	126.73
22	G	610	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
22	g	610	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
22	R	307	CLA	CHC-C1C-C2C	-2.98	118.44	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r	307	CLA	CHC-C1C-C2C	-2.98	118.44	126.73
22	S	310	CLA	CAC-C3C-C2C	-2.98	122.43	127.53
22	s	310	CLA	CAC-C3C-C2C	-2.98	122.43	127.53
22	1	610	CLA	OBD-CAD-C3D	-2.98	121.34	128.52
22	5	610	CLA	OBD-CAD-C3D	-2.98	121.34	128.52
22	b	612	CLA	C3C-C4C-NC	2.98	113.92	110.57
22	N	611	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
22	n	611	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
22	G	610	CLA	CHD-C4C-NC	2.98	128.90	124.20
22	g	610	CLA	CHD-C4C-NC	2.98	128.90	124.20
22	2	612	CLA	CMD-C2D-C3D	2.98	134.47	127.61
22	6	612	CLA	CMD-C2D-C3D	2.98	134.47	127.61
22	B	612	CLA	CMA-C3A-C4A	-2.98	103.76	111.77
22	S	303	CLA	CMD-C2D-C3D	2.98	134.47	127.61
22	s	303	CLA	CMD-C2D-C3D	2.98	134.47	127.61
22	S	305	CLA	CAC-C3C-C2C	-2.98	122.43	127.53
22	s	305	CLA	CAC-C3C-C2C	-2.98	122.43	127.53
25	2	605	CHL	O2D-CGD-CBD	2.98	116.56	111.27
25	6	605	CHL	O2D-CGD-CBD	2.98	116.56	111.27
22	3	310	CLA	CHD-C4C-NC	2.98	128.90	124.20
22	7	310	CLA	CHD-C4C-NC	2.98	128.90	124.20
25	3	309	CHL	O2A-CGA-CBA	2.98	123.60	114.03
25	7	309	CHL	O2A-CGA-CBA	2.98	123.60	114.03
22	S	314	CLA	CHC-C1C-C2C	-2.98	118.46	126.73
22	s	314	CLA	CHC-C1C-C2C	-2.98	118.46	126.73
25	1	608	CHL	O2D-CGD-CBD	2.98	116.56	111.27
25	5	608	CHL	O2D-CGD-CBD	2.98	116.56	111.27
22	N	612	CLA	CHD-C4C-NC	2.98	128.89	124.20
22	n	612	CLA	CHD-C4C-NC	2.98	128.89	124.20
22	3	310	CLA	OBD-CAD-C3D	-2.97	121.36	128.52
22	7	310	CLA	OBD-CAD-C3D	-2.97	121.36	128.52
25	3	302	CHL	O2A-CGA-CBA	2.97	123.58	114.03
25	7	302	CHL	O2A-CGA-CBA	2.97	123.58	114.03
22	Y	611	CLA	CHD-C4C-NC	2.97	128.89	124.20
22	y	611	CLA	CHD-C4C-NC	2.97	128.89	124.20
22	Y	603	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
22	y	603	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
25	G	609	CHL	C3A-C2A-C1A	2.97	105.79	101.34
25	g	609	CHL	C3A-C2A-C1A	2.97	105.79	101.34
22	R	310	CLA	C3C-C4C-NC	2.97	113.90	110.57
22	r	310	CLA	C3C-C4C-NC	2.97	113.90	110.57
22	Y	612	CLA	CMD-C2D-C3D	2.97	134.44	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	y	612	CLA	CMD-C2D-C3D	2.97	134.44	127.61
22	1	610	CLA	CMD-C2D-C3D	2.97	134.44	127.61
22	5	610	CLA	CMD-C2D-C3D	2.97	134.44	127.61
22	S	301	CLA	CHC-C1C-C2C	-2.97	118.48	126.73
22	B	602	CLA	CMD-C2D-C3D	2.97	134.44	127.61
22	G	611	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
22	g	611	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
22	b	607	CLA	CBC-CAC-C3C	-2.97	104.25	112.43
22	C	509	CLA	CMD-C2D-C3D	2.97	134.44	127.61
22	b	613	CLA	CMD-C2D-C3D	2.97	134.44	127.61
22	b	607	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
22	S	311	CLA	C4A-NA-C1A	-2.96	105.37	106.71
22	s	311	CLA	C4A-NA-C1A	-2.96	105.37	106.71
25	3	309	CHL	C2A-C1A-CHA	2.96	129.04	123.86
25	7	309	CHL	C2A-C1A-CHA	2.96	129.04	123.86
22	R	308	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
22	r	308	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
25	R	305	CHL	CAA-CBA-CGA	2.96	120.37	112.51
25	r	305	CHL	CAA-CBA-CGA	2.96	120.37	112.51
22	b	610	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
22	B	615	CLA	CMD-C2D-C3D	2.96	134.43	127.61
22	b	601	CLA	CMD-C2D-C3D	2.96	134.43	127.61
22	b	601	CLA	CHD-C4C-NC	2.96	128.87	124.20
22	b	602	CLA	CHD-C4C-NC	2.96	128.87	124.20
22	b	616	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	B	603	CLA	CHC-C1C-C2C	-2.96	118.51	126.73
25	Y	607	CHL	O2A-CGA-CBA	2.96	123.54	114.03
25	y	607	CHL	O2A-CGA-CBA	2.96	123.54	114.03
22	B	609	CLA	CHC-C1C-C2C	-2.96	118.51	126.73
22	Y	614	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	y	614	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	c	506	CLA	C3B-C2B-C1B	-2.96	103.59	107.16
22	c	502	CLA	C3C-C4C-NC	2.96	113.89	110.57
22	S	314	CLA	CMD-C2D-C3D	2.96	134.42	127.61
22	s	314	CLA	CMD-C2D-C3D	2.96	134.42	127.61
25	2	607	CHL	O2D-CGD-CBD	2.96	116.52	111.27
25	6	607	CHL	O2D-CGD-CBD	2.96	116.52	111.27
22	d	401	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
22	N	602	CLA	C3C-C4C-NC	2.96	113.89	110.57
22	n	602	CLA	C3C-C4C-NC	2.96	113.89	110.57
25	Y	605	CHL	O2D-CGD-CBD	2.96	116.52	111.27
25	y	605	CHL	O2D-CGD-CBD	2.96	116.52	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	R	309	CLA	C3C-C4C-NC	2.95	113.88	110.57
22	r	309	CLA	C3C-C4C-NC	2.95	113.88	110.57
22	C	512	CLA	CBC-CAC-C3C	-2.95	104.30	112.43
22	B	609	CLA	OBD-CAD-C3D	-2.95	121.42	128.52
22	S	303	CLA	C3C-C4C-NC	2.95	113.88	110.57
22	s	303	CLA	C3C-C4C-NC	2.95	113.88	110.57
22	G	612	CLA	CAC-C3C-C2C	-2.95	122.48	127.53
22	g	612	CLA	CAC-C3C-C2C	-2.95	122.48	127.53
22	C	507	CLA	CHC-C1C-C2C	-2.95	118.54	126.73
22	Y	610	CLA	CMD-C2D-C3D	2.95	134.39	127.61
22	y	610	CLA	CMD-C2D-C3D	2.95	134.39	127.61
22	3	312	CLA	CMD-C2D-C3D	2.95	134.39	127.61
22	7	312	CLA	CMD-C2D-C3D	2.95	134.39	127.61
22	G	613	CLA	CMD-C2D-C3D	2.95	134.39	127.61
22	g	613	CLA	CMD-C2D-C3D	2.95	134.39	127.61
22	1	610	CLA	CAC-C3C-C2C	-2.94	122.50	127.53
22	5	610	CLA	CAC-C3C-C2C	-2.94	122.50	127.53
22	S	310	CLA	C3C-C4C-NC	2.94	113.87	110.57
22	s	310	CLA	C3C-C4C-NC	2.94	113.87	110.57
22	b	610	CLA	CGD-CBD-CAD	-2.94	101.21	110.73
22	2	611	CLA	CMD-C2D-C3D	2.94	134.38	127.61
22	6	611	CLA	CMD-C2D-C3D	2.94	134.38	127.61
22	B	601	CLA	CBC-CAC-C3C	-2.94	104.32	112.43
22	c	502	CLA	CMD-C2D-C3D	2.94	134.38	127.61
22	b	610	CLA	CMD-C2D-C3D	2.94	134.38	127.61
22	D	403	CLA	CMC-C2C-C1C	2.94	129.51	125.04
22	2	613	CLA	CAC-C3C-C2C	-2.94	122.50	127.53
22	6	613	CLA	CAC-C3C-C2C	-2.94	122.50	127.53
25	N	609	CHL	C2A-C1A-CHA	2.94	129.00	123.86
25	n	609	CHL	C2A-C1A-CHA	2.94	129.00	123.86
22	D	403	CLA	CGD-CBD-CAD	-2.94	101.22	110.73
22	G	612	CLA	CGD-CBD-CAD	-2.94	101.22	110.73
22	g	612	CLA	CGD-CBD-CAD	-2.94	101.22	110.73
22	B	613	CLA	C4A-NA-C1A	-2.94	105.39	106.71
22	G	610	CLA	CAC-C3C-C2C	-2.93	122.51	127.53
22	g	610	CLA	CAC-C3C-C2C	-2.93	122.51	127.53
22	S	310	CLA	CAA-C2A-C3A	-2.93	104.74	112.78
22	s	310	CLA	CAA-C2A-C3A	-2.93	104.74	112.78
22	G	604	CLA	C4A-NA-C1A	-2.93	105.39	106.71
22	g	604	CLA	C4A-NA-C1A	-2.93	105.39	106.71
22	B	616	CLA	C3C-C4C-NC	2.93	113.86	110.57
22	1	603	CLA	C3C-C4C-NC	2.93	113.86	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	603	CLA	C3C-C4C-NC	2.93	113.86	110.57
22	4	303	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
22	8	303	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
22	c	508	CLA	C3B-C2B-C1B	-2.93	103.62	107.16
22	B	615	CLA	CED-O2D-CGD	2.93	122.57	115.94
22	a	402	CLA	CMD-C2D-C3D	2.93	134.36	127.61
22	s	301	CLA	C3C-C4C-NC	2.93	113.86	110.57
22	2	604	CLA	C3C-C4C-NC	2.93	113.86	110.57
22	6	604	CLA	C3C-C4C-NC	2.93	113.86	110.57
22	4	305	CLA	CMD-C2D-C3D	2.93	134.36	127.61
22	8	305	CLA	CMD-C2D-C3D	2.93	134.36	127.61
22	b	615	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
22	4	301	CLA	CAC-C3C-C2C	-2.93	122.52	127.53
22	8	301	CLA	CAC-C3C-C2C	-2.93	122.52	127.53
25	N	607	CHL	O2A-CGA-CBA	2.93	123.43	114.03
25	n	607	CHL	O2A-CGA-CBA	2.93	123.43	114.03
22	B	613	CLA	CMA-C3A-C4A	-2.93	103.91	111.77
25	S	308	CHL	O2A-CGA-CBA	2.93	123.43	114.03
25	s	308	CHL	O2A-CGA-CBA	2.93	123.43	114.03
22	G	610	CLA	CMD-C2D-C3D	2.92	134.34	127.61
22	g	610	CLA	CMD-C2D-C3D	2.92	134.34	127.61
22	Y	603	CLA	CHD-C4C-NC	2.92	128.81	124.20
22	y	603	CLA	CHD-C4C-NC	2.92	128.81	124.20
22	3	313	CLA	CMD-C2D-C3D	2.92	134.34	127.61
22	7	313	CLA	CMD-C2D-C3D	2.92	134.34	127.61
22	B	609	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
22	C	508	CLA	OBD-CAD-C3D	-2.92	121.49	128.52
25	S	302	CHL	O2A-CGA-CBA	2.92	123.42	114.03
25	s	302	CHL	O2A-CGA-CBA	2.92	123.42	114.03
22	R	301	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	r	301	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	S	303	CLA	CHD-C4C-NC	2.92	128.81	124.20
22	s	303	CLA	CHD-C4C-NC	2.92	128.81	124.20
22	B	613	CLA	OBD-CAD-C3D	-2.92	121.49	128.52
22	c	503	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
22	C	508	CLA	C2D-C1D-ND	2.92	112.25	110.10
22	B	610	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
22	d	404	CLA	CAC-C3C-C2C	-2.92	122.54	127.53
22	1	613	CLA	C3C-C4C-NC	2.92	113.84	110.57
22	5	613	CLA	C3C-C4C-NC	2.92	113.84	110.57
25	3	301	CHL	O1D-CGD-CBD	-2.92	118.52	124.48
25	7	301	CHL	O1D-CGD-CBD	-2.92	118.52	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	403	CLA	C4A-NA-C1A	-2.92	105.39	106.71
22	G	602	CLA	CMD-C2D-C3D	2.92	134.32	127.61
22	g	602	CLA	CMD-C2D-C3D	2.92	134.32	127.61
22	C	506	CLA	C3B-C2B-C1B	-2.92	103.64	107.16
22	N	614	CLA	CHC-C1C-C2C	-2.91	118.64	126.73
22	n	614	CLA	CHC-C1C-C2C	-2.91	118.64	126.73
22	c	505	CLA	C3C-C4C-NC	2.91	113.84	110.57
22	c	510	CLA	CAC-C3C-C2C	-2.91	122.55	127.53
22	S	313	CLA	C4A-NA-C1A	-2.91	105.40	106.71
22	s	313	CLA	C4A-NA-C1A	-2.91	105.40	106.71
22	B	604	CLA	CMD-C2D-C3D	2.91	134.31	127.61
22	D	404	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
25	G	609	CHL	CAA-CBA-CGA	2.91	120.23	112.51
25	g	609	CHL	CAA-CBA-CGA	2.91	120.23	112.51
22	S	312	CLA	CGD-CBD-CAD	-2.91	101.31	110.73
22	s	312	CLA	CGD-CBD-CAD	-2.91	101.31	110.73
22	N	610	CLA	CAC-C3C-C2C	-2.91	122.56	127.53
22	n	610	CLA	CAC-C3C-C2C	-2.91	122.56	127.53
22	B	613	CLA	CMD-C2D-C3D	2.91	134.30	127.61
22	b	610	CLA	C4A-NA-C1A	-2.91	105.40	106.71
22	B	606	CLA	OBD-CAD-C3D	-2.91	121.52	128.52
22	Y	613	CLA	CAC-C3C-C2C	-2.91	122.56	127.53
22	y	613	CLA	CAC-C3C-C2C	-2.91	122.56	127.53
25	N	606	CHL	CHC-C4B-NB	2.91	127.33	124.26
25	n	606	CHL	CHC-C4B-NB	2.91	127.33	124.26
22	B	608	CLA	CGD-CBD-CAD	-2.91	101.32	110.73
22	b	614	CLA	C4A-NA-C1A	-2.90	105.40	106.71
22	Y	611	CLA	CHC-C1C-C2C	-2.90	118.66	126.73
22	y	611	CLA	CHC-C1C-C2C	-2.90	118.66	126.73
22	b	606	CLA	C1D-CHD-C4C	-2.90	119.79	126.06
25	3	301	CHL	CGD-CBD-CAD	-2.90	101.33	110.73
25	7	301	CHL	CGD-CBD-CAD	-2.90	101.33	110.73
22	1	612	CLA	C3C-C4C-NC	2.90	113.83	110.57
22	5	612	CLA	C3C-C4C-NC	2.90	113.83	110.57
22	S	313	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	s	313	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	3	304	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
22	7	304	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
22	N	612	CLA	CGD-CBD-CAD	-2.90	101.35	110.73
22	n	612	CLA	CGD-CBD-CAD	-2.90	101.35	110.73
22	d	401	CLA	CGD-CBD-CAD	-2.90	101.35	110.73
22	S	311	CLA	CHD-C4C-NC	2.89	128.76	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	s	311	CLA	CHD-C4C-NC	2.89	128.76	124.20
22	S	301	CLA	CMD-C2D-C3D	2.89	134.27	127.61
22	4	301	CLA	CMD-C2D-C3D	2.89	134.27	127.61
22	8	301	CLA	CMD-C2D-C3D	2.89	134.27	127.61
25	1	601	CHL	O2D-CGD-CBD	2.89	116.41	111.27
25	5	601	CHL	O2D-CGD-CBD	2.89	116.41	111.27
22	b	612	CLA	CBC-CAC-C3C	-2.89	104.46	112.43
22	N	612	CLA	CMD-C2D-C3D	2.89	134.26	127.61
22	n	612	CLA	CMD-C2D-C3D	2.89	134.26	127.61
22	c	505	CLA	C4D-CHA-C1A	-2.89	117.73	121.25
25	2	608	CHL	O2A-CGA-CBA	2.89	123.31	114.03
25	6	608	CHL	O2A-CGA-CBA	2.89	123.31	114.03
22	2	603	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
22	6	603	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
22	D	404	CLA	CMD-C2D-C3D	2.89	134.26	127.61
22	N	602	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
22	n	602	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
22	1	604	CLA	C3C-C4C-NC	2.89	113.81	110.57
22	5	604	CLA	C3C-C4C-NC	2.89	113.81	110.57
22	S	305	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
22	s	305	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
22	1	613	CLA	CMD-C2D-C3D	2.89	134.26	127.61
22	5	613	CLA	CMD-C2D-C3D	2.89	134.26	127.61
22	1	603	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
22	5	603	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
22	2	604	CLA	CAA-C2A-C3A	-2.88	104.88	112.78
22	6	604	CLA	CAA-C2A-C3A	-2.88	104.88	112.78
22	B	605	CLA	C3C-C4C-NC	2.88	113.81	110.57
25	R	306	CHL	CAA-C2A-C3A	-2.88	104.88	112.78
25	r	306	CHL	CAA-C2A-C3A	-2.88	104.88	112.78
22	B	609	CLA	C4A-NA-C1A	-2.88	105.41	106.71
22	S	305	CLA	C3C-C4C-NC	2.88	113.80	110.57
22	s	305	CLA	C3C-C4C-NC	2.88	113.80	110.57
22	R	309	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
22	r	309	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
22	R	303	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
22	r	303	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
22	G	611	CLA	C3C-C4C-NC	2.88	113.80	110.57
22	g	611	CLA	C3C-C4C-NC	2.88	113.80	110.57
24	e	101	HEM	C3D-C4D-ND	-2.88	106.96	110.17
22	A	402	CLA	CAC-C3C-C2C	-2.88	122.61	127.53
22	C	501	CLA	C3C-C4C-NC	2.88	113.80	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	616	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	2	610	CLA	CMD-C2D-C3D	2.88	134.23	127.61
22	6	610	CLA	CMD-C2D-C3D	2.88	134.23	127.61
22	b	604	CLA	CMA-C3A-C4A	-2.88	104.04	111.77
25	2	606	CHL	O2D-CGD-CBD	2.88	116.38	111.27
25	6	606	CHL	O2D-CGD-CBD	2.88	116.38	111.27
22	N	611	CLA	C3C-C4C-NC	2.87	113.80	110.57
22	n	611	CLA	C3C-C4C-NC	2.87	113.80	110.57
22	B	614	CLA	CAC-C3C-C2C	-2.87	122.61	127.53
22	4	311	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
22	8	311	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
22	c	511	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
22	b	616	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	a	405	CLA	CMD-C2D-C3D	2.87	134.22	127.61
22	2	613	CLA	C3C-C4C-NC	2.87	113.79	110.57
22	6	613	CLA	C3C-C4C-NC	2.87	113.79	110.57
22	3	305	CLA	CAA-C2A-C3A	-2.87	104.93	112.78
22	7	305	CLA	CAA-C2A-C3A	-2.87	104.93	112.78
25	R	305	CHL	O2D-CGD-CBD	2.87	116.36	111.27
25	r	305	CHL	O2D-CGD-CBD	2.87	116.36	111.27
22	A	405	CLA	CMD-C2D-C3D	2.87	134.21	127.61
22	2	610	CLA	CAC-C3C-C2C	-2.86	122.63	127.53
22	6	610	CLA	CAC-C3C-C2C	-2.86	122.63	127.53
22	Y	610	CLA	CBC-CAC-C3C	-2.86	104.53	112.43
22	y	610	CLA	CBC-CAC-C3C	-2.86	104.53	112.43
25	2	607	CHL	O2A-CGA-CBA	2.86	123.23	114.03
25	6	607	CHL	O2A-CGA-CBA	2.86	123.23	114.03
22	Y	610	CLA	CHD-C4C-NC	2.86	128.71	124.20
22	y	610	CLA	CHD-C4C-NC	2.86	128.71	124.20
22	S	313	CLA	C3C-C4C-NC	2.86	113.78	110.57
22	s	313	CLA	C3C-C4C-NC	2.86	113.78	110.57
22	G	611	CLA	CGD-CBD-CAD	-2.86	101.46	110.73
22	g	611	CLA	CGD-CBD-CAD	-2.86	101.46	110.73
22	1	612	CLA	CAC-C3C-C2C	-2.86	122.63	127.53
22	5	612	CLA	CAC-C3C-C2C	-2.86	122.63	127.53
22	4	305	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
22	8	305	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
22	Y	603	CLA	CGD-CBD-CAD	-2.86	101.47	110.73
22	y	603	CLA	CGD-CBD-CAD	-2.86	101.47	110.73
22	S	313	CLA	CHC-C1C-C2C	-2.86	118.79	126.73
22	s	313	CLA	CHC-C1C-C2C	-2.86	118.79	126.73
22	4	310	CLA	CHD-C4C-NC	2.86	128.71	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	310	CLA	CHD-C4C-NC	2.86	128.71	124.20
22	S	312	CLA	CMD-C2D-C3D	2.86	134.19	127.61
22	s	312	CLA	CMD-C2D-C3D	2.86	134.19	127.61
22	G	613	CLA	OBD-CAD-C3D	-2.86	121.64	128.52
22	g	613	CLA	OBD-CAD-C3D	-2.86	121.64	128.52
22	B	612	CLA	CAC-C3C-C2C	-2.86	122.64	127.53
22	G	612	CLA	CMD-C2D-C3D	2.86	134.19	127.61
22	g	612	CLA	CMD-C2D-C3D	2.86	134.19	127.61
22	b	603	CLA	CHC-C1C-C2C	-2.85	118.80	126.73
22	Y	610	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	y	610	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	2	609	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	6	609	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	C	506	CLA	OBD-CAD-C3D	-2.85	121.66	128.52
22	Y	603	CLA	OBD-CAD-C3D	-2.85	121.66	128.52
22	y	603	CLA	OBD-CAD-C3D	-2.85	121.66	128.52
22	3	305	CLA	CMD-C2D-C3D	2.85	134.17	127.61
22	7	305	CLA	CMD-C2D-C3D	2.85	134.17	127.61
22	D	404	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	B	611	CLA	C3C-C4C-NC	2.85	113.77	110.57
22	B	615	CLA	OBD-CAD-C3D	-2.85	121.67	128.52
22	C	508	CLA	CMD-C2D-C3D	2.85	134.16	127.61
22	c	512	CLA	CMD-C2D-C3D	2.84	134.16	127.61
22	R	303	CLA	CMD-C2D-C3D	2.84	134.16	127.61
22	r	303	CLA	CMD-C2D-C3D	2.84	134.16	127.61
22	b	615	CLA	CAC-C3C-C2C	-2.84	122.66	127.53
22	1	611	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
22	5	611	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
22	1	613	CLA	OBD-CAD-C3D	-2.84	121.68	128.52
22	5	613	CLA	OBD-CAD-C3D	-2.84	121.68	128.52
22	3	312	CLA	CAC-C3C-C2C	-2.84	122.67	127.53
22	7	312	CLA	CAC-C3C-C2C	-2.84	122.67	127.53
22	Y	604	CLA	OBD-CAD-C3D	-2.84	121.68	128.52
22	y	604	CLA	OBD-CAD-C3D	-2.84	121.68	128.52
25	1	609	CHL	O2A-CGA-CBA	2.84	123.16	114.03
25	5	609	CHL	O2A-CGA-CBA	2.84	123.16	114.03
22	a	405	CLA	OBD-CAD-C3D	-2.84	121.68	128.52
22	S	304	CLA	CMD-C2D-C3D	2.84	134.15	127.61
22	s	304	CLA	CMD-C2D-C3D	2.84	134.15	127.61
22	Y	612	CLA	CGD-CBD-CAD	-2.84	101.54	110.73
22	y	612	CLA	CGD-CBD-CAD	-2.84	101.54	110.73
22	G	612	CLA	CHC-C1C-C2C	-2.84	118.85	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	612	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
22	b	603	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	a	405	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
22	4	310	CLA	CMC-C2C-C1C	2.84	129.36	125.04
22	8	310	CLA	CMC-C2C-C1C	2.84	129.36	125.04
22	G	604	CLA	C3C-C4C-NC	2.84	113.75	110.57
22	g	604	CLA	C3C-C4C-NC	2.84	113.75	110.57
22	C	502	CLA	C3C-C4C-NC	2.84	113.75	110.57
22	B	610	CLA	CAC-C3C-C2C	-2.84	122.68	127.53
22	C	511	CLA	C3C-C4C-NC	2.84	113.75	110.57
22	b	609	CLA	CMA-C3A-C4A	-2.84	104.15	111.77
22	Y	602	CLA	CAC-C3C-C2C	-2.83	122.68	127.53
22	y	602	CLA	CAC-C3C-C2C	-2.83	122.68	127.53
22	3	304	CLA	CMD-C2D-C3D	2.83	134.13	127.61
22	7	304	CLA	CMD-C2D-C3D	2.83	134.13	127.61
25	R	304	CHL	CHC-C4B-NB	2.83	127.26	124.26
25	r	304	CHL	CHC-C4B-NB	2.83	127.26	124.26
22	c	512	CLA	OBD-CAD-C3D	-2.83	121.70	128.52
22	C	510	CLA	CMD-C2D-C3D	2.83	134.13	127.61
22	d	404	CLA	C3C-C4C-NC	2.83	113.75	110.57
22	N	610	CLA	CHD-C4C-NC	2.83	128.66	124.20
22	n	610	CLA	CHD-C4C-NC	2.83	128.66	124.20
22	R	308	CLA	CHD-C4C-NC	2.83	128.66	124.20
22	r	308	CLA	CHD-C4C-NC	2.83	128.66	124.20
22	D	401	CLA	CMC-C2C-C3C	2.83	133.80	126.12
25	3	306	CHL	C2B-C1B-NB	-2.83	108.34	110.23
25	7	306	CHL	C2B-C1B-NB	-2.83	108.34	110.23
22	b	608	CLA	C3C-C4C-NC	2.83	113.74	110.57
22	3	313	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
22	7	313	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
25	S	306	CHL	O2A-CGA-CBA	2.83	123.11	114.03
25	s	306	CHL	O2A-CGA-CBA	2.83	123.11	114.03
22	Y	603	CLA	CMB-C2B-C1B	2.83	129.67	125.37
22	y	603	CLA	CMB-C2B-C1B	2.83	129.67	125.37
22	S	309	CLA	OBD-CAD-C3D	-2.82	121.72	128.52
22	s	309	CLA	OBD-CAD-C3D	-2.82	121.72	128.52
22	3	305	CLA	CHC-C1C-C2C	-2.82	118.88	126.73
22	7	305	CLA	CHC-C1C-C2C	-2.82	118.88	126.73
25	4	309	CHL	O2D-CGD-CBD	2.82	116.29	111.27
25	8	309	CHL	O2D-CGD-CBD	2.82	116.29	111.27
22	a	402	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
22	R	308	CLA	CAC-C3C-C2C	-2.82	122.70	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r	308	CLA	CAC-C3C-C2C	-2.82	122.70	127.53
22	R	310	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
22	r	310	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
22	3	311	CLA	CMD-C2D-C3D	2.82	134.10	127.61
22	7	311	CLA	CMD-C2D-C3D	2.82	134.10	127.61
22	Y	602	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
22	y	602	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
22	b	608	CLA	CGD-CBD-CAD	-2.82	101.60	110.73
22	S	304	CLA	C3B-C4B-NB	2.82	113.13	110.52
22	s	304	CLA	C3B-C4B-NB	2.82	113.13	110.52
22	B	607	CLA	CMD-C2D-C3D	2.82	134.10	127.61
22	Y	603	CLA	C3C-C4C-NC	2.82	113.73	110.57
22	y	603	CLA	C3C-C4C-NC	2.82	113.73	110.57
22	C	512	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
22	c	508	CLA	OBD-CAD-C3D	-2.82	121.74	128.52
22	R	309	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	r	309	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	3	310	CLA	CMD-C2D-C3D	2.82	134.09	127.61
22	7	310	CLA	CMD-C2D-C3D	2.82	134.09	127.61
22	N	614	CLA	CMD-C2D-C3D	2.82	134.09	127.61
22	n	614	CLA	CMD-C2D-C3D	2.82	134.09	127.61
22	B	608	CLA	CMD-C2D-C3D	2.81	134.08	127.61
22	4	310	CLA	CBC-CAC-C3C	-2.81	104.68	112.43
22	8	310	CLA	CBC-CAC-C3C	-2.81	104.68	112.43
22	C	508	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	A	405	CLA	OBD-CAD-C3D	-2.81	121.75	128.52
22	2	610	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
22	6	610	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
22	A	402	CLA	CAA-C2A-C3A	-2.81	105.08	112.78
22	C	505	CLA	C3C-C4C-NC	2.81	113.72	110.57
22	G	614	CLA	C3C-C4C-NC	2.81	113.72	110.57
22	g	614	CLA	C3C-C4C-NC	2.81	113.72	110.57
22	1	613	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
22	5	613	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
22	b	611	CLA	OBD-CAD-C3D	-2.81	121.76	128.52
22	S	303	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
22	s	303	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
22	b	605	CLA	C3C-C4C-NC	2.81	113.72	110.57
22	2	603	CLA	C3C-C4C-NC	2.81	113.72	110.57
22	6	603	CLA	C3C-C4C-NC	2.81	113.72	110.57
22	2	611	CLA	CHD-C4C-NC	2.81	128.63	124.20
22	6	611	CLA	CHD-C4C-NC	2.81	128.63	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	d	404	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
22	S	311	CLA	CGD-CBD-CAD	-2.81	101.64	110.73
22	s	311	CLA	CGD-CBD-CAD	-2.81	101.64	110.73
25	3	301	CHL	C2B-C1B-NB	-2.81	108.35	110.23
25	7	301	CHL	C2B-C1B-NB	-2.81	108.35	110.23
25	N	609	CHL	O2A-CGA-CBA	2.81	123.04	114.03
25	n	609	CHL	O2A-CGA-CBA	2.81	123.04	114.03
22	C	511	CLA	C4A-NA-C1A	-2.80	105.44	106.71
22	G	610	CLA	CBC-CAC-C3C	-2.80	104.70	112.43
22	g	610	CLA	CBC-CAC-C3C	-2.80	104.70	112.43
22	a	403	CLA	CAA-C2A-C3A	-2.80	105.10	112.78
25	Y	609	CHL	O2A-CGA-CBA	2.80	123.04	114.03
25	y	609	CHL	O2A-CGA-CBA	2.80	123.04	114.03
22	C	502	CLA	C4D-CHA-C1A	-2.80	117.84	121.25
25	G	609	CHL	O2A-CGA-CBA	2.80	123.03	114.03
25	g	609	CHL	O2A-CGA-CBA	2.80	123.03	114.03
25	N	605	CHL	O2D-CGD-CBD	2.80	116.25	111.27
25	n	605	CHL	O2D-CGD-CBD	2.80	116.25	111.27
22	d	404	CLA	CMD-C2D-C3D	2.80	134.06	127.61
22	s	301	CLA	C4D-CHA-C1A	-2.80	117.84	121.25
22	G	610	CLA	CMC-C2C-C1C	2.80	129.30	125.04
22	g	610	CLA	CMC-C2C-C1C	2.80	129.30	125.04
22	d	404	CLA	CHC-C1C-C2C	-2.80	118.95	126.73
22	A	402	CLA	CHD-C4C-NC	2.80	128.61	124.20
22	B	602	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
22	A	403	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
22	C	509	CLA	CGD-CBD-CAD	-2.80	101.68	110.73
22	2	612	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
22	6	612	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
25	R	305	CHL	C2B-C1B-NB	-2.80	108.36	110.23
25	r	305	CHL	C2B-C1B-NB	-2.80	108.36	110.23
22	R	310	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
22	r	310	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
22	1	604	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
22	5	604	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
22	d	403	CLA	C4A-NA-C1A	-2.79	105.45	106.71
22	3	314	CLA	C4A-NA-C1A	-2.79	105.45	106.71
22	7	314	CLA	C4A-NA-C1A	-2.79	105.45	106.71
22	2	604	CLA	CMD-C2D-C3D	2.79	134.04	127.61
22	6	604	CLA	CMD-C2D-C3D	2.79	134.04	127.61
25	N	607	CHL	O1D-CGD-CBD	-2.79	118.77	124.48
25	n	607	CHL	O1D-CGD-CBD	-2.79	118.77	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	612	CLA	OBD-CAD-C3D	-2.79	121.80	128.52
25	N	607	CHL	CGD-CBD-CAD	-2.79	101.69	110.73
25	n	607	CHL	CGD-CBD-CAD	-2.79	101.69	110.73
22	3	305	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	7	305	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	R	301	CLA	CMD-C2D-C3D	2.79	134.03	127.61
22	r	301	CLA	CMD-C2D-C3D	2.79	134.03	127.61
22	4	310	CLA	CMD-C2D-C3D	2.79	134.03	127.61
22	8	310	CLA	CMD-C2D-C3D	2.79	134.03	127.61
22	G	613	CLA	CAC-C3C-C2C	-2.79	122.76	127.53
22	g	613	CLA	CAC-C3C-C2C	-2.79	122.76	127.53
22	C	504	CLA	CMB-C2B-C1B	2.79	129.62	125.37
22	c	512	CLA	CGD-CBD-CAD	-2.79	101.70	110.73
22	R	308	CLA	CMA-C3A-C2A	-2.79	102.58	113.83
22	r	308	CLA	CMA-C3A-C2A	-2.79	102.58	113.83
22	R	303	CLA	C3C-C4C-NC	2.79	113.70	110.57
22	r	303	CLA	C3C-C4C-NC	2.79	113.70	110.57
22	N	603	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
22	n	603	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
22	C	504	CLA	C3C-C4C-NC	2.79	113.69	110.57
22	B	603	CLA	C4D-CHA-C1A	-2.79	117.86	121.25
22	B	604	CLA	CHC-C4B-C3B	-2.78	115.32	127.71
22	A	402	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
22	B	609	CLA	CHA-C1A-NA	-2.78	120.02	126.40
22	1	610	CLA	CMC-C2C-C1C	2.78	129.28	125.04
22	5	610	CLA	CMC-C2C-C1C	2.78	129.28	125.04
22	4	305	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
22	8	305	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
22	4	304	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
22	8	304	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
22	4	305	CLA	CBA-CAA-C2A	2.78	122.07	113.86
22	8	305	CLA	CBA-CAA-C2A	2.78	122.07	113.86
22	B	616	CLA	CBC-CAC-C3C	-2.78	104.76	112.43
25	2	605	CHL	C2B-C1B-NB	-2.78	108.37	110.23
25	6	605	CHL	C2B-C1B-NB	-2.78	108.37	110.23
22	d	403	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
22	B	613	CLA	C3C-C4C-NC	2.78	113.69	110.57
22	Y	614	CLA	CHD-C4C-NC	2.78	128.58	124.20
22	y	614	CLA	CHD-C4C-NC	2.78	128.58	124.20
22	R	303	CLA	CAC-C3C-C2C	-2.78	122.78	127.53
22	r	303	CLA	CAC-C3C-C2C	-2.78	122.78	127.53
22	B	606	CLA	CHC-C1C-C2C	-2.78	119.01	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	611	CLA	CMD-C2D-C3D	2.78	134.00	127.61
22	n	611	CLA	CMD-C2D-C3D	2.78	134.00	127.61
22	b	606	CLA	OBD-CAD-C3D	-2.78	121.84	128.52
22	A	405	CLA	CHC-C1C-C2C	-2.77	119.02	126.73
22	3	311	CLA	CHC-C1C-C2C	-2.77	119.02	126.73
22	7	311	CLA	CHC-C1C-C2C	-2.77	119.02	126.73
25	G	606	CHL	O2D-CGD-CBD	2.77	116.20	111.27
25	g	606	CHL	O2D-CGD-CBD	2.77	116.20	111.27
22	N	604	CLA	C3C-C4C-NC	2.77	113.68	110.57
22	n	604	CLA	C3C-C4C-NC	2.77	113.68	110.57
22	4	303	CLA	CMA-C3A-C2A	-2.77	102.64	113.83
22	8	303	CLA	CMA-C3A-C2A	-2.77	102.64	113.83
22	c	502	CLA	CHD-C4C-NC	2.77	128.57	124.20
25	3	309	CHL	C3A-C2A-C1A	2.77	105.49	101.34
25	7	309	CHL	C3A-C2A-C1A	2.77	105.49	101.34
22	S	309	CLA	C3C-C4C-NC	2.77	113.68	110.57
22	s	309	CLA	C3C-C4C-NC	2.77	113.68	110.57
22	A	402	CLA	CGD-CBD-CAD	-2.77	101.77	110.73
22	c	508	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	N	603	CLA	CMB-C2B-C1B	2.77	129.58	125.37
22	n	603	CLA	CMB-C2B-C1B	2.77	129.58	125.37
22	c	511	CLA	C3C-C4C-NC	2.77	113.67	110.57
22	c	502	CLA	CAC-C3C-C2C	-2.77	122.80	127.53
22	b	616	CLA	CGD-CBD-CAD	-2.77	101.77	110.73
25	3	307	CHL	O2D-CGD-CBD	2.77	116.18	111.27
25	7	307	CHL	O2D-CGD-CBD	2.77	116.18	111.27
25	N	609	CHL	CHC-C4B-NB	2.76	127.18	124.26
25	n	609	CHL	CHC-C4B-NB	2.76	127.18	124.26
22	C	503	CLA	CGD-CBD-CAD	-2.76	101.78	110.73
22	3	305	CLA	C3C-C4C-NC	2.76	113.67	110.57
22	7	305	CLA	C3C-C4C-NC	2.76	113.67	110.57
22	b	607	CLA	CMD-C2D-C3D	2.76	133.97	127.61
22	2	604	CLA	CHC-C1C-C2C	-2.76	119.06	126.73
22	6	604	CLA	CHC-C1C-C2C	-2.76	119.06	126.73
22	R	301	CLA	CAC-C3C-C2C	-2.76	122.80	127.53
22	r	301	CLA	CAC-C3C-C2C	-2.76	122.80	127.53
22	3	303	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	7	303	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	G	603	CLA	CMD-C2D-C3D	2.76	133.96	127.61
22	g	603	CLA	CMD-C2D-C3D	2.76	133.96	127.61
22	1	602	CLA	CMD-C2D-C3D	2.76	133.96	127.61
22	5	602	CLA	CMD-C2D-C3D	2.76	133.96	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	403	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	S	302	CHL	CHB-C1B-NB	2.76	127.18	124.26
25	s	302	CHL	CHB-C1B-NB	2.76	127.18	124.26
22	1	612	CLA	C4A-NA-C1A	-2.76	105.47	106.71
22	5	612	CLA	C4A-NA-C1A	-2.76	105.47	106.71
22	B	611	CLA	CHC-C1C-C2C	-2.76	119.07	126.73
24	F	101	HEM	C4A-NA-C1A	2.76	108.05	105.35
22	G	602	CLA	CMC-C2C-C1C	2.76	129.24	125.04
22	g	602	CLA	CMC-C2C-C1C	2.76	129.24	125.04
22	C	512	CLA	CAC-C3C-C2C	-2.75	122.82	127.53
22	B	613	CLA	CHC-C1C-C2C	-2.75	119.08	126.73
22	S	304	CLA	C4A-NA-C1A	-2.75	105.47	106.71
22	s	304	CLA	C4A-NA-C1A	-2.75	105.47	106.71
22	G	611	CLA	CHD-C4C-NC	2.75	128.54	124.20
22	g	611	CLA	CHD-C4C-NC	2.75	128.54	124.20
22	N	603	CLA	OBD-CAD-C3D	-2.75	121.90	128.52
22	n	603	CLA	OBD-CAD-C3D	-2.75	121.90	128.52
22	B	608	CLA	OBD-CAD-C3D	-2.75	121.90	128.52
22	4	311	CLA	CMD-C2D-C3D	2.75	133.94	127.61
22	8	311	CLA	CMD-C2D-C3D	2.75	133.94	127.61
25	4	306	CHL	O2D-CGD-CBD	2.75	116.15	111.27
25	8	306	CHL	O2D-CGD-CBD	2.75	116.15	111.27
22	b	601	CLA	OBD-CAD-C3D	-2.75	121.91	128.52
22	1	612	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
22	5	612	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
22	Y	610	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
22	y	610	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
22	N	604	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
22	n	604	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
22	4	303	CLA	C4D-CHA-C1A	-2.75	117.91	121.25
22	8	303	CLA	C4D-CHA-C1A	-2.75	117.91	121.25
22	N	603	CLA	CHD-C4C-NC	2.75	128.53	124.20
22	n	603	CLA	CHD-C4C-NC	2.75	128.53	124.20
25	4	306	CHL	CHB-C1B-NB	2.75	127.16	124.26
25	8	306	CHL	CHB-C1B-NB	2.75	127.16	124.26
22	D	401	CLA	CAA-C2A-C3A	-2.74	105.26	112.78
25	2	608	CHL	CMB-C2B-C1B	-2.74	121.19	125.37
25	6	608	CHL	CMB-C2B-C1B	-2.74	121.19	125.37
22	b	606	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
22	C	501	CLA	CMC-C2C-C3C	2.74	133.56	126.12
22	N	612	CLA	CAC-C3C-C2C	-2.74	122.84	127.53
22	n	612	CLA	CAC-C3C-C2C	-2.74	122.84	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	614	CLA	CHC-C1C-C2C	-2.74	119.12	126.73
22	g	614	CLA	CHC-C1C-C2C	-2.74	119.12	126.73
22	Y	614	CLA	C3C-C4C-NC	2.74	113.64	110.57
22	y	614	CLA	C3C-C4C-NC	2.74	113.64	110.57
22	G	612	CLA	CHD-C4C-NC	2.74	128.52	124.20
22	g	612	CLA	CHD-C4C-NC	2.74	128.52	124.20
22	b	601	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	s	301	CLA	CMD-C2D-C3D	2.74	133.92	127.61
22	b	609	CLA	OBD-CAD-C3D	-2.74	121.93	128.52
22	B	614	CLA	CMD-C2D-C3D	2.74	133.91	127.61
22	G	611	CLA	OBD-CAD-C3D	-2.74	121.93	128.52
22	Y	610	CLA	OBD-CAD-C3D	-2.74	121.93	128.52
22	g	611	CLA	OBD-CAD-C3D	-2.74	121.93	128.52
22	y	610	CLA	OBD-CAD-C3D	-2.74	121.93	128.52
22	b	602	CLA	CBB-CAB-C3B	-2.74	114.01	127.62
22	S	309	CLA	CMC-C2C-C3C	2.74	133.54	126.12
22	s	309	CLA	CMC-C2C-C3C	2.74	133.54	126.12
24	e	101	HEM	C4C-NC-C1C	2.74	108.03	105.35
22	S	305	CLA	C4D-CHA-C1A	-2.74	117.92	121.25
22	s	305	CLA	C4D-CHA-C1A	-2.74	117.92	121.25
22	R	301	CLA	CHD-C4C-NC	2.73	128.51	124.20
22	r	301	CLA	CHD-C4C-NC	2.73	128.51	124.20
22	1	610	CLA	CHD-C4C-NC	2.73	128.51	124.20
22	5	610	CLA	CHD-C4C-NC	2.73	128.51	124.20
22	Y	614	CLA	CGD-CBD-CAD	-2.73	101.88	110.73
22	y	614	CLA	CGD-CBD-CAD	-2.73	101.88	110.73
25	G	607	CHL	CAA-C2A-C3A	-2.73	105.29	112.78
25	g	607	CHL	CAA-C2A-C3A	-2.73	105.29	112.78
22	c	511	CLA	OBD-CAD-C3D	-2.73	121.95	128.52
22	B	602	CLA	CGD-CBD-CAD	-2.73	101.89	110.73
22	G	602	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
22	g	602	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
22	D	403	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
24	e	101	HEM	CAC-C3C-C4C	2.73	131.49	124.90
22	2	602	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	6	602	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	4	301	CLA	CHC-C1C-C2C	-2.73	119.15	126.73
22	8	301	CLA	CHC-C1C-C2C	-2.73	119.15	126.73
25	N	609	CHL	C3A-C2A-C1A	2.73	105.42	101.34
25	n	609	CHL	C3A-C2A-C1A	2.73	105.42	101.34
23	a	404	PHO	CBC-CAC-C3C	-2.73	108.89	112.88
22	B	610	CLA	C4A-NA-C1A	-2.73	105.48	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	614	CLA	CHC-C1C-C2C	-2.73	119.16	126.73
24	F	101	HEM	C4D-ND-C1D	2.73	107.89	105.07
22	2	613	CLA	CMD-C2D-C3D	2.73	133.88	127.61
22	6	613	CLA	CMD-C2D-C3D	2.73	133.88	127.61
22	S	310	CLA	C4D-CHA-C1A	-2.73	117.93	121.25
22	s	310	CLA	C4D-CHA-C1A	-2.73	117.93	121.25
22	D	403	CLA	C3C-C4C-NC	2.72	113.63	110.57
22	R	302	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
22	r	302	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
22	b	608	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
22	b	616	CLA	CMD-C2D-C3D	2.72	133.88	127.61
22	c	501	CLA	CAC-C3C-C2C	-2.72	122.87	127.53
22	B	611	CLA	CHD-C4C-NC	2.72	128.49	124.20
22	3	314	CLA	CMD-C2D-C3D	2.72	133.87	127.61
22	7	314	CLA	CMD-C2D-C3D	2.72	133.87	127.61
22	R	309	CLA	CMD-C2D-C3D	2.72	133.87	127.61
22	r	309	CLA	CMD-C2D-C3D	2.72	133.87	127.61
22	2	613	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
22	6	613	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
25	2	608	CHL	CHB-C1B-NB	2.72	127.14	124.26
25	6	608	CHL	CHB-C1B-NB	2.72	127.14	124.26
25	4	307	CHL	O2D-CGD-CBD	2.72	116.10	111.27
25	8	307	CHL	O2D-CGD-CBD	2.72	116.10	111.27
22	R	310	CLA	OBD-CAD-C3D	-2.72	121.98	128.52
22	r	310	CLA	OBD-CAD-C3D	-2.72	121.98	128.52
22	N	602	CLA	CGD-CBD-CAD	-2.72	101.93	110.73
22	n	602	CLA	CGD-CBD-CAD	-2.72	101.93	110.73
22	S	311	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
22	s	311	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
22	N	611	CLA	CHD-C4C-NC	2.72	128.49	124.20
22	n	611	CLA	CHD-C4C-NC	2.72	128.49	124.20
22	S	305	CLA	OBD-CAD-C3D	-2.72	121.98	128.52
22	s	305	CLA	OBD-CAD-C3D	-2.72	121.98	128.52
22	3	312	CLA	CHC-C1C-C2C	-2.72	119.19	126.73
22	7	312	CLA	CHC-C1C-C2C	-2.72	119.19	126.73
22	C	512	CLA	OBD-CAD-C3D	-2.71	121.99	128.52
22	C	504	CLA	CMD-C2D-C3D	2.71	133.86	127.61
22	2	604	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
22	6	604	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
22	3	303	CLA	CMD-C2D-C3D	2.71	133.85	127.61
22	7	303	CLA	CMD-C2D-C3D	2.71	133.85	127.61
22	1	603	CLA	CGD-CBD-CAD	-2.71	101.95	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	603	CLA	CGD-CBD-CAD	-2.71	101.95	110.73
22	A	403	CLA	CHC-C1C-C2C	-2.71	119.20	126.73
25	3	309	CHL	CHC-C4B-NB	2.71	127.13	124.26
25	7	309	CHL	CHC-C4B-NB	2.71	127.13	124.26
22	b	616	CLA	CHB-C1B-C2B	-2.71	119.58	127.24
25	Y	607	CHL	O1D-CGD-CBD	-2.71	118.94	124.48
25	y	607	CHL	O1D-CGD-CBD	-2.71	118.94	124.48
22	B	607	CLA	OBD-CAD-C3D	-2.71	122.00	128.52
22	c	504	CLA	C4A-NA-C1A	-2.71	105.49	106.71
22	S	303	CLA	CGD-CBD-CAD	-2.71	101.96	110.73
22	s	303	CLA	CGD-CBD-CAD	-2.71	101.96	110.73
25	3	302	CHL	O2D-CGD-CBD	2.71	116.08	111.27
25	7	302	CHL	O2D-CGD-CBD	2.71	116.08	111.27
22	b	612	CLA	CAC-C3C-C2C	-2.71	122.90	127.53
22	2	603	CLA	OBD-CAD-C3D	-2.71	122.00	128.52
22	6	603	CLA	OBD-CAD-C3D	-2.71	122.00	128.52
22	G	612	CLA	C3C-C4C-NC	2.71	113.61	110.57
22	g	612	CLA	C3C-C4C-NC	2.71	113.61	110.57
22	N	611	CLA	CGD-CBD-CAD	-2.71	101.97	110.73
22	n	611	CLA	CGD-CBD-CAD	-2.71	101.97	110.73
22	G	602	CLA	CHD-C4C-NC	2.71	128.47	124.20
22	g	602	CLA	CHD-C4C-NC	2.71	128.47	124.20
22	c	505	CLA	OBD-CAD-C3D	-2.70	122.01	128.52
22	S	303	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
22	s	303	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
22	B	605	CLA	OBD-CAD-C3D	-2.70	122.01	128.52
22	R	302	CLA	OBD-CAD-C3D	-2.70	122.02	128.52
22	r	302	CLA	OBD-CAD-C3D	-2.70	122.02	128.52
22	Y	604	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
22	y	604	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
22	S	312	CLA	C4D-CHA-C1A	-2.70	117.96	121.25
22	s	312	CLA	C4D-CHA-C1A	-2.70	117.96	121.25
22	G	614	CLA	OBD-CAD-C3D	-2.70	122.02	128.52
22	g	614	CLA	OBD-CAD-C3D	-2.70	122.02	128.52
22	C	501	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
25	2	608	CHL	C2B-C1B-NB	-2.70	108.42	110.23
25	6	608	CHL	C2B-C1B-NB	-2.70	108.42	110.23
22	b	613	CLA	C4D-CHA-C1A	-2.70	117.96	121.25
22	c	504	CLA	CMD-C2D-C3D	2.70	133.82	127.61
25	Y	606	CHL	C2B-C1B-NB	-2.70	108.42	110.23
25	y	606	CHL	C2B-C1B-NB	-2.70	108.42	110.23
25	3	306	CHL	O2D-CGD-CBD	2.70	116.06	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	306	CHL	O2D-CGD-CBD	2.70	116.06	111.27
25	Y	609	CHL	C3A-C2A-C1A	2.70	105.38	101.34
25	y	609	CHL	C3A-C2A-C1A	2.70	105.38	101.34
22	B	601	CLA	OBD-CAD-C3D	-2.70	122.03	128.52
22	b	609	CLA	CMB-C2B-C1B	2.69	129.47	125.37
22	B	607	CLA	CAC-C3C-C2C	-2.69	122.92	127.53
22	D	401	CLA	CMD-C2D-C3D	2.69	133.81	127.61
22	S	310	CLA	CHC-C1C-C2C	-2.69	119.25	126.73
22	s	310	CLA	CHC-C1C-C2C	-2.69	119.25	126.73
22	B	615	CLA	CHD-C4C-NC	2.69	128.45	124.20
22	N	610	CLA	CMC-C2C-C1C	2.69	129.14	125.04
22	n	610	CLA	CMC-C2C-C1C	2.69	129.14	125.04
22	c	503	CLA	OBD-CAD-C3D	-2.69	122.04	128.52
22	Y	612	CLA	CMB-C2B-C1B	2.69	129.47	125.37
22	y	612	CLA	CMB-C2B-C1B	2.69	129.47	125.37
22	b	603	CLA	C4D-CHA-C1A	-2.69	117.97	121.25
22	S	314	CLA	OBD-CAD-C3D	-2.69	122.05	128.52
22	s	314	CLA	OBD-CAD-C3D	-2.69	122.05	128.52
22	C	503	CLA	CHC-C1C-C2C	-2.69	119.26	126.73
25	S	307	CHL	CAA-C2A-C3A	-2.69	105.41	112.78
25	s	307	CHL	CAA-C2A-C3A	-2.69	105.41	112.78
22	G	614	CLA	CMD-C2D-C3D	2.69	133.80	127.61
22	g	614	CLA	CMD-C2D-C3D	2.69	133.80	127.61
25	G	601	CHL	CHB-C1B-NB	2.69	127.10	124.26
25	g	601	CHL	CHB-C1B-NB	2.69	127.10	124.26
22	3	305	CLA	OBD-CAD-C3D	-2.69	122.05	128.52
22	7	305	CLA	OBD-CAD-C3D	-2.69	122.05	128.52
22	a	403	CLA	CHC-C1C-C2C	-2.69	119.26	126.73
22	R	310	CLA	CAC-C3C-C2C	-2.69	122.93	127.53
22	r	310	CLA	CAC-C3C-C2C	-2.69	122.93	127.53
22	B	605	CLA	CMD-C2D-C3D	2.69	133.79	127.61
22	B	603	CLA	OBD-CAD-C3D	-2.69	122.06	128.52
22	S	305	CLA	CMD-C2D-C3D	2.69	133.79	127.61
22	s	305	CLA	CMD-C2D-C3D	2.69	133.79	127.61
22	N	604	CLA	CAA-CBA-CGA	2.68	119.63	112.51
22	n	604	CLA	CAA-CBA-CGA	2.68	119.63	112.51
22	G	611	CLA	CMD-C2D-C3D	2.68	133.79	127.61
22	g	611	CLA	CMD-C2D-C3D	2.68	133.79	127.61
22	S	301	CLA	OBD-CAD-C3D	-2.68	122.06	128.52
22	b	609	CLA	CMD-C2D-C3D	2.68	133.78	127.61
22	R	303	CLA	CBA-CAA-C2A	2.68	121.78	113.86
22	r	303	CLA	CBA-CAA-C2A	2.68	121.78	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Y	613	CLA	OBD-CAD-C3D	-2.68	122.07	128.52
22	y	613	CLA	OBD-CAD-C3D	-2.68	122.07	128.52
22	b	612	CLA	OBD-CAD-C3D	-2.68	122.08	128.52
22	S	310	CLA	CHD-C4C-NC	2.68	128.42	124.20
22	s	310	CLA	CHD-C4C-NC	2.68	128.42	124.20
22	2	603	CLA	CMD-C2D-C3D	2.68	133.77	127.61
22	6	603	CLA	CMD-C2D-C3D	2.68	133.77	127.61
22	a	402	CLA	CAC-C3C-C2C	-2.68	122.95	127.53
22	2	602	CLA	CHC-C1C-C2C	-2.68	119.30	126.73
22	6	602	CLA	CHC-C1C-C2C	-2.68	119.30	126.73
22	C	504	CLA	C4D-CHA-C1A	-2.67	117.99	121.25
22	B	603	CLA	CMB-C2B-C3B	2.67	133.06	126.59
22	N	611	CLA	OBD-CAD-C3D	-2.67	122.09	128.52
22	n	611	CLA	OBD-CAD-C3D	-2.67	122.09	128.52
22	1	611	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
22	5	611	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
22	G	614	CLA	CHD-C4C-NC	2.67	128.41	124.20
22	g	614	CLA	CHD-C4C-NC	2.67	128.41	124.20
22	b	612	CLA	CMA-C3A-C2A	-2.67	103.08	113.83
25	G	605	CHL	C2B-C1B-NB	-2.67	108.44	110.23
25	g	605	CHL	C2B-C1B-NB	-2.67	108.44	110.23
22	1	602	CLA	CHC-C1C-C2C	-2.67	119.33	126.73
22	5	602	CLA	CHC-C1C-C2C	-2.67	119.33	126.73
22	Y	604	CLA	CHD-C4C-NC	2.67	128.40	124.20
22	y	604	CLA	CHD-C4C-NC	2.67	128.40	124.20
22	Y	611	CLA	OBD-CAD-C3D	-2.66	122.11	128.52
22	y	611	CLA	OBD-CAD-C3D	-2.66	122.11	128.52
22	b	607	CLA	CED-O2D-CGD	2.66	121.96	115.94
22	c	510	CLA	CMD-C2D-C3D	2.66	133.74	127.61
22	B	607	CLA	CMC-C2C-C3C	2.66	133.34	126.12
25	Y	609	CHL	C2A-C1A-CHA	2.66	128.51	123.86
25	y	609	CHL	C2A-C1A-CHA	2.66	128.51	123.86
22	b	616	CLA	OBD-CAD-C3D	-2.66	122.11	128.52
22	2	610	CLA	OBD-CAD-C3D	-2.66	122.11	128.52
22	6	610	CLA	OBD-CAD-C3D	-2.66	122.11	128.52
22	B	607	CLA	CBB-CAB-C3B	-2.66	114.38	127.62
22	B	604	CLA	C4B-CHC-C1C	-2.66	120.03	126.34
22	4	310	CLA	C4D-CHA-C1A	-2.66	118.01	121.25
22	8	310	CLA	C4D-CHA-C1A	-2.66	118.01	121.25
22	b	612	CLA	C4A-NA-C1A	-2.66	105.51	106.71
22	Y	614	CLA	OBD-CAD-C3D	-2.66	122.12	128.52
22	y	614	CLA	OBD-CAD-C3D	-2.66	122.12	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	506	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	4	303	CLA	CAA-C2A-C1A	2.66	120.69	111.97
22	8	303	CLA	CAA-C2A-C1A	2.66	120.69	111.97
25	Y	601	CHL	O2D-CGD-CBD	2.66	115.99	111.27
25	y	601	CHL	O2D-CGD-CBD	2.66	115.99	111.27
22	3	313	CLA	OBD-CAD-C3D	-2.66	122.12	128.52
22	7	313	CLA	OBD-CAD-C3D	-2.66	122.12	128.52
22	b	603	CLA	C3C-C4C-NC	2.66	113.55	110.57
22	1	611	CLA	OBD-CAD-C3D	-2.66	122.13	128.52
22	5	611	CLA	OBD-CAD-C3D	-2.66	122.13	128.52
22	R	310	CLA	CMD-C2D-C3D	2.66	133.72	127.61
22	r	310	CLA	CMD-C2D-C3D	2.66	133.72	127.61
23	D	402	PHO	C4B-NB-C1B	-2.66	104.72	108.83
22	b	611	CLA	C3B-C4B-NB	2.65	112.98	110.52
22	N	604	CLA	CGD-CBD-CAD	-2.65	102.14	110.73
22	n	604	CLA	CGD-CBD-CAD	-2.65	102.14	110.73
23	D	402	PHO	O2D-CGD-O1D	-2.65	118.65	123.84
22	3	304	CLA	C4A-NA-C1A	-2.65	105.51	106.71
22	7	304	CLA	C4A-NA-C1A	-2.65	105.51	106.71
22	2	602	CLA	CMD-C2D-C3D	2.65	133.72	127.61
22	6	602	CLA	CMD-C2D-C3D	2.65	133.72	127.61
22	b	605	CLA	CHC-C1C-C2C	-2.65	119.36	126.73
22	G	603	CLA	CMB-C2B-C1B	2.65	129.41	125.37
22	g	603	CLA	CMB-C2B-C1B	2.65	129.41	125.37
22	1	603	CLA	OBD-CAD-C3D	-2.65	122.14	128.52
22	5	603	CLA	OBD-CAD-C3D	-2.65	122.14	128.52
22	3	304	CLA	C3C-C4C-NC	2.65	113.54	110.57
22	7	304	CLA	C3C-C4C-NC	2.65	113.54	110.57
22	C	509	CLA	CHC-C1C-C2C	-2.65	119.37	126.73
22	3	304	CLA	OBD-CAD-C3D	-2.65	122.15	128.52
22	7	304	CLA	OBD-CAD-C3D	-2.65	122.15	128.52
22	2	604	CLA	OBD-CAD-C3D	-2.65	122.15	128.52
22	6	604	CLA	OBD-CAD-C3D	-2.65	122.15	128.52
22	A	403	CLA	CAC-C3C-C2C	-2.65	123.00	127.53
22	Y	614	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
22	y	614	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
22	R	310	CLA	CHD-C4C-NC	2.65	128.37	124.20
22	r	310	CLA	CHD-C4C-NC	2.65	128.37	124.20
22	B	602	CLA	CBB-CAB-C3B	-2.65	114.45	127.62
22	G	614	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
22	g	614	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
22	c	508	CLA	CMC-C2C-C3C	2.64	133.30	126.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	601	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
22	B	601	CLA	C4D-CHA-C1A	-2.64	118.03	121.25
22	N	602	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
22	n	602	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
22	d	401	CLA	CAC-C3C-C2C	-2.64	123.01	127.53
25	2	601	CHL	O2D-CGD-CBD	2.64	115.96	111.27
25	6	601	CHL	O2D-CGD-CBD	2.64	115.96	111.27
22	3	303	CLA	CMB-C2B-C1B	2.64	129.39	125.37
22	7	303	CLA	CMB-C2B-C1B	2.64	129.39	125.37
22	S	304	CLA	CGD-CBD-CAD	-2.64	102.19	110.73
22	s	304	CLA	CGD-CBD-CAD	-2.64	102.19	110.73
22	b	613	CLA	CHC-C4B-C3B	-2.64	115.98	127.71
22	1	603	CLA	CMD-C2D-C3D	2.64	133.68	127.61
22	5	603	CLA	CMD-C2D-C3D	2.64	133.68	127.61
25	3	308	CHL	O2D-CGD-CBD	2.64	115.95	111.27
25	7	308	CHL	O2D-CGD-CBD	2.64	115.95	111.27
22	d	401	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
22	B	613	CLA	CED-O2D-CGD	2.64	121.90	115.94
22	R	301	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
22	r	301	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
22	B	611	CLA	OBD-CAD-C3D	-2.63	122.18	128.52
22	C	506	CLA	CMC-C2C-C3C	2.63	133.26	126.12
22	c	501	CLA	CMC-C2C-C3C	2.63	133.26	126.12
22	B	613	CLA	C4D-CHA-C1A	-2.63	118.05	121.25
22	B	608	CLA	C3B-C4B-NB	2.63	112.95	110.52
22	R	301	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
22	r	301	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
25	G	601	CHL	O2D-CGD-CBD	2.63	115.94	111.27
25	g	601	CHL	O2D-CGD-CBD	2.63	115.94	111.27
22	R	303	CLA	C4A-NA-C1A	-2.63	105.52	106.71
22	r	303	CLA	C4A-NA-C1A	-2.63	105.52	106.71
22	G	603	CLA	OBD-CAD-C3D	-2.63	122.19	128.52
22	g	603	CLA	OBD-CAD-C3D	-2.63	122.19	128.52
25	1	615	CHL	C2B-C1B-NB	-2.63	108.47	110.23
25	5	615	CHL	C2B-C1B-NB	-2.63	108.47	110.23
22	3	314	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
22	7	314	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
25	1	609	CHL	CHC-C4B-NB	2.63	127.04	124.26
25	5	609	CHL	CHC-C4B-NB	2.63	127.04	124.26
22	Y	612	CLA	CHD-C4C-NC	2.63	128.34	124.20
22	y	612	CLA	CHD-C4C-NC	2.63	128.34	124.20
22	c	506	CLA	C2B-C1B-NB	2.63	111.99	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Y	602	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	y	602	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	c	509	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	4	301	CLA	OBD-CAD-C3D	-2.62	122.21	128.52
22	8	301	CLA	OBD-CAD-C3D	-2.62	122.21	128.52
22	S	310	CLA	OBD-CAD-C3D	-2.62	122.21	128.52
22	s	310	CLA	OBD-CAD-C3D	-2.62	122.21	128.52
22	N	603	CLA	CGD-CBD-CAD	-2.62	102.24	110.73
22	n	603	CLA	CGD-CBD-CAD	-2.62	102.24	110.73
22	C	509	CLA	C4A-NA-C1A	-2.62	105.53	106.71
22	R	311	CLA	CMB-C2B-C1B	2.62	129.36	125.37
22	r	311	CLA	CMB-C2B-C1B	2.62	129.36	125.37
22	1	612	CLA	OBD-CAD-C3D	-2.62	122.22	128.52
22	5	612	CLA	OBD-CAD-C3D	-2.62	122.22	128.52
22	N	612	CLA	C3C-C4C-NC	2.62	113.51	110.57
22	n	612	CLA	C3C-C4C-NC	2.62	113.51	110.57
25	G	608	CHL	CAA-C2A-C3A	-2.62	105.61	112.78
25	g	608	CHL	CAA-C2A-C3A	-2.62	105.61	112.78
25	1	605	CHL	O2D-CGD-CBD	2.62	115.92	111.27
25	5	605	CHL	O2D-CGD-CBD	2.62	115.92	111.27
22	C	511	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	N	601	CHL	O2D-CGD-CBD	2.62	115.92	111.27
25	n	601	CHL	O2D-CGD-CBD	2.62	115.92	111.27
22	a	402	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
22	4	305	CLA	OBD-CAD-C3D	-2.62	122.23	128.52
22	8	305	CLA	OBD-CAD-C3D	-2.62	122.23	128.52
22	1	613	CLA	CMA-C3A-C4A	-2.62	104.74	111.77
22	5	613	CLA	CMA-C3A-C4A	-2.62	104.74	111.77
23	A	404	PHO	CMC-C2C-C3C	2.61	133.22	126.12
22	b	615	CLA	CGD-CBD-CAD	-2.61	102.26	110.73
22	1	604	CLA	C4D-CHA-C1A	-2.61	118.07	121.25
22	5	604	CLA	C4D-CHA-C1A	-2.61	118.07	121.25
22	1	614	CLA	C2D-C1D-ND	2.61	112.03	110.10
22	5	614	CLA	C2D-C1D-ND	2.61	112.03	110.10
25	Y	607	CHL	C2B-C1B-NB	-2.61	108.48	110.23
25	y	607	CHL	C2B-C1B-NB	-2.61	108.48	110.23
22	N	614	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	n	614	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	R	311	CLA	OBD-CAD-C3D	-2.61	122.24	128.52
22	r	311	CLA	OBD-CAD-C3D	-2.61	122.24	128.52
22	b	614	CLA	CMD-C2D-C3D	2.61	133.62	127.61
25	1	607	CHL	CAA-C2A-C3A	-2.61	105.63	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	607	CHL	CAA-C2A-C3A	-2.61	105.63	112.78
22	s	301	CLA	CHC-C1C-C2C	-2.61	119.48	126.73
22	C	501	CLA	CMD-C2D-C3D	2.61	133.62	127.61
22	1	602	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
22	5	602	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
22	B	614	CLA	CAA-C2A-C1A	2.61	120.52	111.97
22	N	610	CLA	CBC-CAC-C3C	-2.61	105.24	112.43
22	n	610	CLA	CBC-CAC-C3C	-2.61	105.24	112.43
25	4	306	CHL	CAA-CBA-CGA	2.61	119.42	112.51
25	8	306	CHL	CAA-CBA-CGA	2.61	119.42	112.51
25	4	306	CHL	CMB-C2B-C1B	-2.60	121.40	125.37
25	8	306	CHL	CMB-C2B-C1B	-2.60	121.40	125.37
22	c	501	CLA	CHC-C4B-C3B	-2.60	116.13	127.71
22	b	602	CLA	C4D-CHA-C1A	-2.60	118.08	121.25
22	2	611	CLA	OBD-CAD-C3D	-2.60	122.26	128.52
22	6	611	CLA	OBD-CAD-C3D	-2.60	122.26	128.52
22	N	614	CLA	OBD-CAD-C3D	-2.60	122.26	128.52
22	n	614	CLA	OBD-CAD-C3D	-2.60	122.26	128.52
22	3	314	CLA	OBD-CAD-C3D	-2.60	122.26	128.52
22	7	314	CLA	OBD-CAD-C3D	-2.60	122.26	128.52
22	4	305	CLA	CAA-CBA-CGA	2.60	119.41	112.51
22	8	305	CLA	CAA-CBA-CGA	2.60	119.41	112.51
22	B	608	CLA	CHC-C4B-C3B	-2.60	116.14	127.71
22	3	311	CLA	OBD-CAD-C3D	-2.60	122.26	128.52
22	7	311	CLA	OBD-CAD-C3D	-2.60	122.26	128.52
22	D	404	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
22	3	311	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
22	7	311	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
22	c	506	CLA	OBD-CAD-C3D	-2.60	122.27	128.52
22	G	603	CLA	CGD-CBD-CAD	-2.60	102.32	110.73
22	g	603	CLA	CGD-CBD-CAD	-2.60	102.32	110.73
22	b	601	CLA	CMC-C2C-C1C	2.60	129.00	125.04
25	Y	606	CHL	O2A-CGA-O1A	-2.60	116.83	123.30
25	y	606	CHL	O2A-CGA-O1A	-2.60	116.83	123.30
22	Y	613	CLA	C4A-NA-C1A	-2.60	105.54	106.71
22	y	613	CLA	C4A-NA-C1A	-2.60	105.54	106.71
25	1	606	CHL	CAA-C2A-C3A	-2.60	105.67	112.78
25	5	606	CHL	CAA-C2A-C3A	-2.60	105.67	112.78
22	b	606	CLA	CHC-C1C-C2C	-2.59	119.52	126.73
22	N	603	CLA	CMD-C2D-C3D	2.59	133.58	127.61
22	n	603	CLA	CMD-C2D-C3D	2.59	133.58	127.61
22	S	309	CLA	C4D-CHA-C1A	-2.59	118.09	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	s	309	CLA	C4D-CHA-C1A	-2.59	118.09	121.25
22	D	401	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
22	b	615	CLA	CHC-C1C-C2C	-2.59	119.53	126.73
22	R	311	CLA	CHC-C1C-C2C	-2.59	119.53	126.73
22	r	311	CLA	CHC-C1C-C2C	-2.59	119.53	126.73
22	b	607	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
25	3	309	CHL	C3B-C4B-NB	-2.59	108.11	110.52
25	7	309	CHL	C3B-C4B-NB	-2.59	108.11	110.52
25	Y	601	CHL	C1D-ND-C4D	-2.59	104.50	106.33
25	y	601	CHL	C1D-ND-C4D	-2.59	104.50	106.33
22	S	312	CLA	C4A-NA-C1A	-2.59	105.54	106.71
22	s	312	CLA	C4A-NA-C1A	-2.59	105.54	106.71
22	R	309	CLA	CHD-C4C-NC	2.59	128.28	124.20
22	r	309	CLA	CHD-C4C-NC	2.59	128.28	124.20
25	3	309	CHL	CAA-CBA-CGA	2.59	119.38	112.51
25	7	309	CHL	CAA-CBA-CGA	2.59	119.38	112.51
22	2	609	CLA	CMD-C2D-C3D	2.59	133.57	127.61
22	6	609	CLA	CMD-C2D-C3D	2.59	133.57	127.61
22	C	502	CLA	CHC-C1C-C2C	-2.59	119.55	126.73
22	C	504	CLA	CHC-C4B-C3B	-2.59	116.21	127.71
22	B	614	CLA	CHD-C4C-NC	2.58	128.28	124.20
22	4	311	CLA	OBD-CAD-C3D	-2.58	122.30	128.52
22	8	311	CLA	OBD-CAD-C3D	-2.58	122.30	128.52
22	c	503	CLA	CHD-C4C-NC	2.58	128.28	124.20
25	3	301	CHL	CAA-C2A-C3A	-2.58	105.70	112.78
25	7	301	CHL	CAA-C2A-C3A	-2.58	105.70	112.78
22	C	509	CLA	CHD-C4C-NC	2.58	128.27	124.20
22	1	604	CLA	C4A-NA-C1A	-2.58	105.55	106.71
22	5	604	CLA	C4A-NA-C1A	-2.58	105.55	106.71
22	G	604	CLA	OBD-CAD-C3D	-2.58	122.31	128.52
22	g	604	CLA	OBD-CAD-C3D	-2.58	122.31	128.52
22	C	503	CLA	CMD-C2D-C3D	2.58	133.55	127.61
25	1	606	CHL	O2D-CGD-CBD	2.58	115.85	111.27
25	5	606	CHL	O2D-CGD-CBD	2.58	115.85	111.27
23	a	404	PHO	CBA-CAA-C2A	-2.58	106.28	113.81
22	c	501	CLA	C3C-C4C-NC	2.58	113.46	110.57
22	C	506	CLA	C2B-C1B-NB	2.58	111.96	110.23
22	3	312	CLA	CHD-C4C-NC	2.58	128.26	124.20
22	7	312	CLA	CHD-C4C-NC	2.58	128.26	124.20
22	3	312	CLA	OBD-CAD-C3D	-2.58	122.32	128.52
22	7	312	CLA	OBD-CAD-C3D	-2.58	122.32	128.52
22	2	613	CLA	OBD-CAD-C3D	-2.58	122.32	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	613	CLA	OBD-CAD-C3D	-2.58	122.32	128.52
25	G	606	CHL	CHB-C1B-NB	2.58	126.98	124.26
25	g	606	CHL	CHB-C1B-NB	2.58	126.98	124.26
22	2	610	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
22	6	610	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
22	b	616	CLA	CHC-C4B-C3B	-2.58	116.25	127.71
25	Y	601	CHL	CHB-C1B-NB	2.57	126.98	124.26
25	y	601	CHL	CHB-C1B-NB	2.57	126.98	124.26
22	1	613	CLA	CMB-C2B-C1B	2.57	129.29	125.37
22	5	613	CLA	CMB-C2B-C1B	2.57	129.29	125.37
22	b	611	CLA	CHD-C4C-NC	2.57	128.26	124.20
22	S	312	CLA	CED-O2D-CGD	2.57	121.75	115.94
22	s	312	CLA	CED-O2D-CGD	2.57	121.75	115.94
25	N	606	CHL	CAA-C2A-C3A	-2.57	105.74	112.78
25	n	606	CHL	CAA-C2A-C3A	-2.57	105.74	112.78
25	3	308	CHL	C2B-C1B-NB	-2.57	108.51	110.23
25	7	308	CHL	C2B-C1B-NB	-2.57	108.51	110.23
22	B	601	CLA	CAC-C3C-C2C	-2.57	123.13	127.53
22	B	609	CLA	CMA-C3A-C2A	-2.57	103.46	113.83
22	C	511	CLA	OBD-CAD-C3D	-2.57	122.34	128.52
22	4	305	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
22	8	305	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
22	c	510	CLA	CHD-C4C-NC	2.57	128.25	124.20
25	3	308	CHL	CAA-C2A-C3A	-2.57	105.75	112.78
25	7	308	CHL	CAA-C2A-C3A	-2.57	105.75	112.78
22	s	301	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
22	1	613	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
22	5	613	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
22	S	305	CLA	CHD-C4C-NC	2.56	128.25	124.20
22	s	305	CLA	CHD-C4C-NC	2.56	128.25	124.20
22	C	506	CLA	CMB-C2B-C1B	2.56	129.28	125.37
22	B	614	CLA	CMC-C2C-C1C	2.56	128.94	125.04
22	B	616	CLA	CED-O2D-CGD	2.56	121.73	115.94
25	2	608	CHL	C3B-C4B-NB	-2.56	108.14	110.52
25	6	608	CHL	C3B-C4B-NB	-2.56	108.14	110.52
22	S	310	CLA	CGD-CBD-CAD	-2.56	102.44	110.73
22	s	310	CLA	CGD-CBD-CAD	-2.56	102.44	110.73
22	c	509	CLA	OBD-CAD-C3D	-2.56	122.36	128.52
22	S	309	CLA	CHD-C4C-NC	2.56	128.24	124.20
22	s	309	CLA	CHD-C4C-NC	2.56	128.24	124.20
22	4	310	CLA	CMA-C3A-C2A	-2.56	103.50	113.83
22	8	310	CLA	CMA-C3A-C2A	-2.56	103.50	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	510	CLA	CHC-C4B-C3B	-2.56	116.33	127.71
25	G	607	CHL	C2A-C1A-CHA	2.56	128.33	123.86
25	g	607	CHL	C2A-C1A-CHA	2.56	128.33	123.86
22	Y	611	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	y	611	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	b	609	CLA	CMC-C2C-C1C	2.56	128.93	125.04
22	b	616	CLA	CHA-C1A-NA	-2.56	120.54	126.40
25	1	606	CHL	C2B-C1B-NB	-2.56	108.52	110.23
25	5	606	CHL	C2B-C1B-NB	-2.56	108.52	110.23
25	N	609	CHL	C2B-C1B-NB	-2.56	108.52	110.23
25	n	609	CHL	C2B-C1B-NB	-2.56	108.52	110.23
25	Y	605	CHL	CHC-C4B-NB	2.56	126.96	124.26
25	y	605	CHL	CHC-C4B-NB	2.56	126.96	124.26
22	B	603	CLA	CMA-C3A-C4A	-2.55	104.91	111.77
22	c	501	CLA	CMD-C2D-C3D	2.55	133.49	127.61
22	N	602	CLA	CMD-C2D-C3D	2.55	133.49	127.61
22	n	602	CLA	CMD-C2D-C3D	2.55	133.49	127.61
22	A	403	CLA	OBD-CAD-C3D	-2.55	122.37	128.52
22	d	403	CLA	CMD-C2D-C3D	2.55	133.49	127.61
22	S	313	CLA	CMC-C2C-C1C	2.55	128.93	125.04
22	s	313	CLA	CMC-C2C-C1C	2.55	128.93	125.04
25	Y	608	CHL	C3B-C4B-NB	-2.55	108.15	110.52
25	y	608	CHL	C3B-C4B-NB	-2.55	108.15	110.52
22	C	503	CLA	CHD-C4C-NC	2.55	128.23	124.20
22	S	314	CLA	CGD-CBD-CAD	-2.55	102.47	110.73
22	s	314	CLA	CGD-CBD-CAD	-2.55	102.47	110.73
22	2	611	CLA	CHC-C1C-C2C	-2.55	119.64	126.73
22	6	611	CLA	CHC-C1C-C2C	-2.55	119.64	126.73
22	C	509	CLA	CAC-C3C-C2C	-2.55	123.17	127.53
22	A	405	CLA	CHA-C1A-NA	-2.55	120.56	126.40
22	C	502	CLA	C4A-NA-C1A	-2.55	105.56	106.71
22	b	611	CLA	CHC-C4B-C3B	-2.55	116.38	127.71
22	b	607	CLA	C4D-CHA-C1A	-2.55	118.15	121.25
22	R	309	CLA	OBD-CAD-C3D	-2.55	122.39	128.52
22	r	309	CLA	OBD-CAD-C3D	-2.55	122.39	128.52
22	4	303	CLA	OBD-CAD-C3D	-2.55	122.39	128.52
22	8	303	CLA	OBD-CAD-C3D	-2.55	122.39	128.52
22	3	303	CLA	CHC-C1C-C2C	-2.55	119.66	126.73
22	7	303	CLA	CHC-C1C-C2C	-2.55	119.66	126.73
22	Y	604	CLA	CHC-C4B-C3B	-2.55	116.38	127.71
22	y	604	CLA	CHC-C4B-C3B	-2.55	116.38	127.71
25	1	609	CHL	CAA-CBA-CGA	2.55	119.26	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	609	CHL	CAA-CBA-CGA	2.55	119.26	112.51
22	C	511	CLA	CED-O2D-CGD	2.55	121.69	115.94
22	S	313	CLA	OBD-CAD-C3D	-2.54	122.40	128.52
22	s	313	CLA	OBD-CAD-C3D	-2.54	122.40	128.52
22	b	604	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
22	3	312	CLA	CGD-CBD-CAD	-2.54	102.50	110.73
22	7	312	CLA	CGD-CBD-CAD	-2.54	102.50	110.73
22	R	303	CLA	CHD-C4C-NC	2.54	128.21	124.20
22	r	303	CLA	CHD-C4C-NC	2.54	128.21	124.20
22	B	606	CLA	CMD-C2D-C3D	2.54	133.46	127.61
22	c	504	CLA	C4D-CHA-C1A	-2.54	118.16	121.25
22	C	512	CLA	CMD-C2D-C3D	2.54	133.46	127.61
22	c	509	CLA	CHC-C1C-C2C	-2.54	119.68	126.73
22	S	310	CLA	CED-O2D-CGD	2.54	121.68	115.94
22	s	310	CLA	CED-O2D-CGD	2.54	121.68	115.94
22	C	507	CLA	CMD-C2D-C3D	2.54	133.45	127.61
22	B	602	CLA	CED-O2D-CGD	2.54	121.68	115.94
22	N	614	CLA	C3C-C4C-NC	2.54	113.42	110.57
22	n	614	CLA	C3C-C4C-NC	2.54	113.42	110.57
22	C	501	CLA	OBD-CAD-C3D	-2.54	122.42	128.52
22	B	612	CLA	CGD-CBD-CAD	-2.54	102.52	110.73
22	N	602	CLA	CHD-C4C-NC	2.54	128.20	124.20
22	n	602	CLA	CHD-C4C-NC	2.54	128.20	124.20
22	b	609	CLA	C4D-CHA-C1A	-2.53	118.16	121.25
22	B	614	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
22	d	403	CLA	OBD-CAD-C3D	-2.53	122.42	128.52
22	B	606	CLA	CHC-C4B-C3B	-2.53	116.44	127.71
22	B	606	CLA	C4B-CHC-C1C	-2.53	120.33	126.34
22	B	603	CLA	CMD-C2D-C3D	2.53	133.44	127.61
22	4	310	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
22	8	310	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
22	G	612	CLA	OBD-CAD-C3D	-2.53	122.42	128.52
22	g	612	CLA	OBD-CAD-C3D	-2.53	122.42	128.52
22	s	301	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	R	311	CLA	CHD-C4C-NC	2.53	128.19	124.20
22	r	311	CLA	CHD-C4C-NC	2.53	128.19	124.20
22	b	602	CLA	CMC-C2C-C1C	2.53	128.89	125.04
22	c	502	CLA	OBD-CAD-C3D	-2.53	122.43	128.52
25	N	607	CHL	CAA-C2A-C3A	-2.53	105.85	112.78
25	n	607	CHL	CAA-C2A-C3A	-2.53	105.85	112.78
22	b	615	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
22	C	507	CLA	O2D-CGD-O1D	-2.53	118.90	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	501	CLA	CAC-C3C-C2C	-2.53	123.21	127.53
22	1	604	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
22	5	604	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
22	b	616	CLA	C4B-CHC-C1C	-2.53	120.35	126.34
22	b	616	CLA	C3C-C4C-NC	2.53	113.40	110.57
22	d	401	CLA	CHD-C4C-NC	2.52	128.18	124.20
22	R	301	CLA	OBD-CAD-C3D	-2.52	122.44	128.52
22	r	301	CLA	OBD-CAD-C3D	-2.52	122.44	128.52
22	a	405	CLA	CHC-C4B-C3B	-2.52	116.49	127.71
25	2	608	CHL	C3A-C2A-C1A	2.52	105.12	101.34
25	6	608	CHL	C3A-C2A-C1A	2.52	105.12	101.34
22	B	602	CLA	OBD-CAD-C3D	-2.52	122.45	128.52
22	c	512	CLA	CAC-C3C-C2C	-2.52	123.22	127.53
22	S	314	CLA	CHD-C4C-NC	2.52	128.18	124.20
22	s	314	CLA	CHD-C4C-NC	2.52	128.18	124.20
22	C	504	CLA	OBD-CAD-C3D	-2.52	122.45	128.52
22	C	501	CLA	CGD-CBD-CAD	-2.52	102.57	110.73
25	3	307	CHL	C2B-C1B-NB	-2.52	108.54	110.23
25	4	306	CHL	C2B-C1B-NB	-2.52	108.54	110.23
25	7	307	CHL	C2B-C1B-NB	-2.52	108.54	110.23
25	8	306	CHL	C2B-C1B-NB	-2.52	108.54	110.23
22	3	303	CLA	CMC-C2C-C1C	2.52	128.88	125.04
22	7	303	CLA	CMC-C2C-C1C	2.52	128.88	125.04
22	4	310	CLA	OBD-CAD-C3D	-2.52	122.46	128.52
22	8	310	CLA	OBD-CAD-C3D	-2.52	122.46	128.52
22	b	609	CLA	C4A-NA-C1A	-2.52	105.57	106.71
22	a	403	CLA	CHD-C4C-NC	2.52	128.17	124.20
22	C	501	CLA	CMA-C3A-C4A	-2.52	105.01	111.77
22	c	507	CLA	CMD-C2D-C3D	2.52	133.40	127.61
22	B	610	CLA	CGD-CBD-CAD	-2.52	102.59	110.73
22	S	312	CLA	CMB-C2B-C1B	2.52	129.20	125.37
22	s	312	CLA	CMB-C2B-C1B	2.52	129.20	125.37
22	C	508	CLA	CHA-C1A-NA	-2.52	120.64	126.40
22	2	610	CLA	CHD-C4C-NC	2.51	128.17	124.20
22	6	610	CLA	CHD-C4C-NC	2.51	128.17	124.20
22	R	307	CLA	OBD-CAD-C3D	-2.51	122.47	128.52
22	r	307	CLA	OBD-CAD-C3D	-2.51	122.47	128.52
22	4	304	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
22	8	304	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
22	S	311	CLA	OBD-CAD-C3D	-2.51	122.47	128.52
22	s	311	CLA	OBD-CAD-C3D	-2.51	122.47	128.52
22	Y	613	CLA	CBB-CAB-C3B	-2.51	115.11	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	y	613	CLA	CBB-CAB-C3B	-2.51	115.11	127.62
22	N	614	CLA	CHD-C4C-NC	2.51	128.16	124.20
22	n	614	CLA	CHD-C4C-NC	2.51	128.16	124.20
22	C	506	CLA	C4B-CHC-C1C	-2.51	120.38	126.34
25	1	609	CHL	C3A-C2A-C1A	2.51	105.10	101.34
25	5	609	CHL	C3A-C2A-C1A	2.51	105.10	101.34
22	N	604	CLA	OBD-CAD-C3D	-2.51	122.47	128.52
22	n	604	CLA	OBD-CAD-C3D	-2.51	122.47	128.52
22	C	510	CLA	OBD-CAD-C3D	-2.51	122.48	128.52
22	R	310	CLA	C4A-NA-C1A	-2.51	105.58	106.71
22	r	310	CLA	C4A-NA-C1A	-2.51	105.58	106.71
22	4	305	CLA	C4A-NA-C1A	-2.51	105.58	106.71
22	8	305	CLA	C4A-NA-C1A	-2.51	105.58	106.71
22	b	602	CLA	CMB-C2B-C1B	2.51	129.19	125.37
22	1	614	CLA	C3B-C4B-NB	2.51	112.84	110.52
22	5	614	CLA	C3B-C4B-NB	2.51	112.84	110.52
22	b	612	CLA	CHC-C1C-C2C	-2.51	119.76	126.73
25	Y	601	CHL	O2A-CGA-O1A	-2.51	117.04	123.30
25	y	601	CHL	O2A-CGA-O1A	-2.51	117.04	123.30
22	b	615	CLA	OBD-CAD-C3D	-2.51	122.48	128.52
25	2	605	CHL	C2A-C3A-C4A	2.51	104.98	101.78
25	6	605	CHL	C2A-C3A-C4A	2.51	104.98	101.78
22	3	314	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
22	7	314	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
22	b	615	CLA	CHD-C4C-NC	2.51	128.16	124.20
22	b	613	CLA	C3B-C4B-NB	2.51	112.84	110.52
22	R	311	CLA	CMC-C2C-C1C	2.51	128.86	125.04
22	r	311	CLA	CMC-C2C-C1C	2.51	128.86	125.04
22	1	602	CLA	CMC-C2C-C1C	2.51	128.86	125.04
22	5	602	CLA	CMC-C2C-C1C	2.51	128.86	125.04
22	c	507	CLA	CHD-C4C-NC	2.51	128.15	124.20
22	N	613	CLA	CHD-C4C-NC	2.51	128.15	124.20
22	n	613	CLA	CHD-C4C-NC	2.51	128.15	124.20
22	G	603	CLA	C3C-C4C-NC	2.51	113.38	110.57
22	g	603	CLA	C3C-C4C-NC	2.51	113.38	110.57
25	3	306	CHL	C2A-C3A-C4A	2.51	104.98	101.78
25	7	306	CHL	C2A-C3A-C4A	2.51	104.98	101.78
22	d	403	CLA	C3C-C4C-NC	2.50	113.38	110.57
22	R	307	CLA	C4D-CHA-C1A	-2.50	118.20	121.25
22	r	307	CLA	C4D-CHA-C1A	-2.50	118.20	121.25
22	B	608	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	b	602	CLA	CHC-C1C-C2C	-2.50	119.79	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	604	CLA	CAA-CBA-CGA	2.50	119.14	112.51
22	6	604	CLA	CAA-CBA-CGA	2.50	119.14	112.51
22	G	603	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
22	g	603	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
22	b	604	CLA	C4D-CHA-C1A	-2.50	118.21	121.25
22	C	505	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	b	606	CLA	O2A-CGA-O1A	-2.50	117.07	123.30
22	b	602	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
22	G	613	CLA	CHD-C4C-NC	2.50	128.14	124.20
22	g	613	CLA	CHD-C4C-NC	2.50	128.14	124.20
22	4	311	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
22	8	311	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
25	N	606	CHL	CAA-CBA-CGA	2.50	119.13	112.51
25	n	606	CHL	CAA-CBA-CGA	2.50	119.13	112.51
22	C	502	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
22	c	503	CLA	CMD-C2D-C3D	2.50	133.35	127.61
22	B	609	CLA	CGD-CBD-CAD	-2.50	102.65	110.73
22	c	508	CLA	CHA-C1A-NA	-2.50	120.68	126.40
23	a	404	PHO	C4B-NB-C1B	-2.49	104.97	108.83
22	C	512	CLA	C4D-CHA-C1A	-2.49	118.21	121.25
22	2	613	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	6	613	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	1	604	CLA	OBD-CAD-C3D	-2.49	122.53	128.52
22	5	604	CLA	OBD-CAD-C3D	-2.49	122.53	128.52
22	c	506	CLA	CHA-C1A-NA	-2.49	120.69	126.40
22	d	404	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	4	310	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	8	310	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	S	313	CLA	CMA-C3A-C4A	-2.49	105.08	111.77
22	s	313	CLA	CMA-C3A-C4A	-2.49	105.08	111.77
22	1	614	CLA	OBD-CAD-C3D	-2.49	122.53	128.52
22	5	614	CLA	OBD-CAD-C3D	-2.49	122.53	128.52
22	S	310	CLA	CMD-C2D-C3D	2.49	133.34	127.61
22	s	310	CLA	CMD-C2D-C3D	2.49	133.34	127.61
22	R	308	CLA	CMA-C3A-C4A	-2.49	105.09	111.77
22	r	308	CLA	CMA-C3A-C4A	-2.49	105.09	111.77
22	b	615	CLA	CMD-C2D-C3D	2.49	133.34	127.61
22	C	506	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
22	Y	613	CLA	CMB-C2B-C1B	2.49	129.16	125.37
22	y	613	CLA	CMB-C2B-C1B	2.49	129.16	125.37
25	S	307	CHL	CHB-C1B-NB	2.49	126.89	124.26
25	s	307	CHL	CHB-C1B-NB	2.49	126.89	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	504	CLA	OBD-CAD-C3D	-2.49	122.54	128.52
22	c	511	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
22	3	303	CLA	CGD-CBD-CAD	-2.49	102.68	110.73
22	7	303	CLA	CGD-CBD-CAD	-2.49	102.68	110.73
22	C	509	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
22	b	603	CLA	CAA-C2A-C3A	-2.48	105.97	112.78
22	S	310	CLA	CMB-C2B-C1B	2.48	129.15	125.37
22	s	310	CLA	CMB-C2B-C1B	2.48	129.15	125.37
25	N	609	CHL	CAA-CBA-CGA	2.48	119.09	112.51
25	n	609	CHL	CAA-CBA-CGA	2.48	119.09	112.51
22	B	616	CLA	CHD-C4C-NC	2.48	128.11	124.20
22	d	403	CLA	CHC-C4B-C3B	-2.48	116.67	127.71
25	3	302	CHL	C2A-C3A-C4A	2.48	105.88	101.87
25	7	302	CHL	C2A-C3A-C4A	2.48	105.88	101.87
22	N	612	CLA	CMB-C2B-C1B	2.48	129.15	125.37
22	n	612	CLA	CMB-C2B-C1B	2.48	129.15	125.37
22	b	607	CLA	OBD-CAD-C3D	-2.48	122.55	128.52
25	Y	607	CHL	CHC-C4B-NB	2.48	126.88	124.26
25	y	607	CHL	CHC-C4B-NB	2.48	126.88	124.26
22	Y	611	CLA	CHA-C1A-NA	-2.48	120.72	126.40
22	y	611	CLA	CHA-C1A-NA	-2.48	120.72	126.40
22	R	302	CLA	CHC-C1C-C2C	-2.48	119.84	126.73
22	r	302	CLA	CHC-C1C-C2C	-2.48	119.84	126.73
22	3	303	CLA	OBD-CAD-C3D	-2.48	122.56	128.52
22	7	303	CLA	OBD-CAD-C3D	-2.48	122.56	128.52
22	N	602	CLA	CMC-C2C-C1C	2.48	128.81	125.04
22	n	602	CLA	CMC-C2C-C1C	2.48	128.81	125.04
22	2	602	CLA	CMC-C2C-C1C	2.48	128.81	125.04
22	6	602	CLA	CMC-C2C-C1C	2.48	128.81	125.04
22	G	602	CLA	CGD-CBD-CAD	-2.48	102.71	110.73
22	g	602	CLA	CGD-CBD-CAD	-2.48	102.71	110.73
22	B	615	CLA	CHC-C4B-C3B	-2.48	116.69	127.71
22	b	603	CLA	CMD-C2D-C3D	2.48	133.31	127.61
22	C	504	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
22	1	614	CLA	C3C-C4C-NC	2.48	113.35	110.57
22	5	614	CLA	C3C-C4C-NC	2.48	113.35	110.57
22	S	303	CLA	CMC-C2C-C1C	2.47	128.81	125.04
22	s	303	CLA	CMC-C2C-C1C	2.47	128.81	125.04
22	G	613	CLA	CMB-C2B-C1B	2.47	129.13	125.37
22	g	613	CLA	CMB-C2B-C1B	2.47	129.13	125.37
22	N	604	CLA	CHD-C4C-NC	2.47	128.10	124.20
22	n	604	CLA	CHD-C4C-NC	2.47	128.10	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	601	CLA	CHC-C1C-C2C	-2.47	119.87	126.73
22	c	507	CLA	C4B-CHC-C1C	-2.47	120.48	126.34
22	Y	614	CLA	CMD-C2D-C3D	2.47	133.30	127.61
22	y	614	CLA	CMD-C2D-C3D	2.47	133.30	127.61
22	3	313	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
22	7	313	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
22	2	602	CLA	CGD-CBD-CAD	-2.47	102.73	110.73
22	6	602	CLA	CGD-CBD-CAD	-2.47	102.73	110.73
22	Y	602	CLA	CHD-C4C-NC	2.47	128.09	124.20
22	y	602	CLA	CHD-C4C-NC	2.47	128.09	124.20
25	1	609	CHL	C3B-C4B-NB	-2.47	108.22	110.52
25	5	609	CHL	C3B-C4B-NB	-2.47	108.22	110.52
22	a	402	CLA	CED-O2D-CGD	2.47	121.52	115.94
22	c	509	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
22	B	604	CLA	CHA-C1A-NA	-2.47	120.75	126.40
22	B	615	CLA	CMC-C2C-C1C	2.47	128.80	125.04
22	N	612	CLA	OBD-CAD-C3D	-2.47	122.58	128.52
22	n	612	CLA	OBD-CAD-C3D	-2.47	122.58	128.52
22	1	603	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
22	5	603	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
22	Y	613	CLA	CHD-C4C-NC	2.47	128.09	124.20
22	y	613	CLA	CHD-C4C-NC	2.47	128.09	124.20
22	b	601	CLA	C4D-CHA-C1A	-2.46	118.25	121.25
22	S	312	CLA	CHC-C4B-C3B	-2.46	116.75	127.71
22	s	312	CLA	CHC-C4B-C3B	-2.46	116.75	127.71
22	2	602	CLA	CMB-C2B-C1B	2.46	129.12	125.37
22	6	602	CLA	CMB-C2B-C1B	2.46	129.12	125.37
22	2	603	CLA	CHD-C4C-NC	2.46	128.09	124.20
22	6	603	CLA	CHD-C4C-NC	2.46	128.09	124.20
25	4	302	CHL	CAA-CBA-CGA	2.46	119.04	112.51
25	8	302	CHL	CAA-CBA-CGA	2.46	119.04	112.51
22	b	605	CLA	O1D-CGD-CBD	-2.46	119.44	124.48
22	c	511	CLA	CHD-C4C-NC	2.46	128.08	124.20
22	3	303	CLA	CHD-C4C-NC	2.46	128.08	124.20
22	7	303	CLA	CHD-C4C-NC	2.46	128.08	124.20
22	A	403	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	b	609	CLA	C4B-CHC-C1C	-2.46	120.50	126.34
22	S	301	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	C	508	CLA	CGD-CBD-CAD	-2.46	102.77	110.73
22	D	403	CLA	OBD-CAD-C3D	-2.46	122.60	128.52
22	2	611	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	6	611	CLA	O2D-CGD-O1D	-2.46	119.03	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	501	CLA	CHC-C4B-C3B	-2.46	116.78	127.71
22	B	610	CLA	OBD-CAD-C3D	-2.46	122.61	128.52
22	S	309	CLA	C3B-C4B-NB	2.46	112.79	110.52
22	s	309	CLA	C3B-C4B-NB	2.46	112.79	110.52
22	c	506	CLA	CED-O2D-CGD	2.46	121.49	115.94
25	N	608	CHL	CHB-C1B-NB	2.46	126.86	124.26
25	n	608	CHL	CHB-C1B-NB	2.46	126.86	124.26
25	G	605	CHL	C2A-C3A-C4A	2.45	104.91	101.78
25	g	605	CHL	C2A-C3A-C4A	2.45	104.91	101.78
22	a	402	CLA	CHD-C4C-NC	2.45	128.07	124.20
22	A	402	CLA	OBD-CAD-C3D	-2.45	122.62	128.52
22	b	606	CLA	CMD-C2D-C3D	2.45	133.25	127.61
22	2	602	CLA	OBD-CAD-C3D	-2.45	122.62	128.52
22	6	602	CLA	OBD-CAD-C3D	-2.45	122.62	128.52
22	b	609	CLA	CHD-C4C-NC	2.45	128.06	124.20
22	a	402	CLA	OBD-CAD-C3D	-2.45	122.63	128.52
22	R	301	CLA	CMA-C3A-C2A	-2.45	103.95	113.83
22	r	301	CLA	CMA-C3A-C2A	-2.45	103.95	113.83
22	c	510	CLA	OBD-CAD-C3D	-2.45	122.63	128.52
22	C	509	CLA	CMC-C2C-C1C	2.45	128.76	125.04
22	1	610	CLA	CHC-C1C-C2C	-2.45	119.93	126.73
22	5	610	CLA	CHC-C1C-C2C	-2.45	119.93	126.73
22	S	312	CLA	CHD-C4C-NC	2.45	128.06	124.20
22	s	312	CLA	CHD-C4C-NC	2.45	128.06	124.20
22	a	403	CLA	CAC-C3C-C2C	-2.45	123.35	127.53
22	b	609	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
22	3	314	CLA	C3C-C4C-NC	2.44	113.31	110.57
22	7	314	CLA	C3C-C4C-NC	2.44	113.31	110.57
22	b	616	CLA	CED-O2D-CGD	2.44	121.46	115.94
22	N	603	CLA	C3C-C4C-NC	2.44	113.31	110.57
22	n	603	CLA	C3C-C4C-NC	2.44	113.31	110.57
22	b	609	CLA	CED-O2D-CGD	2.44	121.46	115.94
25	G	609	CHL	CHC-C4B-NB	2.44	126.84	124.26
25	g	609	CHL	CHC-C4B-NB	2.44	126.84	124.26
22	Y	612	CLA	CHC-C4B-C3B	-2.44	116.85	127.71
22	y	612	CLA	CHC-C4B-C3B	-2.44	116.85	127.71
22	3	305	CLA	CAA-CBA-CGA	2.44	118.99	112.51
22	7	305	CLA	CAA-CBA-CGA	2.44	118.99	112.51
22	c	504	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
22	c	503	CLA	CGD-CBD-CAD	-2.44	102.83	110.73
22	C	503	CLA	CHA-C1A-NA	-2.44	120.81	126.40
25	4	307	CHL	C2B-C1B-NB	-2.44	108.60	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	307	CHL	C2B-C1B-NB	-2.44	108.60	110.23
22	1	603	CLA	CHD-C4C-NC	2.44	128.05	124.20
22	5	603	CLA	CHD-C4C-NC	2.44	128.05	124.20
22	S	301	CLA	CHA-C1A-NA	-2.44	120.81	126.40
25	1	607	CHL	C2B-C1B-NB	-2.44	108.60	110.23
25	5	607	CHL	C2B-C1B-NB	-2.44	108.60	110.23
22	C	504	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
22	b	613	CLA	C4B-CHC-C1C	-2.44	120.56	126.34
22	c	506	CLA	CMB-C2B-C1B	2.44	129.08	125.37
25	1	601	CHL	C1D-ND-C4D	-2.44	104.61	106.33
25	5	601	CHL	C1D-ND-C4D	-2.44	104.61	106.33
22	Y	611	CLA	C4A-NA-C1A	-2.43	105.61	106.71
22	y	611	CLA	C4A-NA-C1A	-2.43	105.61	106.71
22	b	614	CLA	CHC-C4B-C3B	-2.43	116.89	127.71
22	B	607	CLA	CMB-C2B-C1B	2.43	129.07	125.37
22	c	504	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
22	b	605	CLA	CHD-C4C-NC	2.43	128.03	124.20
22	A	403	CLA	CMB-C2B-C3B	2.43	132.47	126.59
22	S	303	CLA	OBD-CAD-C3D	-2.43	122.67	128.52
22	s	303	CLA	OBD-CAD-C3D	-2.43	122.67	128.52
22	C	508	CLA	CHC-C4B-C3B	-2.43	116.90	127.71
22	2	611	CLA	CGD-CBD-CAD	-2.43	102.86	110.73
22	6	611	CLA	CGD-CBD-CAD	-2.43	102.86	110.73
22	A	402	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
22	b	602	CLA	OBD-CAD-C3D	-2.43	122.68	128.52
23	d	402	PHO	O2D-CGD-O1D	-2.43	119.09	123.84
22	b	603	CLA	CHC-C4B-C3B	-2.43	116.91	127.71
22	4	311	CLA	CAC-C3C-C2C	-2.43	123.38	127.53
22	8	311	CLA	CAC-C3C-C2C	-2.43	123.38	127.53
22	S	314	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
22	s	314	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
22	Y	611	CLA	CMC-C2C-C1C	2.43	128.73	125.04
22	y	611	CLA	CMC-C2C-C1C	2.43	128.73	125.04
22	b	609	CLA	CHC-C4B-C3B	-2.43	116.92	127.71
22	Y	612	CLA	CMC-C2C-C3C	2.43	132.70	126.12
22	y	612	CLA	CMC-C2C-C3C	2.43	132.70	126.12
22	C	507	CLA	CHD-C4C-NC	2.42	128.02	124.20
22	1	602	CLA	CMB-C2B-C1B	2.42	129.06	125.37
22	5	602	CLA	CMB-C2B-C1B	2.42	129.06	125.37
22	C	506	CLA	CHA-C1A-NA	-2.42	120.85	126.40
22	R	308	CLA	CMB-C2B-C1B	2.42	129.06	125.37
22	r	308	CLA	CMB-C2B-C1B	2.42	129.06	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	603	CLA	CHD-C4C-NC	2.42	128.02	124.20
22	g	603	CLA	CHD-C4C-NC	2.42	128.02	124.20
22	c	511	CLA	C4D-CHA-C1A	-2.42	118.30	121.25
22	R	303	CLA	CMB-C2B-C1B	2.42	129.06	125.37
22	r	303	CLA	CMB-C2B-C1B	2.42	129.06	125.37
22	b	607	CLA	CBB-CAB-C3B	-2.42	115.57	127.62
22	C	502	CLA	CGD-CBD-CAD	-2.42	102.89	110.73
22	Y	602	CLA	CMA-C3A-C2A	-2.42	104.06	113.83
22	y	602	CLA	CMA-C3A-C2A	-2.42	104.06	113.83
22	C	505	CLA	OBD-CAD-C3D	-2.42	122.70	128.52
25	N	608	CHL	C2B-C1B-NB	-2.42	108.61	110.23
25	n	608	CHL	C2B-C1B-NB	-2.42	108.61	110.23
22	c	512	CLA	CHD-C4C-NC	2.42	128.02	124.20
22	b	616	CLA	CMC-C2C-C3C	2.42	132.68	126.12
22	C	510	CLA	CHD-C4C-NC	2.42	128.01	124.20
22	S	304	CLA	C4D-CHA-C1A	-2.42	118.31	121.25
22	s	304	CLA	C4D-CHA-C1A	-2.42	118.31	121.25
22	c	505	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	4	310	CLA	CHC-C1C-C2C	-2.42	120.01	126.73
22	8	310	CLA	CHC-C1C-C2C	-2.42	120.01	126.73
22	1	603	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
22	5	603	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
25	N	605	CHL	C2A-C1A-CHA	2.42	128.07	123.85
25	n	605	CHL	C2A-C1A-CHA	2.42	128.07	123.85
22	D	403	CLA	CHC-C4B-C3B	-2.42	116.96	127.71
25	1	606	CHL	CAA-CBA-CGA	2.42	118.92	112.51
25	5	606	CHL	CAA-CBA-CGA	2.42	118.92	112.51
22	a	405	CLA	CHA-C1A-NA	-2.41	120.87	126.40
22	c	501	CLA	C3B-C4B-NB	2.41	112.75	110.52
22	C	504	CLA	CHD-C4C-NC	2.41	128.01	124.20
22	b	614	CLA	CHD-C4C-NC	2.41	128.01	124.20
25	G	608	CHL	CHB-C1B-NB	2.41	126.81	124.26
25	g	608	CHL	CHB-C1B-NB	2.41	126.81	124.26
25	1	605	CHL	OMC-CMC-C2C	-2.41	120.23	125.69
25	5	605	CHL	OMC-CMC-C2C	-2.41	120.23	125.69
22	Y	604	CLA	CHA-C1A-NA	-2.41	120.87	126.40
22	y	604	CLA	CHA-C1A-NA	-2.41	120.87	126.40
22	B	602	CLA	CHA-C1A-NA	-2.41	120.87	126.40
25	4	302	CHL	CAA-C2A-C3A	-2.41	106.17	112.78
25	8	302	CHL	CAA-C2A-C3A	-2.41	106.17	112.78
22	b	609	CLA	CGD-CBD-CAD	-2.41	102.92	110.73
22	c	501	CLA	CHA-C1A-NA	-2.41	120.88	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	306	CHL	C2A-C1A-CHA	2.41	128.06	123.85
25	7	306	CHL	C2A-C1A-CHA	2.41	128.06	123.85
22	c	501	CLA	OBD-CAD-C3D	-2.41	122.72	128.52
25	1	615	CHL	CHB-C1B-NB	2.41	126.81	124.26
25	5	615	CHL	CHB-C1B-NB	2.41	126.81	124.26
22	2	602	CLA	C4D-CHA-C1A	-2.41	118.32	121.25
22	6	602	CLA	C4D-CHA-C1A	-2.41	118.32	121.25
22	B	604	CLA	OBD-CAD-C3D	-2.41	122.72	128.52
22	Y	614	CLA	CHC-C4B-C3B	-2.41	117.00	127.71
22	y	614	CLA	CHC-C4B-C3B	-2.41	117.00	127.71
22	B	608	CLA	CHD-C4C-NC	2.41	128.00	124.20
22	d	403	CLA	CMA-C3A-C4A	-2.41	105.30	111.77
22	b	615	CLA	C3C-C4C-NC	2.41	113.27	110.57
22	1	612	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
22	5	612	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
22	4	301	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
22	8	301	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
22	D	401	CLA	CAC-C3C-C2C	-2.40	123.42	127.53
22	b	601	CLA	CAC-C3C-C2C	-2.40	123.42	127.53
25	1	609	CHL	C2A-C1A-CHA	2.40	128.06	123.86
25	5	609	CHL	C2A-C1A-CHA	2.40	128.06	123.86
22	S	305	CLA	CED-O2D-CGD	2.40	121.37	115.94
22	s	305	CLA	CED-O2D-CGD	2.40	121.37	115.94
22	G	604	CLA	CHC-C4B-C3B	-2.40	117.03	127.71
22	g	604	CLA	CHC-C4B-C3B	-2.40	117.03	127.71
25	N	607	CHL	C2B-C1B-NB	-2.40	108.62	110.23
25	n	607	CHL	C2B-C1B-NB	-2.40	108.62	110.23
22	1	603	CLA	CMB-C2B-C1B	2.40	129.03	125.37
22	5	603	CLA	CMB-C2B-C1B	2.40	129.03	125.37
22	C	502	CLA	CED-O2D-CGD	2.40	121.37	115.94
22	B	602	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
25	1	601	CHL	CAA-C2A-C3A	-2.40	106.20	112.78
25	5	601	CHL	CAA-C2A-C3A	-2.40	106.20	112.78
25	2	606	CHL	CHC-C4B-NB	2.40	126.80	124.26
25	6	606	CHL	CHC-C4B-NB	2.40	126.80	124.26
22	C	507	CLA	CBB-CAB-C3B	-2.40	115.68	127.62
22	4	311	CLA	CGD-CBD-CAD	-2.40	102.96	110.73
22	8	311	CLA	CGD-CBD-CAD	-2.40	102.96	110.73
22	S	311	CLA	CAC-C3C-C2C	-2.40	123.42	127.53
22	s	311	CLA	CAC-C3C-C2C	-2.40	123.42	127.53
24	e	101	HEM	CAC-C3C-C2C	-2.40	120.70	128.60
22	C	501	CLA	CHA-C1A-NA	-2.40	120.90	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	614	CLA	CHC-C4B-C3B	-2.40	117.04	127.71
22	5	614	CLA	CHC-C4B-C3B	-2.40	117.04	127.71
25	Y	606	CHL	O2D-CGD-CBD	2.40	115.53	111.27
25	y	606	CHL	O2D-CGD-CBD	2.40	115.53	111.27
25	N	608	CHL	CAA-CBA-CGA	2.40	118.87	112.51
25	n	608	CHL	CAA-CBA-CGA	2.40	118.87	112.51
22	d	403	CLA	CMC-C2C-C1C	2.40	128.69	125.04
22	c	507	CLA	CBB-CAB-C3B	-2.40	115.69	127.62
22	b	601	CLA	CGD-CBD-CAD	-2.40	102.97	110.73
22	b	603	CLA	OBD-CAD-C3D	-2.40	122.75	128.52
22	B	604	CLA	CHD-C4C-NC	2.40	127.98	124.20
22	d	401	CLA	OBD-CAD-C3D	-2.40	122.75	128.52
25	R	305	CHL	CHB-C1B-NB	2.40	126.79	124.26
25	r	305	CHL	CHB-C1B-NB	2.40	126.79	124.26
22	S	301	CLA	CMB-C2B-C1B	2.40	129.02	125.37
22	Y	612	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
22	y	612	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
22	d	403	CLA	C3B-C4B-NB	2.40	112.74	110.52
25	S	306	CHL	C2A-C1A-CHA	2.39	128.05	123.86
25	s	306	CHL	C2A-C1A-CHA	2.39	128.05	123.86
22	S	310	CLA	CBA-CAA-C2A	2.39	120.92	113.86
22	s	310	CLA	CBA-CAA-C2A	2.39	120.92	113.86
22	G	613	CLA	CBB-CAB-C3B	-2.39	115.72	127.62
22	g	613	CLA	CBB-CAB-C3B	-2.39	115.72	127.62
25	Y	609	CHL	C2B-C1B-NB	-2.39	108.63	110.23
25	y	609	CHL	C2B-C1B-NB	-2.39	108.63	110.23
22	Y	610	CLA	CMC-C2C-C1C	2.39	128.68	125.04
22	y	610	CLA	CMC-C2C-C1C	2.39	128.68	125.04
22	N	604	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
22	n	604	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
22	B	602	CLA	CHD-C4C-NC	2.39	127.97	124.20
22	C	509	CLA	OBD-CAD-C3D	-2.39	122.77	128.52
22	R	308	CLA	CBA-CAA-C2A	2.39	120.91	113.86
22	r	308	CLA	CBA-CAA-C2A	2.39	120.91	113.86
22	2	603	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
22	6	603	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
22	C	510	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
22	S	313	CLA	CHD-C4C-NC	2.39	127.97	124.20
22	s	313	CLA	CHD-C4C-NC	2.39	127.97	124.20
22	2	611	CLA	CMB-C2B-C1B	2.39	129.00	125.37
22	6	611	CLA	CMB-C2B-C1B	2.39	129.00	125.37
25	Y	601	CHL	CAA-CBA-CGA	2.39	118.84	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	601	CHL	CAA-CBA-CGA	2.39	118.84	112.51
22	4	304	CLA	CHD-C4C-NC	2.39	127.96	124.20
22	8	304	CLA	CHD-C4C-NC	2.39	127.96	124.20
22	b	615	CLA	CHA-C1A-NA	-2.39	120.93	126.40
22	Y	604	CLA	CGD-CBD-CAD	-2.39	103.01	110.73
22	y	604	CLA	CGD-CBD-CAD	-2.39	103.01	110.73
22	C	507	CLA	CMB-C2B-C1B	2.39	129.00	125.37
22	s	301	CLA	OBD-CAD-C3D	-2.39	122.78	128.52
22	2	613	CLA	CHD-C4C-NC	2.39	127.96	124.20
22	6	613	CLA	CHD-C4C-NC	2.39	127.96	124.20
22	c	503	CLA	CHA-C1A-NA	-2.39	120.94	126.40
22	s	301	CLA	CMC-C2C-C1C	2.38	128.67	125.04
22	A	403	CLA	CHD-C4C-NC	2.38	127.96	124.20
22	b	605	CLA	CHA-C1A-NA	-2.38	120.94	126.40
22	B	614	CLA	CHA-C1A-NA	-2.38	120.94	126.40
22	B	609	CLA	CHD-C4C-NC	2.38	127.96	124.20
22	S	312	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
22	s	312	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
25	S	302	CHL	O2D-CGD-CBD	2.38	115.50	111.27
25	s	302	CHL	O2D-CGD-CBD	2.38	115.50	111.27
22	B	613	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
25	Y	601	CHL	C3B-C4B-NB	-2.38	108.31	110.52
25	y	601	CHL	C3B-C4B-NB	-2.38	108.31	110.52
22	B	609	CLA	C4B-CHC-C1C	-2.38	120.69	126.34
24	F	101	HEM	CAC-C3C-C4C	2.38	130.64	124.90
22	D	404	CLA	CHD-C4C-NC	2.38	127.95	124.20
22	b	605	CLA	CMA-C3A-C4A	-2.38	105.39	111.77
22	3	304	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
22	7	304	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
25	1	605	CHL	C2A-C3A-C4A	2.38	104.82	101.78
25	5	605	CHL	C2A-C3A-C4A	2.38	104.82	101.78
22	c	507	CLA	CHC-C4B-C3B	-2.38	117.14	127.71
22	S	312	CLA	OBD-CAD-C3D	-2.38	122.80	128.52
22	s	312	CLA	OBD-CAD-C3D	-2.38	122.80	128.52
22	4	301	CLA	CHD-C4C-NC	2.38	127.95	124.20
22	8	301	CLA	CHD-C4C-NC	2.38	127.95	124.20
22	B	601	CLA	C4A-NA-C1A	-2.38	105.64	106.71
25	G	607	CHL	CGD-CBD-CAD	-2.37	103.05	110.73
25	g	607	CHL	CGD-CBD-CAD	-2.37	103.05	110.73
22	2	609	CLA	CED-O2D-CGD	2.37	121.31	115.94
22	6	609	CLA	CED-O2D-CGD	2.37	121.31	115.94
22	G	610	CLA	CMA-C3A-C4A	-2.37	105.39	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	610	CLA	CMA-C3A-C4A	-2.37	105.39	111.77
22	b	607	CLA	CHC-C4B-C3B	-2.37	117.16	127.71
22	C	512	CLA	CHA-C1A-NA	-2.37	120.97	126.40
22	D	404	CLA	OBD-CAD-C3D	-2.37	122.81	128.52
22	b	612	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
22	A	405	CLA	C4A-NA-C1A	-2.37	105.64	106.71
22	c	506	CLA	C4B-CHC-C1C	-2.37	120.72	126.34
25	4	302	CHL	O1D-CGD-CBD	-2.37	119.64	124.48
25	8	302	CHL	O1D-CGD-CBD	-2.37	119.64	124.48
25	R	304	CHL	CHB-C1B-NB	2.37	126.77	124.26
25	r	304	CHL	CHB-C1B-NB	2.37	126.77	124.26
22	S	304	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
22	s	304	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
22	b	614	CLA	OBD-CAD-C3D	-2.37	122.83	128.52
22	C	503	CLA	CED-O2D-CGD	2.37	121.29	115.94
25	G	609	CHL	C3B-C4B-NB	-2.36	108.32	110.52
25	g	609	CHL	C3B-C4B-NB	-2.36	108.32	110.52
22	d	404	CLA	OBD-CAD-C3D	-2.36	122.83	128.52
22	N	610	CLA	CHC-C1C-C2C	-2.36	120.16	126.73
22	n	610	CLA	CHC-C1C-C2C	-2.36	120.16	126.73
22	d	403	CLA	CMA-C3A-C2A	-2.36	104.29	113.83
25	N	605	CHL	C2B-C1B-NB	-2.36	108.65	110.23
25	n	605	CHL	C2B-C1B-NB	-2.36	108.65	110.23
22	A	402	CLA	CHC-C4B-C3B	-2.36	117.19	127.71
25	Y	601	CHL	O1D-CGD-CBD	-2.36	119.65	124.48
25	y	601	CHL	O1D-CGD-CBD	-2.36	119.65	124.48
22	c	504	CLA	CHD-C4C-NC	2.36	127.93	124.20
22	c	512	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
22	B	610	CLA	C4D-CHA-C1A	-2.36	118.37	121.25
22	d	404	CLA	CHD-C4C-NC	2.36	127.93	124.20
23	d	402	PHO	CBA-CAA-C2A	-2.36	106.91	113.81
25	3	309	CHL	C2B-C1B-NB	-2.36	108.65	110.23
25	7	309	CHL	C2B-C1B-NB	-2.36	108.65	110.23
22	N	613	CLA	CBB-CAB-C3B	-2.36	115.87	127.62
22	n	613	CLA	CBB-CAB-C3B	-2.36	115.87	127.62
22	S	313	CLA	CED-O2D-CGD	2.36	121.28	115.94
22	s	313	CLA	CED-O2D-CGD	2.36	121.28	115.94
22	G	610	CLA	CHC-C1C-C2C	-2.36	120.17	126.73
22	g	610	CLA	CHC-C1C-C2C	-2.36	120.17	126.73
24	e	101	HEM	CHC-C1C-NC	2.36	126.99	124.44
22	R	311	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
22	r	311	CLA	O2D-CGD-O1D	-2.36	119.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	602	CLA	CMA-C3A-C2A	-2.36	104.31	113.83
22	5	602	CLA	CMA-C3A-C2A	-2.36	104.31	113.83
22	c	510	CLA	CHA-C1A-NA	-2.36	120.99	126.40
22	c	511	CLA	CGD-CBD-CAD	-2.36	103.09	110.73
22	c	502	CLA	CED-O2D-CGD	2.36	121.27	115.94
22	C	508	CLA	C4B-CHC-C1C	-2.36	120.75	126.34
25	R	305	CHL	CHC-C4B-NB	2.36	126.75	124.26
25	r	305	CHL	CHC-C4B-NB	2.36	126.75	124.26
22	C	506	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
22	B	607	CLA	CHA-C1A-NA	-2.35	121.00	126.40
22	c	506	CLA	CHC-C4B-C3B	-2.35	117.24	127.71
25	N	601	CHL	CHB-C1B-NB	2.35	126.75	124.26
25	n	601	CHL	CHB-C1B-NB	2.35	126.75	124.26
22	3	312	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	7	312	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	c	511	CLA	CMD-C2D-C3D	2.35	133.03	127.61
22	B	607	CLA	CHC-C4B-C3B	-2.35	117.25	127.71
22	G	612	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
22	g	612	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
25	Y	606	CHL	CAA-C2A-C3A	-2.35	106.34	112.78
25	y	606	CHL	CAA-C2A-C3A	-2.35	106.34	112.78
22	3	311	CLA	CHD-C4C-NC	2.35	127.91	124.20
22	4	303	CLA	CHD-C4C-NC	2.35	127.91	124.20
22	7	311	CLA	CHD-C4C-NC	2.35	127.91	124.20
22	8	303	CLA	CHD-C4C-NC	2.35	127.91	124.20
22	C	507	CLA	CHC-C4B-C3B	-2.35	117.26	127.71
22	N	611	CLA	CHC-C4B-C3B	-2.35	117.26	127.71
22	n	611	CLA	CHC-C4B-C3B	-2.35	117.26	127.71
22	N	612	CLA	CHC-C4B-C3B	-2.35	117.26	127.71
22	n	612	CLA	CHC-C4B-C3B	-2.35	117.26	127.71
22	d	403	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
22	B	611	CLA	CHC-C4B-C3B	-2.35	117.27	127.71
22	4	305	CLA	CHD-C4C-NC	2.35	127.90	124.20
22	8	305	CLA	CHD-C4C-NC	2.35	127.90	124.20
22	C	510	CLA	CHA-C1A-NA	-2.35	121.02	126.40
22	R	309	CLA	C4D-CHA-C1A	-2.35	118.39	121.25
22	r	309	CLA	C4D-CHA-C1A	-2.35	118.39	121.25
22	C	504	CLA	C3B-C4B-NB	2.35	112.69	110.52
22	a	403	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
22	C	511	CLA	C4D-CHA-C1A	-2.35	118.39	121.25
22	1	602	CLA	OBD-CAD-C3D	-2.34	122.88	128.52
22	5	602	CLA	OBD-CAD-C3D	-2.34	122.88	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	607	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
25	1	608	CHL	CHB-C1B-NB	2.34	126.74	124.26
25	5	608	CHL	CHB-C1B-NB	2.34	126.74	124.26
25	N	608	CHL	O2A-CGA-O1A	-2.34	117.46	123.30
25	n	608	CHL	O2A-CGA-O1A	-2.34	117.46	123.30
22	S	311	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
22	s	311	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
25	N	609	CHL	C3B-C4B-NB	-2.34	108.34	110.52
25	n	609	CHL	C3B-C4B-NB	-2.34	108.34	110.52
22	b	610	CLA	OBD-CAD-C3D	-2.34	122.88	128.52
22	b	608	CLA	OBD-CAD-C3D	-2.34	122.89	128.52
22	Y	612	CLA	OBD-CAD-C3D	-2.34	122.89	128.52
22	y	612	CLA	OBD-CAD-C3D	-2.34	122.89	128.52
22	S	305	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
22	s	305	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
22	b	613	CLA	CHD-C4C-NC	2.34	127.89	124.20
22	S	305	CLA	CHC-C4B-C3B	-2.34	117.30	127.71
22	s	305	CLA	CHC-C4B-C3B	-2.34	117.30	127.71
22	Y	603	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
22	y	603	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
22	C	510	CLA	C4B-CHC-C1C	-2.34	120.79	126.34
22	B	606	CLA	C3B-C4B-NB	2.34	112.69	110.52
22	2	611	CLA	C4D-CHA-C1A	-2.34	118.40	121.25
22	6	611	CLA	C4D-CHA-C1A	-2.34	118.40	121.25
22	B	606	CLA	CHD-C4C-NC	2.34	127.89	124.20
22	B	614	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
22	N	612	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
22	n	612	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
22	2	611	CLA	CAC-C3C-C2C	-2.34	123.53	127.53
22	6	611	CLA	CAC-C3C-C2C	-2.34	123.53	127.53
22	c	508	CLA	CGD-CBD-CAD	-2.34	103.17	110.73
22	a	402	CLA	CHA-C1A-NA	-2.34	121.05	126.40
22	b	615	CLA	CHB-C1B-C2B	-2.34	120.64	127.24
22	2	612	CLA	CHD-C4C-NC	2.34	127.89	124.20
22	6	612	CLA	CHD-C4C-NC	2.34	127.89	124.20
22	c	512	CLA	CHC-C4B-C3B	-2.34	117.32	127.71
22	N	604	CLA	CHC-C4B-C3B	-2.34	117.32	127.71
22	n	604	CLA	CHC-C4B-C3B	-2.34	117.32	127.71
25	R	306	CHL	C2B-C1B-NB	-2.33	108.67	110.23
25	r	306	CHL	C2B-C1B-NB	-2.33	108.67	110.23
22	b	610	CLA	CAC-C3C-C2C	-2.33	123.54	127.53
22	d	401	CLA	C4A-NA-C1A	-2.33	105.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	613	CLA	CED-O2D-CGD	2.33	121.21	115.94
25	3	308	CHL	CHB-C1B-NB	2.33	126.73	124.26
25	7	308	CHL	CHB-C1B-NB	2.33	126.73	124.26
22	B	616	CLA	CMC-C2C-C3C	2.33	132.45	126.12
22	B	616	CLA	CMD-C2D-C1D	2.33	128.82	124.71
22	B	610	CLA	CHC-C4B-C3B	-2.33	117.34	127.71
22	R	310	CLA	C4D-CHA-C1A	-2.33	118.41	121.25
22	r	310	CLA	C4D-CHA-C1A	-2.33	118.41	121.25
25	2	605	CHL	C2A-C1A-CHA	2.33	127.92	123.85
25	6	605	CHL	C2A-C1A-CHA	2.33	127.92	123.85
22	C	505	CLA	CHD-C4C-NC	2.33	127.88	124.20
22	C	511	CLA	CMC-C2C-C3C	2.33	132.44	126.12
22	R	308	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
22	r	308	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
22	b	610	CLA	CHC-C4B-C3B	-2.33	117.35	127.71
22	b	603	CLA	C3B-C4B-NB	2.33	112.67	110.52
22	1	611	CLA	CHD-C4C-NC	2.33	127.87	124.20
22	5	611	CLA	CHD-C4C-NC	2.33	127.87	124.20
22	B	616	CLA	CMB-C2B-C1B	2.33	128.91	125.37
25	S	308	CHL	CAA-CBA-CGA	2.33	118.68	112.51
25	s	308	CHL	CAA-CBA-CGA	2.33	118.68	112.51
25	G	609	CHL	C2B-C1B-NB	-2.33	108.67	110.23
25	g	609	CHL	C2B-C1B-NB	-2.33	108.67	110.23
22	d	404	CLA	CED-O2D-CGD	2.33	121.20	115.94
22	S	311	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
22	s	311	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
22	S	312	CLA	C3C-C4C-NC	2.33	113.18	110.57
22	s	312	CLA	C3C-C4C-NC	2.33	113.18	110.57
22	4	311	CLA	CHD-C4C-NC	2.33	127.87	124.20
22	8	311	CLA	CHD-C4C-NC	2.33	127.87	124.20
25	Y	605	CHL	C2A-C3A-C4A	2.33	104.75	101.78
25	y	605	CHL	C2A-C3A-C4A	2.33	104.75	101.78
22	R	307	CLA	CGD-CBD-CAD	-2.33	103.20	110.73
22	r	307	CLA	CGD-CBD-CAD	-2.33	103.20	110.73
22	A	403	CLA	CMD-C2D-C3D	2.33	132.96	127.61
25	4	302	CHL	CHD-C1D-ND	-2.33	122.32	124.45
25	8	302	CHL	CHD-C1D-ND	-2.33	122.32	124.45
22	a	405	CLA	CED-O2D-CGD	2.32	121.19	115.94
22	S	309	CLA	CHC-C4B-C3B	-2.32	117.38	127.71
22	s	309	CLA	CHC-C4B-C3B	-2.32	117.38	127.71
22	N	613	CLA	CHC-C4B-C3B	-2.32	117.38	127.71
22	n	613	CLA	CHC-C4B-C3B	-2.32	117.38	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	512	CLA	CHA-C1A-NA	-2.32	121.08	126.40
22	A	403	CLA	CHB-C1B-C2B	-2.32	120.68	127.24
25	G	607	CHL	O1D-CGD-CBD	-2.32	119.73	124.48
25	g	607	CHL	O1D-CGD-CBD	-2.32	119.73	124.48
22	4	311	CLA	C4D-CHA-C1A	-2.32	118.42	121.25
22	8	311	CLA	C4D-CHA-C1A	-2.32	118.42	121.25
22	1	614	CLA	CMD-C2D-C3D	2.32	132.95	127.61
22	5	614	CLA	CMD-C2D-C3D	2.32	132.95	127.61
22	G	604	CLA	CHD-C4C-NC	2.32	127.86	124.20
22	g	604	CLA	CHD-C4C-NC	2.32	127.86	124.20
22	3	314	CLA	C4D-CHA-C1A	-2.32	118.43	121.25
22	7	314	CLA	C4D-CHA-C1A	-2.32	118.43	121.25
22	G	603	CLA	C4A-NA-C1A	-2.32	105.66	106.71
22	g	603	CLA	C4A-NA-C1A	-2.32	105.66	106.71
24	F	101	HEM	CHB-C1B-NB	2.32	127.23	124.37
24	F	101	HEM	C3D-C4D-ND	-2.32	107.59	110.17
22	S	301	CLA	CHD-C4C-NC	2.32	127.86	124.20
22	C	507	CLA	CAC-C3C-C2C	-2.32	123.57	127.53
22	C	512	CLA	CGD-CBD-CAD	-2.32	103.23	110.73
22	b	611	CLA	C4D-CHA-C1A	-2.32	118.43	121.25
22	c	507	CLA	C4D-CHA-C1A	-2.32	118.43	121.25
22	N	612	CLA	C4D-CHA-C1A	-2.31	118.43	121.25
22	n	612	CLA	C4D-CHA-C1A	-2.31	118.43	121.25
22	c	505	CLA	CHD-C4C-NC	2.31	127.85	124.20
22	c	507	CLA	C3B-C4B-NB	2.31	112.66	110.52
22	c	503	CLA	CHC-C4B-C3B	-2.31	117.42	127.71
22	B	601	CLA	CHC-C1C-C2C	-2.31	120.31	126.73
22	B	603	CLA	CGD-CBD-CAD	-2.31	103.25	110.73
22	b	608	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
25	3	302	CHL	CHD-C1D-ND	-2.31	122.33	124.45
25	7	302	CHL	CHD-C1D-ND	-2.31	122.33	124.45
25	S	306	CHL	C2B-C1B-NB	-2.31	108.68	110.23
25	s	306	CHL	C2B-C1B-NB	-2.31	108.68	110.23
25	N	607	CHL	C2A-C1A-CHA	2.31	127.90	123.86
25	n	607	CHL	C2A-C1A-CHA	2.31	127.90	123.86
22	A	405	CLA	CHC-C4B-C3B	-2.31	117.44	127.71
24	F	101	HEM	C4C-NC-C1C	2.31	107.61	105.35
22	c	510	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	c	509	CLA	CGD-CBD-CAD	-2.31	103.26	110.73
22	4	310	CLA	CED-O2D-CGD	2.31	121.16	115.94
22	8	310	CLA	CED-O2D-CGD	2.31	121.16	115.94
22	1	612	CLA	CHD-C4C-NC	2.31	127.84	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	612	CLA	CHD-C4C-NC	2.31	127.84	124.20
22	1	604	CLA	CHC-C4B-C3B	-2.31	117.44	127.71
22	5	604	CLA	CHC-C4B-C3B	-2.31	117.44	127.71
25	G	606	CHL	CAA-C2A-C3A	-2.31	106.46	112.78
25	g	606	CHL	CAA-C2A-C3A	-2.31	106.46	112.78
22	B	614	CLA	OBD-CAD-C3D	-2.31	122.97	128.52
22	1	613	CLA	CHD-C4C-NC	2.31	127.84	124.20
22	5	613	CLA	CHD-C4C-NC	2.31	127.84	124.20
25	Y	606	CHL	O1D-CGD-CBD	-2.31	119.77	124.48
25	y	606	CHL	O1D-CGD-CBD	-2.31	119.77	124.48
22	S	314	CLA	CHC-C4B-C3B	-2.31	117.45	127.71
22	s	314	CLA	CHC-C4B-C3B	-2.31	117.45	127.71
22	S	310	CLA	CAA-CBA-CGA	2.31	118.63	112.51
22	s	310	CLA	CAA-CBA-CGA	2.31	118.63	112.51
22	B	606	CLA	CMC-C2C-C1C	2.30	128.55	125.04
22	R	307	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	r	307	CLA	CHD-C4C-NC	2.30	127.83	124.20
25	2	606	CHL	CAA-C2A-C3A	-2.30	106.47	112.78
25	6	606	CHL	CAA-C2A-C3A	-2.30	106.47	112.78
22	S	301	CLA	CMC-C2C-C1C	2.30	128.55	125.04
22	D	403	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	3	304	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	7	304	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	2	613	CLA	C4D-CHA-C1A	-2.30	118.45	121.25
22	6	613	CLA	C4D-CHA-C1A	-2.30	118.45	121.25
22	1	602	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	5	602	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	N	602	CLA	OBD-CAD-C3D	-2.30	122.98	128.52
22	n	602	CLA	OBD-CAD-C3D	-2.30	122.98	128.52
22	b	602	CLA	CHC-C4B-C3B	-2.30	117.48	127.71
22	3	313	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	7	313	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	b	607	CLA	CGD-CBD-CAD	-2.30	103.29	110.73
22	3	305	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	7	305	CLA	CHD-C4C-NC	2.30	127.83	124.20
25	Y	605	CHL	O1D-CGD-CBD	-2.30	119.78	124.48
25	y	605	CHL	O1D-CGD-CBD	-2.30	119.78	124.48
22	b	610	CLA	CMC-C2C-C3C	2.30	132.36	126.12
22	c	508	CLA	CHC-C4B-C3B	-2.30	117.49	127.71
25	G	607	CHL	C2B-C1B-NB	-2.30	108.69	110.23
25	g	607	CHL	C2B-C1B-NB	-2.30	108.69	110.23
22	Y	613	CLA	CMA-C3A-C4A	-2.30	105.60	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	y	613	CLA	CMA-C3A-C4A	-2.30	105.60	111.77
22	R	308	CLA	CHC-C1C-C2C	-2.30	120.35	126.73
22	r	308	CLA	CHC-C1C-C2C	-2.30	120.35	126.73
22	D	401	CLA	CHA-C1A-NA	-2.30	121.14	126.40
22	B	612	CLA	C4D-CHA-C1A	-2.30	118.45	121.25
25	4	302	CHL	CAC-C3C-C4C	2.30	127.79	124.81
25	8	302	CHL	CAC-C3C-C4C	2.30	127.79	124.81
22	3	314	CLA	CHD-C4C-NC	2.29	127.82	124.20
22	7	314	CLA	CHD-C4C-NC	2.29	127.82	124.20
22	4	301	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
22	8	301	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
22	2	612	CLA	CMC-C2C-C1C	2.29	128.53	125.04
22	6	612	CLA	CMC-C2C-C1C	2.29	128.53	125.04
22	Y	610	CLA	CHC-C4B-C3B	-2.29	117.51	127.71
22	y	610	CLA	CHC-C4B-C3B	-2.29	117.51	127.71
22	b	614	CLA	CHA-C1A-NA	-2.29	121.15	126.40
25	G	608	CHL	CAA-CBA-CGA	2.29	118.59	112.51
25	g	608	CHL	CAA-CBA-CGA	2.29	118.59	112.51
22	C	505	CLA	C4B-CHC-C1C	-2.29	120.91	126.34
22	R	303	CLA	CHC-C4B-C3B	-2.29	117.53	127.71
22	r	303	CLA	CHC-C4B-C3B	-2.29	117.53	127.71
22	s	301	CLA	C4A-NA-C1A	-2.29	105.68	106.71
22	N	613	CLA	CMB-C2B-C1B	2.29	128.85	125.37
22	n	613	CLA	CMB-C2B-C1B	2.29	128.85	125.37
22	C	510	CLA	CGD-CBD-CAD	-2.29	103.33	110.73
22	b	602	CLA	C4B-CHC-C1C	-2.28	120.92	126.34
22	Y	613	CLA	CHC-C4B-C3B	-2.28	117.55	127.71
22	y	613	CLA	CHC-C4B-C3B	-2.28	117.55	127.71
22	B	605	CLA	CMB-C2B-C1B	2.28	128.85	125.37
22	Y	603	CLA	CBB-CAB-C3B	-2.28	116.26	127.62
22	y	603	CLA	CBB-CAB-C3B	-2.28	116.26	127.62
22	B	614	CLA	CMB-C2B-C1B	2.28	128.84	125.37
25	1	607	CHL	CHB-C1B-NB	2.28	126.67	124.26
25	5	607	CHL	CHB-C1B-NB	2.28	126.67	124.26
22	R	303	CLA	CBB-CAB-C3B	-2.28	116.27	127.62
22	r	303	CLA	CBB-CAB-C3B	-2.28	116.27	127.62
22	G	611	CLA	CHC-C4B-C3B	-2.28	117.56	127.71
22	g	611	CLA	CHC-C4B-C3B	-2.28	117.56	127.71
25	S	308	CHL	O2D-CGD-CBD	2.28	115.32	111.27
25	s	308	CHL	O2D-CGD-CBD	2.28	115.32	111.27
22	G	611	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
22	g	611	CLA	O1D-CGD-CBD	-2.28	119.81	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	614	CLA	CMC-C2C-C1C	2.28	128.51	125.04
22	5	614	CLA	CMC-C2C-C1C	2.28	128.51	125.04
22	N	614	CLA	CHC-C4B-C3B	-2.28	117.56	127.71
22	n	614	CLA	CHC-C4B-C3B	-2.28	117.56	127.71
25	S	302	CHL	C3B-C4B-NB	-2.28	108.40	110.52
25	s	302	CHL	C3B-C4B-NB	-2.28	108.40	110.52
22	B	608	CLA	C4B-CHC-C1C	-2.28	120.93	126.34
22	c	507	CLA	OBD-CAD-C3D	-2.28	123.03	128.52
22	2	602	CLA	CHD-C4C-NC	2.28	127.80	124.20
22	6	602	CLA	CHD-C4C-NC	2.28	127.80	124.20
22	Y	603	CLA	CMC-C2C-C1C	2.28	128.51	125.04
22	y	603	CLA	CMC-C2C-C1C	2.28	128.51	125.04
22	1	611	CLA	CHC-C4B-C3B	-2.28	117.57	127.71
22	5	611	CLA	CHC-C4B-C3B	-2.28	117.57	127.71
22	c	501	CLA	CHD-C4C-NC	2.28	127.79	124.20
22	B	610	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
22	Y	603	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
22	y	603	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
22	c	504	CLA	CHC-C4B-C3B	-2.28	117.59	127.71
22	B	613	CLA	CHA-C1A-NA	-2.28	121.19	126.40
22	b	610	CLA	CHA-C1A-NA	-2.28	121.19	126.40
22	a	402	CLA	CHC-C4B-C3B	-2.28	117.59	127.71
22	Y	603	CLA	CHA-C1A-NA	-2.27	121.19	126.40
22	y	603	CLA	CHA-C1A-NA	-2.27	121.19	126.40
25	N	606	CHL	CHB-C1B-NB	2.27	126.67	124.26
25	n	606	CHL	CHB-C1B-NB	2.27	126.67	124.26
22	S	305	CLA	C4B-CHC-C1C	-2.27	120.94	126.34
22	s	305	CLA	C4B-CHC-C1C	-2.27	120.94	126.34
22	2	604	CLA	CHD-C4C-NC	2.27	127.78	124.20
22	6	604	CLA	CHD-C4C-NC	2.27	127.78	124.20
22	c	512	CLA	CMC-C2C-C3C	2.27	132.29	126.12
22	B	616	CLA	CHA-C1A-NA	-2.27	121.19	126.40
22	1	604	CLA	CHD-C4C-NC	2.27	127.78	124.20
22	5	604	CLA	CHD-C4C-NC	2.27	127.78	124.20
22	1	612	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
22	5	612	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
25	G	601	CHL	O2A-CGA-O1A	-2.27	117.64	123.30
25	g	601	CHL	O2A-CGA-O1A	-2.27	117.64	123.30
22	Y	602	CLA	OBD-CAD-C3D	-2.27	123.05	128.52
22	y	602	CLA	OBD-CAD-C3D	-2.27	123.05	128.52
22	1	614	CLA	CHA-C1A-NA	-2.27	121.20	126.40
22	5	614	CLA	CHA-C1A-NA	-2.27	121.20	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	603	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
22	n	603	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
22	Y	603	CLA	CHC-C4B-C3B	-2.27	117.61	127.71
22	y	603	CLA	CHC-C4B-C3B	-2.27	117.61	127.71
22	G	603	CLA	CHA-C1A-NA	-2.27	121.20	126.40
22	g	603	CLA	CHA-C1A-NA	-2.27	121.20	126.40
22	R	309	CLA	CHC-C4B-C3B	-2.27	117.62	127.71
22	r	309	CLA	CHC-C4B-C3B	-2.27	117.62	127.71
22	C	503	CLA	CBB-CAB-C3B	-2.27	116.33	127.62
25	4	308	CHL	C2B-C1B-NB	-2.27	108.71	110.23
25	8	308	CHL	C2B-C1B-NB	-2.27	108.71	110.23
22	c	502	CLA	CMB-C2B-C1B	2.27	128.82	125.37
22	R	311	CLA	CHC-C4B-C3B	-2.27	117.62	127.71
22	r	311	CLA	CHC-C4B-C3B	-2.27	117.62	127.71
22	B	610	CLA	CHA-C1A-NA	-2.27	121.20	126.40
22	C	509	CLA	C4D-CHA-C1A	-2.27	118.49	121.25
22	b	604	CLA	CBB-CAB-C3B	-2.27	116.34	127.62
22	c	502	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
22	a	405	CLA	CHD-C4C-NC	2.27	127.78	124.20
25	3	301	CHL	CAA-CBA-CGA	2.27	118.53	112.51
25	7	301	CHL	CAA-CBA-CGA	2.27	118.53	112.51
22	a	403	CLA	CAA-CBA-CGA	2.27	118.52	112.51
25	G	607	CHL	CHA-C1A-NA	-2.27	121.21	126.40
25	g	607	CHL	CHA-C1A-NA	-2.27	121.21	126.40
25	4	302	CHL	C2B-C1B-NB	-2.27	108.71	110.23
25	8	302	CHL	C2B-C1B-NB	-2.27	108.71	110.23
22	C	505	CLA	CHC-C4B-C3B	-2.27	117.63	127.71
25	4	309	CHL	CAA-CBA-CGA	2.26	118.51	112.51
25	8	309	CHL	CAA-CBA-CGA	2.26	118.51	112.51
22	A	405	CLA	CED-O2D-CGD	2.26	121.06	115.94
22	N	602	CLA	CHC-C4B-C3B	-2.26	117.65	127.71
22	n	602	CLA	CHC-C4B-C3B	-2.26	117.65	127.71
22	a	405	CLA	CMC-C2C-C1C	2.26	128.48	125.04
22	S	312	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
22	s	312	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
22	G	613	CLA	CHC-C4B-C3B	-2.26	117.65	127.71
22	g	613	CLA	CHC-C4B-C3B	-2.26	117.65	127.71
22	C	506	CLA	CHC-C4B-C3B	-2.26	117.65	127.71
22	d	401	CLA	CBB-CAB-C3B	-2.26	116.37	127.62
22	3	305	CLA	CHC-C4B-C3B	-2.26	117.65	127.71
22	7	305	CLA	CHC-C4B-C3B	-2.26	117.65	127.71
22	C	511	CLA	CAA-C2A-C3A	-2.26	106.59	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	615	CLA	C4B-CHC-C1C	-2.26	120.98	126.34
22	4	311	CLA	CMC-C2C-C3C	2.26	132.25	126.12
22	8	311	CLA	CMC-C2C-C3C	2.26	132.25	126.12
22	3	313	CLA	CMB-C2B-C1B	2.26	128.81	125.37
22	7	313	CLA	CMB-C2B-C1B	2.26	128.81	125.37
25	1	615	CHL	O1D-CGD-CBD	-2.26	119.86	124.48
25	5	615	CHL	O1D-CGD-CBD	-2.26	119.86	124.48
22	B	605	CLA	CHD-C4C-NC	2.26	127.76	124.20
25	G	608	CHL	C3B-C4B-NB	-2.26	108.42	110.52
25	g	608	CHL	C3B-C4B-NB	-2.26	108.42	110.52
25	N	606	CHL	O2A-CGA-O1A	-2.26	117.67	123.30
25	n	606	CHL	O2A-CGA-O1A	-2.26	117.67	123.30
25	G	601	CHL	C3A-C2A-C1A	2.26	104.72	101.34
25	g	601	CHL	C3A-C2A-C1A	2.26	104.72	101.34
22	D	404	CLA	CHC-C4B-C3B	-2.26	117.68	127.71
22	Y	612	CLA	C4B-CHC-C1C	-2.26	120.99	126.34
22	y	612	CLA	C4B-CHC-C1C	-2.26	120.99	126.34
25	2	605	CHL	C3B-C4B-NB	-2.26	108.42	110.52
25	6	605	CHL	C3B-C4B-NB	-2.26	108.42	110.52
24	F	101	HEM	CHD-C1D-ND	2.25	126.87	124.42
22	C	506	CLA	CBB-CAB-C3B	-2.25	116.40	127.62
23	a	404	PHO	O2D-CGD-O1D	-2.25	119.43	123.84
22	R	307	CLA	CMB-C2B-C1B	2.25	128.80	125.37
22	r	307	CLA	CMB-C2B-C1B	2.25	128.80	125.37
22	Y	613	CLA	CHA-C1A-NA	-2.25	121.24	126.40
22	y	613	CLA	CHA-C1A-NA	-2.25	121.24	126.40
22	B	607	CLA	C4B-CHC-C1C	-2.25	121.00	126.34
22	b	602	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
25	R	304	CHL	CAA-CBA-CGA	2.25	118.48	112.51
25	r	304	CHL	CAA-CBA-CGA	2.25	118.48	112.51
22	c	512	CLA	CMB-C2B-C1B	2.25	128.80	125.37
22	b	613	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
22	Y	612	CLA	C3B-C4B-NB	2.25	112.60	110.52
22	y	612	CLA	C3B-C4B-NB	2.25	112.60	110.52
25	G	605	CHL	C2A-C1A-CHA	2.25	127.78	123.85
25	g	605	CHL	C2A-C1A-CHA	2.25	127.78	123.85
22	b	606	CLA	CMC-C2C-C3C	2.25	132.23	126.12
22	b	603	CLA	CED-O2D-CGD	2.25	121.03	115.94
22	C	504	CLA	C4B-CHC-C1C	-2.25	121.00	126.34
22	B	605	CLA	CMA-C3A-C4A	-2.25	105.73	111.77
22	3	304	CLA	C3B-C4B-NB	2.25	112.60	110.52
22	7	304	CLA	C3B-C4B-NB	2.25	112.60	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	603	CLA	CHC-C4B-C3B	-2.25	117.70	127.71
22	n	603	CLA	CHC-C4B-C3B	-2.25	117.70	127.71
22	S	309	CLA	CMD-C2D-C3D	2.25	132.79	127.61
22	s	309	CLA	CMD-C2D-C3D	2.25	132.79	127.61
22	1	614	CLA	CMB-C2B-C1B	2.25	128.79	125.37
22	5	614	CLA	CMB-C2B-C1B	2.25	128.79	125.37
25	G	606	CHL	O1D-CGD-CBD	-2.25	119.88	124.48
25	g	606	CHL	O1D-CGD-CBD	-2.25	119.88	124.48
22	4	304	CLA	OBD-CAD-C3D	-2.25	123.11	128.52
22	8	304	CLA	OBD-CAD-C3D	-2.25	123.11	128.52
22	B	616	CLA	CGD-CBD-CAD	-2.25	103.45	110.73
25	1	608	CHL	C3B-C4B-NB	-2.25	108.43	110.52
25	5	608	CHL	C3B-C4B-NB	-2.25	108.43	110.52
22	C	507	CLA	CMC-C2C-C3C	2.25	132.22	126.12
25	R	304	CHL	O1D-CGD-CBD	-2.25	119.89	124.48
25	r	304	CHL	O1D-CGD-CBD	-2.25	119.89	124.48
23	d	402	PHO	C4B-NB-C1B	-2.25	105.35	108.83
22	C	511	CLA	CHC-C4B-C3B	-2.25	117.72	127.71
22	B	616	CLA	CHC-C4B-C3B	-2.24	117.72	127.71
22	b	614	CLA	C4B-CHC-C1C	-2.24	121.02	126.34
22	b	606	CLA	CHB-C1B-C2B	-2.24	120.90	127.24
23	d	402	PHO	CAC-C3C-C4C	2.24	129.96	124.27
22	c	502	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
22	B	605	CLA	CHC-C4B-C3B	-2.24	117.74	127.71
22	c	507	CLA	CED-O2D-CGD	2.24	121.01	115.94
22	G	603	CLA	CHC-C4B-C3B	-2.24	117.74	127.71
22	g	603	CLA	CHC-C4B-C3B	-2.24	117.74	127.71
22	B	610	CLA	CHD-C4C-NC	2.24	127.74	124.20
22	B	612	CLA	CMB-C2B-C1B	2.24	128.78	125.37
22	4	303	CLA	CHC-C4B-C3B	-2.24	117.74	127.71
22	8	303	CLA	CHC-C4B-C3B	-2.24	117.74	127.71
22	a	405	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
22	N	604	CLA	C4A-NA-C1A	-2.24	105.70	106.71
22	n	604	CLA	C4A-NA-C1A	-2.24	105.70	106.71
22	G	610	CLA	CMA-C3A-C2A	-2.24	104.79	113.83
22	g	610	CLA	CMA-C3A-C2A	-2.24	104.79	113.83
22	C	509	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
22	C	509	CLA	CHC-C4B-C3B	-2.24	117.75	127.71
22	4	304	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
22	8	304	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
22	C	507	CLA	CED-O2D-CGD	2.24	121.00	115.94
25	4	308	CHL	CAA-CBA-CGA	2.24	118.44	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	308	CHL	CAA-CBA-CGA	2.24	118.44	112.51
22	d	404	CLA	CMB-C2B-C1B	2.24	128.78	125.37
23	D	402	PHO	CBA-CAA-C2A	-2.24	107.28	113.81
23	A	404	PHO	CBA-CAA-C2A	-2.24	107.28	113.81
22	C	507	CLA	OBD-CAD-C3D	-2.24	123.14	128.52
22	B	609	CLA	CHC-C4B-C3B	-2.24	117.77	127.71
22	4	301	CLA	C4A-NA-C1A	-2.24	105.70	106.71
22	8	301	CLA	C4A-NA-C1A	-2.24	105.70	106.71
22	4	301	CLA	CED-O2D-CGD	2.24	120.99	115.94
22	8	301	CLA	CED-O2D-CGD	2.24	120.99	115.94
25	G	607	CHL	C3B-C4B-NB	-2.23	108.44	110.52
25	g	607	CHL	C3B-C4B-NB	-2.23	108.44	110.52
22	c	505	CLA	CHC-C4B-C3B	-2.23	117.77	127.71
25	4	302	CHL	O2A-CGA-O1A	-2.23	117.73	123.30
25	8	302	CHL	O2A-CGA-O1A	-2.23	117.73	123.30
25	N	601	CHL	C2B-C1B-NB	-2.23	108.73	110.23
25	n	601	CHL	C2B-C1B-NB	-2.23	108.73	110.23
25	4	309	CHL	C2A-C3A-C4A	2.23	105.48	101.87
25	8	309	CHL	C2A-C3A-C4A	2.23	105.48	101.87
22	c	502	CLA	CBB-CAB-C3B	-2.23	116.51	127.62
22	1	612	CLA	CED-O2D-CGD	2.23	120.98	115.94
22	5	612	CLA	CED-O2D-CGD	2.23	120.98	115.94
22	2	603	CLA	CMB-C2B-C1B	2.23	128.77	125.37
22	6	603	CLA	CMB-C2B-C1B	2.23	128.77	125.37
22	C	501	CLA	C4D-CHA-C1A	-2.23	118.53	121.25
22	B	602	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
22	b	613	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
22	C	508	CLA	C3B-C4B-NB	2.23	112.58	110.52
22	S	304	CLA	CMC-C2C-C1C	2.23	128.44	125.04
22	s	304	CLA	CMC-C2C-C1C	2.23	128.44	125.04
22	c	505	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
22	B	603	CLA	CHD-C4C-NC	2.23	127.72	124.20
22	B	612	CLA	CHC-C4B-C3B	-2.23	117.80	127.71
22	1	613	CLA	CHC-C4B-C3B	-2.23	117.80	127.71
22	3	304	CLA	CHC-C4B-C3B	-2.23	117.80	127.71
22	5	613	CLA	CHC-C4B-C3B	-2.23	117.80	127.71
22	7	304	CLA	CHC-C4B-C3B	-2.23	117.80	127.71
22	N	614	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
22	n	614	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
22	4	305	CLA	CHC-C4B-C3B	-2.23	117.81	127.71
22	8	305	CLA	CHC-C4B-C3B	-2.23	117.81	127.71
23	d	402	PHO	CAA-C2A-C3A	-2.23	106.68	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	610	CLA	CGD-CBD-CAD	-2.23	103.52	110.73
22	6	610	CLA	CGD-CBD-CAD	-2.23	103.52	110.73
22	D	401	CLA	CHD-C4C-NC	2.23	127.71	124.20
22	3	310	CLA	CHC-C1C-C2C	-2.22	120.55	126.73
22	7	310	CLA	CHC-C1C-C2C	-2.22	120.55	126.73
22	d	401	CLA	CMB-C2B-C1B	2.22	128.76	125.37
22	G	611	CLA	CED-O2D-CGD	2.22	120.97	115.94
22	g	611	CLA	CED-O2D-CGD	2.22	120.97	115.94
22	Y	612	CLA	C3C-C4C-NC	2.22	113.06	110.57
22	y	612	CLA	C3C-C4C-NC	2.22	113.06	110.57
22	N	613	CLA	CHA-C1A-NA	-2.22	121.31	126.40
22	n	613	CLA	CHA-C1A-NA	-2.22	121.31	126.40
22	R	311	CLA	CGD-CBD-CAD	-2.22	103.53	110.73
22	r	311	CLA	CGD-CBD-CAD	-2.22	103.53	110.73
22	B	611	CLA	C3B-C4B-NB	2.22	112.58	110.52
25	S	308	CHL	CHB-C1B-NB	2.22	126.61	124.26
25	s	308	CHL	CHB-C1B-NB	2.22	126.61	124.26
22	b	608	CLA	CHA-C1A-NA	-2.22	121.31	126.40
22	b	614	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
22	b	604	CLA	C3C-C4C-NC	2.22	113.06	110.57
22	1	612	CLA	CHC-C4B-C3B	-2.22	117.84	127.71
22	5	612	CLA	CHC-C4B-C3B	-2.22	117.84	127.71
22	b	608	CLA	CHD-C4C-NC	2.22	127.70	124.20
25	3	301	CHL	C3B-C4B-NB	-2.22	108.46	110.52
25	7	301	CHL	C3B-C4B-NB	-2.22	108.46	110.52
22	D	401	CLA	CED-O2D-CGD	2.22	120.95	115.94
22	B	604	CLA	CGD-CBD-CAD	-2.22	103.55	110.73
22	Y	614	CLA	CED-O2D-CGD	2.22	120.95	115.94
22	y	614	CLA	CED-O2D-CGD	2.22	120.95	115.94
22	C	512	CLA	CHD-C4C-NC	2.22	127.70	124.20
22	1	603	CLA	CMC-C2C-C1C	2.22	128.42	125.04
22	5	603	CLA	CMC-C2C-C1C	2.22	128.42	125.04
22	Y	602	CLA	CHC-C4B-C3B	-2.22	117.85	127.71
22	y	602	CLA	CHC-C4B-C3B	-2.22	117.85	127.71
22	R	308	CLA	CHC-C4B-C3B	-2.22	117.85	127.71
22	r	308	CLA	CHC-C4B-C3B	-2.22	117.85	127.71
22	b	607	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
22	2	612	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
22	6	612	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
22	C	503	CLA	OBD-CAD-C3D	-2.21	123.19	128.52
22	B	606	CLA	CAA-C2A-C3A	-2.21	106.71	112.78
25	1	601	CHL	CHB-C1B-NB	2.21	126.60	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	301	CHL	CHB-C1B-NB	2.21	126.60	124.26
25	5	601	CHL	CHB-C1B-NB	2.21	126.60	124.26
25	7	301	CHL	CHB-C1B-NB	2.21	126.60	124.26
22	3	311	CLA	CHC-C4B-C3B	-2.21	117.86	127.71
22	7	311	CLA	CHC-C4B-C3B	-2.21	117.86	127.71
22	Y	613	CLA	CMC-C2C-C3C	2.21	132.13	126.12
22	y	613	CLA	CMC-C2C-C3C	2.21	132.13	126.12
22	S	304	CLA	OBD-CAD-C3D	-2.21	123.19	128.52
22	s	304	CLA	OBD-CAD-C3D	-2.21	123.19	128.52
25	N	607	CHL	C3B-C4B-NB	-2.21	108.46	110.52
25	n	607	CHL	C3B-C4B-NB	-2.21	108.46	110.52
22	1	603	CLA	CHC-C4B-C3B	-2.21	117.87	127.71
22	5	603	CLA	CHC-C4B-C3B	-2.21	117.87	127.71
22	Y	611	CLA	CHC-C4B-C3B	-2.21	117.87	127.71
22	y	611	CLA	CHC-C4B-C3B	-2.21	117.87	127.71
22	Y	612	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
22	y	612	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
22	c	510	CLA	CHC-C4B-C3B	-2.21	117.87	127.71
22	2	604	CLA	CHA-C1A-NA	-2.21	121.33	126.40
22	6	604	CLA	CHA-C1A-NA	-2.21	121.33	126.40
22	B	613	CLA	CHD-C4C-NC	2.21	127.69	124.20
22	A	402	CLA	CED-O2D-CGD	2.21	120.94	115.94
22	C	505	CLA	C4D-CHA-C1A	-2.21	118.56	121.25
22	b	611	CLA	C4B-CHC-C1C	-2.21	121.10	126.34
22	b	614	CLA	C3B-C4B-NB	2.21	112.56	110.52
22	A	403	CLA	CGD-CBD-CAD	-2.21	103.58	110.73
25	R	305	CHL	C3B-C4B-NB	-2.21	108.47	110.52
25	r	305	CHL	C3B-C4B-NB	-2.21	108.47	110.52
22	Y	612	CLA	CHA-C1A-NA	-2.21	121.34	126.40
22	y	612	CLA	CHA-C1A-NA	-2.21	121.34	126.40
22	b	611	CLA	CED-O2D-CGD	2.21	120.93	115.94
22	R	303	CLA	CMC-C2C-C3C	2.21	132.11	126.12
22	r	303	CLA	CMC-C2C-C3C	2.21	132.11	126.12
25	2	601	CHL	CHD-C1D-ND	-2.21	122.43	124.45
25	6	601	CHL	CHD-C1D-ND	-2.21	122.43	124.45
22	b	612	CLA	CED-O2D-CGD	2.20	120.92	115.94
22	b	612	CLA	CMB-C2B-C3B	2.20	131.93	126.59
22	A	405	CLA	CMC-C2C-C1C	2.20	128.40	125.04
25	2	606	CHL	CHB-C1B-NB	2.20	126.59	124.26
25	6	606	CHL	CHB-C1B-NB	2.20	126.59	124.26
22	S	312	CLA	CMC-C2C-C3C	2.20	132.10	126.12
22	s	312	CLA	CMC-C2C-C3C	2.20	132.10	126.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Y	603	CLA	CED-O2D-CGD	2.20	120.92	115.94
22	y	603	CLA	CED-O2D-CGD	2.20	120.92	115.94
22	S	314	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
22	s	314	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
22	3	303	CLA	CMA-C3A-C2A	-2.20	104.94	113.83
22	7	303	CLA	CMA-C3A-C2A	-2.20	104.94	113.83
22	D	404	CLA	CMB-C2B-C1B	2.20	128.72	125.37
22	b	608	CLA	C4D-CHA-C1A	-2.20	118.57	121.25
22	2	604	CLA	CHC-C4B-C3B	-2.20	117.92	127.71
22	6	604	CLA	CHC-C4B-C3B	-2.20	117.92	127.71
22	d	403	CLA	C4B-CHC-C1C	-2.20	121.12	126.34
22	a	405	CLA	C4D-CHA-C1A	-2.20	118.57	121.25
22	c	505	CLA	C4B-CHC-C1C	-2.20	121.12	126.34
22	b	605	CLA	C3D-C4D-CHA	-2.20	107.69	112.72
22	1	613	CLA	CBB-CAB-C3B	-2.20	116.67	127.62
22	5	613	CLA	CBB-CAB-C3B	-2.20	116.67	127.62
22	c	505	CLA	CMC-C2C-C3C	2.20	132.09	126.12
22	S	312	CLA	CBB-CAB-C3B	-2.20	116.68	127.62
22	s	312	CLA	CBB-CAB-C3B	-2.20	116.68	127.62
22	C	510	CLA	CED-O2D-CGD	2.20	120.91	115.94
25	3	301	CHL	O2A-CGA-O1A	-2.20	117.82	123.30
25	7	301	CHL	O2A-CGA-O1A	-2.20	117.82	123.30
22	1	613	CLA	C4D-CHA-C1A	-2.20	118.57	121.25
22	5	613	CLA	C4D-CHA-C1A	-2.20	118.57	121.25
22	G	612	CLA	CHC-C4B-C3B	-2.20	117.93	127.71
22	g	612	CLA	CHC-C4B-C3B	-2.20	117.93	127.71
25	4	302	CHL	CHB-C1B-NB	2.20	126.58	124.26
25	8	302	CHL	CHB-C1B-NB	2.20	126.58	124.26
22	b	601	CLA	CBB-CAB-C3B	-2.20	116.69	127.62
22	G	602	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
22	g	602	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
22	d	401	CLA	CHC-C4B-C3B	-2.20	117.94	127.71
22	C	501	CLA	C3B-C4B-NB	2.20	112.55	110.52
22	N	611	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
22	n	611	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
25	S	307	CHL	CHC-C4B-NB	2.20	126.58	124.26
25	s	307	CHL	CHC-C4B-NB	2.20	126.58	124.26
22	S	303	CLA	CHC-C4B-C3B	-2.20	117.94	127.71
22	s	303	CLA	CHC-C4B-C3B	-2.20	117.94	127.71
22	S	309	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
22	s	309	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
22	c	502	CLA	CHC-C4B-C3B	-2.20	117.94	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	606	CHL	O2D-CGD-CBD	2.19	115.17	111.27
25	n	606	CHL	O2D-CGD-CBD	2.19	115.17	111.27
22	c	501	CLA	CAA-C2A-C3A	-2.19	106.77	112.78
25	N	606	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
25	n	606	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
22	a	403	CLA	CHA-C1A-NA	-2.19	121.37	126.40
22	C	505	CLA	CMC-C2C-C3C	2.19	132.07	126.12
22	Y	602	CLA	CBB-CAB-C3B	-2.19	116.71	127.62
22	y	602	CLA	CBB-CAB-C3B	-2.19	116.71	127.62
22	G	614	CLA	CHA-C1A-NA	-2.19	121.38	126.40
22	g	614	CLA	CHA-C1A-NA	-2.19	121.38	126.40
22	3	305	CLA	CHA-C1A-NA	-2.19	121.38	126.40
22	7	305	CLA	CHA-C1A-NA	-2.19	121.38	126.40
25	R	306	CHL	CHB-C1B-NB	2.19	126.58	124.26
25	r	306	CHL	CHB-C1B-NB	2.19	126.58	124.26
25	1	608	CHL	C2B-C1B-NB	-2.19	108.76	110.23
25	5	608	CHL	C2B-C1B-NB	-2.19	108.76	110.23
24	F	101	HEM	C1B-NB-C4B	2.19	107.34	105.07
22	b	605	CLA	C4D-CHA-C1A	-2.19	118.58	121.25
22	3	303	CLA	C4D-CHA-C1A	-2.19	118.58	121.25
22	7	303	CLA	C4D-CHA-C1A	-2.19	118.58	121.25
25	1	606	CHL	O2A-CGA-O1A	-2.19	117.84	123.30
25	5	606	CHL	O2A-CGA-O1A	-2.19	117.84	123.30
22	B	605	CLA	CHA-C1A-NA	-2.19	121.38	126.40
22	2	610	CLA	CHC-C4B-C3B	-2.19	117.97	127.71
22	6	610	CLA	CHC-C4B-C3B	-2.19	117.97	127.71
22	b	604	CLA	OBD-CAD-C3D	-2.19	123.25	128.52
22	b	612	CLA	CGD-CBD-CAD	-2.19	103.64	110.73
25	3	302	CHL	CHB-C1B-NB	2.19	126.58	124.26
25	7	302	CHL	CHB-C1B-NB	2.19	126.58	124.26
22	C	503	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
25	4	307	CHL	CHB-C1B-NB	2.19	126.57	124.26
25	8	307	CHL	CHB-C1B-NB	2.19	126.57	124.26
22	d	401	CLA	CMC-C2C-C3C	2.19	132.06	126.12
22	1	603	CLA	C4D-CHA-C1A	-2.19	118.59	121.25
22	5	603	CLA	C4D-CHA-C1A	-2.19	118.59	121.25
22	B	608	CLA	CMC-C2C-C3C	2.19	132.05	126.12
22	4	310	CLA	CHC-C4B-C3B	-2.19	117.98	127.71
22	8	310	CLA	CHC-C4B-C3B	-2.19	117.98	127.71
22	3	304	CLA	CHA-C1A-NA	-2.19	121.39	126.40
22	7	304	CLA	CHA-C1A-NA	-2.19	121.39	126.40
22	S	301	CLA	CHC-C4B-C3B	-2.19	117.98	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	601	CHL	C2A-C1A-CHA	2.19	127.68	123.86
25	6	601	CHL	C2A-C1A-CHA	2.19	127.68	123.86
22	1	612	CLA	CMB-C2B-C1B	2.19	128.70	125.37
22	5	612	CLA	CMB-C2B-C1B	2.19	128.70	125.37
22	G	604	CLA	CHA-C1A-NA	-2.19	121.39	126.40
22	g	604	CLA	CHA-C1A-NA	-2.19	121.39	126.40
22	B	602	CLA	CAC-C3C-C2C	-2.18	123.79	127.53
22	C	510	CLA	CMC-C2C-C1C	2.18	128.37	125.04
22	Y	602	CLA	CGD-CBD-CAD	-2.18	103.66	110.73
22	y	602	CLA	CGD-CBD-CAD	-2.18	103.66	110.73
22	S	310	CLA	CMC-C2C-C1C	2.18	128.37	125.04
22	s	310	CLA	CMC-C2C-C1C	2.18	128.37	125.04
22	C	505	CLA	CBB-CAB-C3B	-2.18	116.76	127.62
23	D	402	PHO	CAA-C2A-C3A	-2.18	106.80	112.78
22	G	603	CLA	CBB-CAB-C3B	-2.18	116.76	127.62
22	g	603	CLA	CBB-CAB-C3B	-2.18	116.76	127.62
22	c	506	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
22	s	301	CLA	CHD-C4C-NC	2.18	127.64	124.20
24	F	101	HEM	CHD-C4C-C3C	2.18	128.99	125.26
22	G	612	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
22	g	612	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
25	2	606	CHL	CAA-CBA-CGA	2.18	118.29	112.51
25	6	606	CHL	CAA-CBA-CGA	2.18	118.29	112.51
25	1	605	CHL	C2A-C1A-CHA	2.18	127.66	123.85
25	5	605	CHL	C2A-C1A-CHA	2.18	127.66	123.85
22	c	503	CLA	CMC-C2C-C1C	2.18	128.36	125.04
22	N	603	CLA	CBB-CAB-C3B	-2.18	116.78	127.62
22	s	301	CLA	CBB-CAB-C3B	-2.18	116.78	127.62
22	n	603	CLA	CBB-CAB-C3B	-2.18	116.78	127.62
22	c	510	CLA	CED-O2D-CGD	2.18	120.87	115.94
22	1	603	CLA	CED-O2D-CGD	2.18	120.86	115.94
22	5	603	CLA	CED-O2D-CGD	2.18	120.86	115.94
22	s	301	CLA	CED-O2D-CGD	2.18	120.86	115.94
22	b	605	CLA	OBD-CAD-C3D	-2.18	123.28	128.52
25	3	306	CHL	C3B-C4B-NB	-2.18	108.50	110.52
25	7	306	CHL	C3B-C4B-NB	-2.18	108.50	110.52
25	N	605	CHL	CHB-C1B-NB	2.18	126.56	124.26
25	n	605	CHL	CHB-C1B-NB	2.18	126.56	124.26
22	R	309	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
22	r	309	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
25	G	601	CHL	O1D-CGD-CBD	-2.18	120.03	124.48
25	g	601	CHL	O1D-CGD-CBD	-2.18	120.03	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	606	CLA	CAA-CBA-CGA	2.18	118.28	112.51
22	2	612	CLA	CHC-C4B-C3B	-2.18	118.03	127.71
22	6	612	CLA	CHC-C4B-C3B	-2.18	118.03	127.71
22	D	403	CLA	C4B-CHC-C1C	-2.18	121.18	126.34
22	a	405	CLA	C4B-CHC-C1C	-2.18	121.18	126.34
25	Y	606	CHL	CHC-C4B-NB	2.18	126.56	124.26
25	y	606	CHL	CHC-C4B-NB	2.18	126.56	124.26
22	B	609	CLA	CMC-C2C-C1C	2.17	128.35	125.04
25	R	305	CHL	O2A-CGA-O1A	-2.17	117.88	123.30
25	r	305	CHL	O2A-CGA-O1A	-2.17	117.88	123.30
22	Y	614	CLA	CMC-C2C-C1C	2.17	128.35	125.04
22	y	614	CLA	CMC-C2C-C1C	2.17	128.35	125.04
22	G	604	CLA	C4B-CHC-C1C	-2.17	121.18	126.34
22	g	604	CLA	C4B-CHC-C1C	-2.17	121.18	126.34
25	N	601	CHL	O2A-CGA-O1A	-2.17	117.88	123.30
25	n	601	CHL	O2A-CGA-O1A	-2.17	117.88	123.30
22	b	614	CLA	CMB-C2B-C1B	2.17	128.68	125.37
22	C	502	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
22	B	613	CLA	CHC-C4B-C3B	-2.17	118.04	127.71
22	D	401	CLA	CHC-C4B-C3B	-2.17	118.04	127.71
22	c	505	CLA	CBB-CAB-C3B	-2.17	116.81	127.62
22	B	603	CLA	CHA-C1A-NA	-2.17	121.42	126.40
22	G	614	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
22	g	614	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
22	s	301	CLA	CMB-C2B-C1B	2.17	128.68	125.37
22	C	507	CLA	CHA-C1A-NA	-2.17	121.42	126.40
22	3	311	CLA	CGD-CBD-CAD	-2.17	103.70	110.73
22	7	311	CLA	CGD-CBD-CAD	-2.17	103.70	110.73
22	N	603	CLA	C4A-NA-C1A	-2.17	105.73	106.71
22	n	603	CLA	C4A-NA-C1A	-2.17	105.73	106.71
25	R	304	CHL	C2A-C3A-C4A	2.17	105.38	101.87
25	r	304	CHL	C2A-C3A-C4A	2.17	105.38	101.87
22	Y	612	CLA	CBB-CAB-C3B	-2.17	116.82	127.62
22	y	612	CLA	CBB-CAB-C3B	-2.17	116.82	127.62
22	4	301	CLA	CHA-C1A-NA	-2.17	121.43	126.40
22	8	301	CLA	CHA-C1A-NA	-2.17	121.43	126.40
22	b	609	CLA	CHA-C1A-NA	-2.17	121.43	126.40
22	c	506	CLA	CMC-C2C-C1C	2.17	128.34	125.04
22	c	510	CLA	CMC-C2C-C1C	2.17	128.34	125.04
25	1	601	CHL	C3B-C4B-NB	-2.17	108.50	110.52
25	5	601	CHL	C3B-C4B-NB	-2.17	108.50	110.52
25	4	307	CHL	CAA-CBA-CGA	2.17	118.26	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	307	CHL	CAA-CBA-CGA	2.17	118.26	112.51
25	Y	601	CHL	C2D-C1D-ND	2.17	111.70	110.10
25	y	601	CHL	C2D-C1D-ND	2.17	111.70	110.10
22	d	401	CLA	CHA-C1A-NA	-2.17	121.43	126.40
22	D	403	CLA	CHA-C1A-NA	-2.17	121.43	126.40
22	C	507	CLA	C4B-CHC-C1C	-2.17	121.20	126.34
22	N	604	CLA	C3B-C4B-NB	2.17	112.53	110.52
22	n	604	CLA	C3B-C4B-NB	2.17	112.53	110.52
25	Y	609	CHL	C2C-C3C-C4C	2.17	108.03	106.49
25	y	609	CHL	C2C-C3C-C4C	2.17	108.03	106.49
25	2	607	CHL	CHB-C1B-NB	2.17	126.55	124.26
25	6	607	CHL	CHB-C1B-NB	2.17	126.55	124.26
22	2	613	CLA	CED-O2D-CGD	2.17	120.84	115.94
22	6	613	CLA	CED-O2D-CGD	2.17	120.84	115.94
22	B	610	CLA	C4B-CHC-C1C	-2.17	121.20	126.34
22	3	303	CLA	CMA-C3A-C4A	-2.17	105.95	111.77
22	7	303	CLA	CMA-C3A-C4A	-2.17	105.95	111.77
22	C	502	CLA	CBB-CAB-C3B	-2.17	116.85	127.62
22	S	304	CLA	C4B-CHC-C1C	-2.16	121.20	126.34
22	s	304	CLA	C4B-CHC-C1C	-2.16	121.20	126.34
22	B	604	CLA	CAC-C3C-C2C	-2.16	123.83	127.53
22	b	610	CLA	CED-O2D-CGD	2.16	120.83	115.94
22	R	311	CLA	CBB-CAB-C3B	-2.16	116.85	127.62
22	r	311	CLA	CBB-CAB-C3B	-2.16	116.85	127.62
22	G	611	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
22	g	611	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
22	B	614	CLA	CHC-C1C-C2C	-2.16	120.72	126.73
22	2	609	CLA	CHC-C1C-C2C	-2.16	120.72	126.73
22	6	609	CLA	CHC-C1C-C2C	-2.16	120.72	126.73
22	c	507	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
22	C	507	CLA	C4A-NA-C1A	-2.16	105.73	106.71
22	G	604	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
22	g	604	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
22	R	307	CLA	CHC-C4B-C3B	-2.16	118.09	127.71
22	r	307	CLA	CHC-C4B-C3B	-2.16	118.09	127.71
22	B	607	CLA	CGD-CBD-CAD	-2.16	103.73	110.73
22	4	311	CLA	CED-O2D-CGD	2.16	120.83	115.94
22	8	311	CLA	CED-O2D-CGD	2.16	120.83	115.94
22	N	604	CLA	CBB-CAB-C3B	-2.16	116.87	127.62
22	n	604	CLA	CBB-CAB-C3B	-2.16	116.87	127.62
22	d	403	CLA	CHA-C1A-NA	-2.16	121.45	126.40
22	S	311	CLA	CHA-C1A-NA	-2.16	121.45	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	s	311	CLA	CHA-C1A-NA	-2.16	121.45	126.40
22	b	601	CLA	CHC-C4B-C3B	-2.16	118.10	127.71
22	A	405	CLA	CHD-C4C-NC	2.16	127.61	124.20
22	B	607	CLA	CHD-C4C-NC	2.16	127.60	124.20
22	4	304	CLA	CMB-C2B-C1B	2.16	128.66	125.37
22	8	304	CLA	CMB-C2B-C1B	2.16	128.66	125.37
22	c	511	CLA	CHC-C4B-C3B	-2.16	118.11	127.71
22	S	312	CLA	C4B-CHC-C1C	-2.16	121.22	126.34
22	s	312	CLA	C4B-CHC-C1C	-2.16	121.22	126.34
22	B	603	CLA	CHC-C4B-C3B	-2.16	118.11	127.71
22	3	304	CLA	CMC-C2C-C1C	2.16	128.32	125.04
22	7	304	CLA	CMC-C2C-C1C	2.16	128.32	125.04
22	G	612	CLA	CMB-C2B-C1B	2.16	128.65	125.37
22	g	612	CLA	CMB-C2B-C1B	2.16	128.65	125.37
22	3	312	CLA	CMB-C2B-C1B	2.16	128.65	125.37
22	7	312	CLA	CMB-C2B-C1B	2.16	128.65	125.37
22	2	602	CLA	CHC-C4B-C3B	-2.16	118.12	127.71
22	6	602	CLA	CHC-C4B-C3B	-2.16	118.12	127.71
22	A	403	CLA	CHA-C1A-NA	-2.16	121.46	126.40
22	A	403	CLA	CBA-CAA-C2A	2.16	120.23	113.86
25	S	307	CHL	C2B-C1B-NB	-2.16	108.79	110.23
25	s	307	CHL	C2B-C1B-NB	-2.16	108.79	110.23
25	N	601	CHL	O1D-CGD-CBD	-2.15	120.08	124.48
25	n	601	CHL	O1D-CGD-CBD	-2.15	120.08	124.48
22	3	311	CLA	C4D-CHA-C1A	-2.15	118.63	121.25
22	7	311	CLA	C4D-CHA-C1A	-2.15	118.63	121.25
22	D	401	CLA	CBB-CAB-C3B	-2.15	116.91	127.62
25	G	601	CHL	CHD-C1D-ND	-2.15	122.47	124.45
25	g	601	CHL	CHD-C1D-ND	-2.15	122.47	124.45
22	c	503	CLA	CBB-CAB-C3B	-2.15	116.91	127.62
22	3	303	CLA	CHC-C4B-C3B	-2.15	118.14	127.71
22	7	303	CLA	CHC-C4B-C3B	-2.15	118.14	127.71
22	b	602	CLA	CGD-CBD-CAD	-2.15	103.77	110.73
22	C	505	CLA	CMB-C2B-C1B	2.15	128.64	125.37
25	Y	605	CHL	CMA-C3A-C2A	-2.15	111.08	116.10
25	y	605	CHL	CMA-C3A-C2A	-2.15	111.08	116.10
22	c	508	CLA	C4B-CHC-C1C	-2.15	121.24	126.34
22	C	501	CLA	CED-O2D-CGD	2.15	120.80	115.94
22	b	601	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
25	G	608	CHL	O2A-CGA-O1A	-2.15	117.94	123.30
25	g	608	CHL	O2A-CGA-O1A	-2.15	117.94	123.30
22	3	312	CLA	CHC-C4B-C3B	-2.15	118.15	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	312	CLA	CHC-C4B-C3B	-2.15	118.15	127.71
22	1	602	CLA	CGD-CBD-CAD	-2.15	103.77	110.73
22	5	602	CLA	CGD-CBD-CAD	-2.15	103.77	110.73
22	C	505	CLA	CHA-C1A-NA	-2.15	121.48	126.40
22	3	312	CLA	CMC-C2C-C1C	2.15	128.31	125.04
22	7	312	CLA	CMC-C2C-C1C	2.15	128.31	125.04
22	B	612	CLA	C3B-C4B-NB	2.15	112.51	110.52
22	S	309	CLA	CED-O2D-CGD	2.15	120.79	115.94
22	s	309	CLA	CED-O2D-CGD	2.15	120.79	115.94
22	c	501	CLA	CGD-CBD-CAD	-2.15	103.78	110.73
22	S	311	CLA	CHC-C4B-C3B	-2.15	118.17	127.71
22	s	311	CLA	CHC-C4B-C3B	-2.15	118.17	127.71
22	S	314	CLA	CMC-C2C-C1C	2.15	128.31	125.04
22	s	314	CLA	CMC-C2C-C1C	2.15	128.31	125.04
22	2	610	CLA	CED-O2D-CGD	2.14	120.79	115.94
22	6	610	CLA	CED-O2D-CGD	2.14	120.79	115.94
22	S	309	CLA	CAC-C3C-C2C	-2.14	123.86	127.53
22	s	309	CLA	CAC-C3C-C2C	-2.14	123.86	127.53
25	4	309	CHL	C2B-C1B-NB	-2.14	108.80	110.23
25	8	309	CHL	C2B-C1B-NB	-2.14	108.80	110.23
22	N	614	CLA	C3B-C4B-NB	2.14	112.50	110.52
22	n	614	CLA	C3B-C4B-NB	2.14	112.50	110.52
22	4	305	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	8	305	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	3	314	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
22	7	314	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
25	N	601	CHL	C2A-C1A-CHA	2.14	127.61	123.86
25	n	601	CHL	C2A-C1A-CHA	2.14	127.61	123.86
22	Y	614	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	y	614	CLA	CHA-C1A-NA	-2.14	121.49	126.40
24	F	101	HEM	CHC-C1C-NC	2.14	126.76	124.44
22	Y	603	CLA	C4B-CHC-C1C	-2.14	121.26	126.34
22	y	603	CLA	C4B-CHC-C1C	-2.14	121.26	126.34
22	b	607	CLA	CHD-C4C-NC	2.14	127.58	124.20
22	R	302	CLA	CHD-C1D-C2D	-2.14	120.99	125.48
22	r	302	CLA	CHD-C1D-C2D	-2.14	120.99	125.48
22	b	613	CLA	CHA-C1A-NA	-2.14	121.50	126.40
22	B	612	CLA	CHA-C1A-NA	-2.14	121.50	126.40
22	d	404	CLA	C4D-CHA-C1A	-2.14	118.65	121.25
23	D	402	PHO	CAC-C3C-C4C	2.14	129.69	124.27
22	b	611	CLA	CHA-C1A-NA	-2.14	121.50	126.40
22	S	310	CLA	CHC-C4B-C3B	-2.14	118.20	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	s	310	CLA	CHC-C4B-C3B	-2.14	118.20	127.71
22	d	404	CLA	CHC-C4B-C3B	-2.14	118.21	127.71
25	2	608	CHL	CHA-C1A-NA	-2.14	121.51	126.40
25	6	608	CHL	CHA-C1A-NA	-2.14	121.51	126.40
22	S	313	CLA	CHA-C1A-NA	-2.14	121.51	126.40
22	s	313	CLA	CHA-C1A-NA	-2.14	121.51	126.40
22	B	614	CLA	C4D-CHA-C1A	-2.14	118.65	121.25
22	b	610	CLA	C4D-CHA-C1A	-2.14	118.65	121.25
22	N	612	CLA	CMC-C2C-C3C	2.14	131.91	126.12
22	n	612	CLA	CMC-C2C-C3C	2.14	131.91	126.12
22	N	603	CLA	CMC-C2C-C1C	2.14	128.29	125.04
22	n	603	CLA	CMC-C2C-C1C	2.14	128.29	125.04
22	N	611	CLA	CHA-C1A-NA	-2.14	121.51	126.40
22	n	611	CLA	CHA-C1A-NA	-2.14	121.51	126.40
22	1	612	CLA	CHA-C1A-NA	-2.14	121.51	126.40
22	5	612	CLA	CHA-C1A-NA	-2.14	121.51	126.40
22	S	310	CLA	O2D-CGD-O1D	-2.13	119.66	123.84
22	N	613	CLA	O2D-CGD-O1D	-2.13	119.66	123.84
22	s	310	CLA	O2D-CGD-O1D	-2.13	119.66	123.84
22	n	613	CLA	O2D-CGD-O1D	-2.13	119.66	123.84
22	C	501	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
22	G	614	CLA	C4A-NA-C1A	-2.13	105.75	106.71
22	g	614	CLA	C4A-NA-C1A	-2.13	105.75	106.71
25	S	307	CHL	O2A-CGA-O1A	-2.13	117.98	123.30
25	s	307	CHL	O2A-CGA-O1A	-2.13	117.98	123.30
22	G	602	CLA	CHC-C4B-C3B	-2.13	118.22	127.71
22	g	602	CLA	CHC-C4B-C3B	-2.13	118.22	127.71
22	B	614	CLA	CBB-CAB-C3B	-2.13	117.01	127.62
22	C	509	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	1	613	CLA	CMC-C2C-C1C	2.13	128.29	125.04
22	5	613	CLA	CMC-C2C-C1C	2.13	128.29	125.04
25	Y	607	CHL	CHB-C1B-NB	2.13	126.51	124.26
25	y	607	CHL	CHB-C1B-NB	2.13	126.51	124.26
22	b	604	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	R	302	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	r	302	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	G	612	CLA	CED-O2D-CGD	2.13	120.76	115.94
22	g	612	CLA	CED-O2D-CGD	2.13	120.76	115.94
22	3	313	CLA	CHC-C4B-C3B	-2.13	118.23	127.71
22	7	313	CLA	CHC-C4B-C3B	-2.13	118.23	127.71
25	G	608	CHL	C2B-C1B-NB	-2.13	108.80	110.23
25	g	608	CHL	C2B-C1B-NB	-2.13	108.80	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	607	CHL	CHB-C1B-NB	2.13	126.51	124.26
25	n	607	CHL	CHB-C1B-NB	2.13	126.51	124.26
22	1	602	CLA	CHC-C4B-C3B	-2.13	118.23	127.71
22	5	602	CLA	CHC-C4B-C3B	-2.13	118.23	127.71
22	S	309	CLA	CMB-C2B-C1B	2.13	128.61	125.37
22	s	309	CLA	CMB-C2B-C1B	2.13	128.61	125.37
22	c	507	CLA	CMB-C2B-C1B	2.13	128.61	125.37
22	D	403	CLA	CMA-C3A-C4A	-2.13	106.05	111.77
25	2	601	CHL	C3A-C2A-C1A	2.13	104.53	101.34
25	6	601	CHL	C3A-C2A-C1A	2.13	104.53	101.34
23	A	404	PHO	C4B-NB-C1B	-2.13	105.53	108.83
25	2	605	CHL	C1D-ND-C4D	-2.13	104.82	106.33
25	6	605	CHL	C1D-ND-C4D	-2.13	104.82	106.33
22	B	603	CLA	CMC-C2C-C1C	2.13	128.28	125.04
22	s	301	CLA	CGD-CBD-CAD	-2.13	103.85	110.73
25	2	607	CHL	C2A-C1A-CHA	2.12	127.57	123.86
25	6	607	CHL	C2A-C1A-CHA	2.12	127.57	123.86
22	2	612	CLA	CBB-CAB-C3B	-2.12	117.05	127.62
22	6	612	CLA	CBB-CAB-C3B	-2.12	117.05	127.62
22	G	611	CLA	C4D-CHA-C1A	-2.12	118.66	121.25
22	g	611	CLA	C4D-CHA-C1A	-2.12	118.66	121.25
22	B	603	CLA	C4B-CHC-C1C	-2.12	121.30	126.34
22	b	604	CLA	CHC-C4B-C3B	-2.12	118.27	127.71
22	2	602	CLA	CMA-C3A-C4A	-2.12	106.07	111.77
22	6	602	CLA	CMA-C3A-C4A	-2.12	106.07	111.77
22	B	606	CLA	CMB-C2B-C1B	2.12	128.60	125.37
25	R	305	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
25	r	305	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
22	S	313	CLA	C4D-CHA-C1A	-2.12	118.67	121.25
22	s	313	CLA	C4D-CHA-C1A	-2.12	118.67	121.25
24	F	101	HEM	C2A-C1A-NA	-2.12	107.78	110.15
22	A	402	CLA	C4B-CHC-C1C	-2.12	121.31	126.34
22	a	403	CLA	CBB-CAB-C3B	-2.12	117.07	127.62
22	B	612	CLA	CHD-C1D-C2D	-2.12	121.03	125.48
22	C	503	CLA	CMC-C2C-C1C	2.12	128.27	125.04
22	R	307	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
22	r	307	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
22	1	611	CLA	CMB-C2B-C1B	2.12	128.60	125.37
22	5	611	CLA	CMB-C2B-C1B	2.12	128.60	125.37
22	G	603	CLA	CED-O2D-CGD	2.12	120.73	115.94
22	g	603	CLA	CED-O2D-CGD	2.12	120.73	115.94
22	c	504	CLA	C4B-CHC-C1C	-2.12	121.31	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	612	CLA	C4B-CHC-C1C	-2.12	121.31	126.34
22	n	612	CLA	C4B-CHC-C1C	-2.12	121.31	126.34
22	3	311	CLA	C4A-NA-C1A	-2.12	105.75	106.71
22	7	311	CLA	C4A-NA-C1A	-2.12	105.75	106.71
25	R	306	CHL	C3A-C2A-C1A	2.12	104.51	101.34
25	r	306	CHL	C3A-C2A-C1A	2.12	104.51	101.34
22	C	511	CLA	CGD-CBD-CAD	-2.12	103.88	110.73
22	2	611	CLA	CHC-C4B-C3B	-2.12	118.30	127.71
22	6	611	CLA	CHC-C4B-C3B	-2.12	118.30	127.71
22	c	507	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
22	B	615	CLA	CBB-CAB-C3B	-2.12	117.09	127.62
22	C	511	CLA	C4B-CHC-C1C	-2.12	121.32	126.34
22	D	401	CLA	CMB-C2B-C1B	2.12	128.59	125.37
22	b	608	CLA	CHB-C1B-C2B	-2.12	121.26	127.24
22	b	603	CLA	CBB-CAB-C3B	-2.11	117.10	127.62
25	2	608	CHL	CHC-C4B-NB	2.11	126.50	124.26
25	6	608	CHL	CHC-C4B-NB	2.11	126.50	124.26
22	4	301	CLA	CGD-CBD-CAD	-2.11	103.88	110.73
22	8	301	CLA	CGD-CBD-CAD	-2.11	103.88	110.73
22	1	610	CLA	CHC-C4B-C3B	-2.11	118.30	127.71
22	5	610	CLA	CHC-C4B-C3B	-2.11	118.30	127.71
22	D	403	CLA	C3B-C4B-NB	2.11	112.48	110.52
22	G	610	CLA	CHC-C4B-C3B	-2.11	118.31	127.71
22	g	610	CLA	CHC-C4B-C3B	-2.11	118.31	127.71
22	G	613	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
22	g	613	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
22	1	611	CLA	CHA-C1A-NA	-2.11	121.56	126.40
22	5	611	CLA	CHA-C1A-NA	-2.11	121.56	126.40
22	R	301	CLA	CGD-CBD-CAD	-2.11	103.89	110.73
22	r	301	CLA	CGD-CBD-CAD	-2.11	103.89	110.73
22	C	503	CLA	CHC-C4B-C3B	-2.11	118.32	127.71
25	2	606	CHL	O2A-CGA-O1A	-2.11	118.04	123.30
25	6	606	CHL	O2A-CGA-O1A	-2.11	118.04	123.30
25	1	606	CHL	CHB-C1B-NB	2.11	126.49	124.26
25	5	606	CHL	CHB-C1B-NB	2.11	126.49	124.26
22	S	301	CLA	CBB-CAB-C3B	-2.11	117.13	127.62
22	S	313	CLA	CHC-C4B-C3B	-2.11	118.33	127.71
22	s	313	CLA	CHC-C4B-C3B	-2.11	118.33	127.71
22	b	612	CLA	C3D-C4D-CHA	-2.11	107.90	112.72
22	2	603	CLA	CHC-C4B-C3B	-2.11	118.34	127.71
22	6	603	CLA	CHC-C4B-C3B	-2.11	118.34	127.71
22	N	612	CLA	CED-O2D-CGD	2.11	120.70	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	n	612	CLA	CED-O2D-CGD	2.11	120.70	115.94
22	4	304	CLA	CHC-C4B-C3B	-2.11	118.34	127.71
22	8	304	CLA	CHC-C4B-C3B	-2.11	118.34	127.71
25	R	304	CHL	O2A-CGA-O1A	-2.11	118.05	123.30
25	r	304	CHL	O2A-CGA-O1A	-2.11	118.05	123.30
22	1	611	CLA	C4A-NA-C1A	-2.11	105.76	106.71
22	5	611	CLA	C4A-NA-C1A	-2.11	105.76	106.71
22	3	312	CLA	C4D-CHA-C1A	-2.11	118.69	121.25
22	7	312	CLA	C4D-CHA-C1A	-2.11	118.69	121.25
22	G	614	CLA	CED-O2D-CGD	2.10	120.70	115.94
22	g	614	CLA	CED-O2D-CGD	2.10	120.70	115.94
22	c	502	CLA	C4B-CHC-C1C	-2.10	121.35	126.34
22	s	301	CLA	CHC-C4B-C3B	-2.10	118.35	127.71
25	1	605	CHL	CHB-C1B-NB	2.10	126.48	124.26
25	5	605	CHL	CHB-C1B-NB	2.10	126.48	124.26
25	4	306	CHL	C2A-C1A-CHA	2.10	127.54	123.86
25	8	306	CHL	C2A-C1A-CHA	2.10	127.54	123.86
22	3	313	CLA	CMC-C2C-C1C	2.10	128.24	125.04
22	7	313	CLA	CMC-C2C-C1C	2.10	128.24	125.04
22	B	611	CLA	C4D-CHA-C1A	-2.10	118.69	121.25
25	Y	607	CHL	O2A-CGA-O1A	-2.10	118.05	123.30
25	y	607	CHL	O2A-CGA-O1A	-2.10	118.05	123.30
22	2	613	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	6	613	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	S	313	CLA	CBB-CAB-C3B	-2.10	117.15	127.62
22	s	313	CLA	CBB-CAB-C3B	-2.10	117.15	127.62
25	N	601	CHL	C3A-C2A-C1A	2.10	104.49	101.34
25	n	601	CHL	C3A-C2A-C1A	2.10	104.49	101.34
22	R	302	CLA	CHC-C4B-C3B	-2.10	118.35	127.71
22	r	302	CLA	CHC-C4B-C3B	-2.10	118.35	127.71
22	B	603	CLA	CHB-C1B-C2B	-2.10	121.30	127.24
22	C	511	CLA	CAA-CBA-CGA	2.10	118.09	112.51
22	R	307	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	r	307	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	b	602	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	R	303	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
22	r	303	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
25	1	615	CHL	C3A-C2A-C1A	2.10	104.49	101.34
25	5	615	CHL	C3A-C2A-C1A	2.10	104.49	101.34
24	e	101	HEM	CAA-CBA-CGA	-2.10	109.08	113.60
22	1	612	CLA	CGD-CBD-CAD	-2.10	103.93	110.73
22	5	612	CLA	CGD-CBD-CAD	-2.10	103.93	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	610	CLA	CHC-C4B-C3B	-2.10	118.36	127.71
22	n	610	CLA	CHC-C4B-C3B	-2.10	118.36	127.71
22	N	611	CLA	C3B-C4B-NB	2.10	112.46	110.52
22	n	611	CLA	C3B-C4B-NB	2.10	112.46	110.52
22	C	504	CLA	CMC-C2C-C1C	2.10	128.24	125.04
22	A	405	CLA	C4D-CHA-C1A	-2.10	118.69	121.25
24	F	101	HEM	CAC-C3C-C2C	-2.10	121.69	128.60
22	c	505	CLA	CMA-C3A-C2A	-2.10	105.36	113.83
25	Y	605	CHL	C2A-C1A-CHA	2.10	127.52	123.85
25	y	605	CHL	C2A-C1A-CHA	2.10	127.52	123.85
22	4	303	CLA	CMC-C2C-C1C	2.10	128.24	125.04
22	8	303	CLA	CMC-C2C-C1C	2.10	128.24	125.04
22	2	604	CLA	CMC-C2C-C1C	2.10	128.24	125.04
22	6	604	CLA	CMC-C2C-C1C	2.10	128.24	125.04
22	Y	610	CLA	C4B-CHC-C1C	-2.10	121.36	126.34
22	y	610	CLA	C4B-CHC-C1C	-2.10	121.36	126.34
22	B	616	CLA	CMD-C2D-C3D	2.10	132.44	127.61
22	G	614	CLA	CHC-C4B-C3B	-2.10	118.38	127.71
22	g	614	CLA	CHC-C4B-C3B	-2.10	118.38	127.71
25	3	308	CHL	C3B-C4B-NB	-2.10	108.57	110.52
25	7	308	CHL	C3B-C4B-NB	-2.10	108.57	110.52
22	S	314	CLA	CHA-C1A-NA	-2.10	121.60	126.40
22	s	314	CLA	CHA-C1A-NA	-2.10	121.60	126.40
22	d	403	CLA	CMB-C2B-C3B	2.10	131.66	126.59
22	B	602	CLA	CHC-C4B-C3B	-2.10	118.39	127.71
22	B	616	CLA	OBD-CAD-C3D	-2.10	123.48	128.52
23	a	404	PHO	CAA-C2A-C3A	-2.09	107.04	112.78
22	Y	602	CLA	CMB-C2B-C1B	2.09	128.56	125.37
22	y	602	CLA	CMB-C2B-C1B	2.09	128.56	125.37
22	c	512	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
22	R	302	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
22	r	302	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
22	1	614	CLA	CHD-C4C-NC	2.09	127.50	124.20
22	5	614	CLA	CHD-C4C-NC	2.09	127.50	124.20
22	C	502	CLA	CMB-C2B-C1B	2.09	128.56	125.37
22	G	604	CLA	O2A-CGA-CBA	2.09	120.75	114.03
22	g	604	CLA	O2A-CGA-CBA	2.09	120.75	114.03
22	G	613	CLA	CGD-CBD-CAD	-2.09	103.96	110.73
22	g	613	CLA	CGD-CBD-CAD	-2.09	103.96	110.73
22	Y	613	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
22	y	613	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
22	G	602	CLA	OBD-CAD-C3D	-2.09	123.49	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	602	CLA	OBD-CAD-C3D	-2.09	123.49	128.52
22	c	512	CLA	C3B-C4B-NB	2.09	112.45	110.52
22	3	310	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
22	7	310	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
22	a	402	CLA	CMC-C2C-C3C	2.09	131.79	126.12
22	b	603	CLA	CHA-C1A-NA	-2.09	121.61	126.40
22	c	512	CLA	C4B-CHC-C1C	-2.09	121.38	126.34
22	D	403	CLA	C4A-NA-C1A	-2.09	105.77	106.71
22	4	311	CLA	CHA-C1A-NA	-2.09	121.61	126.40
22	8	311	CLA	CHA-C1A-NA	-2.09	121.61	126.40
22	C	511	CLA	CHD-C4C-NC	2.09	127.49	124.20
25	Y	607	CHL	C2A-C1A-CHA	2.09	127.51	123.86
25	y	607	CHL	C2A-C1A-CHA	2.09	127.51	123.86
22	R	307	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
22	r	307	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
25	1	601	CHL	CHD-C1D-ND	-2.09	122.54	124.45
25	5	601	CHL	CHD-C1D-ND	-2.09	122.54	124.45
22	c	511	CLA	CHA-C1A-NA	-2.09	121.62	126.40
22	3	313	CLA	CBB-CAB-C3B	-2.08	117.25	127.62
22	7	313	CLA	CBB-CAB-C3B	-2.08	117.25	127.62
22	4	311	CLA	CHC-C4B-C3B	-2.08	118.44	127.71
22	8	311	CLA	CHC-C4B-C3B	-2.08	118.44	127.71
25	1	607	CHL	O2A-CGA-O1A	-2.08	118.11	123.30
25	5	607	CHL	O2A-CGA-O1A	-2.08	118.11	123.30
22	G	602	CLA	CBB-CAB-C3B	-2.08	117.25	127.62
22	g	602	CLA	CBB-CAB-C3B	-2.08	117.25	127.62
25	1	615	CHL	C3B-C4B-NB	-2.08	108.58	110.52
25	5	615	CHL	C3B-C4B-NB	-2.08	108.58	110.52
25	3	306	CHL	C1D-ND-C4D	-2.08	104.86	106.33
25	7	306	CHL	C1D-ND-C4D	-2.08	104.86	106.33
22	2	610	CLA	CHA-C1A-NA	-2.08	121.63	126.40
22	6	610	CLA	CHA-C1A-NA	-2.08	121.63	126.40
25	G	607	CHL	CHB-C1B-NB	2.08	126.46	124.26
25	g	607	CHL	CHB-C1B-NB	2.08	126.46	124.26
22	N	602	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
22	n	602	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
22	4	301	CLA	CHC-C4B-C3B	-2.08	118.45	127.71
22	8	301	CLA	CHC-C4B-C3B	-2.08	118.45	127.71
22	R	301	CLA	CMC-C2C-C1C	2.08	128.21	125.04
22	r	301	CLA	CMC-C2C-C1C	2.08	128.21	125.04
22	b	614	CLA	CBB-CAB-C3B	-2.08	117.27	127.62
22	S	313	CLA	CMB-C2B-C1B	2.08	128.54	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	s	313	CLA	CMB-C2B-C1B	2.08	128.54	125.37
22	B	611	CLA	CHA-C1A-NA	-2.08	121.63	126.40
22	4	301	CLA	C4D-CHA-C1A	-2.08	118.72	121.25
22	8	301	CLA	C4D-CHA-C1A	-2.08	118.72	121.25
22	3	304	CLA	CED-O2D-CGD	2.08	120.64	115.94
22	7	304	CLA	CED-O2D-CGD	2.08	120.64	115.94
22	B	603	CLA	C4A-NA-C1A	-2.08	105.77	106.71
22	S	313	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
22	s	313	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
22	c	506	CLA	CBB-CAB-C3B	-2.08	117.28	127.62
25	3	308	CHL	O2A-CGA-O1A	-2.08	118.12	123.30
25	7	308	CHL	O2A-CGA-O1A	-2.08	118.12	123.30
22	b	614	CLA	C4D-CHA-C1A	-2.08	118.72	121.25
22	C	512	CLA	CMC-C2C-C3C	2.08	131.76	126.12
22	A	402	CLA	CHA-C1A-NA	-2.08	121.64	126.40
22	G	613	CLA	CMC-C2C-C3C	2.08	131.76	126.12
22	g	613	CLA	CMC-C2C-C3C	2.08	131.76	126.12
22	C	502	CLA	CAC-C3C-C2C	-2.08	123.97	127.53
22	R	301	CLA	CMB-C2B-C1B	2.08	128.53	125.37
22	r	301	CLA	CMB-C2B-C1B	2.08	128.53	125.37
22	c	502	CLA	CGD-CBD-CAD	-2.08	104.00	110.73
25	3	307	CHL	CAA-C2A-C3A	-2.08	107.09	112.78
25	7	307	CHL	CAA-C2A-C3A	-2.08	107.09	112.78
25	S	306	CHL	CHA-C1A-NA	-2.08	121.64	126.40
25	s	306	CHL	CHA-C1A-NA	-2.08	121.64	126.40
25	3	308	CHL	C2A-C1A-CHA	2.08	127.49	123.86
25	7	308	CHL	C2A-C1A-CHA	2.08	127.49	123.86
25	Y	608	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
25	y	608	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
25	Y	607	CHL	C3A-C2A-C1A	2.08	104.45	101.34
25	y	607	CHL	C3A-C2A-C1A	2.08	104.45	101.34
25	S	306	CHL	CAA-CBA-CGA	2.08	118.02	112.51
25	s	306	CHL	CAA-CBA-CGA	2.08	118.02	112.51
22	b	607	CLA	C4B-CHC-C1C	-2.08	121.41	126.34
25	Y	606	CHL	C2A-C3A-C4A	2.08	105.22	101.87
25	y	606	CHL	C2A-C3A-C4A	2.08	105.22	101.87
22	3	314	CLA	CHA-C1A-NA	-2.08	121.64	126.40
22	7	314	CLA	CHA-C1A-NA	-2.08	121.64	126.40
22	C	512	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
25	4	306	CHL	CHD-C1D-ND	-2.08	122.55	124.45
25	8	306	CHL	CHD-C1D-ND	-2.08	122.55	124.45
22	1	611	CLA	CMC-C2C-C1C	2.08	128.20	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	611	CLA	CMC-C2C-C1C	2.08	128.20	125.04
25	1	608	CHL	O2A-CGA-O1A	-2.07	118.13	123.30
25	5	608	CHL	O2A-CGA-O1A	-2.07	118.13	123.30
22	G	611	CLA	CMC-C2C-C1C	2.07	128.20	125.04
22	g	611	CLA	CMC-C2C-C1C	2.07	128.20	125.04
22	G	604	CLA	CMC-C2C-C3C	2.07	131.75	126.12
22	g	604	CLA	CMC-C2C-C3C	2.07	131.75	126.12
22	G	602	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
22	g	602	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
25	R	306	CHL	O2A-CGA-O1A	-2.07	118.13	123.30
25	r	306	CHL	O2A-CGA-O1A	-2.07	118.13	123.30
22	G	613	CLA	CHA-C1A-NA	-2.07	121.65	126.40
22	g	613	CLA	CHA-C1A-NA	-2.07	121.65	126.40
25	G	608	CHL	C2C-C3C-C4C	2.07	107.97	106.49
25	g	608	CHL	C2C-C3C-C4C	2.07	107.97	106.49
22	3	313	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
22	7	313	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
22	b	601	CLA	CMB-C2B-C1B	2.07	128.52	125.37
22	R	301	CLA	CHC-C4B-C3B	-2.07	118.50	127.71
22	r	301	CLA	CHC-C4B-C3B	-2.07	118.50	127.71
25	1	606	CHL	CHC-C4B-NB	2.07	126.45	124.26
25	5	606	CHL	CHC-C4B-NB	2.07	126.45	124.26
22	2	612	CLA	CMB-C2B-C1B	2.07	128.52	125.37
22	6	612	CLA	CMB-C2B-C1B	2.07	128.52	125.37
22	a	403	CLA	CHC-C4B-C3B	-2.07	118.50	127.71
25	2	606	CHL	C2A-C3A-C4A	2.07	105.21	101.87
25	6	606	CHL	C2A-C3A-C4A	2.07	105.21	101.87
22	b	612	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	B	612	CLA	CHD-C4C-NC	2.07	127.46	124.20
22	R	301	CLA	CBB-CAB-C3B	-2.07	117.33	127.62
22	r	301	CLA	CBB-CAB-C3B	-2.07	117.33	127.62
22	N	603	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	n	603	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	R	309	CLA	C3B-C4B-NB	2.07	112.43	110.52
22	r	309	CLA	C3B-C4B-NB	2.07	112.43	110.52
22	N	612	CLA	CBB-CAB-C3B	-2.07	117.33	127.62
22	n	612	CLA	CBB-CAB-C3B	-2.07	117.33	127.62
22	S	301	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
22	B	604	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
22	Y	604	CLA	CMB-C2B-C1B	2.07	128.52	125.37
22	y	604	CLA	CMB-C2B-C1B	2.07	128.52	125.37
22	c	509	CLA	CHC-C4B-C3B	-2.07	118.52	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	610	CLA	C4B-CHC-C1C	-2.07	121.44	126.34
22	S	301	CLA	C4B-CHC-C1C	-2.07	121.44	126.34
25	Y	608	CHL	O2A-CGA-O1A	-2.07	118.15	123.30
25	y	608	CHL	O2A-CGA-O1A	-2.07	118.15	123.30
22	b	606	CLA	C2D-C1D-ND	2.07	111.63	110.10
22	B	601	CLA	CHC-C4B-C3B	-2.06	118.53	127.71
22	2	603	CLA	CED-O2D-CGD	2.06	120.61	115.94
22	6	603	CLA	CED-O2D-CGD	2.06	120.61	115.94
25	N	607	CHL	CHC-C4B-NB	2.06	126.44	124.26
25	n	607	CHL	CHC-C4B-NB	2.06	126.44	124.26
22	b	603	CLA	CMB-C2B-C1B	2.06	128.51	125.37
22	R	310	CLA	CMB-C2B-C1B	2.06	128.51	125.37
22	r	310	CLA	CMB-C2B-C1B	2.06	128.51	125.37
22	S	311	CLA	CMC-C2C-C1C	2.06	128.18	125.04
22	s	311	CLA	CMC-C2C-C1C	2.06	128.18	125.04
22	S	301	CLA	CED-O2D-CGD	2.06	120.60	115.94
25	4	307	CHL	O2A-CGA-O1A	-2.06	118.16	123.30
25	8	307	CHL	O2A-CGA-O1A	-2.06	118.16	123.30
22	B	608	CLA	CED-O2D-CGD	2.06	120.60	115.94
22	b	608	CLA	CHC-C4B-C3B	-2.06	118.54	127.71
22	B	609	CLA	CBB-CAB-C3B	-2.06	117.37	127.62
22	2	603	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
22	6	603	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
22	N	611	CLA	CMC-C2C-C1C	2.06	128.18	125.04
22	n	611	CLA	CMC-C2C-C1C	2.06	128.18	125.04
22	2	613	CLA	CHC-C4B-C3B	-2.06	118.55	127.71
22	6	613	CLA	CHC-C4B-C3B	-2.06	118.55	127.71
22	3	314	CLA	CED-O2D-CGD	2.06	120.60	115.94
22	7	314	CLA	CED-O2D-CGD	2.06	120.60	115.94
22	S	305	CLA	C4A-NA-C1A	-2.06	105.78	106.71
22	s	305	CLA	C4A-NA-C1A	-2.06	105.78	106.71
22	G	602	CLA	CHA-C1A-NA	-2.06	121.68	126.40
22	g	602	CLA	CHA-C1A-NA	-2.06	121.68	126.40
22	3	311	CLA	CHA-C1A-NA	-2.06	121.68	126.40
22	7	311	CLA	CHA-C1A-NA	-2.06	121.68	126.40
22	D	404	CLA	CED-O2D-CGD	2.06	120.59	115.94
25	3	302	CHL	C2A-C1A-CHA	2.06	127.46	123.86
25	7	302	CHL	C2A-C1A-CHA	2.06	127.46	123.86
22	4	310	CLA	CBA-CAA-C2A	2.06	119.94	113.86
22	8	310	CLA	CBA-CAA-C2A	2.06	119.94	113.86
22	C	506	CLA	CED-O2D-CGD	2.06	120.59	115.94
22	b	601	CLA	CED-O2D-CGD	2.06	120.59	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	R	311	CLA	C4D-CHA-C1A	-2.06	118.75	121.25
22	r	311	CLA	C4D-CHA-C1A	-2.06	118.75	121.25
25	S	306	CHL	C3B-C4B-NB	-2.06	108.61	110.52
25	s	306	CHL	C3B-C4B-NB	-2.06	108.61	110.52
22	4	304	CLA	CHA-C1A-NA	-2.06	121.69	126.40
22	8	304	CLA	CHA-C1A-NA	-2.06	121.69	126.40
22	c	504	CLA	CED-O2D-CGD	2.06	120.59	115.94
22	B	601	CLA	CBB-CAB-C3B	-2.06	117.39	127.62
22	B	605	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
25	G	609	CHL	O2D-CGD-O1D	-2.06	119.82	123.84
25	g	609	CHL	O2D-CGD-O1D	-2.06	119.82	123.84
22	b	608	CLA	CMB-C2B-C3B	2.05	131.56	126.59
22	D	401	CLA	CHB-C1B-C2B	-2.05	121.43	127.24
25	S	306	CHL	CHC-C4B-NB	2.05	126.43	124.26
25	s	306	CHL	CHC-C4B-NB	2.05	126.43	124.26
22	N	604	CLA	CMB-C2B-C1B	2.05	128.50	125.37
22	n	604	CLA	CMB-C2B-C1B	2.05	128.50	125.37
22	3	311	CLA	CMB-C2B-C1B	2.05	128.50	125.37
22	7	311	CLA	CMB-C2B-C1B	2.05	128.50	125.37
25	2	606	CHL	O1D-CGD-CBD	-2.05	120.28	124.48
25	6	606	CHL	O1D-CGD-CBD	-2.05	120.28	124.48
22	G	603	CLA	C4B-CHC-C1C	-2.05	121.47	126.34
22	g	603	CLA	C4B-CHC-C1C	-2.05	121.47	126.34
22	1	613	CLA	CED-O2D-CGD	2.05	120.58	115.94
22	5	613	CLA	CED-O2D-CGD	2.05	120.58	115.94
22	S	312	CLA	C3B-C4B-NB	2.05	112.42	110.52
22	s	312	CLA	C3B-C4B-NB	2.05	112.42	110.52
25	3	307	CHL	C2A-C3A-C4A	2.05	105.18	101.87
25	7	307	CHL	C2A-C3A-C4A	2.05	105.18	101.87
25	1	606	CHL	O1D-CGD-CBD	-2.05	120.28	124.48
25	5	606	CHL	O1D-CGD-CBD	-2.05	120.28	124.48
22	2	610	CLA	C4D-CHA-C1A	-2.05	118.75	121.25
22	6	610	CLA	C4D-CHA-C1A	-2.05	118.75	121.25
22	3	311	CLA	CMC-C2C-C1C	2.05	128.16	125.04
22	7	311	CLA	CMC-C2C-C1C	2.05	128.16	125.04
22	b	607	CLA	CHA-C1A-NA	-2.05	121.70	126.40
24	e	101	HEM	C1B-NB-C4B	2.05	107.19	105.07
22	R	310	CLA	CHC-C4B-C3B	-2.05	118.59	127.71
22	r	310	CLA	CHC-C4B-C3B	-2.05	118.59	127.71
22	Y	614	CLA	C4B-CHC-C1C	-2.05	121.48	126.34
22	y	614	CLA	C4B-CHC-C1C	-2.05	121.48	126.34
22	G	614	CLA	CMC-C2C-C1C	2.05	128.16	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	614	CLA	CMC-C2C-C1C	2.05	128.16	125.04
22	c	510	CLA	CGD-CBD-CAD	-2.05	104.10	110.73
22	b	603	CLA	C4B-CHC-C1C	-2.05	121.48	126.34
22	b	613	CLA	CMC-C2C-C3C	2.05	131.67	126.12
22	c	503	CLA	CMB-C2B-C1B	2.05	128.49	125.37
22	d	404	CLA	CBB-CAB-C3B	-2.05	117.44	127.62
22	N	611	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
22	n	611	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
22	d	403	CLA	CHD-C4C-NC	2.04	127.42	124.20
22	3	304	CLA	CMB-C2B-C1B	2.04	128.48	125.37
22	7	304	CLA	CMB-C2B-C1B	2.04	128.48	125.37
22	2	603	CLA	C4D-CHA-C1A	-2.04	118.76	121.25
22	6	603	CLA	C4D-CHA-C1A	-2.04	118.76	121.25
22	C	504	CLA	CMC-C2C-C3C	2.04	131.66	126.12
25	G	607	CHL	C2A-C3A-C4A	2.04	105.17	101.87
25	g	607	CHL	C2A-C3A-C4A	2.04	105.17	101.87
22	R	309	CLA	CMC-C2C-C1C	2.04	128.15	125.04
22	r	309	CLA	CMC-C2C-C1C	2.04	128.15	125.04
22	C	503	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
25	1	601	CHL	O2A-CGA-O1A	-2.04	118.21	123.30
25	5	601	CHL	O2A-CGA-O1A	-2.04	118.21	123.30
22	S	310	CLA	C3D-C4D-CHA	-2.04	108.06	112.72
22	s	310	CLA	C3D-C4D-CHA	-2.04	108.06	112.72
22	b	613	CLA	CGD-CBD-CAD	-2.04	104.13	110.73
22	4	303	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	8	303	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	B	614	CLA	CHC-C4B-C3B	-2.04	118.64	127.71
22	C	509	CLA	C3B-C4B-NB	2.04	112.41	110.52
22	N	603	CLA	CED-O2D-CGD	2.04	120.55	115.94
22	n	603	CLA	CED-O2D-CGD	2.04	120.55	115.94
22	N	611	CLA	CMB-C2B-C1B	2.04	128.47	125.37
22	n	611	CLA	CMB-C2B-C1B	2.04	128.47	125.37
22	S	304	CLA	CMB-C2B-C1B	2.04	128.47	125.37
22	s	304	CLA	CMB-C2B-C1B	2.04	128.47	125.37
25	S	302	CHL	C3A-C2A-C1A	2.04	104.39	101.34
25	s	302	CHL	C3A-C2A-C1A	2.04	104.39	101.34
25	G	601	CHL	C2A-C1A-CHA	2.04	127.42	123.86
25	g	601	CHL	C2A-C1A-CHA	2.04	127.42	123.86
22	c	509	CLA	CMC-C2C-C3C	2.04	131.64	126.12
25	S	302	CHL	C2B-C1B-NB	-2.03	108.87	110.23
25	s	302	CHL	C2B-C1B-NB	-2.03	108.87	110.23
22	R	311	CLA	CED-O2D-CGD	2.03	120.54	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r	311	CLA	CED-O2D-CGD	2.03	120.54	115.94
22	Y	613	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
22	y	613	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
25	1	601	CHL	C3A-C2A-C1A	2.03	104.39	101.34
25	5	601	CHL	C3A-C2A-C1A	2.03	104.39	101.34
25	2	607	CHL	C2B-C1B-NB	-2.03	108.87	110.23
25	6	607	CHL	C2B-C1B-NB	-2.03	108.87	110.23
25	Y	601	CHL	CMA-C3A-C4A	-2.03	106.31	111.77
25	y	601	CHL	CMA-C3A-C4A	-2.03	106.31	111.77
22	D	404	CLA	CGD-CBD-CAD	-2.03	104.15	110.73
25	4	306	CHL	O2A-CGA-O1A	-2.03	118.23	123.30
25	8	306	CHL	O2A-CGA-O1A	-2.03	118.23	123.30
22	B	603	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
22	G	604	CLA	C3B-C4B-NB	2.03	112.40	110.52
22	g	604	CLA	C3B-C4B-NB	2.03	112.40	110.52
25	2	601	CHL	CHB-C1B-NB	2.03	126.41	124.26
25	6	601	CHL	CHB-C1B-NB	2.03	126.41	124.26
22	2	612	CLA	CHA-C1A-NA	-2.03	121.75	126.40
22	6	612	CLA	CHA-C1A-NA	-2.03	121.75	126.40
22	G	612	CLA	CMC-C2C-C3C	2.03	131.63	126.12
22	g	612	CLA	CMC-C2C-C3C	2.03	131.63	126.12
22	2	613	CLA	C4A-NA-C1A	-2.03	105.79	106.71
22	6	613	CLA	C4A-NA-C1A	-2.03	105.79	106.71
25	2	607	CHL	C3A-C2A-C1A	2.03	104.38	101.34
25	6	607	CHL	C3A-C2A-C1A	2.03	104.38	101.34
22	C	511	CLA	CMB-C2B-C1B	2.03	128.46	125.37
22	1	610	CLA	CED-O2D-CGD	2.03	120.53	115.94
22	5	610	CLA	CED-O2D-CGD	2.03	120.53	115.94
22	B	604	CLA	C3C-C4C-NC	2.03	112.85	110.57
22	C	502	CLA	OBD-CAD-C3D	-2.03	123.64	128.52
25	3	307	CHL	CHB-C1B-NB	2.03	126.40	124.26
25	7	307	CHL	CHB-C1B-NB	2.03	126.40	124.26
22	B	611	CLA	CAA-CBA-CGA	-2.03	107.13	112.51
22	b	606	CLA	CHC-C4B-C3B	-2.03	118.69	127.71
22	a	402	CLA	CGD-CBD-CAD	-2.03	104.17	110.73
22	c	511	CLA	CMC-C2C-C3C	2.03	131.62	126.12
25	S	308	CHL	C3A-C2A-C1A	2.03	104.37	101.34
25	s	308	CHL	C3A-C2A-C1A	2.03	104.37	101.34
25	Y	607	CHL	CAA-CBA-CGA	2.03	117.88	112.51
25	y	607	CHL	CAA-CBA-CGA	2.03	117.88	112.51
22	N	603	CLA	C4B-CHC-C1C	-2.03	121.53	126.34
22	n	603	CLA	C4B-CHC-C1C	-2.03	121.53	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	402	PHO	CBC-CAC-C3C	-2.02	109.92	112.88
22	c	512	CLA	CBB-CAB-C3B	-2.02	117.55	127.62
22	2	603	CLA	CHA-C1A-NA	-2.02	121.76	126.40
22	6	603	CLA	CHA-C1A-NA	-2.02	121.76	126.40
22	b	607	CLA	CMC-C2C-C1C	2.02	128.12	125.04
22	c	504	CLA	CMC-C2C-C3C	2.02	131.61	126.12
22	C	503	CLA	CMB-C2B-C1B	2.02	128.45	125.37
22	G	612	CLA	CHA-C1A-NA	-2.02	121.77	126.40
22	g	612	CLA	CHA-C1A-NA	-2.02	121.77	126.40
25	3	308	CHL	CHA-C1A-NA	-2.02	121.77	126.40
25	7	308	CHL	CHA-C1A-NA	-2.02	121.77	126.40
22	D	404	CLA	CMC-C2C-C3C	2.02	131.61	126.12
22	3	310	CLA	CED-O2D-CGD	2.02	120.51	115.94
22	7	310	CLA	CED-O2D-CGD	2.02	120.51	115.94
22	d	404	CLA	CHA-C1A-NA	-2.02	121.77	126.40
25	1	615	CHL	C2A-C1A-CHA	2.02	127.39	123.86
25	5	615	CHL	C2A-C1A-CHA	2.02	127.39	123.86
25	Y	605	CHL	C4D-CHA-C1A	2.02	123.71	121.25
25	y	605	CHL	C4D-CHA-C1A	2.02	123.71	121.25
25	2	601	CHL	O2A-CGA-O1A	-2.02	118.27	123.30
25	6	601	CHL	O2A-CGA-O1A	-2.02	118.27	123.30
22	S	303	CLA	CHA-C1A-NA	-2.02	121.77	126.40
22	s	303	CLA	CHA-C1A-NA	-2.02	121.77	126.40
22	3	312	CLA	CHA-C1A-NA	-2.02	121.77	126.40
22	7	312	CLA	CHA-C1A-NA	-2.02	121.77	126.40
22	R	309	CLA	CMB-C2B-C1B	2.02	128.44	125.37
22	r	309	CLA	CMB-C2B-C1B	2.02	128.44	125.37
22	N	611	CLA	C4B-CHC-C1C	-2.02	121.55	126.34
22	n	611	CLA	C4B-CHC-C1C	-2.02	121.55	126.34
25	G	605	CHL	O1D-CGD-CBD	-2.02	120.36	124.48
25	g	605	CHL	O1D-CGD-CBD	-2.02	120.36	124.48
22	G	603	CLA	C3B-C4B-NB	2.02	112.39	110.52
22	g	603	CLA	C3B-C4B-NB	2.02	112.39	110.52
22	A	403	CLA	CMC-C2C-C3C	2.02	131.59	126.12
25	4	307	CHL	C3B-C4B-NB	-2.02	108.64	110.52
25	8	307	CHL	C3B-C4B-NB	-2.02	108.64	110.52
25	G	601	CHL	C4D-CHA-C1A	2.02	123.70	121.25
25	g	601	CHL	C4D-CHA-C1A	2.02	123.70	121.25
22	c	507	CLA	CHA-C1A-NA	-2.02	121.78	126.40
24	F	101	HEM	CAB-C3B-C2B	-2.02	121.96	128.60
22	B	602	CLA	C4B-CHC-C1C	-2.02	121.56	126.34
22	N	611	CLA	C4A-NA-C1A	-2.02	105.80	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	n	611	CLA	C4A-NA-C1A	-2.02	105.80	106.71
22	b	608	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
22	N	611	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
22	n	611	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
22	N	610	CLA	CMA-C3A-C2A	-2.01	105.70	113.83
22	n	610	CLA	CMA-C3A-C2A	-2.01	105.70	113.83
22	1	614	CLA	C4B-CHC-C1C	-2.01	121.56	126.34
22	5	614	CLA	C4B-CHC-C1C	-2.01	121.56	126.34
22	D	404	CLA	CBB-CAB-C3B	-2.01	117.60	127.62
22	4	305	CLA	CED-O2D-CGD	2.01	120.49	115.94
22	8	305	CLA	CED-O2D-CGD	2.01	120.49	115.94
22	2	611	CLA	CBB-CAB-C3B	-2.01	117.61	127.62
22	6	611	CLA	CBB-CAB-C3B	-2.01	117.61	127.62
25	S	306	CHL	C2A-C3A-C4A	2.01	105.12	101.87
25	s	306	CHL	C2A-C3A-C4A	2.01	105.12	101.87
22	N	602	CLA	CBB-CAB-C3B	-2.01	117.61	127.62
22	n	602	CLA	CBB-CAB-C3B	-2.01	117.61	127.62
25	1	609	CHL	C2B-C1B-NB	-2.01	108.88	110.23
25	5	609	CHL	C2B-C1B-NB	-2.01	108.88	110.23
22	N	614	CLA	CMC-C2C-C3C	2.01	131.58	126.12
22	n	614	CLA	CMC-C2C-C3C	2.01	131.58	126.12
22	2	603	CLA	CMC-C2C-C1C	2.01	128.10	125.04
22	6	603	CLA	CMC-C2C-C1C	2.01	128.10	125.04
22	c	502	CLA	CMC-C2C-C3C	2.01	131.58	126.12
25	S	307	CHL	C2A-C1A-CHA	2.01	127.38	123.86
25	s	307	CHL	C2A-C1A-CHA	2.01	127.38	123.86
22	b	603	CLA	CMC-C2C-C1C	2.01	128.10	125.04
22	c	503	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
22	R	307	CLA	CHD-C1D-C2D	-2.01	121.26	125.48
22	r	307	CLA	CHD-C1D-C2D	-2.01	121.26	125.48
25	1	605	CHL	C4D-C3D-CAD	-2.01	105.73	108.10
25	5	605	CHL	C4D-C3D-CAD	-2.01	105.73	108.10
22	B	614	CLA	C4A-NA-C1A	-2.01	105.80	106.71
22	G	611	CLA	C4B-CHC-C1C	-2.01	121.57	126.34
22	g	611	CLA	C4B-CHC-C1C	-2.01	121.57	126.34
22	G	603	CLA	CMC-C2C-C1C	2.01	128.10	125.04
22	g	603	CLA	CMC-C2C-C1C	2.01	128.10	125.04
22	C	512	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
22	N	602	CLA	CMA-C3A-C2A	-2.01	105.72	113.83
22	n	602	CLA	CMA-C3A-C2A	-2.01	105.72	113.83
22	B	605	CLA	CAA-CBA-CGA	2.01	117.84	112.51
25	4	306	CHL	C3B-C4B-NB	-2.01	108.65	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	306	CHL	C3B-C4B-NB	-2.01	108.65	110.52
22	C	505	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
22	S	314	CLA	CMB-C2B-C1B	2.01	128.43	125.37
22	s	314	CLA	CMB-C2B-C1B	2.01	128.43	125.37
25	N	608	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
25	n	608	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
22	B	604	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
22	Y	610	CLA	CMA-C3A-C4A	-2.01	106.38	111.77
22	y	610	CLA	CMA-C3A-C4A	-2.01	106.38	111.77
25	R	305	CHL	C3A-C2A-C1A	2.01	104.35	101.34
25	r	305	CHL	C3A-C2A-C1A	2.01	104.35	101.34
25	4	308	CHL	CHB-C1B-NB	2.01	126.38	124.26
25	8	308	CHL	CHB-C1B-NB	2.01	126.38	124.26
25	S	306	CHL	O2D-CGD-CBD	2.01	114.84	111.27
25	s	306	CHL	O2D-CGD-CBD	2.01	114.84	111.27
22	3	314	CLA	CHC-C4B-C3B	-2.01	118.78	127.71
22	7	314	CLA	CHC-C4B-C3B	-2.01	118.78	127.71
22	a	402	CLA	CMB-C2B-C3B	2.01	131.45	126.59
22	b	605	CLA	CHC-C4B-C3B	-2.01	118.78	127.71
22	D	404	CLA	C4D-CHA-C1A	-2.01	118.81	121.25
22	R	303	CLA	C4B-CHC-C1C	-2.01	121.58	126.34
22	r	303	CLA	C4B-CHC-C1C	-2.01	121.58	126.34
25	1	615	CHL	O2A-CGA-O1A	-2.01	118.30	123.30
25	5	615	CHL	O2A-CGA-O1A	-2.01	118.30	123.30
22	3	311	CLA	CED-O2D-CGD	2.01	120.47	115.94
22	7	311	CLA	CED-O2D-CGD	2.01	120.47	115.94
22	b	611	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
22	Y	604	CLA	C3B-C4B-NB	2.00	112.38	110.52
22	y	604	CLA	C3B-C4B-NB	2.00	112.38	110.52
22	S	309	CLA	C4B-CHC-C1C	-2.00	121.58	126.34
22	s	309	CLA	C4B-CHC-C1C	-2.00	121.58	126.34
22	G	611	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	g	611	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	1	614	CLA	C4A-NA-C1A	-2.00	105.81	106.71
22	5	614	CLA	C4A-NA-C1A	-2.00	105.81	106.71
22	1	614	CLA	CGD-CBD-CAD	-2.00	104.24	110.73
22	5	614	CLA	CGD-CBD-CAD	-2.00	104.24	110.73
22	c	506	CLA	CGD-CBD-CAD	-2.00	104.25	110.73
22	Y	602	CLA	CMC-C2C-C3C	2.00	131.55	126.12
22	y	602	CLA	CMC-C2C-C3C	2.00	131.55	126.12
22	b	615	CLA	CBB-CAB-C3B	-2.00	117.66	127.62
22	G	610	CLA	CHD-C1D-C2D	-2.00	121.28	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	610	CLA	CHD-C1D-C2D	-2.00	121.28	125.48
22	R	302	CLA	CMB-C2B-C1B	2.00	128.42	125.37
22	r	302	CLA	CMB-C2B-C1B	2.00	128.42	125.37
22	N	603	CLA	C3B-C4B-NB	2.00	112.37	110.52
22	n	603	CLA	C3B-C4B-NB	2.00	112.37	110.52
25	N	606	CHL	C2A-C3A-C4A	2.00	105.10	101.87
25	n	606	CHL	C2A-C3A-C4A	2.00	105.10	101.87
22	4	304	CLA	CMC-C2C-C1C	2.00	128.09	125.04
22	8	304	CLA	CMC-C2C-C1C	2.00	128.09	125.04
22	d	403	CLA	C4D-CHA-C1A	-2.00	118.81	121.25

There are no chirality outliers.

All (2559) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	402	CLA	CBD-CGD-O2D-CED
22	A	403	CLA	C1A-C2A-CAA-CBA
22	A	405	CLA	C3A-C2A-CAA-CBA
22	B	601	CLA	CHA-CBD-CGD-O1D
22	B	601	CLA	CAD-CBD-CGD-O1D
22	B	602	CLA	C2B-C3B-CAB-CBB
22	B	602	CLA	C4B-C3B-CAB-CBB
22	B	604	CLA	C2B-C3B-CAB-CBB
22	B	604	CLA	C4B-C3B-CAB-CBB
22	B	605	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	C2B-C3B-CAB-CBB
22	B	606	CLA	C4B-C3B-CAB-CBB
22	B	609	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	C2B-C3B-CAB-CBB
22	B	609	CLA	C4B-C3B-CAB-CBB
22	B	610	CLA	C1A-C2A-CAA-CBA
22	B	610	CLA	C3A-C2A-CAA-CBA
22	B	610	CLA	C2B-C3B-CAB-CBB
22	B	610	CLA	C4B-C3B-CAB-CBB
22	B	611	CLA	C1A-C2A-CAA-CBA
22	B	611	CLA	CBD-CGD-O2D-CED
22	B	612	CLA	CBD-CGD-O2D-CED
22	B	613	CLA	CBD-CGD-O2D-CED
22	B	614	CLA	C1A-C2A-CAA-CBA
22	B	614	CLA	C2B-C3B-CAB-CBB
22	B	614	CLA	C4B-C3B-CAB-CBB
22	B	615	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	616	CLA	C1A-C2A-CAA-CBA
22	B	616	CLA	C3A-C2A-CAA-CBA
22	B	616	CLA	CBD-CGD-O2D-CED
22	C	502	CLA	C2B-C3B-CAB-CBB
22	C	502	CLA	C4B-C3B-CAB-CBB
22	C	505	CLA	C2B-C3B-CAB-CBB
22	C	505	CLA	C4B-C3B-CAB-CBB
22	C	507	CLA	C1A-C2A-CAA-CBA
22	C	507	CLA	C3A-C2A-CAA-CBA
22	C	507	CLA	C2B-C3B-CAB-CBB
22	C	507	CLA	C4B-C3B-CAB-CBB
22	C	507	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CBD-CGD-O2D-CED
22	C	509	CLA	C1A-C2A-CAA-CBA
22	C	510	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	C2B-C3B-CAB-CBB
22	C	511	CLA	C4B-C3B-CAB-CBB
22	C	511	CLA	CBD-CGD-O2D-CED
22	D	401	CLA	C2B-C3B-CAB-CBB
22	D	401	CLA	C4B-C3B-CAB-CBB
22	D	403	CLA	CBD-CGD-O2D-CED
22	D	404	CLA	C2B-C3B-CAB-CBB
22	D	404	CLA	C4B-C3B-CAB-CBB
22	a	402	CLA	CBD-CGD-O2D-CED
22	a	403	CLA	C1A-C2A-CAA-CBA
22	a	403	CLA	CBD-CGD-O2D-CED
22	a	405	CLA	C1A-C2A-CAA-CBA
22	a	405	CLA	C3A-C2A-CAA-CBA
22	b	601	CLA	CHA-CBD-CGD-O1D
22	b	601	CLA	CHA-CBD-CGD-O2D
22	b	601	CLA	CAD-CBD-CGD-O1D
22	b	601	CLA	CAD-CBD-CGD-O2D
22	b	601	CLA	CBD-CGD-O2D-CED
22	b	602	CLA	C3A-C2A-CAA-CBA
22	b	602	CLA	C2B-C3B-CAB-CBB
22	b	602	CLA	C4B-C3B-CAB-CBB
22	b	602	CLA	CBD-CGD-O2D-CED
22	b	603	CLA	C2B-C3B-CAB-CBB
22	b	603	CLA	C4B-C3B-CAB-CBB
22	b	603	CLA	CBD-CGD-O2D-CED
22	b	604	CLA	C2B-C3B-CAB-CBB
22	b	604	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	b	604	CLA	CHA-CBD-CGD-O1D
22	b	604	CLA	CHA-CBD-CGD-O2D
22	b	604	CLA	CAD-CBD-CGD-O1D
22	b	604	CLA	CAD-CBD-CGD-O2D
22	b	606	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	C2B-C3B-CAB-CBB
22	b	609	CLA	C4B-C3B-CAB-CBB
22	b	609	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	C1A-C2A-CAA-CBA
22	b	610	CLA	C3A-C2A-CAA-CBA
22	b	610	CLA	C2B-C3B-CAB-CBB
22	b	610	CLA	C4B-C3B-CAB-CBB
22	b	611	CLA	CBD-CGD-O2D-CED
22	b	612	CLA	CHA-CBD-CGD-O1D
22	b	612	CLA	CHA-CBD-CGD-O2D
22	b	612	CLA	CAD-CBD-CGD-O1D
22	b	613	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	C1A-C2A-CAA-CBA
22	b	614	CLA	C2B-C3B-CAB-CBB
22	b	614	CLA	C4B-C3B-CAB-CBB
22	b	616	CLA	C3A-C2A-CAA-CBA
22	b	616	CLA	CAD-CBD-CGD-O1D
22	d	401	CLA	C2B-C3B-CAB-CBB
22	d	401	CLA	C4B-C3B-CAB-CBB
22	d	403	CLA	CBD-CGD-O2D-CED
22	d	404	CLA	C2B-C3B-CAB-CBB
22	d	404	CLA	C4B-C3B-CAB-CBB
22	c	501	CLA	CBD-CGD-O2D-CED
22	c	502	CLA	C2B-C3B-CAB-CBB
22	c	502	CLA	C4B-C3B-CAB-CBB
22	c	503	CLA	CBD-CGD-O2D-CED
22	c	504	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	C2B-C3B-CAB-CBB
22	c	505	CLA	C4B-C3B-CAB-CBB
22	c	507	CLA	C1A-C2A-CAA-CBA
22	c	507	CLA	C3A-C2A-CAA-CBA
22	c	507	CLA	C2B-C3B-CAB-CBB
22	c	507	CLA	C4B-C3B-CAB-CBB
22	c	508	CLA	CBD-CGD-O2D-CED
22	c	509	CLA	C1A-C2A-CAA-CBA
22	c	510	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C4B-C3B-CAB-CBB
22	c	511	CLA	CHA-CBD-CGD-O1D
22	c	511	CLA	CHA-CBD-CGD-O2D
22	c	511	CLA	CBD-CGD-O2D-CED
22	R	301	CLA	C1A-C2A-CAA-CBA
22	R	302	CLA	C1A-C2A-CAA-CBA
22	R	303	CLA	C1A-C2A-CAA-CBA
22	R	303	CLA	C2B-C3B-CAB-CBB
22	R	303	CLA	C4B-C3B-CAB-CBB
22	R	303	CLA	CBD-CGD-O2D-CED
22	R	307	CLA	C1A-C2A-CAA-CBA
22	R	307	CLA	C3A-C2A-CAA-CBA
22	R	307	CLA	CHA-CBD-CGD-O1D
22	R	307	CLA	CBD-CGD-O2D-CED
22	R	308	CLA	C1A-C2A-CAA-CBA
22	R	309	CLA	CBD-CGD-O2D-CED
22	R	309	CLA	O1D-CGD-O2D-CED
22	R	310	CLA	C2B-C3B-CAB-CBB
22	R	310	CLA	C4B-C3B-CAB-CBB
22	R	311	CLA	CBD-CGD-O2D-CED
22	S	303	CLA	C1A-C2A-CAA-CBA
22	S	303	CLA	C3A-C2A-CAA-CBA
22	S	303	CLA	CBD-CGD-O2D-CED
22	S	304	CLA	C2B-C3B-CAB-CBB
22	S	304	CLA	C4B-C3B-CAB-CBB
22	S	305	CLA	CAD-CBD-CGD-O2D
22	S	305	CLA	CBD-CGD-O2D-CED
22	S	309	CLA	C2B-C3B-CAB-CBB
22	S	309	CLA	C4B-C3B-CAB-CBB
22	S	309	CLA	CBD-CGD-O2D-CED
22	S	310	CLA	C1A-C2A-CAA-CBA
22	S	310	CLA	C2B-C3B-CAB-CBB
22	S	310	CLA	C4B-C3B-CAB-CBB
22	S	310	CLA	CBD-CGD-O2D-CED
22	S	311	CLA	C1A-C2A-CAA-CBA
22	S	312	CLA	C2B-C3B-CAB-CBB
22	S	312	CLA	C4B-C3B-CAB-CBB
22	S	312	CLA	CBD-CGD-O2D-CED
22	S	313	CLA	CBD-CGD-O2D-CED
22	S	314	CLA	C2B-C3B-CAB-CBB
22	S	314	CLA	C4B-C3B-CAB-CBB
22	S	314	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	S	314	CLA	O1D-CGD-O2D-CED
22	G	602	CLA	C2B-C3B-CAB-CBB
22	G	602	CLA	C4B-C3B-CAB-CBB
22	G	603	CLA	CBD-CGD-O2D-CED
22	G	604	CLA	C1A-C2A-CAA-CBA
22	G	610	CLA	CBD-CGD-O2D-CED
22	G	612	CLA	C2B-C3B-CAB-CBB
22	G	612	CLA	C4B-C3B-CAB-CBB
22	G	613	CLA	C2B-C3B-CAB-CBB
22	G	613	CLA	C4B-C3B-CAB-CBB
22	G	613	CLA	CBD-CGD-O2D-CED
22	G	613	CLA	O1D-CGD-O2D-CED
22	G	614	CLA	C1A-C2A-CAA-CBA
22	G	614	CLA	CBD-CGD-O2D-CED
22	N	602	CLA	C2B-C3B-CAB-CBB
22	N	602	CLA	C4B-C3B-CAB-CBB
22	N	603	CLA	CBD-CGD-O2D-CED
22	N	604	CLA	C1A-C2A-CAA-CBA
22	N	610	CLA	CBD-CGD-O2D-CED
22	N	612	CLA	C2B-C3B-CAB-CBB
22	N	612	CLA	C4B-C3B-CAB-CBB
22	N	613	CLA	C2B-C3B-CAB-CBB
22	N	613	CLA	C4B-C3B-CAB-CBB
22	N	613	CLA	CBD-CGD-O2D-CED
22	N	613	CLA	O1D-CGD-O2D-CED
22	N	614	CLA	C1A-C2A-CAA-CBA
22	N	614	CLA	CBD-CGD-O2D-CED
22	Y	602	CLA	C2B-C3B-CAB-CBB
22	Y	602	CLA	C4B-C3B-CAB-CBB
22	Y	602	CLA	CBD-CGD-O2D-CED
22	Y	603	CLA	C2B-C3B-CAB-CBB
22	Y	603	CLA	C4B-C3B-CAB-CBB
22	Y	604	CLA	C1A-C2A-CAA-CBA
22	Y	610	CLA	CBD-CGD-O2D-CED
22	Y	611	CLA	CBD-CGD-O2D-CED
22	Y	612	CLA	C2B-C3B-CAB-CBB
22	Y	612	CLA	C4B-C3B-CAB-CBB
22	Y	613	CLA	C2B-C3B-CAB-CBB
22	Y	613	CLA	C4B-C3B-CAB-CBB
22	Y	613	CLA	CBD-CGD-O2D-CED
22	Y	614	CLA	C1A-C2A-CAA-CBA
22	Y	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	r	301	CLA	C1A-C2A-CAA-CBA
22	r	302	CLA	C1A-C2A-CAA-CBA
22	r	303	CLA	C1A-C2A-CAA-CBA
22	r	303	CLA	C2B-C3B-CAB-CBB
22	r	303	CLA	C4B-C3B-CAB-CBB
22	r	303	CLA	CBD-CGD-O2D-CED
22	r	307	CLA	C1A-C2A-CAA-CBA
22	r	307	CLA	C3A-C2A-CAA-CBA
22	r	307	CLA	CHA-CBD-CGD-O1D
22	r	307	CLA	CBD-CGD-O2D-CED
22	r	308	CLA	C1A-C2A-CAA-CBA
22	r	309	CLA	CBD-CGD-O2D-CED
22	r	309	CLA	O1D-CGD-O2D-CED
22	r	310	CLA	C2B-C3B-CAB-CBB
22	r	310	CLA	C4B-C3B-CAB-CBB
22	r	311	CLA	CBD-CGD-O2D-CED
22	s	301	CLA	CBD-CGD-O2D-CED
22	s	303	CLA	C1A-C2A-CAA-CBA
22	s	303	CLA	C3A-C2A-CAA-CBA
22	s	303	CLA	CBD-CGD-O2D-CED
22	s	304	CLA	C2B-C3B-CAB-CBB
22	s	304	CLA	C4B-C3B-CAB-CBB
22	s	305	CLA	CAD-CBD-CGD-O2D
22	s	305	CLA	CBD-CGD-O2D-CED
22	s	309	CLA	C2B-C3B-CAB-CBB
22	s	309	CLA	C4B-C3B-CAB-CBB
22	s	309	CLA	CBD-CGD-O2D-CED
22	s	310	CLA	C1A-C2A-CAA-CBA
22	s	310	CLA	C2B-C3B-CAB-CBB
22	s	310	CLA	C4B-C3B-CAB-CBB
22	s	310	CLA	CBD-CGD-O2D-CED
22	s	311	CLA	C1A-C2A-CAA-CBA
22	s	312	CLA	C2B-C3B-CAB-CBB
22	s	312	CLA	C4B-C3B-CAB-CBB
22	s	312	CLA	CBD-CGD-O2D-CED
22	s	313	CLA	CBD-CGD-O2D-CED
22	s	314	CLA	C2B-C3B-CAB-CBB
22	s	314	CLA	C4B-C3B-CAB-CBB
22	s	314	CLA	CBD-CGD-O2D-CED
22	s	314	CLA	O1D-CGD-O2D-CED
22	g	602	CLA	C2B-C3B-CAB-CBB
22	g	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	g	603	CLA	CBD-CGD-O2D-CED
22	g	604	CLA	C1A-C2A-CAA-CBA
22	g	610	CLA	CBD-CGD-O2D-CED
22	g	612	CLA	C2B-C3B-CAB-CBB
22	g	612	CLA	C4B-C3B-CAB-CBB
22	g	613	CLA	C2B-C3B-CAB-CBB
22	g	613	CLA	C4B-C3B-CAB-CBB
22	g	613	CLA	CBD-CGD-O2D-CED
22	g	613	CLA	O1D-CGD-O2D-CED
22	g	614	CLA	C1A-C2A-CAA-CBA
22	g	614	CLA	CBD-CGD-O2D-CED
22	n	602	CLA	C2B-C3B-CAB-CBB
22	n	602	CLA	C4B-C3B-CAB-CBB
22	n	603	CLA	CBD-CGD-O2D-CED
22	n	604	CLA	C1A-C2A-CAA-CBA
22	n	610	CLA	CBD-CGD-O2D-CED
22	n	612	CLA	C2B-C3B-CAB-CBB
22	n	612	CLA	C4B-C3B-CAB-CBB
22	n	613	CLA	C2B-C3B-CAB-CBB
22	n	613	CLA	C4B-C3B-CAB-CBB
22	n	613	CLA	CBD-CGD-O2D-CED
22	n	613	CLA	O1D-CGD-O2D-CED
22	n	614	CLA	C1A-C2A-CAA-CBA
22	n	614	CLA	CBD-CGD-O2D-CED
22	y	602	CLA	C2B-C3B-CAB-CBB
22	y	602	CLA	C4B-C3B-CAB-CBB
22	y	602	CLA	CBD-CGD-O2D-CED
22	y	603	CLA	C2B-C3B-CAB-CBB
22	y	603	CLA	C4B-C3B-CAB-CBB
22	y	604	CLA	C1A-C2A-CAA-CBA
22	y	610	CLA	CBD-CGD-O2D-CED
22	y	611	CLA	CBD-CGD-O2D-CED
22	y	612	CLA	C2B-C3B-CAB-CBB
22	y	612	CLA	C4B-C3B-CAB-CBB
22	y	613	CLA	C2B-C3B-CAB-CBB
22	y	613	CLA	C4B-C3B-CAB-CBB
22	y	613	CLA	CBD-CGD-O2D-CED
22	y	614	CLA	C1A-C2A-CAA-CBA
22	y	614	CLA	CBD-CGD-O2D-CED
22	1	602	CLA	C2B-C3B-CAB-CBB
22	1	602	CLA	C4B-C3B-CAB-CBB
22	1	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	1	610	CLA	CBD-CGD-O2D-CED
22	1	611	CLA	CBD-CGD-O2D-CED
22	1	612	CLA	C2B-C3B-CAB-CBB
22	1	612	CLA	C4B-C3B-CAB-CBB
22	1	613	CLA	C2B-C3B-CAB-CBB
22	1	613	CLA	C4B-C3B-CAB-CBB
22	1	613	CLA	CBD-CGD-O2D-CED
22	1	614	CLA	C1A-C2A-CAA-CBA
22	1	614	CLA	CBD-CGD-O2D-CED
22	1	614	CLA	O1D-CGD-O2D-CED
22	2	602	CLA	C1A-C2A-CAA-CBA
22	2	602	CLA	C3A-C2A-CAA-CBA
22	2	602	CLA	C2B-C3B-CAB-CBB
22	2	602	CLA	C4B-C3B-CAB-CBB
22	2	603	CLA	CBD-CGD-O2D-CED
22	2	604	CLA	C1A-C2A-CAA-CBA
22	2	609	CLA	CBD-CGD-O2D-CED
22	2	611	CLA	C2B-C3B-CAB-CBB
22	2	611	CLA	C4B-C3B-CAB-CBB
22	2	612	CLA	C2B-C3B-CAB-CBB
22	2	612	CLA	C4B-C3B-CAB-CBB
22	2	612	CLA	CBD-CGD-O2D-CED
22	2	613	CLA	C1A-C2A-CAA-CBA
22	2	613	CLA	CBD-CGD-O2D-CED
22	3	303	CLA	C2B-C3B-CAB-CBB
22	3	303	CLA	C4B-C3B-CAB-CBB
22	3	304	CLA	CBD-CGD-O2D-CED
22	3	305	CLA	C1A-C2A-CAA-CBA
22	3	310	CLA	CBD-CGD-O2D-CED
22	3	312	CLA	C2B-C3B-CAB-CBB
22	3	312	CLA	C4B-C3B-CAB-CBB
22	3	313	CLA	C2B-C3B-CAB-CBB
22	3	313	CLA	C4B-C3B-CAB-CBB
22	3	313	CLA	CBD-CGD-O2D-CED
22	3	314	CLA	C1A-C2A-CAA-CBA
22	3	314	CLA	CBD-CGD-O2D-CED
22	4	301	CLA	CBD-CGD-O2D-CED
22	4	303	CLA	C2B-C3B-CAB-CBB
22	4	303	CLA	C4B-C3B-CAB-CBB
22	4	304	CLA	C2B-C3B-CAB-CBB
22	4	304	CLA	C4B-C3B-CAB-CBB
22	4	304	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	4	305	CLA	C1A-C2A-CAA-CBA
22	4	305	CLA	C3A-C2A-CAA-CBA
22	4	310	CLA	C1A-C2A-CAA-CBA
22	4	310	CLA	CBD-CGD-O2D-CED
22	4	311	CLA	CBD-CGD-O2D-CED
22	5	602	CLA	C2B-C3B-CAB-CBB
22	5	602	CLA	C4B-C3B-CAB-CBB
22	5	603	CLA	CBD-CGD-O2D-CED
22	5	610	CLA	CBD-CGD-O2D-CED
22	5	611	CLA	CBD-CGD-O2D-CED
22	5	612	CLA	C2B-C3B-CAB-CBB
22	5	612	CLA	C4B-C3B-CAB-CBB
22	5	613	CLA	C2B-C3B-CAB-CBB
22	5	613	CLA	C4B-C3B-CAB-CBB
22	5	613	CLA	CBD-CGD-O2D-CED
22	5	614	CLA	C1A-C2A-CAA-CBA
22	5	614	CLA	CBD-CGD-O2D-CED
22	5	614	CLA	O1D-CGD-O2D-CED
22	6	602	CLA	C1A-C2A-CAA-CBA
22	6	602	CLA	C3A-C2A-CAA-CBA
22	6	602	CLA	C2B-C3B-CAB-CBB
22	6	602	CLA	C4B-C3B-CAB-CBB
22	6	603	CLA	CBD-CGD-O2D-CED
22	6	604	CLA	C1A-C2A-CAA-CBA
22	6	609	CLA	CBD-CGD-O2D-CED
22	6	611	CLA	C2B-C3B-CAB-CBB
22	6	611	CLA	C4B-C3B-CAB-CBB
22	6	612	CLA	C2B-C3B-CAB-CBB
22	6	612	CLA	C4B-C3B-CAB-CBB
22	6	612	CLA	CBD-CGD-O2D-CED
22	6	613	CLA	C1A-C2A-CAA-CBA
22	6	613	CLA	CBD-CGD-O2D-CED
22	7	303	CLA	C2B-C3B-CAB-CBB
22	7	303	CLA	C4B-C3B-CAB-CBB
22	7	304	CLA	CBD-CGD-O2D-CED
22	7	305	CLA	C1A-C2A-CAA-CBA
22	7	310	CLA	CBD-CGD-O2D-CED
22	7	312	CLA	C2B-C3B-CAB-CBB
22	7	312	CLA	C4B-C3B-CAB-CBB
22	7	313	CLA	C2B-C3B-CAB-CBB
22	7	313	CLA	C4B-C3B-CAB-CBB
22	7	313	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	7	314	CLA	C1A-C2A-CAA-CBA
22	7	314	CLA	CBD-CGD-O2D-CED
22	8	301	CLA	CBD-CGD-O2D-CED
22	8	303	CLA	C2B-C3B-CAB-CBB
22	8	303	CLA	C4B-C3B-CAB-CBB
22	8	304	CLA	C2B-C3B-CAB-CBB
22	8	304	CLA	C4B-C3B-CAB-CBB
22	8	304	CLA	CBD-CGD-O2D-CED
22	8	305	CLA	C1A-C2A-CAA-CBA
22	8	305	CLA	C3A-C2A-CAA-CBA
22	8	310	CLA	C1A-C2A-CAA-CBA
22	8	310	CLA	CBD-CGD-O2D-CED
22	8	311	CLA	CBD-CGD-O2D-CED
23	A	404	PHO	C3A-C2A-CAA-CBA
25	R	304	CHL	C1A-C2A-CAA-CBA
25	R	304	CHL	C3A-C2A-CAA-CBA
25	R	304	CHL	C4B-C3B-CAB-CBB
25	R	304	CHL	CHA-CBD-CGD-O1D
25	R	304	CHL	CHA-CBD-CGD-O2D
25	R	305	CHL	C1A-C2A-CAA-CBA
25	R	305	CHL	C2B-C3B-CAB-CBB
25	R	305	CHL	C4B-C3B-CAB-CBB
25	R	305	CHL	C1C-C2C-CMC-OMC
25	R	305	CHL	C3C-C2C-CMC-OMC
25	R	305	CHL	CBD-CGD-O2D-CED
25	R	305	CHL	O1D-CGD-O2D-CED
25	R	306	CHL	C2B-C3B-CAB-CBB
25	R	306	CHL	C4B-C3B-CAB-CBB
25	R	306	CHL	C1C-C2C-CMC-OMC
25	R	306	CHL	C3C-C2C-CMC-OMC
25	R	306	CHL	CHA-CBD-CGD-O1D
25	R	306	CHL	CHA-CBD-CGD-O2D
25	R	306	CHL	CAD-CBD-CGD-O1D
25	R	306	CHL	CBD-CGD-O2D-CED
25	S	302	CHL	C2B-C3B-CAB-CBB
25	S	302	CHL	C4B-C3B-CAB-CBB
25	S	302	CHL	C1C-C2C-CMC-OMC
25	S	302	CHL	C3C-C2C-CMC-OMC
25	S	306	CHL	C2B-C3B-CAB-CBB
25	S	306	CHL	C4B-C3B-CAB-CBB
25	S	307	CHL	C1C-C2C-CMC-OMC
25	S	307	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
25	S	307	CHL	CBD-CGD-O2D-CED
25	S	308	CHL	C2B-C3B-CAB-CBB
25	S	308	CHL	C4B-C3B-CAB-CBB
25	S	308	CHL	C1C-C2C-CMC-OMC
25	S	308	CHL	C3C-C2C-CMC-OMC
25	G	601	CHL	C1C-C2C-CMC-OMC
25	G	601	CHL	C3C-C2C-CMC-OMC
25	G	605	CHL	C1C-C2C-CMC-OMC
25	G	605	CHL	C3C-C2C-CMC-OMC
25	G	605	CHL	CBD-CGD-O2D-CED
25	G	606	CHL	C1A-C2A-CAA-CBA
25	G	606	CHL	C4B-C3B-CAB-CBB
25	G	606	CHL	CBD-CGD-O2D-CED
25	G	607	CHL	C2B-C3B-CAB-CBB
25	G	607	CHL	C4B-C3B-CAB-CBB
25	G	607	CHL	C1C-C2C-CMC-OMC
25	G	607	CHL	C3C-C2C-CMC-OMC
25	G	607	CHL	CBD-CGD-O2D-CED
25	G	608	CHL	C1C-C2C-CMC-OMC
25	G	608	CHL	C3C-C2C-CMC-OMC
25	G	609	CHL	C1A-C2A-CAA-CBA
25	G	609	CHL	C2B-C3B-CAB-CBB
25	G	609	CHL	C4B-C3B-CAB-CBB
25	G	609	CHL	C1C-C2C-CMC-OMC
25	G	609	CHL	C3C-C2C-CMC-OMC
25	G	609	CHL	CAD-CBD-CGD-O1D
25	G	609	CHL	CAD-CBD-CGD-O2D
25	N	601	CHL	C2B-C3B-CAB-CBB
25	N	601	CHL	C4B-C3B-CAB-CBB
25	N	601	CHL	C1C-C2C-CMC-OMC
25	N	601	CHL	C3C-C2C-CMC-OMC
25	N	601	CHL	CBD-CGD-O2D-CED
25	N	605	CHL	C2B-C3B-CAB-CBB
25	N	605	CHL	C4B-C3B-CAB-CBB
25	N	605	CHL	C1C-C2C-CMC-OMC
25	N	605	CHL	C3C-C2C-CMC-OMC
25	N	605	CHL	CBD-CGD-O2D-CED
25	N	606	CHL	C1A-C2A-CAA-CBA
25	N	606	CHL	C3A-C2A-CAA-CBA
25	N	606	CHL	CBD-CGD-O2D-CED
25	N	607	CHL	C2B-C3B-CAB-CBB
25	N	607	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	N	607	CHL	C1C-C2C-CMC-OMC
25	N	607	CHL	C3C-C2C-CMC-OMC
25	N	607	CHL	CBD-CGD-O2D-CED
25	N	608	CHL	C1C-C2C-CMC-OMC
25	N	608	CHL	C3C-C2C-CMC-OMC
25	N	609	CHL	C1A-C2A-CAA-CBA
25	N	609	CHL	C1C-C2C-CMC-OMC
25	N	609	CHL	C3C-C2C-CMC-OMC
25	N	609	CHL	CAD-CBD-CGD-O1D
25	N	609	CHL	CAD-CBD-CGD-O2D
25	N	609	CHL	CBD-CGD-O2D-CED
25	Y	601	CHL	C1A-C2A-CAA-CBA
25	Y	601	CHL	C2B-C3B-CAB-CBB
25	Y	601	CHL	C4B-C3B-CAB-CBB
25	Y	601	CHL	C1C-C2C-CMC-OMC
25	Y	601	CHL	C3C-C2C-CMC-OMC
25	Y	605	CHL	C2B-C3B-CAB-CBB
25	Y	605	CHL	C4B-C3B-CAB-CBB
25	Y	605	CHL	C1C-C2C-CMC-OMC
25	Y	605	CHL	C3C-C2C-CMC-OMC
25	Y	606	CHL	C1A-C2A-CAA-CBA
25	Y	606	CHL	C3A-C2A-CAA-CBA
25	Y	606	CHL	CBD-CGD-O2D-CED
25	Y	607	CHL	C2B-C3B-CAB-CBB
25	Y	607	CHL	C4B-C3B-CAB-CBB
25	Y	607	CHL	C1C-C2C-CMC-OMC
25	Y	607	CHL	C3C-C2C-CMC-OMC
25	Y	607	CHL	CBD-CGD-O2D-CED
25	Y	608	CHL	C1C-C2C-CMC-OMC
25	Y	608	CHL	C3C-C2C-CMC-OMC
25	Y	609	CHL	C1A-C2A-CAA-CBA
25	Y	609	CHL	C2B-C3B-CAB-CBB
25	Y	609	CHL	C4B-C3B-CAB-CBB
25	Y	609	CHL	C1C-C2C-CMC-OMC
25	Y	609	CHL	C3C-C2C-CMC-OMC
25	Y	609	CHL	CHA-CBD-CGD-O1D
25	Y	609	CHL	CHA-CBD-CGD-O2D
25	Y	609	CHL	CAD-CBD-CGD-O1D
25	Y	609	CHL	CAD-CBD-CGD-O2D
25	Y	609	CHL	CBD-CGD-O2D-CED
25	r	304	CHL	C1A-C2A-CAA-CBA
25	r	304	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	r	304	CHL	C4B-C3B-CAB-CBB
25	r	304	CHL	CHA-CBD-CGD-O1D
25	r	304	CHL	CHA-CBD-CGD-O2D
25	r	305	CHL	C1A-C2A-CAA-CBA
25	r	305	CHL	C2B-C3B-CAB-CBB
25	r	305	CHL	C4B-C3B-CAB-CBB
25	r	305	CHL	C1C-C2C-CMC-OMC
25	r	305	CHL	C3C-C2C-CMC-OMC
25	r	305	CHL	CBD-CGD-O2D-CED
25	r	305	CHL	O1D-CGD-O2D-CED
25	r	306	CHL	C2B-C3B-CAB-CBB
25	r	306	CHL	C4B-C3B-CAB-CBB
25	r	306	CHL	C1C-C2C-CMC-OMC
25	r	306	CHL	C3C-C2C-CMC-OMC
25	r	306	CHL	CHA-CBD-CGD-O1D
25	r	306	CHL	CHA-CBD-CGD-O2D
25	r	306	CHL	CAD-CBD-CGD-O1D
25	r	306	CHL	CBD-CGD-O2D-CED
25	s	302	CHL	C2B-C3B-CAB-CBB
25	s	302	CHL	C4B-C3B-CAB-CBB
25	s	302	CHL	C1C-C2C-CMC-OMC
25	s	302	CHL	C3C-C2C-CMC-OMC
25	s	306	CHL	C2B-C3B-CAB-CBB
25	s	306	CHL	C4B-C3B-CAB-CBB
25	s	307	CHL	C1C-C2C-CMC-OMC
25	s	307	CHL	C3C-C2C-CMC-OMC
25	s	307	CHL	CBD-CGD-O2D-CED
25	s	308	CHL	C2B-C3B-CAB-CBB
25	s	308	CHL	C4B-C3B-CAB-CBB
25	s	308	CHL	C1C-C2C-CMC-OMC
25	s	308	CHL	C3C-C2C-CMC-OMC
25	g	601	CHL	C1C-C2C-CMC-OMC
25	g	601	CHL	C3C-C2C-CMC-OMC
25	g	605	CHL	C1C-C2C-CMC-OMC
25	g	605	CHL	C3C-C2C-CMC-OMC
25	g	605	CHL	CBD-CGD-O2D-CED
25	g	606	CHL	C1A-C2A-CAA-CBA
25	g	606	CHL	C4B-C3B-CAB-CBB
25	g	606	CHL	CBD-CGD-O2D-CED
25	g	607	CHL	C2B-C3B-CAB-CBB
25	g	607	CHL	C4B-C3B-CAB-CBB
25	g	607	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
25	g	607	CHL	C3C-C2C-CMC-OMC
25	g	607	CHL	CBD-CGD-O2D-CED
25	g	608	CHL	C1C-C2C-CMC-OMC
25	g	608	CHL	C3C-C2C-CMC-OMC
25	g	609	CHL	C1A-C2A-CAA-CBA
25	g	609	CHL	C2B-C3B-CAB-CBB
25	g	609	CHL	C4B-C3B-CAB-CBB
25	g	609	CHL	C1C-C2C-CMC-OMC
25	g	609	CHL	C3C-C2C-CMC-OMC
25	g	609	CHL	CAD-CBD-CGD-O1D
25	g	609	CHL	CAD-CBD-CGD-O2D
25	n	601	CHL	C2B-C3B-CAB-CBB
25	n	601	CHL	C4B-C3B-CAB-CBB
25	n	601	CHL	C1C-C2C-CMC-OMC
25	n	601	CHL	C3C-C2C-CMC-OMC
25	n	601	CHL	CBD-CGD-O2D-CED
25	n	605	CHL	C2B-C3B-CAB-CBB
25	n	605	CHL	C4B-C3B-CAB-CBB
25	n	605	CHL	C1C-C2C-CMC-OMC
25	n	605	CHL	C3C-C2C-CMC-OMC
25	n	605	CHL	CBD-CGD-O2D-CED
25	n	606	CHL	C1A-C2A-CAA-CBA
25	n	606	CHL	C3A-C2A-CAA-CBA
25	n	606	CHL	CBD-CGD-O2D-CED
25	n	607	CHL	C2B-C3B-CAB-CBB
25	n	607	CHL	C4B-C3B-CAB-CBB
25	n	607	CHL	C1C-C2C-CMC-OMC
25	n	607	CHL	C3C-C2C-CMC-OMC
25	n	607	CHL	CBD-CGD-O2D-CED
25	n	608	CHL	C1C-C2C-CMC-OMC
25	n	608	CHL	C3C-C2C-CMC-OMC
25	n	609	CHL	C1A-C2A-CAA-CBA
25	n	609	CHL	C1C-C2C-CMC-OMC
25	n	609	CHL	C3C-C2C-CMC-OMC
25	n	609	CHL	CAD-CBD-CGD-O1D
25	n	609	CHL	CAD-CBD-CGD-O2D
25	n	609	CHL	CBD-CGD-O2D-CED
25	y	601	CHL	C1A-C2A-CAA-CBA
25	y	601	CHL	C2B-C3B-CAB-CBB
25	y	601	CHL	C4B-C3B-CAB-CBB
25	y	601	CHL	C1C-C2C-CMC-OMC
25	y	601	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
25	y	605	CHL	C2B-C3B-CAB-CBB
25	y	605	CHL	C4B-C3B-CAB-CBB
25	y	605	CHL	C1C-C2C-CMC-OMC
25	y	605	CHL	C3C-C2C-CMC-OMC
25	y	606	CHL	C1A-C2A-CAA-CBA
25	y	606	CHL	C3A-C2A-CAA-CBA
25	y	606	CHL	CBD-CGD-O2D-CED
25	y	607	CHL	C2B-C3B-CAB-CBB
25	y	607	CHL	C4B-C3B-CAB-CBB
25	y	607	CHL	C1C-C2C-CMC-OMC
25	y	607	CHL	C3C-C2C-CMC-OMC
25	y	607	CHL	CBD-CGD-O2D-CED
25	y	608	CHL	C1C-C2C-CMC-OMC
25	y	608	CHL	C3C-C2C-CMC-OMC
25	y	609	CHL	C1A-C2A-CAA-CBA
25	y	609	CHL	C2B-C3B-CAB-CBB
25	y	609	CHL	C4B-C3B-CAB-CBB
25	y	609	CHL	C1C-C2C-CMC-OMC
25	y	609	CHL	C3C-C2C-CMC-OMC
25	y	609	CHL	CHA-CBD-CGD-O1D
25	y	609	CHL	CHA-CBD-CGD-O2D
25	y	609	CHL	CAD-CBD-CGD-O1D
25	y	609	CHL	CAD-CBD-CGD-O2D
25	y	609	CHL	CBD-CGD-O2D-CED
25	1	601	CHL	C1A-C2A-CAA-CBA
25	1	601	CHL	C2B-C3B-CAB-CBB
25	1	601	CHL	C4B-C3B-CAB-CBB
25	1	601	CHL	C1C-C2C-CMC-OMC
25	1	601	CHL	C3C-C2C-CMC-OMC
25	1	601	CHL	CBD-CGD-O2D-CED
25	1	605	CHL	C2B-C3B-CAB-CBB
25	1	605	CHL	C4B-C3B-CAB-CBB
25	1	605	CHL	C1C-C2C-CMC-OMC
25	1	605	CHL	C3C-C2C-CMC-OMC
25	1	605	CHL	CBD-CGD-O2D-CED
25	1	606	CHL	C1A-C2A-CAA-CBA
25	1	606	CHL	C3A-C2A-CAA-CBA
25	1	606	CHL	CBD-CGD-O2D-CED
25	1	607	CHL	C2B-C3B-CAB-CBB
25	1	607	CHL	C4B-C3B-CAB-CBB
25	1	607	CHL	C1C-C2C-CMC-OMC
25	1	607	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
25	1	607	CHL	CBD-CGD-O2D-CED
25	1	608	CHL	C1C-C2C-CMC-OMC
25	1	608	CHL	C3C-C2C-CMC-OMC
25	1	609	CHL	C1A-C2A-CAA-CBA
25	1	609	CHL	C2B-C3B-CAB-CBB
25	1	609	CHL	C4B-C3B-CAB-CBB
25	1	609	CHL	C1C-C2C-CMC-OMC
25	1	609	CHL	C3C-C2C-CMC-OMC
25	1	609	CHL	CHA-CBD-CGD-O1D
25	1	609	CHL	CHA-CBD-CGD-O2D
25	1	609	CHL	CAD-CBD-CGD-O1D
25	1	609	CHL	CAD-CBD-CGD-O2D
25	1	609	CHL	CBD-CGD-O2D-CED
25	1	615	CHL	C2B-C3B-CAB-CBB
25	1	615	CHL	C4B-C3B-CAB-CBB
25	1	615	CHL	C1C-C2C-CMC-OMC
25	1	615	CHL	C3C-C2C-CMC-OMC
25	1	615	CHL	CHA-CBD-CGD-O1D
25	1	615	CHL	CHA-CBD-CGD-O2D
25	1	615	CHL	CBD-CGD-O2D-CED
25	2	601	CHL	C2B-C3B-CAB-CBB
25	2	601	CHL	C4B-C3B-CAB-CBB
25	2	601	CHL	C1C-C2C-CMC-OMC
25	2	601	CHL	C3C-C2C-CMC-OMC
25	2	605	CHL	C4B-C3B-CAB-CBB
25	2	605	CHL	C1C-C2C-CMC-OMC
25	2	605	CHL	C3C-C2C-CMC-OMC
25	2	605	CHL	CBD-CGD-O2D-CED
25	2	606	CHL	C1A-C2A-CAA-CBA
25	2	606	CHL	C3A-C2A-CAA-CBA
25	2	606	CHL	C2B-C3B-CAB-CBB
25	2	606	CHL	C4B-C3B-CAB-CBB
25	2	606	CHL	CBD-CGD-O2D-CED
25	2	607	CHL	C1C-C2C-CMC-OMC
25	2	607	CHL	C3C-C2C-CMC-OMC
25	2	608	CHL	C1A-C2A-CAA-CBA
25	2	608	CHL	C2B-C3B-CAB-CBB
25	2	608	CHL	C4B-C3B-CAB-CBB
25	2	608	CHL	C1C-C2C-CMC-OMC
25	2	608	CHL	C3C-C2C-CMC-OMC
25	2	608	CHL	CHA-CBD-CGD-O1D
25	2	608	CHL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	2	608	CHL	CAD-CBD-CGD-O2D
25	2	608	CHL	CBD-CGD-O2D-CED
25	3	301	CHL	C2B-C3B-CAB-CBB
25	3	301	CHL	C4B-C3B-CAB-CBB
25	3	301	CHL	C1C-C2C-CMC-OMC
25	3	301	CHL	C3C-C2C-CMC-OMC
25	3	301	CHL	CBD-CGD-O2D-CED
25	3	302	CHL	C1A-C2A-CAA-CBA
25	3	302	CHL	C2B-C3B-CAB-CBB
25	3	302	CHL	C4B-C3B-CAB-CBB
25	3	302	CHL	C1C-C2C-CMC-OMC
25	3	302	CHL	C3C-C2C-CMC-OMC
25	3	302	CHL	CBD-CGD-O2D-CED
25	3	306	CHL	C4B-C3B-CAB-CBB
25	3	306	CHL	C1C-C2C-CMC-OMC
25	3	306	CHL	C3C-C2C-CMC-OMC
25	3	306	CHL	CBD-CGD-O2D-CED
25	3	307	CHL	C1A-C2A-CAA-CBA
25	3	307	CHL	C3A-C2A-CAA-CBA
25	3	307	CHL	C2B-C3B-CAB-CBB
25	3	307	CHL	C4B-C3B-CAB-CBB
25	3	307	CHL	CBD-CGD-O2D-CED
25	3	308	CHL	C1C-C2C-CMC-OMC
25	3	308	CHL	C3C-C2C-CMC-OMC
25	3	309	CHL	C1A-C2A-CAA-CBA
25	3	309	CHL	C2B-C3B-CAB-CBB
25	3	309	CHL	C4B-C3B-CAB-CBB
25	3	309	CHL	C1C-C2C-CMC-OMC
25	3	309	CHL	C3C-C2C-CMC-OMC
25	3	309	CHL	CAD-CBD-CGD-O1D
25	3	309	CHL	CAD-CBD-CGD-O2D
25	3	309	CHL	CBD-CGD-O2D-CED
25	4	302	CHL	C2B-C3B-CAB-CBB
25	4	302	CHL	C4B-C3B-CAB-CBB
25	4	302	CHL	C1C-C2C-CMC-OMC
25	4	302	CHL	C3C-C2C-CMC-OMC
25	4	306	CHL	C1A-C2A-CAA-CBA
25	4	306	CHL	C1C-C2C-CMC-OMC
25	4	306	CHL	C3C-C2C-CMC-OMC
25	4	306	CHL	CBD-CGD-O2D-CED
25	4	307	CHL	C1A-C2A-CAA-CBA
25	4	307	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	4	307	CHL	C4B-C3B-CAB-CBB
25	4	307	CHL	C1C-C2C-CMC-OMC
25	4	307	CHL	C3C-C2C-CMC-OMC
25	4	307	CHL	CBD-CGD-O2D-CED
25	4	308	CHL	C2B-C3B-CAB-CBB
25	4	308	CHL	C4B-C3B-CAB-CBB
25	4	308	CHL	C1C-C2C-CMC-OMC
25	4	308	CHL	C3C-C2C-CMC-OMC
25	4	309	CHL	C1C-C2C-CMC-OMC
25	4	309	CHL	C3C-C2C-CMC-OMC
25	4	309	CHL	CBD-CGD-O2D-CED
25	5	601	CHL	C1A-C2A-CAA-CBA
25	5	601	CHL	C2B-C3B-CAB-CBB
25	5	601	CHL	C4B-C3B-CAB-CBB
25	5	601	CHL	C1C-C2C-CMC-OMC
25	5	601	CHL	C3C-C2C-CMC-OMC
25	5	601	CHL	CBD-CGD-O2D-CED
25	5	605	CHL	C2B-C3B-CAB-CBB
25	5	605	CHL	C4B-C3B-CAB-CBB
25	5	605	CHL	C1C-C2C-CMC-OMC
25	5	605	CHL	C3C-C2C-CMC-OMC
25	5	605	CHL	CBD-CGD-O2D-CED
25	5	606	CHL	C1A-C2A-CAA-CBA
25	5	606	CHL	C3A-C2A-CAA-CBA
25	5	606	CHL	CBD-CGD-O2D-CED
25	5	607	CHL	C2B-C3B-CAB-CBB
25	5	607	CHL	C4B-C3B-CAB-CBB
25	5	607	CHL	C1C-C2C-CMC-OMC
25	5	607	CHL	C3C-C2C-CMC-OMC
25	5	607	CHL	CBD-CGD-O2D-CED
25	5	608	CHL	C1C-C2C-CMC-OMC
25	5	608	CHL	C3C-C2C-CMC-OMC
25	5	609	CHL	C1A-C2A-CAA-CBA
25	5	609	CHL	C2B-C3B-CAB-CBB
25	5	609	CHL	C4B-C3B-CAB-CBB
25	5	609	CHL	C1C-C2C-CMC-OMC
25	5	609	CHL	C3C-C2C-CMC-OMC
25	5	609	CHL	CHA-CBD-CGD-O1D
25	5	609	CHL	CHA-CBD-CGD-O2D
25	5	609	CHL	CAD-CBD-CGD-O1D
25	5	609	CHL	CAD-CBD-CGD-O2D
25	5	609	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	5	615	CHL	C2B-C3B-CAB-CBB
25	5	615	CHL	C4B-C3B-CAB-CBB
25	5	615	CHL	C1C-C2C-CMC-OMC
25	5	615	CHL	C3C-C2C-CMC-OMC
25	5	615	CHL	CHA-CBD-CGD-O1D
25	5	615	CHL	CHA-CBD-CGD-O2D
25	5	615	CHL	CBD-CGD-O2D-CED
25	6	601	CHL	C2B-C3B-CAB-CBB
25	6	601	CHL	C4B-C3B-CAB-CBB
25	6	601	CHL	C1C-C2C-CMC-OMC
25	6	601	CHL	C3C-C2C-CMC-OMC
25	6	605	CHL	C4B-C3B-CAB-CBB
25	6	605	CHL	C1C-C2C-CMC-OMC
25	6	605	CHL	C3C-C2C-CMC-OMC
25	6	605	CHL	CBD-CGD-O2D-CED
25	6	606	CHL	C1A-C2A-CAA-CBA
25	6	606	CHL	C3A-C2A-CAA-CBA
25	6	606	CHL	C2B-C3B-CAB-CBB
25	6	606	CHL	C4B-C3B-CAB-CBB
25	6	606	CHL	CBD-CGD-O2D-CED
25	6	607	CHL	C1C-C2C-CMC-OMC
25	6	607	CHL	C3C-C2C-CMC-OMC
25	6	608	CHL	C1A-C2A-CAA-CBA
25	6	608	CHL	C2B-C3B-CAB-CBB
25	6	608	CHL	C4B-C3B-CAB-CBB
25	6	608	CHL	C1C-C2C-CMC-OMC
25	6	608	CHL	C3C-C2C-CMC-OMC
25	6	608	CHL	CHA-CBD-CGD-O1D
25	6	608	CHL	CAD-CBD-CGD-O1D
25	6	608	CHL	CAD-CBD-CGD-O2D
25	6	608	CHL	CBD-CGD-O2D-CED
25	7	301	CHL	C2B-C3B-CAB-CBB
25	7	301	CHL	C4B-C3B-CAB-CBB
25	7	301	CHL	C1C-C2C-CMC-OMC
25	7	301	CHL	C3C-C2C-CMC-OMC
25	7	301	CHL	CBD-CGD-O2D-CED
25	7	302	CHL	C1A-C2A-CAA-CBA
25	7	302	CHL	C2B-C3B-CAB-CBB
25	7	302	CHL	C4B-C3B-CAB-CBB
25	7	302	CHL	C1C-C2C-CMC-OMC
25	7	302	CHL	C3C-C2C-CMC-OMC
25	7	302	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	7	306	CHL	C4B-C3B-CAB-CBB
25	7	306	CHL	C1C-C2C-CMC-OMC
25	7	306	CHL	C3C-C2C-CMC-OMC
25	7	306	CHL	CBD-CGD-O2D-CED
25	7	307	CHL	C1A-C2A-CAA-CBA
25	7	307	CHL	C3A-C2A-CAA-CBA
25	7	307	CHL	C2B-C3B-CAB-CBB
25	7	307	CHL	C4B-C3B-CAB-CBB
25	7	307	CHL	CBD-CGD-O2D-CED
25	7	308	CHL	C1C-C2C-CMC-OMC
25	7	308	CHL	C3C-C2C-CMC-OMC
25	7	309	CHL	C1A-C2A-CAA-CBA
25	7	309	CHL	C2B-C3B-CAB-CBB
25	7	309	CHL	C4B-C3B-CAB-CBB
25	7	309	CHL	C1C-C2C-CMC-OMC
25	7	309	CHL	C3C-C2C-CMC-OMC
25	7	309	CHL	CAD-CBD-CGD-O1D
25	7	309	CHL	CAD-CBD-CGD-O2D
25	7	309	CHL	CBD-CGD-O2D-CED
25	8	302	CHL	C2B-C3B-CAB-CBB
25	8	302	CHL	C4B-C3B-CAB-CBB
25	8	302	CHL	C1C-C2C-CMC-OMC
25	8	302	CHL	C3C-C2C-CMC-OMC
25	8	306	CHL	C1A-C2A-CAA-CBA
25	8	306	CHL	C1C-C2C-CMC-OMC
25	8	306	CHL	C3C-C2C-CMC-OMC
25	8	306	CHL	CBD-CGD-O2D-CED
25	8	307	CHL	C1A-C2A-CAA-CBA
25	8	307	CHL	C2B-C3B-CAB-CBB
25	8	307	CHL	C4B-C3B-CAB-CBB
25	8	307	CHL	C1C-C2C-CMC-OMC
25	8	307	CHL	C3C-C2C-CMC-OMC
25	8	307	CHL	CBD-CGD-O2D-CED
25	8	308	CHL	C2B-C3B-CAB-CBB
25	8	308	CHL	C4B-C3B-CAB-CBB
25	8	308	CHL	C1C-C2C-CMC-OMC
25	8	308	CHL	C3C-C2C-CMC-OMC
25	8	309	CHL	C1C-C2C-CMC-OMC
25	8	309	CHL	C3C-C2C-CMC-OMC
25	8	309	CHL	CBD-CGD-O2D-CED
22	A	403	CLA	O1D-CGD-O2D-CED
22	B	606	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	608	CLA	O1D-CGD-O2D-CED
22	C	502	CLA	O1D-CGD-O2D-CED
22	a	403	CLA	O1D-CGD-O2D-CED
22	b	606	CLA	O1D-CGD-O2D-CED
22	b	607	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	O1D-CGD-O2D-CED
22	c	502	CLA	O1D-CGD-O2D-CED
22	c	506	CLA	O1D-CGD-O2D-CED
22	R	307	CLA	O1D-CGD-O2D-CED
22	S	309	CLA	O1D-CGD-O2D-CED
22	N	612	CLA	O1D-CGD-O2D-CED
22	N	614	CLA	O1D-CGD-O2D-CED
22	Y	612	CLA	O1D-CGD-O2D-CED
22	Y	613	CLA	O1D-CGD-O2D-CED
22	r	307	CLA	O1D-CGD-O2D-CED
22	s	301	CLA	O1D-CGD-O2D-CED
22	s	309	CLA	O1D-CGD-O2D-CED
22	n	612	CLA	O1D-CGD-O2D-CED
22	n	614	CLA	O1D-CGD-O2D-CED
22	y	612	CLA	O1D-CGD-O2D-CED
22	y	613	CLA	O1D-CGD-O2D-CED
22	1	612	CLA	O1D-CGD-O2D-CED
22	2	611	CLA	O1D-CGD-O2D-CED
22	3	314	CLA	O1D-CGD-O2D-CED
22	5	612	CLA	O1D-CGD-O2D-CED
22	6	611	CLA	O1D-CGD-O2D-CED
22	7	314	CLA	O1D-CGD-O2D-CED
25	S	307	CHL	O1D-CGD-O2D-CED
25	s	307	CHL	O1D-CGD-O2D-CED
25	1	607	CHL	O1D-CGD-O2D-CED
25	2	601	CHL	O1D-CGD-O2D-CED
25	4	307	CHL	O1D-CGD-O2D-CED
25	4	308	CHL	O1D-CGD-O2D-CED
25	5	607	CHL	O1D-CGD-O2D-CED
25	6	601	CHL	O1D-CGD-O2D-CED
25	8	307	CHL	O1D-CGD-O2D-CED
25	8	308	CHL	O1D-CGD-O2D-CED
22	A	402	CLA	O1D-CGD-O2D-CED
22	C	503	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED
22	b	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	b	616	CLA	O1D-CGD-O2D-CED
22	d	403	CLA	O1D-CGD-O2D-CED
22	c	511	CLA	O1D-CGD-O2D-CED
22	S	305	CLA	O1D-CGD-O2D-CED
22	S	312	CLA	O1D-CGD-O2D-CED
22	G	612	CLA	O1D-CGD-O2D-CED
22	Y	614	CLA	O1D-CGD-O2D-CED
22	s	305	CLA	O1D-CGD-O2D-CED
22	s	312	CLA	O1D-CGD-O2D-CED
22	g	612	CLA	O1D-CGD-O2D-CED
22	y	614	CLA	O1D-CGD-O2D-CED
22	1	613	CLA	O1D-CGD-O2D-CED
22	2	612	CLA	O1D-CGD-O2D-CED
22	2	613	CLA	O1D-CGD-O2D-CED
22	3	311	CLA	O1D-CGD-O2D-CED
22	3	312	CLA	O1D-CGD-O2D-CED
22	3	313	CLA	O1D-CGD-O2D-CED
22	4	301	CLA	O1D-CGD-O2D-CED
22	5	613	CLA	O1D-CGD-O2D-CED
22	6	612	CLA	O1D-CGD-O2D-CED
22	6	613	CLA	O1D-CGD-O2D-CED
22	7	311	CLA	O1D-CGD-O2D-CED
22	7	312	CLA	O1D-CGD-O2D-CED
22	7	313	CLA	O1D-CGD-O2D-CED
22	8	301	CLA	O1D-CGD-O2D-CED
25	G	607	CHL	O1D-CGD-O2D-CED
25	N	607	CHL	O1D-CGD-O2D-CED
25	Y	606	CHL	O1D-CGD-O2D-CED
25	Y	607	CHL	O1D-CGD-O2D-CED
25	g	607	CHL	O1D-CGD-O2D-CED
25	n	607	CHL	O1D-CGD-O2D-CED
25	y	606	CHL	O1D-CGD-O2D-CED
25	y	607	CHL	O1D-CGD-O2D-CED
25	1	615	CHL	O1D-CGD-O2D-CED
25	2	606	CHL	O1D-CGD-O2D-CED
25	3	301	CHL	O1D-CGD-O2D-CED
25	5	615	CHL	O1D-CGD-O2D-CED
25	6	606	CHL	O1D-CGD-O2D-CED
25	7	301	CHL	O1D-CGD-O2D-CED
22	A	403	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	CBD-CGD-O2D-CED
22	B	604	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	CBD-CGD-O2D-CED
22	B	607	CLA	CBD-CGD-O2D-CED
22	B	608	CLA	CBD-CGD-O2D-CED
22	C	501	CLA	CBD-CGD-O2D-CED
22	C	502	CLA	CBD-CGD-O2D-CED
22	C	503	CLA	CBD-CGD-O2D-CED
22	C	504	CLA	CBD-CGD-O2D-CED
22	C	506	CLA	CBD-CGD-O2D-CED
22	C	509	CLA	CBD-CGD-O2D-CED
22	C	512	CLA	CBD-CGD-O2D-CED
22	D	401	CLA	CBD-CGD-O2D-CED
22	D	404	CLA	CBD-CGD-O2D-CED
22	b	605	CLA	CBD-CGD-O2D-CED
22	b	607	CLA	CBD-CGD-O2D-CED
22	b	608	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
22	b	612	CLA	CBD-CGD-O2D-CED
22	b	616	CLA	CBD-CGD-O2D-CED
22	d	401	CLA	CBD-CGD-O2D-CED
22	d	404	CLA	CBD-CGD-O2D-CED
22	c	502	CLA	CBD-CGD-O2D-CED
22	c	506	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED
22	c	509	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
22	R	308	CLA	CBD-CGD-O2D-CED
22	R	310	CLA	CBD-CGD-O2D-CED
22	G	602	CLA	CBD-CGD-O2D-CED
22	G	611	CLA	CBD-CGD-O2D-CED
22	G	612	CLA	CBD-CGD-O2D-CED
22	N	602	CLA	CBD-CGD-O2D-CED
22	N	611	CLA	CBD-CGD-O2D-CED
22	N	612	CLA	CBD-CGD-O2D-CED
22	Y	603	CLA	CBD-CGD-O2D-CED
22	Y	612	CLA	CBD-CGD-O2D-CED
22	r	308	CLA	CBD-CGD-O2D-CED
22	r	310	CLA	CBD-CGD-O2D-CED
22	g	602	CLA	CBD-CGD-O2D-CED
22	g	611	CLA	CBD-CGD-O2D-CED
22	g	612	CLA	CBD-CGD-O2D-CED
22	n	602	CLA	CBD-CGD-O2D-CED
22	n	611	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	n	612	CLA	CBD-CGD-O2D-CED
22	y	603	CLA	CBD-CGD-O2D-CED
22	y	612	CLA	CBD-CGD-O2D-CED
22	1	602	CLA	CBD-CGD-O2D-CED
22	1	612	CLA	CBD-CGD-O2D-CED
22	2	602	CLA	CBD-CGD-O2D-CED
22	2	610	CLA	CBD-CGD-O2D-CED
22	2	611	CLA	CBD-CGD-O2D-CED
22	3	303	CLA	CBD-CGD-O2D-CED
22	3	311	CLA	CBD-CGD-O2D-CED
22	3	312	CLA	CBD-CGD-O2D-CED
22	4	303	CLA	CBD-CGD-O2D-CED
22	5	602	CLA	CBD-CGD-O2D-CED
22	5	612	CLA	CBD-CGD-O2D-CED
22	6	602	CLA	CBD-CGD-O2D-CED
22	6	610	CLA	CBD-CGD-O2D-CED
22	6	611	CLA	CBD-CGD-O2D-CED
22	7	303	CLA	CBD-CGD-O2D-CED
22	7	311	CLA	CBD-CGD-O2D-CED
22	7	312	CLA	CBD-CGD-O2D-CED
22	8	303	CLA	CBD-CGD-O2D-CED
23	A	404	PHO	CBD-CGD-O2D-CED
23	a	404	PHO	CBD-CGD-O2D-CED
23	d	402	PHO	CBD-CGD-O2D-CED
25	S	306	CHL	CBD-CGD-O2D-CED
25	G	601	CHL	CBD-CGD-O2D-CED
25	G	609	CHL	CBD-CGD-O2D-CED
25	N	608	CHL	CBD-CGD-O2D-CED
25	Y	601	CHL	CBD-CGD-O2D-CED
25	Y	605	CHL	CBD-CGD-O2D-CED
25	Y	608	CHL	CBD-CGD-O2D-CED
25	s	306	CHL	CBD-CGD-O2D-CED
25	g	601	CHL	CBD-CGD-O2D-CED
25	g	609	CHL	CBD-CGD-O2D-CED
25	n	608	CHL	CBD-CGD-O2D-CED
25	y	601	CHL	CBD-CGD-O2D-CED
25	y	605	CHL	CBD-CGD-O2D-CED
25	y	608	CHL	CBD-CGD-O2D-CED
25	2	601	CHL	CBD-CGD-O2D-CED
25	4	308	CHL	CBD-CGD-O2D-CED
25	6	601	CHL	CBD-CGD-O2D-CED
25	8	308	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	607	CLA	O1D-CGD-O2D-CED
22	B	611	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	O1D-CGD-O2D-CED
22	C	507	CLA	O1D-CGD-O2D-CED
22	C	511	CLA	O1D-CGD-O2D-CED
22	D	403	CLA	O1D-CGD-O2D-CED
22	a	402	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	O1D-CGD-O2D-CED
22	R	303	CLA	O1D-CGD-O2D-CED
22	G	611	CLA	O1D-CGD-O2D-CED
22	N	603	CLA	O1D-CGD-O2D-CED
22	N	611	CLA	O1D-CGD-O2D-CED
22	Y	603	CLA	O1D-CGD-O2D-CED
22	r	303	CLA	O1D-CGD-O2D-CED
22	g	611	CLA	O1D-CGD-O2D-CED
22	n	603	CLA	O1D-CGD-O2D-CED
22	n	611	CLA	O1D-CGD-O2D-CED
22	y	603	CLA	O1D-CGD-O2D-CED
22	2	603	CLA	O1D-CGD-O2D-CED
22	2	610	CLA	O1D-CGD-O2D-CED
22	6	603	CLA	O1D-CGD-O2D-CED
22	6	610	CLA	O1D-CGD-O2D-CED
25	R	306	CHL	O1D-CGD-O2D-CED
25	r	306	CHL	O1D-CGD-O2D-CED
22	B	605	CLA	O1D-CGD-O2D-CED
22	B	612	CLA	O1D-CGD-O2D-CED
22	C	501	CLA	O1D-CGD-O2D-CED
22	D	404	CLA	O1D-CGD-O2D-CED
22	b	602	CLA	O1D-CGD-O2D-CED
22	b	609	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
22	c	501	CLA	O1D-CGD-O2D-CED
22	c	503	CLA	O1D-CGD-O2D-CED
22	R	311	CLA	O1D-CGD-O2D-CED
22	S	303	CLA	O1D-CGD-O2D-CED
22	S	310	CLA	O1D-CGD-O2D-CED
22	S	313	CLA	O1D-CGD-O2D-CED
22	G	603	CLA	O1D-CGD-O2D-CED
22	G	610	CLA	O1D-CGD-O2D-CED
22	G	614	CLA	O1D-CGD-O2D-CED
22	Y	610	CLA	O1D-CGD-O2D-CED
22	Y	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	r	311	CLA	O1D-CGD-O2D-CED
22	s	303	CLA	O1D-CGD-O2D-CED
22	s	310	CLA	O1D-CGD-O2D-CED
22	s	313	CLA	O1D-CGD-O2D-CED
22	g	603	CLA	O1D-CGD-O2D-CED
22	g	610	CLA	O1D-CGD-O2D-CED
22	g	614	CLA	O1D-CGD-O2D-CED
22	y	610	CLA	O1D-CGD-O2D-CED
22	y	611	CLA	O1D-CGD-O2D-CED
22	1	603	CLA	O1D-CGD-O2D-CED
22	1	611	CLA	O1D-CGD-O2D-CED
22	2	609	CLA	O1D-CGD-O2D-CED
22	3	304	CLA	O1D-CGD-O2D-CED
22	4	304	CLA	O1D-CGD-O2D-CED
22	4	310	CLA	O1D-CGD-O2D-CED
22	4	311	CLA	O1D-CGD-O2D-CED
22	5	603	CLA	O1D-CGD-O2D-CED
22	5	611	CLA	O1D-CGD-O2D-CED
22	6	609	CLA	O1D-CGD-O2D-CED
22	7	304	CLA	O1D-CGD-O2D-CED
22	8	304	CLA	O1D-CGD-O2D-CED
22	8	310	CLA	O1D-CGD-O2D-CED
22	8	311	CLA	O1D-CGD-O2D-CED
25	G	601	CHL	O1D-CGD-O2D-CED
25	G	605	CHL	O1D-CGD-O2D-CED
25	G	606	CHL	O1D-CGD-O2D-CED
25	G	609	CHL	O1D-CGD-O2D-CED
25	N	601	CHL	O1D-CGD-O2D-CED
25	N	605	CHL	O1D-CGD-O2D-CED
25	N	606	CHL	O1D-CGD-O2D-CED
25	N	609	CHL	O1D-CGD-O2D-CED
25	g	601	CHL	O1D-CGD-O2D-CED
25	g	605	CHL	O1D-CGD-O2D-CED
25	g	606	CHL	O1D-CGD-O2D-CED
25	g	609	CHL	O1D-CGD-O2D-CED
25	n	601	CHL	O1D-CGD-O2D-CED
25	n	605	CHL	O1D-CGD-O2D-CED
25	n	606	CHL	O1D-CGD-O2D-CED
25	n	609	CHL	O1D-CGD-O2D-CED
25	1	605	CHL	O1D-CGD-O2D-CED
25	1	606	CHL	O1D-CGD-O2D-CED
25	1	609	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	2	605	CHL	O1D-CGD-O2D-CED
25	3	306	CHL	O1D-CGD-O2D-CED
25	3	307	CHL	O1D-CGD-O2D-CED
25	3	309	CHL	O1D-CGD-O2D-CED
25	4	309	CHL	O1D-CGD-O2D-CED
25	5	605	CHL	O1D-CGD-O2D-CED
25	5	606	CHL	O1D-CGD-O2D-CED
25	5	609	CHL	O1D-CGD-O2D-CED
25	6	605	CHL	O1D-CGD-O2D-CED
25	7	306	CHL	O1D-CGD-O2D-CED
25	7	307	CHL	O1D-CGD-O2D-CED
25	7	309	CHL	O1D-CGD-O2D-CED
25	8	309	CHL	O1D-CGD-O2D-CED
22	B	601	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED
22	R	302	CLA	CBD-CGD-O2D-CED
22	r	302	CLA	CBD-CGD-O2D-CED
23	D	402	PHO	CBD-CGD-O2D-CED
25	R	304	CHL	CBD-CGD-O2D-CED
25	S	308	CHL	CBD-CGD-O2D-CED
25	G	608	CHL	CBD-CGD-O2D-CED
25	r	304	CHL	CBD-CGD-O2D-CED
25	s	308	CHL	CBD-CGD-O2D-CED
25	g	608	CHL	CBD-CGD-O2D-CED
25	1	608	CHL	CBD-CGD-O2D-CED
25	3	308	CHL	CBD-CGD-O2D-CED
25	5	608	CHL	CBD-CGD-O2D-CED
25	7	308	CHL	CBD-CGD-O2D-CED
22	B	615	CLA	O1D-CGD-O2D-CED
22	b	603	CLA	O1D-CGD-O2D-CED
22	N	610	CLA	O1D-CGD-O2D-CED
22	n	610	CLA	O1D-CGD-O2D-CED
22	1	610	CLA	O1D-CGD-O2D-CED
22	5	610	CLA	O1D-CGD-O2D-CED
25	Y	609	CHL	O1D-CGD-O2D-CED
25	y	609	CHL	O1D-CGD-O2D-CED
25	2	608	CHL	O1D-CGD-O2D-CED
25	3	302	CHL	O1D-CGD-O2D-CED
25	4	306	CHL	O1D-CGD-O2D-CED
25	6	608	CHL	O1D-CGD-O2D-CED
25	7	302	CHL	O1D-CGD-O2D-CED
25	8	306	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	O1D-CGD-O2D-CED
22	B	614	CLA	CBD-CGD-O2D-CED
22	G	604	CLA	CBD-CGD-O2D-CED
22	g	604	CLA	CBD-CGD-O2D-CED
25	S	302	CHL	CBD-CGD-O2D-CED
25	s	302	CHL	CBD-CGD-O2D-CED
22	B	616	CLA	O1D-CGD-O2D-CED
22	C	504	CLA	O1D-CGD-O2D-CED
22	C	508	CLA	O1D-CGD-O2D-CED
22	c	504	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED
22	G	602	CLA	O1D-CGD-O2D-CED
22	Y	602	CLA	O1D-CGD-O2D-CED
22	g	602	CLA	O1D-CGD-O2D-CED
22	y	602	CLA	O1D-CGD-O2D-CED
22	1	602	CLA	O1D-CGD-O2D-CED
22	3	310	CLA	O1D-CGD-O2D-CED
22	5	602	CLA	O1D-CGD-O2D-CED
22	7	310	CLA	O1D-CGD-O2D-CED
25	1	601	CHL	O1D-CGD-O2D-CED
25	5	601	CHL	O1D-CGD-O2D-CED
22	B	604	CLA	O1D-CGD-O2D-CED
22	d	401	CLA	O1D-CGD-O2D-CED
22	d	404	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	O1D-CGD-O2D-CED
22	2	602	CLA	O1D-CGD-O2D-CED
22	6	602	CLA	O1D-CGD-O2D-CED
22	b	604	CLA	CBD-CGD-O2D-CED
22	S	304	CLA	CBD-CGD-O2D-CED
22	s	304	CLA	CBD-CGD-O2D-CED
22	B	614	CLA	C2A-CAA-CBA-CGA
22	a	405	CLA	C2A-CAA-CBA-CGA
22	b	609	CLA	C2A-CAA-CBA-CGA
22	b	614	CLA	C2A-CAA-CBA-CGA
22	R	310	CLA	C2A-CAA-CBA-CGA
22	S	301	CLA	C2A-CAA-CBA-CGA
22	r	310	CLA	C2A-CAA-CBA-CGA
22	4	304	CLA	C2A-CAA-CBA-CGA
22	8	304	CLA	C2A-CAA-CBA-CGA
25	G	601	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	g	601	CHL	C2A-CAA-CBA-CGA
25	1	601	CHL	C2A-CAA-CBA-CGA
25	2	601	CHL	C2A-CAA-CBA-CGA
25	3	302	CHL	C2A-CAA-CBA-CGA
25	4	302	CHL	C2A-CAA-CBA-CGA
25	5	601	CHL	C2A-CAA-CBA-CGA
25	6	601	CHL	C2A-CAA-CBA-CGA
25	7	302	CHL	C2A-CAA-CBA-CGA
25	8	302	CHL	C2A-CAA-CBA-CGA
22	3	303	CLA	O1D-CGD-O2D-CED
22	7	303	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	O1D-CGD-O2D-CED
22	C	512	CLA	O1D-CGD-O2D-CED
22	c	512	CLA	O1D-CGD-O2D-CED
22	R	310	CLA	O1D-CGD-O2D-CED
22	N	602	CLA	O1D-CGD-O2D-CED
22	r	310	CLA	O1D-CGD-O2D-CED
22	n	602	CLA	O1D-CGD-O2D-CED
25	N	608	CHL	O1D-CGD-O2D-CED
25	n	608	CHL	O1D-CGD-O2D-CED
22	b	615	CLA	CBD-CGD-O2D-CED
25	2	607	CHL	CBD-CGD-O2D-CED
25	6	607	CHL	CBD-CGD-O2D-CED
22	b	610	CLA	O1D-CGD-O2D-CED
23	A	404	PHO	O1D-CGD-O2D-CED
25	Y	605	CHL	O1D-CGD-O2D-CED
25	y	605	CHL	O1D-CGD-O2D-CED
22	4	303	CLA	O1D-CGD-O2D-CED
22	8	303	CLA	O1D-CGD-O2D-CED
23	d	402	PHO	O1D-CGD-O2D-CED
25	S	306	CHL	O1D-CGD-O2D-CED
25	Y	601	CHL	O1D-CGD-O2D-CED
25	Y	608	CHL	O1D-CGD-O2D-CED
25	s	306	CHL	O1D-CGD-O2D-CED
25	y	601	CHL	O1D-CGD-O2D-CED
25	y	608	CHL	O1D-CGD-O2D-CED
22	R	301	CLA	CBD-CGD-O2D-CED
22	N	604	CLA	CBD-CGD-O2D-CED
22	r	301	CLA	CBD-CGD-O2D-CED
22	n	604	CLA	CBD-CGD-O2D-CED
22	2	604	CLA	CBD-CGD-O2D-CED
22	6	604	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	509	CLA	O1D-CGD-O2D-CED
22	R	308	CLA	O1D-CGD-O2D-CED
22	r	308	CLA	O1D-CGD-O2D-CED
22	B	603	CLA	CBD-CGD-O2D-CED
22	B	603	CLA	C2A-CAA-CBA-CGA
22	B	606	CLA	C2A-CAA-CBA-CGA
22	B	613	CLA	C2A-CAA-CBA-CGA
22	S	309	CLA	C2A-CAA-CBA-CGA
22	s	309	CLA	C2A-CAA-CBA-CGA
22	1	604	CLA	C2A-CAA-CBA-CGA
22	5	604	CLA	C2A-CAA-CBA-CGA
25	S	306	CHL	C2A-CAA-CBA-CGA
25	s	306	CHL	C2A-CAA-CBA-CGA
22	C	509	CLA	O1D-CGD-O2D-CED
22	D	401	CLA	O1D-CGD-O2D-CED
23	a	404	PHO	O1D-CGD-O2D-CED
22	B	601	CLA	O1D-CGD-O2D-CED
22	B	610	CLA	O1D-CGD-O2D-CED
25	3	308	CHL	O1D-CGD-O2D-CED
25	7	308	CHL	O1D-CGD-O2D-CED
23	D	402	PHO	O1D-CGD-O2D-CED
25	G	608	CHL	O1D-CGD-O2D-CED
25	g	608	CHL	O1D-CGD-O2D-CED
25	S	308	CHL	O1D-CGD-O2D-CED
25	s	308	CHL	O1D-CGD-O2D-CED
25	R	304	CHL	O1D-CGD-O2D-CED
25	r	304	CHL	O1D-CGD-O2D-CED
22	a	402	CLA	C2A-CAA-CBA-CGA
22	S	305	CLA	C2A-CAA-CBA-CGA
22	s	305	CLA	C2A-CAA-CBA-CGA
25	Y	601	CHL	C2A-CAA-CBA-CGA
25	y	601	CHL	C2A-CAA-CBA-CGA
25	2	607	CHL	C2A-CAA-CBA-CGA
25	6	607	CHL	C2A-CAA-CBA-CGA
25	1	608	CHL	O1D-CGD-O2D-CED
25	5	608	CHL	O1D-CGD-O2D-CED
22	c	505	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	CBD-CGD-O2D-CED
24	e	101	HEM	C2A-CAA-CBA-CGA
22	A	402	CLA	C2A-CAA-CBA-CGA
22	B	612	CLA	C2A-CAA-CBA-CGA
22	C	506	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	b	603	CLA	C2A-CAA-CBA-CGA
22	b	607	CLA	C2A-CAA-CBA-CGA
22	b	612	CLA	C2A-CAA-CBA-CGA
22	N	604	CLA	C2A-CAA-CBA-CGA
22	s	301	CLA	C2A-CAA-CBA-CGA
22	n	604	CLA	C2A-CAA-CBA-CGA
22	3	311	CLA	C2A-CAA-CBA-CGA
22	7	311	CLA	C2A-CAA-CBA-CGA
25	3	308	CHL	C2A-CAA-CBA-CGA
25	7	308	CHL	C2A-CAA-CBA-CGA
22	R	302	CLA	O1D-CGD-O2D-CED
22	G	604	CLA	O1D-CGD-O2D-CED
22	r	302	CLA	O1D-CGD-O2D-CED
22	g	604	CLA	O1D-CGD-O2D-CED
25	S	302	CHL	O1D-CGD-O2D-CED
25	s	302	CHL	O1D-CGD-O2D-CED
22	B	614	CLA	O1D-CGD-O2D-CED
22	S	304	CLA	O1D-CGD-O2D-CED
22	s	304	CLA	O1D-CGD-O2D-CED
22	b	604	CLA	O1D-CGD-O2D-CED
22	R	307	CLA	C2A-CAA-CBA-CGA
22	r	307	CLA	C2A-CAA-CBA-CGA
25	G	608	CHL	C2A-CAA-CBA-CGA
25	N	601	CHL	C2A-CAA-CBA-CGA
25	g	608	CHL	C2A-CAA-CBA-CGA
25	n	601	CHL	C2A-CAA-CBA-CGA
25	1	607	CHL	C2A-CAA-CBA-CGA
25	1	615	CHL	C2A-CAA-CBA-CGA
25	5	607	CHL	C2A-CAA-CBA-CGA
25	5	615	CHL	C2A-CAA-CBA-CGA
22	b	615	CLA	O1D-CGD-O2D-CED
25	2	607	CHL	O1D-CGD-O2D-CED
25	6	607	CHL	O1D-CGD-O2D-CED
22	c	506	CLA	C2A-CAA-CBA-CGA
22	Y	604	CLA	C2A-CAA-CBA-CGA
22	y	604	CLA	C2A-CAA-CBA-CGA
25	4	309	CHL	C2A-CAA-CBA-CGA
25	8	309	CHL	C2A-CAA-CBA-CGA
22	B	605	CLA	C4B-C3B-CAB-CBB
22	B	607	CLA	C4B-C3B-CAB-CBB
22	b	607	CLA	C4B-C3B-CAB-CBB
22	b	616	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	c	503	CLA	C4B-C3B-CAB-CBB
22	G	603	CLA	C4B-C3B-CAB-CBB
22	N	603	CLA	C4B-C3B-CAB-CBB
22	g	603	CLA	C4B-C3B-CAB-CBB
22	n	603	CLA	C4B-C3B-CAB-CBB
25	S	307	CHL	C4B-C3B-CAB-CBB
25	G	601	CHL	C4B-C3B-CAB-CBB
25	G	605	CHL	C4B-C3B-CAB-CBB
25	N	609	CHL	C4B-C3B-CAB-CBB
25	s	307	CHL	C4B-C3B-CAB-CBB
25	g	601	CHL	C4B-C3B-CAB-CBB
25	g	605	CHL	C4B-C3B-CAB-CBB
25	n	609	CHL	C4B-C3B-CAB-CBB
25	4	309	CHL	C4B-C3B-CAB-CBB
25	8	309	CHL	C4B-C3B-CAB-CBB
22	A	402	CLA	C3A-C2A-CAA-CBA
22	B	602	CLA	C3A-C2A-CAA-CBA
22	B	614	CLA	C3A-C2A-CAA-CBA
22	B	615	CLA	C3A-C2A-CAA-CBA
22	C	509	CLA	C3A-C2A-CAA-CBA
22	D	403	CLA	C3A-C2A-CAA-CBA
22	a	402	CLA	C3A-C2A-CAA-CBA
22	b	615	CLA	C3A-C2A-CAA-CBA
22	d	403	CLA	C3A-C2A-CAA-CBA
22	c	509	CLA	C3A-C2A-CAA-CBA
22	R	302	CLA	C3A-C2A-CAA-CBA
22	R	309	CLA	C3A-C2A-CAA-CBA
22	S	311	CLA	C3A-C2A-CAA-CBA
22	S	312	CLA	C3A-C2A-CAA-CBA
22	N	612	CLA	C3A-C2A-CAA-CBA
22	Y	602	CLA	C3A-C2A-CAA-CBA
22	Y	612	CLA	C3A-C2A-CAA-CBA
22	r	302	CLA	C3A-C2A-CAA-CBA
22	r	309	CLA	C3A-C2A-CAA-CBA
22	s	311	CLA	C3A-C2A-CAA-CBA
22	s	312	CLA	C3A-C2A-CAA-CBA
22	n	612	CLA	C3A-C2A-CAA-CBA
22	y	602	CLA	C3A-C2A-CAA-CBA
22	y	612	CLA	C3A-C2A-CAA-CBA
22	2	604	CLA	C3A-C2A-CAA-CBA
22	2	611	CLA	C3A-C2A-CAA-CBA
22	3	305	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	4	304	CLA	C3A-C2A-CAA-CBA
22	6	604	CLA	C3A-C2A-CAA-CBA
22	6	611	CLA	C3A-C2A-CAA-CBA
22	7	305	CLA	C3A-C2A-CAA-CBA
22	8	304	CLA	C3A-C2A-CAA-CBA
23	a	404	PHO	C3A-C2A-CAA-CBA
23	d	402	PHO	C3A-C2A-CAA-CBA
25	R	305	CHL	C3A-C2A-CAA-CBA
25	G	601	CHL	C3A-C2A-CAA-CBA
25	N	601	CHL	C3A-C2A-CAA-CBA
25	Y	601	CHL	C3A-C2A-CAA-CBA
25	r	305	CHL	C3A-C2A-CAA-CBA
25	g	601	CHL	C3A-C2A-CAA-CBA
25	n	601	CHL	C3A-C2A-CAA-CBA
25	y	601	CHL	C3A-C2A-CAA-CBA
25	1	601	CHL	C3A-C2A-CAA-CBA
25	1	609	CHL	C3A-C2A-CAA-CBA
25	2	601	CHL	C3A-C2A-CAA-CBA
25	2	608	CHL	C3A-C2A-CAA-CBA
25	3	302	CHL	C3A-C2A-CAA-CBA
25	3	309	CHL	C3A-C2A-CAA-CBA
25	4	306	CHL	C3A-C2A-CAA-CBA
25	5	601	CHL	C3A-C2A-CAA-CBA
25	5	609	CHL	C3A-C2A-CAA-CBA
25	6	601	CHL	C3A-C2A-CAA-CBA
25	6	608	CHL	C3A-C2A-CAA-CBA
25	7	302	CHL	C3A-C2A-CAA-CBA
25	7	309	CHL	C3A-C2A-CAA-CBA
25	8	306	CHL	C3A-C2A-CAA-CBA
25	4	309	CHL	C2C-C3C-CAC-CBC
25	8	309	CHL	C2C-C3C-CAC-CBC
25	S	306	CHL	C2C-C3C-CAC-CBC
25	s	306	CHL	C2C-C3C-CAC-CBC
22	B	605	CLA	C2B-C3B-CAB-CBB
22	B	607	CLA	C2B-C3B-CAB-CBB
22	C	503	CLA	C2B-C3B-CAB-CBB
22	b	607	CLA	C2B-C3B-CAB-CBB
22	b	616	CLA	C2B-C3B-CAB-CBB
22	c	503	CLA	C2B-C3B-CAB-CBB
22	G	603	CLA	C2B-C3B-CAB-CBB
22	N	603	CLA	C2B-C3B-CAB-CBB
22	g	603	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	n	603	CLA	C2B-C3B-CAB-CBB
25	R	304	CHL	C2B-C3B-CAB-CBB
25	S	307	CHL	C2B-C3B-CAB-CBB
25	G	601	CHL	C2B-C3B-CAB-CBB
25	G	605	CHL	C2B-C3B-CAB-CBB
25	G	606	CHL	C2B-C3B-CAB-CBB
25	N	609	CHL	C2B-C3B-CAB-CBB
25	r	304	CHL	C2B-C3B-CAB-CBB
25	s	307	CHL	C2B-C3B-CAB-CBB
25	g	601	CHL	C2B-C3B-CAB-CBB
25	g	605	CHL	C2B-C3B-CAB-CBB
25	g	606	CHL	C2B-C3B-CAB-CBB
25	n	609	CHL	C2B-C3B-CAB-CBB
25	1	606	CHL	C2B-C3B-CAB-CBB
25	2	605	CHL	C2B-C3B-CAB-CBB
25	3	306	CHL	C2B-C3B-CAB-CBB
25	4	309	CHL	C2B-C3B-CAB-CBB
25	5	606	CHL	C2B-C3B-CAB-CBB
25	6	605	CHL	C2B-C3B-CAB-CBB
25	7	306	CHL	C2B-C3B-CAB-CBB
25	8	309	CHL	C2B-C3B-CAB-CBB
24	F	101	HEM	C2A-CAA-CBA-CGA
24	e	101	HEM	C3D-CAD-CBD-CGD
22	N	604	CLA	O1D-CGD-O2D-CED
22	n	604	CLA	O1D-CGD-O2D-CED
22	C	504	CLA	C2A-CAA-CBA-CGA
22	D	401	CLA	C2A-CAA-CBA-CGA
22	b	606	CLA	C2A-CAA-CBA-CGA
22	c	505	CLA	C2A-CAA-CBA-CGA
22	S	314	CLA	C2A-CAA-CBA-CGA
22	G	611	CLA	C2A-CAA-CBA-CGA
22	Y	602	CLA	C2A-CAA-CBA-CGA
22	s	314	CLA	C2A-CAA-CBA-CGA
22	g	611	CLA	C2A-CAA-CBA-CGA
22	y	602	CLA	C2A-CAA-CBA-CGA
22	1	602	CLA	C2A-CAA-CBA-CGA
22	3	303	CLA	C2A-CAA-CBA-CGA
22	4	311	CLA	C2A-CAA-CBA-CGA
22	5	602	CLA	C2A-CAA-CBA-CGA
22	7	303	CLA	C2A-CAA-CBA-CGA
22	8	311	CLA	C2A-CAA-CBA-CGA
25	Y	606	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	y	606	CHL	C2A-CAA-CBA-CGA
25	1	608	CHL	C2A-CAA-CBA-CGA
25	5	608	CHL	C2A-CAA-CBA-CGA
22	B	603	CLA	O1D-CGD-O2D-CED
22	2	604	CLA	O1D-CGD-O2D-CED
22	6	604	CLA	O1D-CGD-O2D-CED
22	R	301	CLA	O1D-CGD-O2D-CED
22	r	301	CLA	O1D-CGD-O2D-CED
25	4	307	CHL	C2C-C3C-CAC-CBC
25	8	307	CHL	C2C-C3C-CAC-CBC
24	e	101	HEM	C4C-C3C-CAC-CBC
22	d	404	CLA	C2A-CAA-CBA-CGA
22	c	503	CLA	C2A-CAA-CBA-CGA
22	G	602	CLA	C2A-CAA-CBA-CGA
22	N	602	CLA	C2A-CAA-CBA-CGA
22	g	602	CLA	C2A-CAA-CBA-CGA
22	n	602	CLA	C2A-CAA-CBA-CGA
22	1	611	CLA	C2A-CAA-CBA-CGA
22	5	611	CLA	C2A-CAA-CBA-CGA
25	N	608	CHL	C2A-CAA-CBA-CGA
25	Y	607	CHL	C2A-CAA-CBA-CGA
25	Y	608	CHL	C2A-CAA-CBA-CGA
25	Y	609	CHL	C2A-CAA-CBA-CGA
25	n	608	CHL	C2A-CAA-CBA-CGA
25	y	607	CHL	C2A-CAA-CBA-CGA
25	y	608	CHL	C2A-CAA-CBA-CGA
25	y	609	CHL	C2A-CAA-CBA-CGA
22	A	402	CLA	C1A-C2A-CAA-CBA
22	A	405	CLA	C1A-C2A-CAA-CBA
22	B	602	CLA	C1A-C2A-CAA-CBA
22	B	615	CLA	C1A-C2A-CAA-CBA
22	C	501	CLA	C1A-C2A-CAA-CBA
22	C	503	CLA	C1A-C2A-CAA-CBA
22	C	506	CLA	C1A-C2A-CAA-CBA
22	D	401	CLA	C1A-C2A-CAA-CBA
22	D	403	CLA	C1A-C2A-CAA-CBA
22	D	404	CLA	C1A-C2A-CAA-CBA
22	a	402	CLA	C1A-C2A-CAA-CBA
22	b	602	CLA	C1A-C2A-CAA-CBA
22	b	611	CLA	C1A-C2A-CAA-CBA
22	b	615	CLA	C1A-C2A-CAA-CBA
22	b	616	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	d	401	CLA	C1A-C2A-CAA-CBA
22	d	404	CLA	C1A-C2A-CAA-CBA
22	c	503	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C1A-C2A-CAA-CBA
22	R	309	CLA	C1A-C2A-CAA-CBA
22	S	305	CLA	C1A-C2A-CAA-CBA
22	Y	602	CLA	C1A-C2A-CAA-CBA
22	Y	612	CLA	C1A-C2A-CAA-CBA
22	r	309	CLA	C1A-C2A-CAA-CBA
22	s	305	CLA	C1A-C2A-CAA-CBA
22	y	602	CLA	C1A-C2A-CAA-CBA
22	y	612	CLA	C1A-C2A-CAA-CBA
22	1	604	CLA	C1A-C2A-CAA-CBA
22	2	611	CLA	C1A-C2A-CAA-CBA
22	3	310	CLA	C1A-C2A-CAA-CBA
22	4	304	CLA	C1A-C2A-CAA-CBA
22	5	604	CLA	C1A-C2A-CAA-CBA
22	6	611	CLA	C1A-C2A-CAA-CBA
22	7	310	CLA	C1A-C2A-CAA-CBA
22	8	304	CLA	C1A-C2A-CAA-CBA
25	R	306	CHL	C1A-C2A-CAA-CBA
25	S	306	CHL	C1A-C2A-CAA-CBA
25	G	601	CHL	C1A-C2A-CAA-CBA
25	N	601	CHL	C1A-C2A-CAA-CBA
25	r	306	CHL	C1A-C2A-CAA-CBA
25	s	306	CHL	C1A-C2A-CAA-CBA
25	g	601	CHL	C1A-C2A-CAA-CBA
25	n	601	CHL	C1A-C2A-CAA-CBA
25	2	601	CHL	C1A-C2A-CAA-CBA
25	4	308	CHL	C1A-C2A-CAA-CBA
25	6	601	CHL	C1A-C2A-CAA-CBA
25	8	308	CHL	C1A-C2A-CAA-CBA
22	B	604	CLA	C2C-C3C-CAC-CBC
22	c	505	CLA	O1D-CGD-O2D-CED
22	R	302	CLA	C2A-CAA-CBA-CGA
22	r	302	CLA	C2A-CAA-CBA-CGA
22	C	505	CLA	O1D-CGD-O2D-CED
23	D	402	PHO	CHA-CBD-CGD-O1D
23	D	402	PHO	CHA-CBD-CGD-O2D
22	C	503	CLA	C4B-C3B-CAB-CBB
22	C	506	CLA	C4B-C3B-CAB-CBB
22	a	403	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	C4B-C3B-CAB-CBB
22	c	506	CLA	C4B-C3B-CAB-CBB
22	c	512	CLA	C4B-C3B-CAB-CBB
22	R	301	CLA	C4B-C3B-CAB-CBB
22	R	311	CLA	C4B-C3B-CAB-CBB
22	S	301	CLA	C4B-C3B-CAB-CBB
22	S	303	CLA	C4B-C3B-CAB-CBB
22	S	313	CLA	C4B-C3B-CAB-CBB
22	N	604	CLA	C4B-C3B-CAB-CBB
22	r	301	CLA	C4B-C3B-CAB-CBB
22	r	311	CLA	C4B-C3B-CAB-CBB
22	s	301	CLA	C4B-C3B-CAB-CBB
22	s	303	CLA	C4B-C3B-CAB-CBB
22	s	313	CLA	C4B-C3B-CAB-CBB
22	n	604	CLA	C4B-C3B-CAB-CBB
22	2	603	CLA	C4B-C3B-CAB-CBB
22	6	603	CLA	C4B-C3B-CAB-CBB
25	N	606	CHL	C4B-C3B-CAB-CBB
25	n	606	CHL	C4B-C3B-CAB-CBB
25	1	606	CHL	C4B-C3B-CAB-CBB
25	5	606	CHL	C4B-C3B-CAB-CBB
22	C	511	CLA	C3A-C2A-CAA-CBA
22	c	511	CLA	C3A-C2A-CAA-CBA
22	R	303	CLA	C3A-C2A-CAA-CBA
22	R	310	CLA	C3A-C2A-CAA-CBA
22	G	602	CLA	C3A-C2A-CAA-CBA
22	G	610	CLA	C3A-C2A-CAA-CBA
22	N	602	CLA	C3A-C2A-CAA-CBA
22	Y	611	CLA	C3A-C2A-CAA-CBA
22	r	303	CLA	C3A-C2A-CAA-CBA
22	r	310	CLA	C3A-C2A-CAA-CBA
22	g	602	CLA	C3A-C2A-CAA-CBA
22	g	610	CLA	C3A-C2A-CAA-CBA
22	n	602	CLA	C3A-C2A-CAA-CBA
22	y	611	CLA	C3A-C2A-CAA-CBA
22	1	602	CLA	C3A-C2A-CAA-CBA
22	3	303	CLA	C3A-C2A-CAA-CBA
22	3	310	CLA	C3A-C2A-CAA-CBA
22	4	310	CLA	C3A-C2A-CAA-CBA
22	5	602	CLA	C3A-C2A-CAA-CBA
22	7	303	CLA	C3A-C2A-CAA-CBA
22	7	310	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	8	310	CLA	C3A-C2A-CAA-CBA
25	S	306	CHL	C3A-C2A-CAA-CBA
25	G	606	CHL	C3A-C2A-CAA-CBA
25	s	306	CHL	C3A-C2A-CAA-CBA
25	g	606	CHL	C3A-C2A-CAA-CBA
25	1	615	CHL	C3A-C2A-CAA-CBA
25	5	615	CHL	C3A-C2A-CAA-CBA
22	b	602	CLA	C2A-CAA-CBA-CGA
25	R	306	CHL	C2C-C3C-CAC-CBC
25	r	306	CHL	C2C-C3C-CAC-CBC
25	4	309	CHL	C4C-C3C-CAC-CBC
25	8	309	CHL	C4C-C3C-CAC-CBC
22	C	506	CLA	C2B-C3B-CAB-CBB
22	a	403	CLA	C2B-C3B-CAB-CBB
22	b	601	CLA	C2B-C3B-CAB-CBB
22	c	512	CLA	C2B-C3B-CAB-CBB
22	S	301	CLA	C2B-C3B-CAB-CBB
25	N	606	CHL	C2B-C3B-CAB-CBB
25	n	606	CHL	C2B-C3B-CAB-CBB
25	S	306	CHL	C4C-C3C-CAC-CBC
25	s	306	CHL	C4C-C3C-CAC-CBC
23	A	404	PHO	C1A-C2A-CAA-CBA
22	A	405	CLA	C2A-CAA-CBA-CGA
25	G	609	CHL	C2A-CAA-CBA-CGA
25	g	609	CHL	C2A-CAA-CBA-CGA
25	R	304	CHL	C2C-C3C-CAC-CBC
25	r	304	CHL	C2C-C3C-CAC-CBC
22	C	501	CLA	C2A-CAA-CBA-CGA
22	b	615	CLA	C2A-CAA-CBA-CGA
22	c	508	CLA	C2A-CAA-CBA-CGA
22	A	405	CLA	CAD-CBD-CGD-O2D
22	B	615	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	C	510	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	b	612	CLA	CAD-CBD-CGD-O2D
22	c	510	CLA	CAD-CBD-CGD-O2D
22	N	614	CLA	CAD-CBD-CGD-O2D
22	n	614	CLA	CAD-CBD-CGD-O2D
22	2	604	CLA	CAD-CBD-CGD-O2D
22	3	305	CLA	CAD-CBD-CGD-O2D
22	6	604	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	7	305	CLA	CAD-CBD-CGD-O2D
25	R	306	CHL	CAD-CBD-CGD-O2D
25	S	307	CHL	CAD-CBD-CGD-O2D
25	G	608	CHL	CAD-CBD-CGD-O2D
25	Y	606	CHL	CAD-CBD-CGD-O2D
25	r	306	CHL	CAD-CBD-CGD-O2D
25	s	307	CHL	CAD-CBD-CGD-O2D
25	g	608	CHL	CAD-CBD-CGD-O2D
25	y	606	CHL	CAD-CBD-CGD-O2D
25	2	606	CHL	CAD-CBD-CGD-O2D
25	2	607	CHL	CAD-CBD-CGD-O2D
25	3	308	CHL	CAD-CBD-CGD-O2D
25	4	306	CHL	CAD-CBD-CGD-O2D
25	4	308	CHL	CAD-CBD-CGD-O2D
25	6	606	CHL	CAD-CBD-CGD-O2D
25	6	607	CHL	CAD-CBD-CGD-O2D
25	7	308	CHL	CAD-CBD-CGD-O2D
25	8	306	CHL	CAD-CBD-CGD-O2D
25	8	308	CHL	CAD-CBD-CGD-O2D
24	F	101	HEM	C4C-C3C-CAC-CBC
24	e	101	HEM	C4B-C3B-CAB-CBB
22	B	616	CLA	C2A-CAA-CBA-CGA
22	C	503	CLA	C2A-CAA-CBA-CGA
22	c	504	CLA	C2A-CAA-CBA-CGA
22	3	305	CLA	C2A-CAA-CBA-CGA
22	7	305	CLA	C2A-CAA-CBA-CGA
25	3	301	CHL	C2A-CAA-CBA-CGA
25	7	301	CHL	C2A-CAA-CBA-CGA
25	4	307	CHL	C4C-C3C-CAC-CBC
25	8	307	CHL	C4C-C3C-CAC-CBC
22	B	601	CLA	CHA-CBD-CGD-O2D
22	B	604	CLA	CHA-CBD-CGD-O1D
22	B	604	CLA	CHA-CBD-CGD-O2D
22	B	609	CLA	CHA-CBD-CGD-O1D
22	B	609	CLA	CHA-CBD-CGD-O2D
22	B	612	CLA	CHA-CBD-CGD-O1D
22	B	612	CLA	CHA-CBD-CGD-O2D
22	B	614	CLA	CHA-CBD-CGD-O1D
22	B	615	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CHA-CBD-CGD-O2D
22	C	505	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	CHA-CBD-CGD-O2D
22	b	616	CLA	CHA-CBD-CGD-O1D
22	b	616	CLA	CHA-CBD-CGD-O2D
22	c	501	CLA	CHA-CBD-CGD-O1D
22	c	503	CLA	CHA-CBD-CGD-O1D
22	c	505	CLA	CHA-CBD-CGD-O1D
22	c	505	CLA	CHA-CBD-CGD-O2D
22	R	301	CLA	CHA-CBD-CGD-O1D
22	R	301	CLA	CHA-CBD-CGD-O2D
22	R	302	CLA	CHA-CBD-CGD-O1D
22	R	302	CLA	CHA-CBD-CGD-O2D
22	R	307	CLA	CHA-CBD-CGD-O2D
22	N	612	CLA	CHA-CBD-CGD-O1D
22	N	612	CLA	CHA-CBD-CGD-O2D
22	Y	603	CLA	CHA-CBD-CGD-O1D
22	Y	603	CLA	CHA-CBD-CGD-O2D
22	Y	612	CLA	CHA-CBD-CGD-O1D
22	Y	612	CLA	CHA-CBD-CGD-O2D
22	r	301	CLA	CHA-CBD-CGD-O1D
22	r	301	CLA	CHA-CBD-CGD-O2D
22	r	302	CLA	CHA-CBD-CGD-O1D
22	r	302	CLA	CHA-CBD-CGD-O2D
22	r	307	CLA	CHA-CBD-CGD-O2D
22	n	612	CLA	CHA-CBD-CGD-O1D
22	n	612	CLA	CHA-CBD-CGD-O2D
22	y	603	CLA	CHA-CBD-CGD-O1D
22	y	603	CLA	CHA-CBD-CGD-O2D
22	y	612	CLA	CHA-CBD-CGD-O1D
22	y	612	CLA	CHA-CBD-CGD-O2D
22	1	603	CLA	CHA-CBD-CGD-O1D
22	2	611	CLA	CHA-CBD-CGD-O1D
22	4	305	CLA	CHA-CBD-CGD-O1D
22	5	603	CLA	CHA-CBD-CGD-O1D
22	6	611	CLA	CHA-CBD-CGD-O1D
22	8	305	CLA	CHA-CBD-CGD-O1D
25	S	302	CHL	CHA-CBD-CGD-O1D
25	S	302	CHL	CHA-CBD-CGD-O2D
25	S	308	CHL	CHA-CBD-CGD-O1D
25	S	308	CHL	CHA-CBD-CGD-O2D
25	G	605	CHL	CHA-CBD-CGD-O1D
25	G	605	CHL	CHA-CBD-CGD-O2D
25	N	605	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	N	605	CHL	CHA-CBD-CGD-O2D
25	Y	605	CHL	CHA-CBD-CGD-O1D
25	s	302	CHL	CHA-CBD-CGD-O1D
25	s	302	CHL	CHA-CBD-CGD-O2D
25	s	308	CHL	CHA-CBD-CGD-O1D
25	s	308	CHL	CHA-CBD-CGD-O2D
25	g	605	CHL	CHA-CBD-CGD-O1D
25	g	605	CHL	CHA-CBD-CGD-O2D
25	n	605	CHL	CHA-CBD-CGD-O1D
25	n	605	CHL	CHA-CBD-CGD-O2D
25	y	605	CHL	CHA-CBD-CGD-O1D
25	1	605	CHL	CHA-CBD-CGD-O1D
25	1	605	CHL	CHA-CBD-CGD-O2D
25	2	608	CHL	CHA-CBD-CGD-O2D
25	3	306	CHL	CHA-CBD-CGD-O1D
25	3	306	CHL	CHA-CBD-CGD-O2D
25	5	605	CHL	CHA-CBD-CGD-O1D
25	5	605	CHL	CHA-CBD-CGD-O2D
25	6	608	CHL	CHA-CBD-CGD-O2D
25	7	306	CHL	CHA-CBD-CGD-O1D
25	7	306	CHL	CHA-CBD-CGD-O2D
22	Y	611	CLA	C2A-CAA-CBA-CGA
22	y	611	CLA	C2A-CAA-CBA-CGA
22	2	602	CLA	C2A-CAA-CBA-CGA
22	6	602	CLA	C2A-CAA-CBA-CGA
22	B	607	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	511	CLA	C1A-C2A-CAA-CBA
22	b	604	CLA	C1A-C2A-CAA-CBA
22	b	607	CLA	C1A-C2A-CAA-CBA
22	c	501	CLA	C1A-C2A-CAA-CBA
22	c	505	CLA	C1A-C2A-CAA-CBA
22	R	310	CLA	C1A-C2A-CAA-CBA
22	S	312	CLA	C1A-C2A-CAA-CBA
22	G	610	CLA	C1A-C2A-CAA-CBA
22	N	612	CLA	C1A-C2A-CAA-CBA
22	r	310	CLA	C1A-C2A-CAA-CBA
22	s	312	CLA	C1A-C2A-CAA-CBA
22	g	610	CLA	C1A-C2A-CAA-CBA
22	n	612	CLA	C1A-C2A-CAA-CBA
25	Y	606	CHL	C4B-C3B-CAB-CBB
25	y	606	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	N	609	CHL	C2A-CAA-CBA-CGA
25	n	609	CHL	C2A-CAA-CBA-CGA
22	B	604	CLA	C4C-C3C-CAC-CBC
22	B	603	CLA	CAD-CBD-CGD-O1D
22	B	604	CLA	CAD-CBD-CGD-O1D
22	B	609	CLA	CAD-CBD-CGD-O1D
22	B	612	CLA	CAD-CBD-CGD-O1D
22	C	501	CLA	CAD-CBD-CGD-O1D
22	C	503	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O1D
22	c	505	CLA	CAD-CBD-CGD-O1D
22	R	301	CLA	CAD-CBD-CGD-O1D
22	G	603	CLA	CAD-CBD-CGD-O1D
22	Y	603	CLA	CAD-CBD-CGD-O1D
22	r	301	CLA	CAD-CBD-CGD-O1D
22	g	603	CLA	CAD-CBD-CGD-O1D
22	y	603	CLA	CAD-CBD-CGD-O1D
22	4	305	CLA	CAD-CBD-CGD-O1D
22	8	305	CLA	CAD-CBD-CGD-O1D
25	S	308	CHL	CAD-CBD-CGD-O1D
25	G	605	CHL	CAD-CBD-CGD-O1D
25	N	605	CHL	CAD-CBD-CGD-O1D
25	Y	605	CHL	CAD-CBD-CGD-O1D
25	s	308	CHL	CAD-CBD-CGD-O1D
25	g	605	CHL	CAD-CBD-CGD-O1D
25	n	605	CHL	CAD-CBD-CGD-O1D
25	y	605	CHL	CAD-CBD-CGD-O1D
25	1	605	CHL	CAD-CBD-CGD-O1D
25	2	605	CHL	CAD-CBD-CGD-O1D
25	3	306	CHL	CAD-CBD-CGD-O1D
25	5	605	CHL	CAD-CBD-CGD-O1D
25	6	605	CHL	CAD-CBD-CGD-O1D
25	7	306	CHL	CAD-CBD-CGD-O1D
25	4	302	CHL	CBD-CGD-O2D-CED
25	8	302	CHL	CBD-CGD-O2D-CED
22	C	505	CLA	C2A-CAA-CBA-CGA
22	G	604	CLA	C2A-CAA-CBA-CGA
22	g	604	CLA	C2A-CAA-CBA-CGA
25	2	601	CHL	C2C-C3C-CAC-CBC
25	6	601	CHL	C2C-C3C-CAC-CBC
22	B	615	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	C2B-C3B-CAB-CBB
22	R	301	CLA	C2B-C3B-CAB-CBB
22	R	302	CLA	C2B-C3B-CAB-CBB
22	R	311	CLA	C2B-C3B-CAB-CBB
22	S	303	CLA	C2B-C3B-CAB-CBB
22	S	313	CLA	C2B-C3B-CAB-CBB
22	G	604	CLA	C2B-C3B-CAB-CBB
22	N	604	CLA	C2B-C3B-CAB-CBB
22	Y	604	CLA	C2B-C3B-CAB-CBB
22	r	301	CLA	C2B-C3B-CAB-CBB
22	r	302	CLA	C2B-C3B-CAB-CBB
22	r	311	CLA	C2B-C3B-CAB-CBB
22	s	301	CLA	C2B-C3B-CAB-CBB
22	s	303	CLA	C2B-C3B-CAB-CBB
22	s	313	CLA	C2B-C3B-CAB-CBB
22	g	604	CLA	C2B-C3B-CAB-CBB
22	n	604	CLA	C2B-C3B-CAB-CBB
22	y	604	CLA	C2B-C3B-CAB-CBB
22	1	603	CLA	C2B-C3B-CAB-CBB
22	1	611	CLA	C2B-C3B-CAB-CBB
22	2	603	CLA	C2B-C3B-CAB-CBB
22	5	603	CLA	C2B-C3B-CAB-CBB
22	5	611	CLA	C2B-C3B-CAB-CBB
22	6	603	CLA	C2B-C3B-CAB-CBB
25	Y	606	CHL	C2B-C3B-CAB-CBB
25	y	606	CHL	C2B-C3B-CAB-CBB
22	C	508	CLA	C2A-CAA-CBA-CGA
22	N	611	CLA	C2A-CAA-CBA-CGA
22	Y	603	CLA	C2A-CAA-CBA-CGA
22	n	611	CLA	C2A-CAA-CBA-CGA
22	y	603	CLA	C2A-CAA-CBA-CGA
25	R	305	CHL	C2A-CAA-CBA-CGA
25	r	305	CHL	C2A-CAA-CBA-CGA
22	B	611	CLA	C2A-CAA-CBA-CGA
23	d	402	PHO	CHA-CBD-CGD-O1D
23	d	402	PHO	CHA-CBD-CGD-O2D
25	R	306	CHL	C4C-C3C-CAC-CBC
25	r	306	CHL	C4C-C3C-CAC-CBC
22	4	305	CLA	CBD-CGD-O2D-CED
22	8	305	CLA	CBD-CGD-O2D-CED
22	G	602	CLA	CAA-CBA-CGA-O1A
22	Y	602	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	Y	604	CLA	CAA-CBA-CGA-O1A
22	g	602	CLA	CAA-CBA-CGA-O1A
22	y	602	CLA	CAA-CBA-CGA-O1A
22	y	604	CLA	CAA-CBA-CGA-O1A
22	1	602	CLA	CAA-CBA-CGA-O1A
22	1	604	CLA	CAA-CBA-CGA-O2A
22	5	602	CLA	CAA-CBA-CGA-O1A
22	5	604	CLA	CAA-CBA-CGA-O2A
25	4	302	CHL	O1D-CGD-O2D-CED
25	8	302	CHL	O1D-CGD-O2D-CED
22	B	615	CLA	C4B-C3B-CAB-CBB
22	C	512	CLA	C4B-C3B-CAB-CBB
22	R	302	CLA	C4B-C3B-CAB-CBB
22	R	307	CLA	C4B-C3B-CAB-CBB
22	R	309	CLA	C4B-C3B-CAB-CBB
22	G	604	CLA	C4B-C3B-CAB-CBB
22	Y	604	CLA	C4B-C3B-CAB-CBB
22	r	302	CLA	C4B-C3B-CAB-CBB
22	r	307	CLA	C4B-C3B-CAB-CBB
22	r	309	CLA	C4B-C3B-CAB-CBB
22	g	604	CLA	C4B-C3B-CAB-CBB
22	y	604	CLA	C4B-C3B-CAB-CBB
22	1	603	CLA	C4B-C3B-CAB-CBB
22	1	611	CLA	C4B-C3B-CAB-CBB
22	1	614	CLA	C4B-C3B-CAB-CBB
22	5	603	CLA	C4B-C3B-CAB-CBB
22	5	611	CLA	C4B-C3B-CAB-CBB
22	5	614	CLA	C4B-C3B-CAB-CBB
22	B	602	CLA	C2A-CAA-CBA-CGA
22	b	601	CLA	C2A-CAA-CBA-CGA
22	S	303	CLA	C2A-CAA-CBA-CGA
22	s	303	CLA	C2A-CAA-CBA-CGA
22	B	615	CLA	CAA-CBA-CGA-O1A
22	R	309	CLA	CAA-CBA-CGA-O2A
22	N	602	CLA	CAA-CBA-CGA-O1A
22	N	604	CLA	CAA-CBA-CGA-O1A
22	r	309	CLA	CAA-CBA-CGA-O2A
22	n	602	CLA	CAA-CBA-CGA-O1A
22	n	604	CLA	CAA-CBA-CGA-O1A
25	R	305	CHL	C2C-C3C-CAC-CBC
25	r	305	CHL	C2C-C3C-CAC-CBC
25	R	304	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	r	304	CHL	C4C-C3C-CAC-CBC
25	4	308	CHL	CAA-CBA-CGA-O2A
25	8	308	CHL	CAA-CBA-CGA-O2A
22	S	304	CLA	CAA-CBA-CGA-O2A
22	s	304	CLA	CAA-CBA-CGA-O2A
22	c	509	CLA	CAA-CBA-CGA-O1A
25	N	606	CHL	CAA-CBA-CGA-O1A
25	n	606	CHL	CAA-CBA-CGA-O1A
24	F	101	HEM	CAD-CBD-CGD-O1D
25	2	608	CHL	CAA-CBA-CGA-O2A
25	6	608	CHL	CAA-CBA-CGA-O2A
22	B	601	CLA	C2A-CAA-CBA-CGA
22	C	502	CLA	C2A-CAA-CBA-CGA
22	D	404	CLA	C2A-CAA-CBA-CGA
22	d	401	CLA	C2A-CAA-CBA-CGA
22	R	309	CLA	C2A-CAA-CBA-CGA
22	S	313	CLA	C2A-CAA-CBA-CGA
22	r	309	CLA	C2A-CAA-CBA-CGA
22	s	313	CLA	C2A-CAA-CBA-CGA
22	2	604	CLA	C2A-CAA-CBA-CGA
22	6	604	CLA	C2A-CAA-CBA-CGA
25	G	607	CHL	C2A-CAA-CBA-CGA
25	g	607	CHL	C2A-CAA-CBA-CGA
22	R	308	CLA	C3A-C2A-CAA-CBA
22	S	310	CLA	C3A-C2A-CAA-CBA
22	G	614	CLA	C3A-C2A-CAA-CBA
22	N	614	CLA	C3A-C2A-CAA-CBA
22	Y	610	CLA	C3A-C2A-CAA-CBA
22	r	308	CLA	C3A-C2A-CAA-CBA
22	s	310	CLA	C3A-C2A-CAA-CBA
22	g	614	CLA	C3A-C2A-CAA-CBA
22	n	614	CLA	C3A-C2A-CAA-CBA
22	y	610	CLA	C3A-C2A-CAA-CBA
22	1	610	CLA	C3A-C2A-CAA-CBA
22	2	609	CLA	C3A-C2A-CAA-CBA
22	2	613	CLA	C3A-C2A-CAA-CBA
22	5	610	CLA	C3A-C2A-CAA-CBA
22	6	609	CLA	C3A-C2A-CAA-CBA
22	6	613	CLA	C3A-C2A-CAA-CBA
25	Y	609	CHL	C3A-C2A-CAA-CBA
25	y	609	CHL	C3A-C2A-CAA-CBA
25	4	307	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	8	307	CHL	C3A-C2A-CAA-CBA
22	b	616	CLA	CAA-CBA-CGA-O2A
22	4	305	CLA	O1D-CGD-O2D-CED
22	8	305	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	CAA-CBA-CGA-O1A
22	C	503	CLA	CAA-CBA-CGA-O2A
22	C	505	CLA	CAA-CBA-CGA-O1A
22	S	304	CLA	CAA-CBA-CGA-O1A
22	s	304	CLA	CAA-CBA-CGA-O1A
22	1	604	CLA	CAA-CBA-CGA-O1A
22	3	310	CLA	CAA-CBA-CGA-O1A
22	5	604	CLA	CAA-CBA-CGA-O1A
22	7	310	CLA	CAA-CBA-CGA-O1A
25	Y	606	CHL	CAA-CBA-CGA-O2A
25	y	606	CHL	CAA-CBA-CGA-O2A
25	2	606	CHL	CAA-CBA-CGA-O2A
25	6	606	CHL	CAA-CBA-CGA-O2A
22	b	601	CLA	CAA-CBA-CGA-O1A
22	R	309	CLA	CAA-CBA-CGA-O1A
22	N	611	CLA	CAA-CBA-CGA-O1A
22	Y	611	CLA	CAA-CBA-CGA-O2A
22	r	309	CLA	CAA-CBA-CGA-O1A
22	n	611	CLA	CAA-CBA-CGA-O1A
22	y	611	CLA	CAA-CBA-CGA-O2A
22	1	613	CLA	CAA-CBA-CGA-O2A
22	5	613	CLA	CAA-CBA-CGA-O2A
22	B	601	CLA	CAA-CBA-CGA-O1A
22	C	509	CLA	CAA-CBA-CGA-O1A
22	a	403	CLA	CAA-CBA-CGA-O1A
22	c	502	CLA	CAA-CBA-CGA-O1A
22	G	603	CLA	C2A-CAA-CBA-CGA
22	g	603	CLA	C2A-CAA-CBA-CGA
22	c	509	CLA	CAA-CBA-CGA-O2A
22	R	310	CLA	CAA-CBA-CGA-O1A
22	S	305	CLA	CAA-CBA-CGA-O1A
22	Y	602	CLA	CAA-CBA-CGA-O2A
22	r	310	CLA	CAA-CBA-CGA-O1A
22	s	305	CLA	CAA-CBA-CGA-O1A
22	y	602	CLA	CAA-CBA-CGA-O2A
22	3	303	CLA	CAA-CBA-CGA-O1A
22	3	304	CLA	CAA-CBA-CGA-O1A
22	7	303	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	7	304	CLA	CAA-CBA-CGA-O1A
25	S	306	CHL	CAA-CBA-CGA-O1A
25	Y	606	CHL	CAA-CBA-CGA-O1A
25	s	306	CHL	CAA-CBA-CGA-O1A
25	y	606	CHL	CAA-CBA-CGA-O1A
25	2	608	CHL	CAA-CBA-CGA-O1A
25	6	608	CHL	CAA-CBA-CGA-O1A
22	B	603	CLA	CAA-CBA-CGA-O1A
22	B	613	CLA	CAA-CBA-CGA-O2A
22	b	615	CLA	CAA-CBA-CGA-O1A
22	b	615	CLA	CAA-CBA-CGA-O2A
22	b	616	CLA	CAA-CBA-CGA-O1A
22	R	308	CLA	CAA-CBA-CGA-O1A
22	N	602	CLA	CAA-CBA-CGA-O2A
22	r	308	CLA	CAA-CBA-CGA-O1A
22	n	602	CLA	CAA-CBA-CGA-O2A
22	1	613	CLA	CAA-CBA-CGA-O1A
22	3	312	CLA	CAA-CBA-CGA-O1A
22	5	613	CLA	CAA-CBA-CGA-O1A
22	7	312	CLA	CAA-CBA-CGA-O1A
25	R	306	CHL	CAA-CBA-CGA-O1A
25	r	306	CHL	CAA-CBA-CGA-O1A
22	d	403	CLA	C1A-C2A-CAA-CBA
22	G	602	CLA	C1A-C2A-CAA-CBA
22	G	612	CLA	C1A-C2A-CAA-CBA
22	Y	611	CLA	C1A-C2A-CAA-CBA
22	g	602	CLA	C1A-C2A-CAA-CBA
22	g	612	CLA	C1A-C2A-CAA-CBA
22	y	611	CLA	C1A-C2A-CAA-CBA
22	1	602	CLA	C1A-C2A-CAA-CBA
22	5	602	CLA	C1A-C2A-CAA-CBA
25	1	615	CHL	C1A-C2A-CAA-CBA
25	5	615	CHL	C1A-C2A-CAA-CBA
22	A	403	CLA	CAA-CBA-CGA-O1A
22	B	608	CLA	CAA-CBA-CGA-O1A
22	B	612	CLA	CAA-CBA-CGA-O1A
22	B	615	CLA	CAA-CBA-CGA-O2A
22	C	505	CLA	CAA-CBA-CGA-O2A
22	b	603	CLA	CAA-CBA-CGA-O1A
22	R	301	CLA	CAA-CBA-CGA-O2A
22	S	305	CLA	CAA-CBA-CGA-O2A
22	G	614	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	Y	604	CLA	CAA-CBA-CGA-O2A
22	r	301	CLA	CAA-CBA-CGA-O2A
22	s	305	CLA	CAA-CBA-CGA-O2A
22	g	614	CLA	CAA-CBA-CGA-O1A
22	y	604	CLA	CAA-CBA-CGA-O2A
22	1	603	CLA	CAA-CBA-CGA-O1A
22	5	603	CLA	CAA-CBA-CGA-O1A
25	4	302	CHL	CAA-CBA-CGA-O2A
25	8	302	CHL	CAA-CBA-CGA-O2A
22	B	601	CLA	CAA-CBA-CGA-O2A
22	B	610	CLA	CAA-CBA-CGA-O2A
22	C	509	CLA	CAA-CBA-CGA-O2A
22	R	301	CLA	CAA-CBA-CGA-O1A
22	N	603	CLA	CAA-CBA-CGA-O1A
22	r	301	CLA	CAA-CBA-CGA-O1A
22	n	603	CLA	CAA-CBA-CGA-O1A
22	3	310	CLA	CAA-CBA-CGA-O2A
22	7	310	CLA	CAA-CBA-CGA-O2A
25	4	302	CHL	CAA-CBA-CGA-O1A
25	8	302	CHL	CAA-CBA-CGA-O1A
22	G	613	CLA	C2A-CAA-CBA-CGA
22	g	613	CLA	C2A-CAA-CBA-CGA
22	2	610	CLA	C2A-CAA-CBA-CGA
22	6	610	CLA	C2A-CAA-CBA-CGA
25	4	308	CHL	C2A-CAA-CBA-CGA
25	8	308	CHL	C2A-CAA-CBA-CGA
22	1	614	CLA	CAA-CBA-CGA-O2A
22	3	314	CLA	CAA-CBA-CGA-O1A
22	4	303	CLA	CAA-CBA-CGA-O1A
22	4	303	CLA	CAA-CBA-CGA-O2A
22	5	614	CLA	CAA-CBA-CGA-O2A
22	7	314	CLA	CAA-CBA-CGA-O1A
22	8	303	CLA	CAA-CBA-CGA-O1A
22	8	303	CLA	CAA-CBA-CGA-O2A
24	F	101	HEM	CAD-CBD-CGD-O2D
25	R	306	CHL	CAA-CBA-CGA-O2A
25	N	606	CHL	CAA-CBA-CGA-O2A
25	r	306	CHL	CAA-CBA-CGA-O2A
25	n	606	CHL	CAA-CBA-CGA-O2A
22	b	608	CLA	CAA-CBA-CGA-O1A
22	c	507	CLA	CAA-CBA-CGA-O2A
22	R	307	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	R	307	CLA	CAA-CBA-CGA-O2A
22	Y	611	CLA	CAA-CBA-CGA-O1A
22	r	307	CLA	CAA-CBA-CGA-O1A
22	r	307	CLA	CAA-CBA-CGA-O2A
22	y	611	CLA	CAA-CBA-CGA-O1A
22	2	613	CLA	CAA-CBA-CGA-O2A
22	3	303	CLA	CAA-CBA-CGA-O2A
22	4	301	CLA	CAA-CBA-CGA-O2A
22	4	304	CLA	CAA-CBA-CGA-O2A
22	6	613	CLA	CAA-CBA-CGA-O2A
22	7	303	CLA	CAA-CBA-CGA-O2A
22	8	301	CLA	CAA-CBA-CGA-O2A
22	8	304	CLA	CAA-CBA-CGA-O2A
25	4	308	CHL	CAA-CBA-CGA-O1A
25	8	308	CHL	CAA-CBA-CGA-O1A
22	C	512	CLA	C2B-C3B-CAB-CBB
22	R	309	CLA	C2B-C3B-CAB-CBB
22	r	309	CLA	C2B-C3B-CAB-CBB
22	1	614	CLA	C2B-C3B-CAB-CBB
22	4	310	CLA	C2B-C3B-CAB-CBB
22	5	614	CLA	C2B-C3B-CAB-CBB
22	8	310	CLA	C2B-C3B-CAB-CBB
22	B	610	CLA	CAA-CBA-CGA-O1A
22	a	403	CLA	CAA-CBA-CGA-O2A
22	S	311	CLA	CAA-CBA-CGA-O1A
22	S	312	CLA	CAA-CBA-CGA-O2A
22	N	604	CLA	CAA-CBA-CGA-O2A
22	N	612	CLA	CAA-CBA-CGA-O1A
22	N	612	CLA	CAA-CBA-CGA-O2A
22	Y	614	CLA	CAA-CBA-CGA-O1A
22	s	311	CLA	CAA-CBA-CGA-O1A
22	s	312	CLA	CAA-CBA-CGA-O2A
22	n	604	CLA	CAA-CBA-CGA-O2A
22	n	612	CLA	CAA-CBA-CGA-O1A
22	n	612	CLA	CAA-CBA-CGA-O2A
22	y	614	CLA	CAA-CBA-CGA-O1A
22	1	612	CLA	CAA-CBA-CGA-O1A
22	5	612	CLA	CAA-CBA-CGA-O1A
25	4	307	CHL	CAA-CBA-CGA-O1A
25	8	307	CHL	CAA-CBA-CGA-O1A
22	B	603	CLA	CAA-CBA-CGA-O2A
22	C	510	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	CAA-CBA-CGA-O2A
22	G	602	CLA	CAA-CBA-CGA-O2A
22	G	612	CLA	CAA-CBA-CGA-O1A
22	g	602	CLA	CAA-CBA-CGA-O2A
22	g	612	CLA	CAA-CBA-CGA-O1A
22	1	614	CLA	CAA-CBA-CGA-O1A
22	4	304	CLA	CAA-CBA-CGA-O1A
22	5	614	CLA	CAA-CBA-CGA-O1A
22	8	304	CLA	CAA-CBA-CGA-O1A
22	B	612	CLA	CAA-CBA-CGA-O2A
22	C	503	CLA	CAA-CBA-CGA-O1A
22	R	302	CLA	CAA-CBA-CGA-O1A
22	S	311	CLA	CAA-CBA-CGA-O2A
22	G	612	CLA	CAA-CBA-CGA-O2A
22	N	614	CLA	CAA-CBA-CGA-O2A
22	r	302	CLA	CAA-CBA-CGA-O1A
22	s	311	CLA	CAA-CBA-CGA-O2A
22	g	612	CLA	CAA-CBA-CGA-O2A
22	n	614	CLA	CAA-CBA-CGA-O2A
22	1	602	CLA	CAA-CBA-CGA-O2A
22	3	312	CLA	CAA-CBA-CGA-O2A
22	3	313	CLA	CAA-CBA-CGA-O1A
22	3	314	CLA	CAA-CBA-CGA-O2A
22	5	602	CLA	CAA-CBA-CGA-O2A
22	7	312	CLA	CAA-CBA-CGA-O2A
22	7	313	CLA	CAA-CBA-CGA-O1A
22	7	314	CLA	CAA-CBA-CGA-O2A
24	e	101	HEM	CAD-CBD-CGD-O2D
25	4	307	CHL	CAA-CBA-CGA-O2A
25	8	307	CHL	CAA-CBA-CGA-O2A
22	C	507	CLA	CAA-CBA-CGA-O2A
22	b	608	CLA	CAA-CBA-CGA-O2A
22	b	610	CLA	CAA-CBA-CGA-O2A
22	R	308	CLA	CAA-CBA-CGA-O2A
22	Y	612	CLA	CAA-CBA-CGA-O1A
22	r	308	CLA	CAA-CBA-CGA-O2A
22	y	612	CLA	CAA-CBA-CGA-O1A
22	2	613	CLA	CAA-CBA-CGA-O1A
22	6	613	CLA	CAA-CBA-CGA-O1A
25	S	306	CHL	CAA-CBA-CGA-O2A
25	G	606	CHL	CAA-CBA-CGA-O2A
25	s	306	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	g	606	CHL	CAA-CBA-CGA-O2A
25	2	606	CHL	CAA-CBA-CGA-O1A
25	6	606	CHL	CAA-CBA-CGA-O1A
22	b	610	CLA	CAA-CBA-CGA-O1A
22	c	502	CLA	CAA-CBA-CGA-O2A
22	c	507	CLA	CAA-CBA-CGA-O1A
22	R	310	CLA	CAA-CBA-CGA-O2A
22	Y	613	CLA	CAA-CBA-CGA-O2A
22	r	310	CLA	CAA-CBA-CGA-O2A
22	y	613	CLA	CAA-CBA-CGA-O2A
22	3	304	CLA	CAA-CBA-CGA-O2A
22	3	311	CLA	CAA-CBA-CGA-O2A
22	4	301	CLA	CAA-CBA-CGA-O1A
22	7	304	CLA	CAA-CBA-CGA-O2A
22	7	311	CLA	CAA-CBA-CGA-O2A
22	8	301	CLA	CAA-CBA-CGA-O1A
25	1	606	CHL	CAA-CBA-CGA-O2A
25	5	606	CHL	CAA-CBA-CGA-O2A
22	A	403	CLA	CAA-CBA-CGA-O2A
22	B	608	CLA	CAA-CBA-CGA-O2A
22	b	601	CLA	CAA-CBA-CGA-O2A
22	b	603	CLA	CAA-CBA-CGA-O2A
22	b	613	CLA	CAA-CBA-CGA-O2A
22	c	504	CLA	CAA-CBA-CGA-O2A
22	R	302	CLA	CAA-CBA-CGA-O2A
22	S	312	CLA	CAA-CBA-CGA-O1A
22	N	611	CLA	CAA-CBA-CGA-O2A
22	r	302	CLA	CAA-CBA-CGA-O2A
22	s	312	CLA	CAA-CBA-CGA-O1A
22	n	611	CLA	CAA-CBA-CGA-O2A
22	2	612	CLA	CAA-CBA-CGA-O2A
22	6	612	CLA	CAA-CBA-CGA-O2A
23	d	402	PHO	C1A-C2A-CAA-CBA
22	R	311	CLA	C2A-CAA-CBA-CGA
22	r	311	CLA	C2A-CAA-CBA-CGA
22	D	404	CLA	CAA-CBA-CGA-O2A
22	G	610	CLA	CAA-CBA-CGA-O1A
22	N	603	CLA	CAA-CBA-CGA-O2A
22	Y	612	CLA	CAA-CBA-CGA-O2A
22	g	610	CLA	CAA-CBA-CGA-O1A
22	n	603	CLA	CAA-CBA-CGA-O2A
22	y	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	1	603	CLA	CAA-CBA-CGA-O2A
22	1	612	CLA	CAA-CBA-CGA-O2A
22	5	603	CLA	CAA-CBA-CGA-O2A
22	5	612	CLA	CAA-CBA-CGA-O2A
22	C	502	CLA	CAA-CBA-CGA-O2A
22	C	510	CLA	CAA-CBA-CGA-O1A
22	d	401	CLA	CAA-CBA-CGA-O2A
22	c	510	CLA	CAA-CBA-CGA-O1A
22	G	613	CLA	CAA-CBA-CGA-O2A
22	Y	614	CLA	CAA-CBA-CGA-O2A
22	g	613	CLA	CAA-CBA-CGA-O2A
22	y	614	CLA	CAA-CBA-CGA-O2A
22	R	311	CLA	CAA-CBA-CGA-O2A
22	G	614	CLA	CAA-CBA-CGA-O2A
22	N	614	CLA	CAA-CBA-CGA-O1A
22	r	311	CLA	CAA-CBA-CGA-O2A
22	g	614	CLA	CAA-CBA-CGA-O2A
22	n	614	CLA	CAA-CBA-CGA-O1A
22	3	313	CLA	CAA-CBA-CGA-O2A
22	7	313	CLA	CAA-CBA-CGA-O2A
22	d	404	CLA	CAA-CBA-CGA-O2A
22	G	613	CLA	CAA-CBA-CGA-O1A
22	N	613	CLA	CAA-CBA-CGA-O2A
22	g	613	CLA	CAA-CBA-CGA-O1A
22	n	613	CLA	CAA-CBA-CGA-O2A
25	G	609	CHL	CAA-CBA-CGA-O2A
25	g	609	CHL	CAA-CBA-CGA-O2A
22	b	612	CLA	CAA-CBA-CGA-O2A
22	d	401	CLA	CAA-CBA-CGA-O1A
22	Y	613	CLA	CAA-CBA-CGA-O1A
22	y	613	CLA	CAA-CBA-CGA-O1A
22	2	609	CLA	CAA-CBA-CGA-O1A
22	2	611	CLA	CAA-CBA-CGA-O2A
22	2	612	CLA	CAA-CBA-CGA-O1A
22	6	609	CLA	CAA-CBA-CGA-O1A
22	6	611	CLA	CAA-CBA-CGA-O2A
22	6	612	CLA	CAA-CBA-CGA-O1A
25	G	606	CHL	CAA-CBA-CGA-O1A
25	g	606	CHL	CAA-CBA-CGA-O1A
25	1	606	CHL	CAA-CBA-CGA-O1A
25	5	606	CHL	CAA-CBA-CGA-O1A
22	C	502	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	b	613	CLA	CAA-CBA-CGA-O1A
22	c	504	CLA	CAA-CBA-CGA-O1A
22	c	505	CLA	CAA-CBA-CGA-O2A
22	2	603	CLA	CAA-CBA-CGA-O2A
22	3	311	CLA	CAA-CBA-CGA-O1A
22	6	603	CLA	CAA-CBA-CGA-O2A
22	7	311	CLA	CAA-CBA-CGA-O1A
24	e	101	HEM	CAD-CBD-CGD-O1D
22	4	301	CLA	C4B-C3B-CAB-CBB
22	4	310	CLA	C4B-C3B-CAB-CBB
22	8	301	CLA	C4B-C3B-CAB-CBB
22	8	310	CLA	C4B-C3B-CAB-CBB
22	D	403	CLA	CAA-CBA-CGA-O1A
25	N	609	CHL	CAA-CBA-CGA-O1A
25	n	609	CHL	CAA-CBA-CGA-O1A
25	3	307	CHL	CAA-CBA-CGA-O1A
25	3	307	CHL	CAA-CBA-CGA-O2A
25	7	307	CHL	CAA-CBA-CGA-O1A
25	7	307	CHL	CAA-CBA-CGA-O2A
25	N	609	CHL	CAA-CBA-CGA-O2A
25	n	609	CHL	CAA-CBA-CGA-O2A
25	1	609	CHL	CAA-CBA-CGA-O1A
25	3	309	CHL	CAA-CBA-CGA-O1A
25	5	609	CHL	CAA-CBA-CGA-O1A
25	7	309	CHL	CAA-CBA-CGA-O1A
22	C	507	CLA	CAA-CBA-CGA-O1A
22	2	611	CLA	CAA-CBA-CGA-O1A
22	6	611	CLA	CAA-CBA-CGA-O1A
25	3	309	CHL	CAA-CBA-CGA-O2A
25	7	309	CHL	CAA-CBA-CGA-O2A
22	D	404	CLA	CAA-CBA-CGA-O1A
22	d	404	CLA	CAA-CBA-CGA-O1A
22	c	503	CLA	CAA-CBA-CGA-O2A
22	S	313	CLA	CAA-CBA-CGA-O2A
22	G	611	CLA	CAA-CBA-CGA-O2A
22	s	313	CLA	CAA-CBA-CGA-O2A
22	g	611	CLA	CAA-CBA-CGA-O2A
25	G	609	CHL	CAA-CBA-CGA-O1A
25	g	609	CHL	CAA-CBA-CGA-O1A
25	1	609	CHL	CAA-CBA-CGA-O2A
25	5	609	CHL	CAA-CBA-CGA-O2A
22	d	403	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	N	613	CLA	CAA-CBA-CGA-O1A
22	n	613	CLA	CAA-CBA-CGA-O1A
22	b	612	CLA	CAA-CBA-CGA-O1A
22	c	505	CLA	CAA-CBA-CGA-O1A
22	G	604	CLA	CAA-CBA-CGA-O1A
22	g	604	CLA	CAA-CBA-CGA-O1A
25	S	307	CHL	CAA-CBA-CGA-O1A
25	s	307	CHL	CAA-CBA-CGA-O1A
22	A	403	CLA	C3A-C2A-CAA-CBA
22	a	403	CLA	C3A-C2A-CAA-CBA
22	b	614	CLA	C3A-C2A-CAA-CBA
22	R	301	CLA	C3A-C2A-CAA-CBA
22	G	604	CLA	C3A-C2A-CAA-CBA
22	G	612	CLA	C3A-C2A-CAA-CBA
22	N	610	CLA	C3A-C2A-CAA-CBA
22	Y	604	CLA	C3A-C2A-CAA-CBA
22	Y	614	CLA	C3A-C2A-CAA-CBA
22	r	301	CLA	C3A-C2A-CAA-CBA
22	g	604	CLA	C3A-C2A-CAA-CBA
22	g	612	CLA	C3A-C2A-CAA-CBA
22	n	610	CLA	C3A-C2A-CAA-CBA
22	y	604	CLA	C3A-C2A-CAA-CBA
22	y	614	CLA	C3A-C2A-CAA-CBA
22	1	614	CLA	C3A-C2A-CAA-CBA
22	3	314	CLA	C3A-C2A-CAA-CBA
22	5	614	CLA	C3A-C2A-CAA-CBA
22	7	314	CLA	C3A-C2A-CAA-CBA
22	B	602	CLA	CAA-CBA-CGA-O2A
22	C	504	CLA	CAA-CBA-CGA-O2A
22	Y	603	CLA	CAA-CBA-CGA-O2A
22	y	603	CLA	CAA-CBA-CGA-O2A
22	2	603	CLA	CAA-CBA-CGA-O1A
22	6	603	CLA	CAA-CBA-CGA-O1A
22	B	601	CLA	CAD-CBD-CGD-O2D
22	a	405	CLA	CAD-CBD-CGD-O2D
22	b	606	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	CAD-CBD-CGD-O2D
22	R	309	CLA	CAD-CBD-CGD-O2D
22	S	301	CLA	CAD-CBD-CGD-O2D
22	S	309	CLA	CAD-CBD-CGD-O2D
22	G	604	CLA	CAD-CBD-CGD-O2D
22	G	610	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	N	610	CLA	CAD-CBD-CGD-O2D
22	Y	610	CLA	CAD-CBD-CGD-O2D
22	Y	614	CLA	CAD-CBD-CGD-O2D
22	r	309	CLA	CAD-CBD-CGD-O2D
22	s	309	CLA	CAD-CBD-CGD-O2D
22	g	604	CLA	CAD-CBD-CGD-O2D
22	g	610	CLA	CAD-CBD-CGD-O2D
22	n	610	CLA	CAD-CBD-CGD-O2D
22	y	610	CLA	CAD-CBD-CGD-O2D
22	y	614	CLA	CAD-CBD-CGD-O2D
22	2	603	CLA	CAD-CBD-CGD-O2D
22	3	304	CLA	CAD-CBD-CGD-O2D
22	3	310	CLA	CAD-CBD-CGD-O2D
22	4	303	CLA	CAD-CBD-CGD-O2D
22	4	304	CLA	CAD-CBD-CGD-O2D
22	4	311	CLA	CAD-CBD-CGD-O2D
22	6	603	CLA	CAD-CBD-CGD-O2D
22	7	304	CLA	CAD-CBD-CGD-O2D
22	7	310	CLA	CAD-CBD-CGD-O2D
22	8	303	CLA	CAD-CBD-CGD-O2D
22	8	304	CLA	CAD-CBD-CGD-O2D
22	8	311	CLA	CAD-CBD-CGD-O2D
25	N	608	CHL	CAD-CBD-CGD-O2D
25	Y	608	CHL	CAD-CBD-CGD-O2D
25	n	608	CHL	CAD-CBD-CGD-O2D
25	y	608	CHL	CAD-CBD-CGD-O2D
25	1	608	CHL	CAD-CBD-CGD-O2D
25	5	608	CHL	CAD-CBD-CGD-O2D
22	c	503	CLA	CAA-CBA-CGA-O1A
22	S	314	CLA	CAA-CBA-CGA-O2A
22	G	603	CLA	CAA-CBA-CGA-O2A
22	s	314	CLA	CAA-CBA-CGA-O2A
22	g	603	CLA	CAA-CBA-CGA-O2A
22	1	611	CLA	CAA-CBA-CGA-O2A
22	4	310	CLA	CAA-CBA-CGA-O2A
22	5	611	CLA	CAA-CBA-CGA-O2A
22	8	310	CLA	CAA-CBA-CGA-O2A
22	G	611	CLA	CAA-CBA-CGA-O1A
22	g	611	CLA	CAA-CBA-CGA-O1A
22	1	610	CLA	CAA-CBA-CGA-O1A
22	1	611	CLA	CAA-CBA-CGA-O1A
22	4	310	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	5	610	CLA	CAA-CBA-CGA-O1A
22	5	611	CLA	CAA-CBA-CGA-O1A
22	8	310	CLA	CAA-CBA-CGA-O1A
22	b	604	CLA	C2C-C3C-CAC-CBC
22	Y	603	CLA	CAA-CBA-CGA-O1A
22	y	603	CLA	CAA-CBA-CGA-O1A
22	R	311	CLA	CAA-CBA-CGA-O1A
22	S	314	CLA	CAA-CBA-CGA-O1A
22	r	311	CLA	CAA-CBA-CGA-O1A
22	s	314	CLA	CAA-CBA-CGA-O1A
22	1	610	CLA	CAA-CBA-CGA-O2A
22	5	610	CLA	CAA-CBA-CGA-O2A
25	Y	609	CHL	CAA-CBA-CGA-O2A
25	y	609	CHL	CAA-CBA-CGA-O2A
22	A	403	CLA	CHA-CBD-CGD-O1D
22	A	403	CLA	CHA-CBD-CGD-O2D
22	B	607	CLA	CHA-CBD-CGD-O1D
22	B	610	CLA	CHA-CBD-CGD-O1D
22	B	610	CLA	CHA-CBD-CGD-O2D
22	B	614	CLA	CHA-CBD-CGD-O2D
22	B	615	CLA	CHA-CBD-CGD-O2D
22	C	502	CLA	CHA-CBD-CGD-O1D
22	C	502	CLA	CHA-CBD-CGD-O2D
22	C	504	CLA	CHA-CBD-CGD-O2D
22	C	506	CLA	CHA-CBD-CGD-O1D
22	C	506	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	C	511	CLA	CHA-CBD-CGD-O1D
22	C	511	CLA	CHA-CBD-CGD-O2D
22	C	512	CLA	CHA-CBD-CGD-O1D
22	D	401	CLA	CHA-CBD-CGD-O1D
22	D	401	CLA	CHA-CBD-CGD-O2D
22	a	403	CLA	CHA-CBD-CGD-O1D
22	a	403	CLA	CHA-CBD-CGD-O2D
22	b	607	CLA	CHA-CBD-CGD-O1D
22	b	607	CLA	CHA-CBD-CGD-O2D
22	b	610	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	b	610	CLA	CHA-CBD-CGD-O2D
22	b	615	CLA	CHA-CBD-CGD-O1D
22	b	615	CLA	CHA-CBD-CGD-O2D
22	c	502	CLA	CHA-CBD-CGD-O1D
22	c	502	CLA	CHA-CBD-CGD-O2D
22	c	503	CLA	CHA-CBD-CGD-O2D
22	c	506	CLA	CHA-CBD-CGD-O1D
22	c	506	CLA	CHA-CBD-CGD-O2D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
22	S	303	CLA	CHA-CBD-CGD-O1D
22	S	303	CLA	CHA-CBD-CGD-O2D
22	S	304	CLA	CHA-CBD-CGD-O2D
22	S	305	CLA	CHA-CBD-CGD-O1D
22	S	310	CLA	CHA-CBD-CGD-O1D
22	S	310	CLA	CHA-CBD-CGD-O2D
22	G	602	CLA	CHA-CBD-CGD-O1D
22	G	602	CLA	CHA-CBD-CGD-O2D
22	G	612	CLA	CHA-CBD-CGD-O1D
22	G	612	CLA	CHA-CBD-CGD-O2D
22	N	602	CLA	CHA-CBD-CGD-O1D
22	N	602	CLA	CHA-CBD-CGD-O2D
22	N	604	CLA	CHA-CBD-CGD-O1D
22	N	604	CLA	CHA-CBD-CGD-O2D
22	Y	602	CLA	CHA-CBD-CGD-O1D
22	Y	602	CLA	CHA-CBD-CGD-O2D
22	s	303	CLA	CHA-CBD-CGD-O1D
22	s	303	CLA	CHA-CBD-CGD-O2D
22	s	304	CLA	CHA-CBD-CGD-O2D
22	s	305	CLA	CHA-CBD-CGD-O1D
22	s	310	CLA	CHA-CBD-CGD-O1D
22	s	310	CLA	CHA-CBD-CGD-O2D
22	g	602	CLA	CHA-CBD-CGD-O1D
22	g	602	CLA	CHA-CBD-CGD-O2D
22	g	612	CLA	CHA-CBD-CGD-O1D
22	g	612	CLA	CHA-CBD-CGD-O2D
22	n	602	CLA	CHA-CBD-CGD-O1D
22	n	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	n	604	CLA	CHA-CBD-CGD-O1D
22	n	604	CLA	CHA-CBD-CGD-O2D
22	y	602	CLA	CHA-CBD-CGD-O1D
22	y	602	CLA	CHA-CBD-CGD-O2D
22	1	602	CLA	CHA-CBD-CGD-O1D
22	1	612	CLA	CHA-CBD-CGD-O1D
22	1	612	CLA	CHA-CBD-CGD-O2D
22	2	602	CLA	CHA-CBD-CGD-O1D
22	2	602	CLA	CHA-CBD-CGD-O2D
22	2	611	CLA	CHA-CBD-CGD-O2D
22	3	303	CLA	CHA-CBD-CGD-O1D
22	3	303	CLA	CHA-CBD-CGD-O2D
22	3	312	CLA	CHA-CBD-CGD-O1D
22	3	312	CLA	CHA-CBD-CGD-O2D
22	4	305	CLA	CHA-CBD-CGD-O2D
22	5	602	CLA	CHA-CBD-CGD-O1D
22	5	612	CLA	CHA-CBD-CGD-O1D
22	5	612	CLA	CHA-CBD-CGD-O2D
22	6	602	CLA	CHA-CBD-CGD-O1D
22	6	602	CLA	CHA-CBD-CGD-O2D
22	6	611	CLA	CHA-CBD-CGD-O2D
22	7	303	CLA	CHA-CBD-CGD-O1D
22	7	303	CLA	CHA-CBD-CGD-O2D
22	7	312	CLA	CHA-CBD-CGD-O1D
22	7	312	CLA	CHA-CBD-CGD-O2D
22	8	305	CLA	CHA-CBD-CGD-O2D
25	G	609	CHL	CHA-CBD-CGD-O2D
25	N	609	CHL	CHA-CBD-CGD-O1D
25	N	609	CHL	CHA-CBD-CGD-O2D
25	Y	605	CHL	CHA-CBD-CGD-O2D
25	g	609	CHL	CHA-CBD-CGD-O2D
25	n	609	CHL	CHA-CBD-CGD-O1D
25	n	609	CHL	CHA-CBD-CGD-O2D
25	y	605	CHL	CHA-CBD-CGD-O2D
25	2	605	CHL	CHA-CBD-CGD-O1D
25	3	301	CHL	CHA-CBD-CGD-O1D
25	3	301	CHL	CHA-CBD-CGD-O2D
25	3	309	CHL	CHA-CBD-CGD-O1D
25	3	309	CHL	CHA-CBD-CGD-O2D
25	4	307	CHL	CHA-CBD-CGD-O1D
25	4	307	CHL	CHA-CBD-CGD-O2D
25	6	605	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	7	301	CHL	CHA-CBD-CGD-O1D
25	7	301	CHL	CHA-CBD-CGD-O2D
25	7	309	CHL	CHA-CBD-CGD-O1D
25	7	309	CHL	CHA-CBD-CGD-O2D
25	8	307	CHL	CHA-CBD-CGD-O1D
25	8	307	CHL	CHA-CBD-CGD-O2D
22	C	504	CLA	CAA-CBA-CGA-O1A
22	S	303	CLA	CAA-CBA-CGA-O2A
22	S	313	CLA	CAA-CBA-CGA-O1A
22	G	603	CLA	CAA-CBA-CGA-O1A
22	s	303	CLA	CAA-CBA-CGA-O2A
22	s	313	CLA	CAA-CBA-CGA-O1A
22	g	603	CLA	CAA-CBA-CGA-O1A
25	S	307	CHL	CAA-CBA-CGA-O2A
25	s	307	CHL	CAA-CBA-CGA-O2A
22	N	603	CLA	C2A-CAA-CBA-CGA
22	N	613	CLA	C2A-CAA-CBA-CGA
22	n	603	CLA	C2A-CAA-CBA-CGA
22	n	613	CLA	C2A-CAA-CBA-CGA
22	2	603	CLA	C2A-CAA-CBA-CGA
22	4	301	CLA	C2A-CAA-CBA-CGA
22	6	603	CLA	C2A-CAA-CBA-CGA
22	8	301	CLA	C2A-CAA-CBA-CGA
25	N	607	CHL	C2A-CAA-CBA-CGA
25	n	607	CHL	C2A-CAA-CBA-CGA
25	Y	609	CHL	CAA-CBA-CGA-O1A
25	y	609	CHL	CAA-CBA-CGA-O1A
22	3	305	CLA	CAA-CBA-CGA-O1A
22	7	305	CLA	CAA-CBA-CGA-O1A
25	G	606	CHL	C2C-C3C-CAC-CBC
25	g	606	CHL	C2C-C3C-CAC-CBC
22	G	610	CLA	CAA-CBA-CGA-O2A
22	N	610	CLA	CAA-CBA-CGA-O1A
22	g	610	CLA	CAA-CBA-CGA-O2A
22	n	610	CLA	CAA-CBA-CGA-O1A
22	d	403	CLA	C2B-C3B-CAB-CBB
22	G	604	CLA	CAA-CBA-CGA-O2A
22	g	604	CLA	CAA-CBA-CGA-O2A
22	S	304	CLA	C2A-CAA-CBA-CGA
22	s	304	CLA	C2A-CAA-CBA-CGA
22	2	612	CLA	C2A-CAA-CBA-CGA
22	6	612	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	2	604	CLA	CAA-CBA-CGA-O1A
22	6	604	CLA	CAA-CBA-CGA-O1A
25	G	608	CHL	CAA-CBA-CGA-O1A
25	g	608	CHL	CAA-CBA-CGA-O1A
22	B	602	CLA	CAA-CBA-CGA-O1A
22	D	403	CLA	CAA-CBA-CGA-O2A
22	c	511	CLA	C1A-C2A-CAA-CBA
22	N	602	CLA	C1A-C2A-CAA-CBA
22	N	610	CLA	C1A-C2A-CAA-CBA
22	Y	610	CLA	C1A-C2A-CAA-CBA
22	n	602	CLA	C1A-C2A-CAA-CBA
22	n	610	CLA	C1A-C2A-CAA-CBA
22	y	610	CLA	C1A-C2A-CAA-CBA
22	1	610	CLA	C1A-C2A-CAA-CBA
22	1	612	CLA	C1A-C2A-CAA-CBA
22	2	609	CLA	C1A-C2A-CAA-CBA
22	3	303	CLA	C1A-C2A-CAA-CBA
22	3	312	CLA	C1A-C2A-CAA-CBA
22	5	610	CLA	C1A-C2A-CAA-CBA
22	5	612	CLA	C1A-C2A-CAA-CBA
22	6	609	CLA	C1A-C2A-CAA-CBA
22	7	303	CLA	C1A-C2A-CAA-CBA
22	7	312	CLA	C1A-C2A-CAA-CBA
25	4	302	CHL	C1A-C2A-CAA-CBA
25	8	302	CHL	C1A-C2A-CAA-CBA
22	2	609	CLA	CAA-CBA-CGA-O2A
22	6	609	CLA	CAA-CBA-CGA-O2A
22	b	613	CLA	C2A-CAA-CBA-CGA
22	3	313	CLA	C2A-CAA-CBA-CGA
22	7	313	CLA	C2A-CAA-CBA-CGA
22	d	403	CLA	CAA-CBA-CGA-O2A
22	S	303	CLA	CAA-CBA-CGA-O1A
22	Y	610	CLA	CAA-CBA-CGA-O2A
22	s	303	CLA	CAA-CBA-CGA-O1A
22	y	610	CLA	CAA-CBA-CGA-O2A
25	N	608	CHL	CAA-CBA-CGA-O2A
25	n	608	CHL	CAA-CBA-CGA-O2A
25	1	608	CHL	CAA-CBA-CGA-O2A
25	5	608	CHL	CAA-CBA-CGA-O2A
25	2	607	CHL	CAA-CBA-CGA-O2A
25	6	607	CHL	CAA-CBA-CGA-O2A
22	3	311	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	7	311	CLA	C4B-C3B-CAB-CBB
25	4	309	CHL	CAA-CBA-CGA-O2A
25	8	309	CHL	CAA-CBA-CGA-O2A
22	Y	612	CLA	C2A-CAA-CBA-CGA
22	y	612	CLA	C2A-CAA-CBA-CGA
22	3	304	CLA	C2A-CAA-CBA-CGA
22	7	304	CLA	C2A-CAA-CBA-CGA
22	S	310	CLA	CAA-CBA-CGA-O2A
22	s	310	CLA	CAA-CBA-CGA-O2A
22	d	403	CLA	CAA-CBA-CGA-O1A
22	3	305	CLA	CAA-CBA-CGA-O2A
22	7	305	CLA	CAA-CBA-CGA-O2A
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O1D
22	B	616	CLA	CAD-CBD-CGD-O1D
22	R	308	CLA	CAD-CBD-CGD-O1D
22	S	305	CLA	CAD-CBD-CGD-O1D
22	N	611	CLA	CAD-CBD-CGD-O1D
22	Y	604	CLA	CAD-CBD-CGD-O1D
22	r	308	CLA	CAD-CBD-CGD-O1D
22	s	305	CLA	CAD-CBD-CGD-O1D
22	n	611	CLA	CAD-CBD-CGD-O1D
22	y	604	CLA	CAD-CBD-CGD-O1D
25	1	607	CHL	CAD-CBD-CGD-O1D
25	4	308	CHL	CAD-CBD-CGD-O1D
25	5	607	CHL	CAD-CBD-CGD-O1D
25	8	308	CHL	CAD-CBD-CGD-O1D
22	b	604	CLA	C4C-C3C-CAC-CBC
25	Y	608	CHL	CAA-CBA-CGA-O2A
25	y	608	CHL	CAA-CBA-CGA-O2A
22	Y	613	CLA	C2A-CAA-CBA-CGA
22	y	613	CLA	C2A-CAA-CBA-CGA
25	G	609	CHL	C3A-C2A-CAA-CBA
25	N	609	CHL	C3A-C2A-CAA-CBA
25	g	609	CHL	C3A-C2A-CAA-CBA
25	n	609	CHL	C3A-C2A-CAA-CBA
25	N	608	CHL	CAA-CBA-CGA-O1A
25	n	608	CHL	CAA-CBA-CGA-O1A
22	N	610	CLA	CAA-CBA-CGA-O2A
22	n	610	CLA	CAA-CBA-CGA-O2A
22	2	604	CLA	CAA-CBA-CGA-O2A
22	6	604	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	R	304	CHL	CAA-CBA-CGA-O1A
25	G	608	CHL	CAA-CBA-CGA-O2A
25	r	304	CHL	CAA-CBA-CGA-O1A
25	g	608	CHL	CAA-CBA-CGA-O2A
25	G	606	CHL	C4C-C3C-CAC-CBC
25	g	606	CHL	C4C-C3C-CAC-CBC
25	R	304	CHL	CAA-CBA-CGA-O2A
25	r	304	CHL	CAA-CBA-CGA-O2A
22	S	310	CLA	CAA-CBA-CGA-O1A
22	s	310	CLA	CAA-CBA-CGA-O1A
25	3	308	CHL	CAA-CBA-CGA-O1A
25	7	308	CHL	CAA-CBA-CGA-O1A

There are no ring outliers.

215 monomers are involved in 496 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	609	CLA	2	0
25	6	606	CHL	2	0
25	r	305	CHL	1	0
22	r	311	CLA	2	0
22	s	304	CLA	1	0
22	5	612	CLA	1	0
25	n	605	CHL	1	0
22	G	611	CLA	2	0
22	r	302	CLA	2	0
25	G	609	CHL	2	0
22	R	302	CLA	22	0
22	4	305	CLA	1	0
22	b	606	CLA	1	0
25	4	302	CHL	10	0
22	C	509	CLA	1	0
25	4	309	CHL	1	0
22	a	405	CLA	1	0
22	b	607	CLA	1	0
22	6	613	CLA	17	0
22	Y	614	CLA	4	0
22	b	611	CLA	3	0
22	b	610	CLA	1	0
25	2	606	CHL	2	0
22	B	614	CLA	2	0
22	2	610	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Y	608	CHL	2	0
22	C	507	CLA	1	0
22	C	511	CLA	1	0
25	4	306	CHL	2	0
22	R	308	CLA	1	0
22	r	307	CLA	2	0
22	8	305	CLA	1	0
25	N	606	CHL	3	0
22	C	506	CLA	2	0
23	d	402	PHO	2	0
24	F	101	HEM	3	0
25	Y	605	CHL	3	0
25	R	304	CHL	1	0
22	6	612	CLA	1	0
22	b	609	CLA	1	0
22	C	512	CLA	1	0
25	3	308	CHL	4	0
22	b	608	CLA	1	0
25	Y	601	CHL	2	0
25	R	306	CHL	2	0
22	B	611	CLA	3	0
25	g	607	CHL	1	0
22	d	403	CLA	4	0
22	3	313	CLA	1	0
25	Y	606	CHL	3	0
23	a	404	PHO	2	0
25	N	605	CHL	1	0
22	r	303	CLA	1	0
22	Y	611	CLA	1	0
22	Y	602	CLA	1	0
25	8	306	CHL	1	0
25	7	301	CHL	1	0
25	8	309	CHL	1	0
22	5	610	CLA	1	0
22	S	301	CLA	6	0
25	4	307	CHL	2	0
22	b	601	CLA	1	0
22	a	403	CLA	1	0
22	c	512	CLA	1	0
25	R	305	CHL	4	0
22	D	403	CLA	3	0
25	6	601	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	301	CLA	38	0
25	S	302	CHL	1	0
22	3	311	CLA	1	0
22	R	307	CLA	2	0
25	N	608	CHL	3	0
22	C	508	CLA	5	0
25	1	609	CHL	1	0
25	G	606	CHL	2	0
22	2	609	CLA	1	0
22	B	613	CLA	1	0
25	n	608	CHL	3	0
22	B	615	CLA	1	0
24	e	101	HEM	3	0
22	B	607	CLA	1	0
22	G	602	CLA	1	0
22	y	614	CLA	2	0
25	1	615	CHL	2	0
23	D	402	PHO	1	0
25	7	306	CHL	1	0
22	Y	613	CLA	1	0
22	4	310	CLA	2	0
25	6	607	CHL	5	0
25	7	308	CHL	4	0
22	1	614	CLA	1	0
22	7	313	CLA	1	0
25	1	608	CHL	3	0
22	8	301	CLA	40	0
22	c	502	CLA	1	0
25	1	606	CHL	1	0
25	5	606	CHL	1	0
25	8	302	CHL	12	0
25	n	609	CHL	1	0
25	n	606	CHL	2	0
22	s	303	CLA	3	0
25	r	306	CHL	2	0
22	1	611	CLA	1	0
22	G	610	CLA	1	0
22	B	608	CLA	1	0
25	n	607	CHL	2	0
25	r	304	CHL	1	0
22	B	616	CLA	3	0
22	c	509	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	2	611	CLA	1	0
25	G	607	CHL	1	0
22	G	612	CLA	2	0
22	G	613	CLA	1	0
22	8	310	CLA	2	0
25	g	605	CHL	1	0
22	B	601	CLA	1	0
22	S	313	CLA	2	0
22	c	507	CLA	1	0
25	1	601	CHL	1	0
22	c	506	CLA	3	0
23	A	404	PHO	2	0
22	b	605	CLA	1	0
25	6	608	CHL	1	0
22	N	611	CLA	1	0
25	3	301	CHL	1	0
22	1	612	CLA	1	0
25	6	605	CHL	2	0
22	4	303	CLA	2	0
22	c	511	CLA	1	0
22	g	611	CLA	2	0
22	y	611	CLA	1	0
25	5	605	CHL	1	0
22	2	612	CLA	1	0
22	B	602	CLA	5	0
25	g	601	CHL	2	0
25	2	607	CHL	5	0
22	c	508	CLA	4	0
22	8	303	CLA	2	0
25	2	601	CHL	3	0
22	a	402	CLA	1	0
25	2	608	CHL	1	0
25	g	609	CHL	2	0
22	6	610	CLA	2	0
25	s	306	CHL	1	0
22	S	310	CLA	1	0
25	g	608	CHL	4	0
25	s	308	CHL	1	0
22	R	311	CLA	1	0
22	s	313	CLA	2	0
25	N	609	CHL	1	0
22	y	602	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	N	607	CHL	2	0
25	y	601	CHL	2	0
22	Y	610	CLA	1	0
25	s	302	CHL	1	0
25	y	609	CHL	2	0
25	g	606	CHL	2	0
22	C	502	CLA	2	0
22	n	602	CLA	1	0
22	6	602	CLA	1	0
25	5	609	CHL	1	0
25	S	308	CHL	2	0
25	3	306	CHL	1	0
22	b	614	CLA	3	0
22	2	602	CLA	1	0
22	s	310	CLA	1	0
22	C	501	CLA	2	0
22	S	314	CLA	1	0
25	N	601	CHL	1	0
25	n	601	CHL	1	0
22	b	613	CLA	1	0
22	A	403	CLA	1	0
22	s	301	CLA	17	0
22	2	613	CLA	16	0
22	g	610	CLA	1	0
25	8	307	CHL	2	0
22	y	613	CLA	1	0
22	6	611	CLA	1	0
22	R	303	CLA	1	0
25	Y	607	CHL	1	0
22	A	405	CLA	1	0
22	c	505	CLA	1	0
22	N	602	CLA	1	0
25	2	605	CHL	2	0
22	g	613	CLA	1	0
25	y	608	CHL	2	0
22	N	610	CLA	1	0
22	b	604	CLA	3	0
22	N	613	CLA	1	0
22	B	604	CLA	1	0
25	G	608	CHL	4	0
22	B	603	CLA	1	0
22	n	610	CLA	2	0

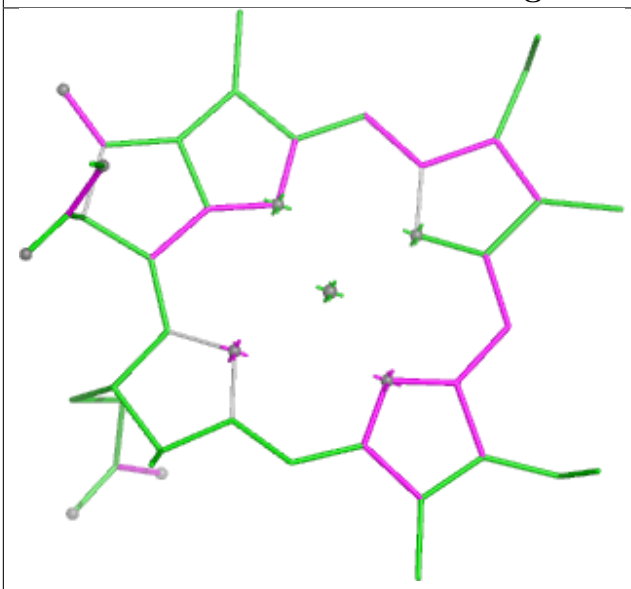
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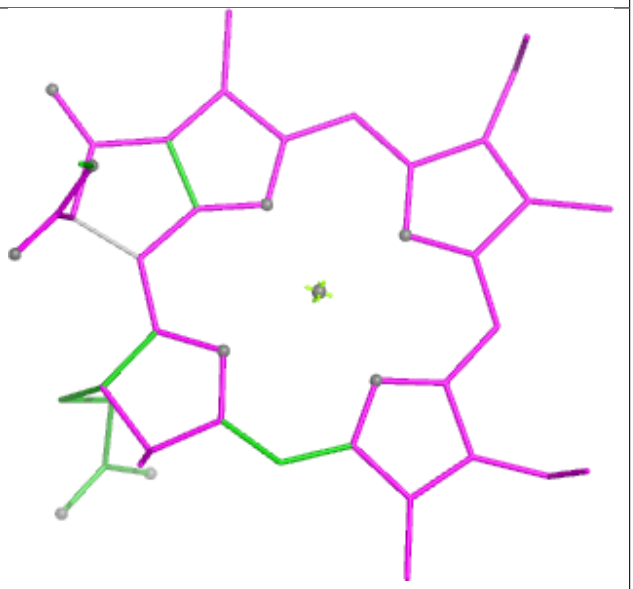
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	n	611	CLA	1	0
22	7	311	CLA	1	0
22	b	602	CLA	3	0
22	A	402	CLA	2	0
25	5	608	CHL	3	0
22	S	304	CLA	1	0
25	7	307	CHL	1	0
22	r	308	CLA	1	0
22	B	606	CLA	2	0
22	B	612	CLA	1	0
25	G	605	CHL	1	0
25	1	605	CHL	1	0
25	G	601	CHL	2	0
25	y	606	CHL	2	0
25	Y	609	CHL	2	0
25	y	605	CHL	3	0
22	b	603	CLA	1	0
22	5	614	CLA	1	0
25	5	601	CHL	1	0
22	g	612	CLA	2	0
25	S	306	CHL	1	0
22	S	303	CLA	3	0

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

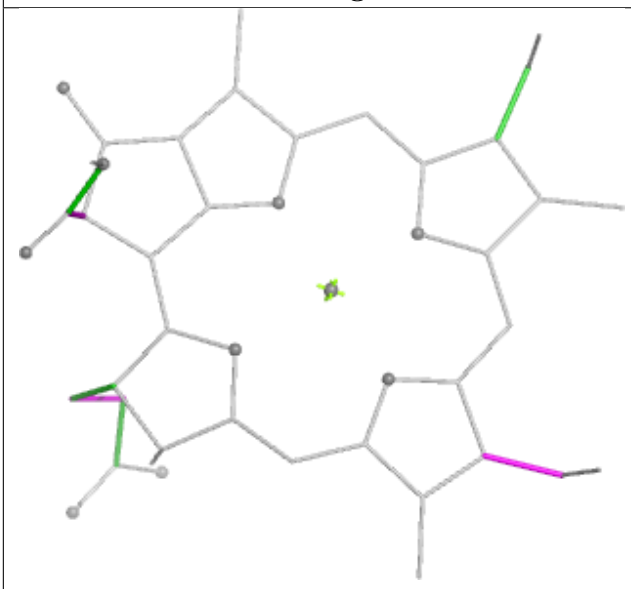
Ligand CLA B 609



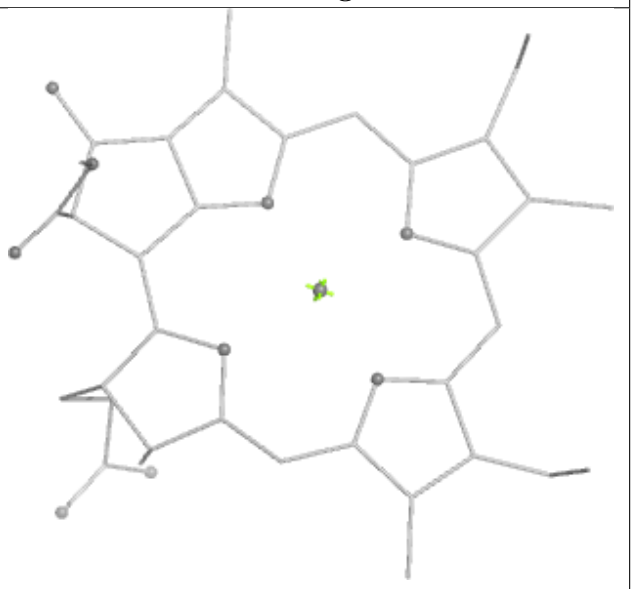
Bond lengths



Bond angles

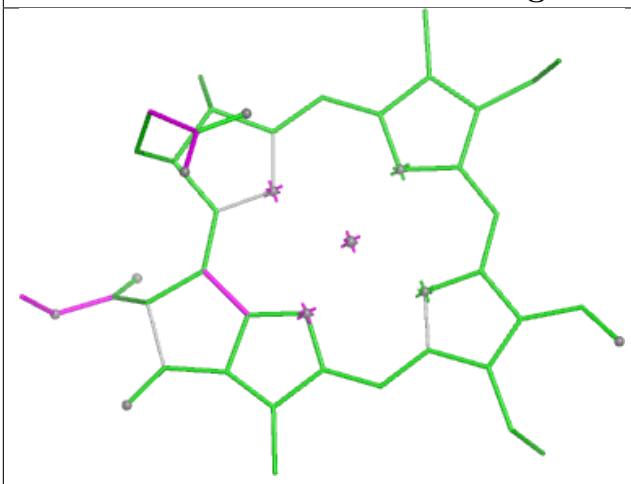


Torsions

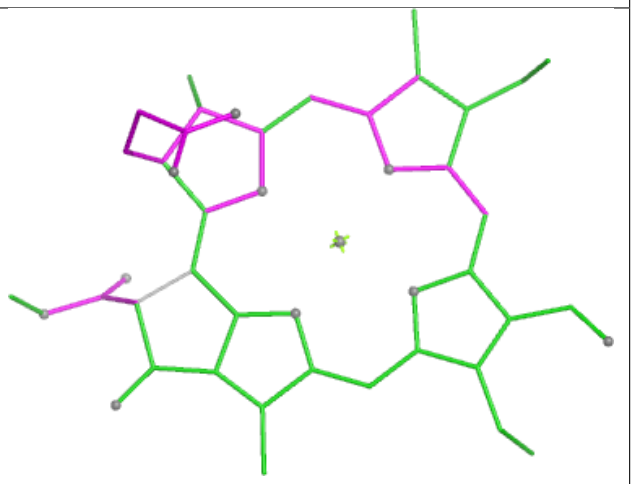


Rings

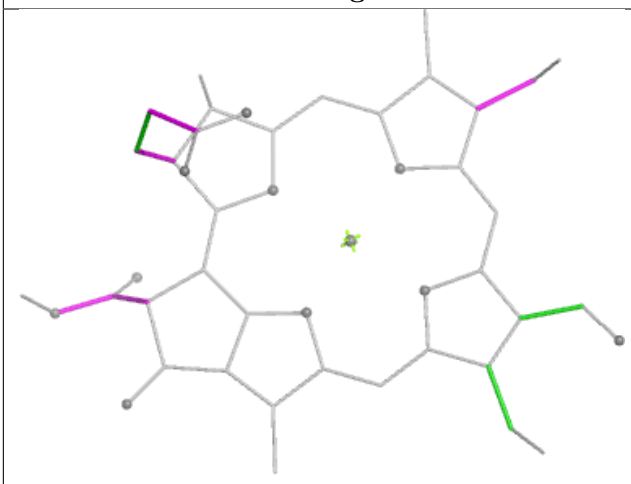
Ligand CHL 6 606



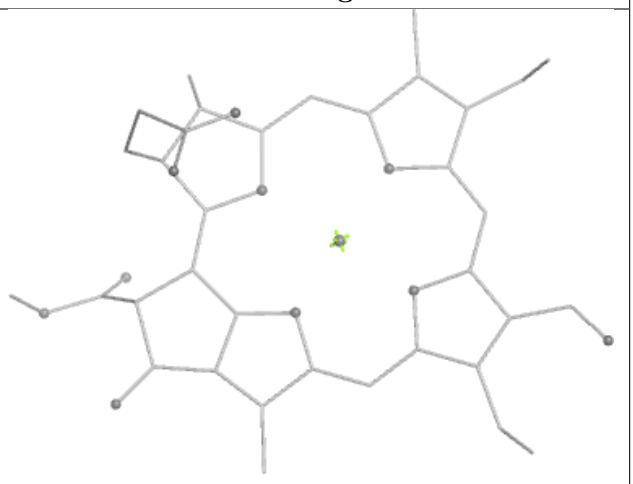
Bond lengths



Bond angles

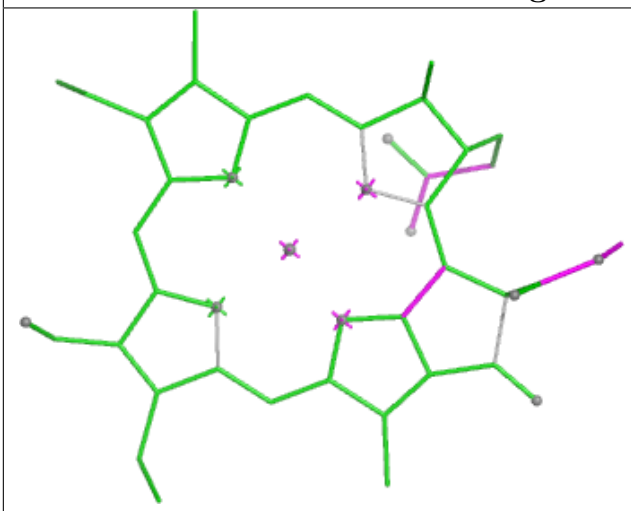


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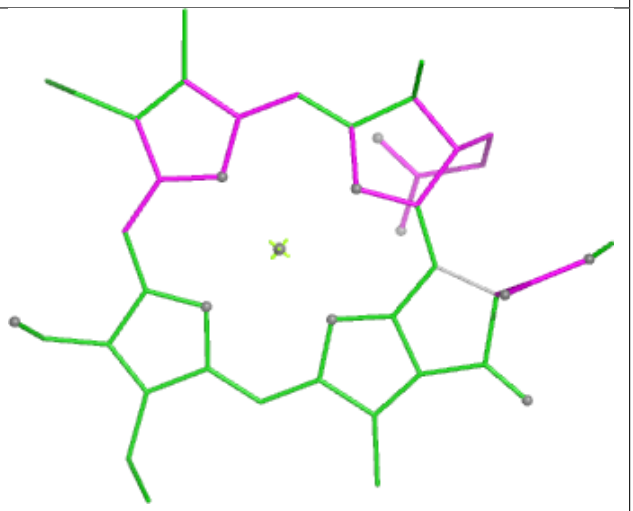


Rings

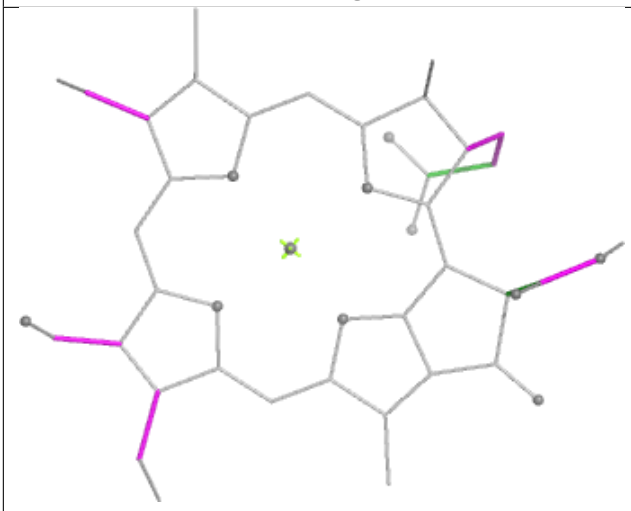
Ligand CHL r 305



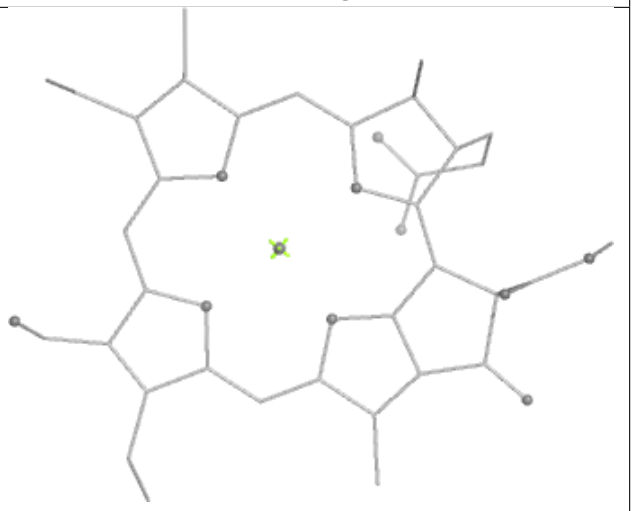
Bond lengths



Bond angles

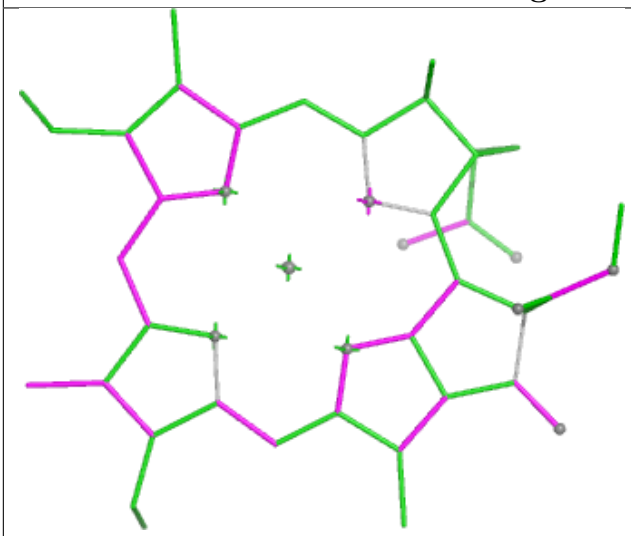


Torsions

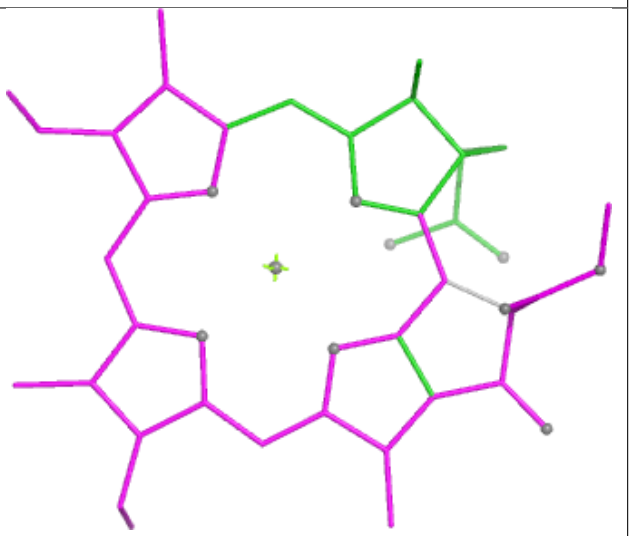


Rings

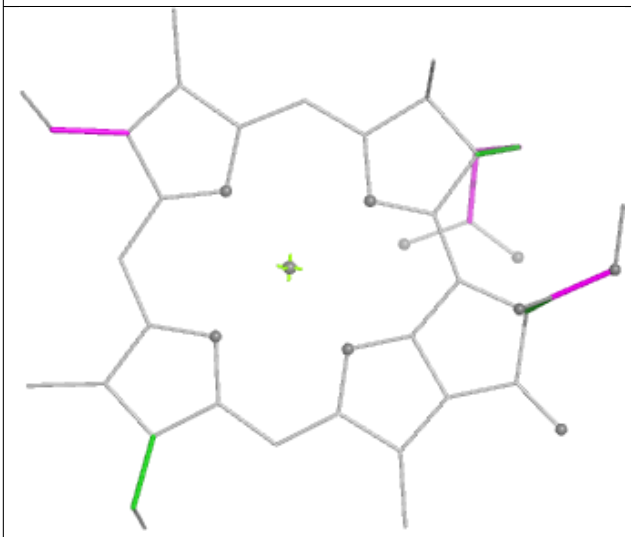
Ligand CLA r 311



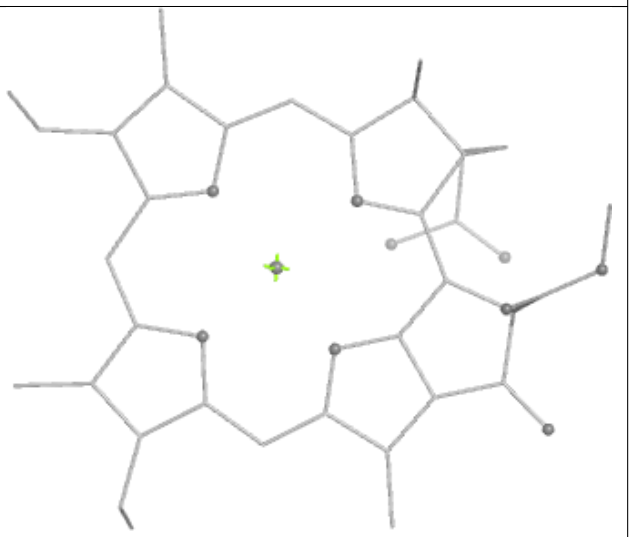
Bond lengths



Bond angles

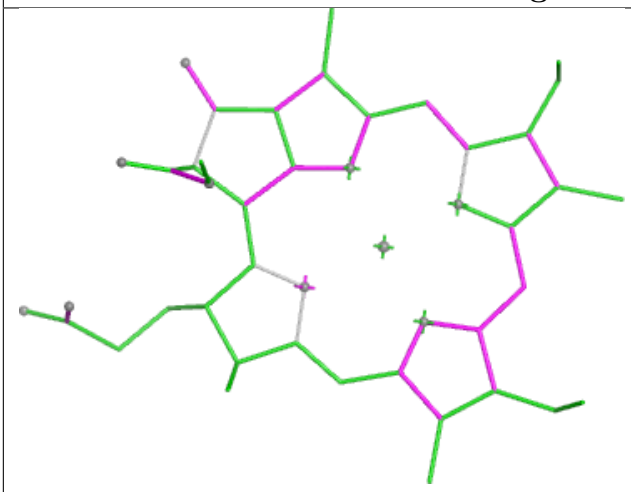


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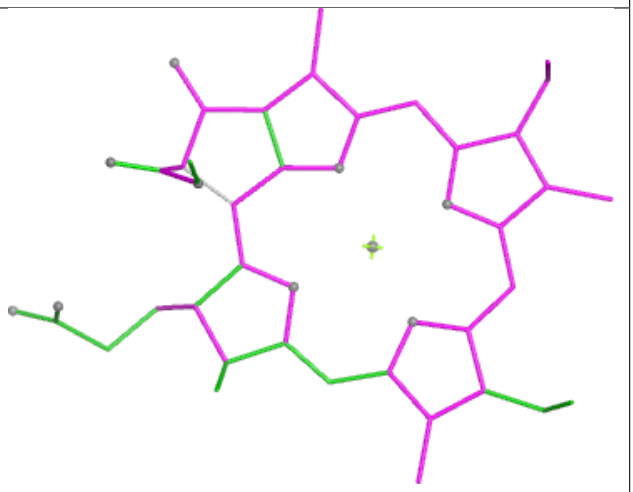


Rings

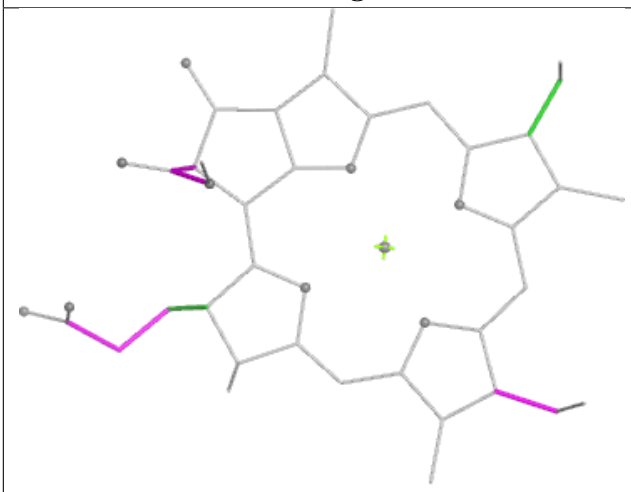
Ligand CLA s 304



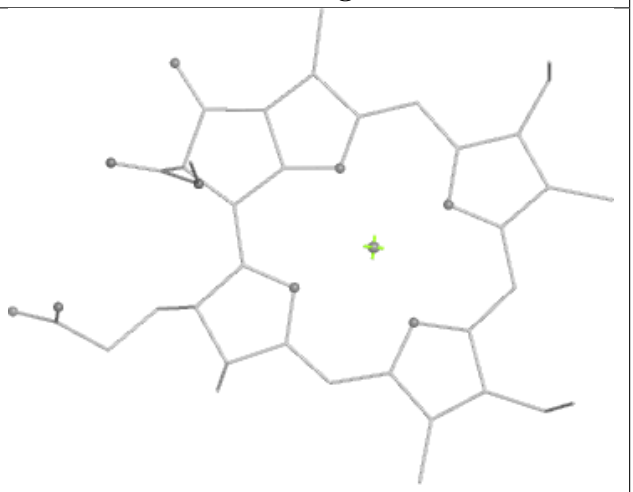
Bond lengths



Bond angles

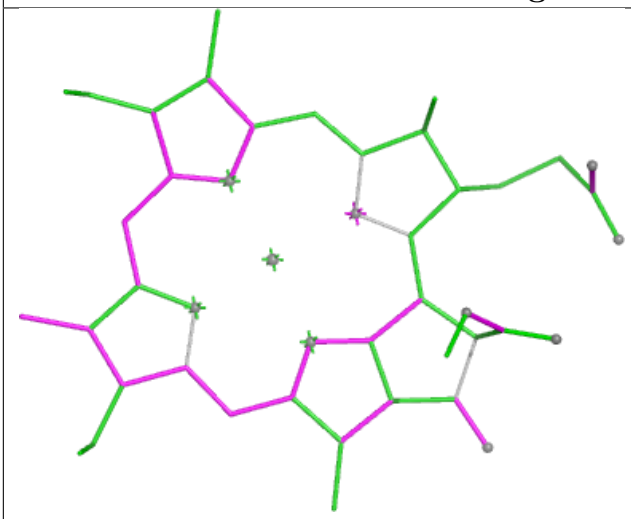


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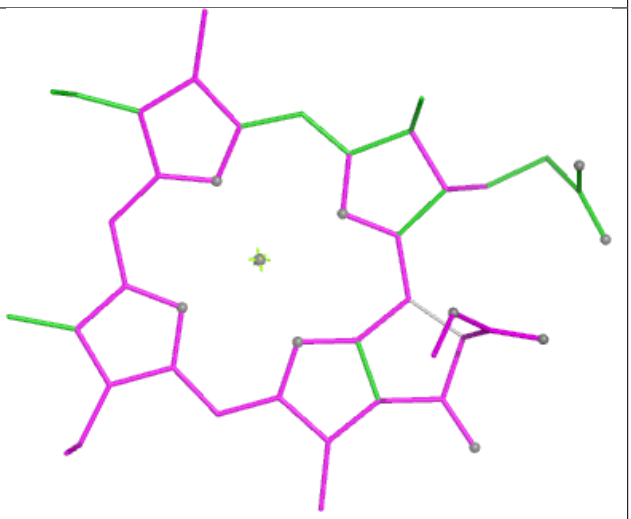


Rings

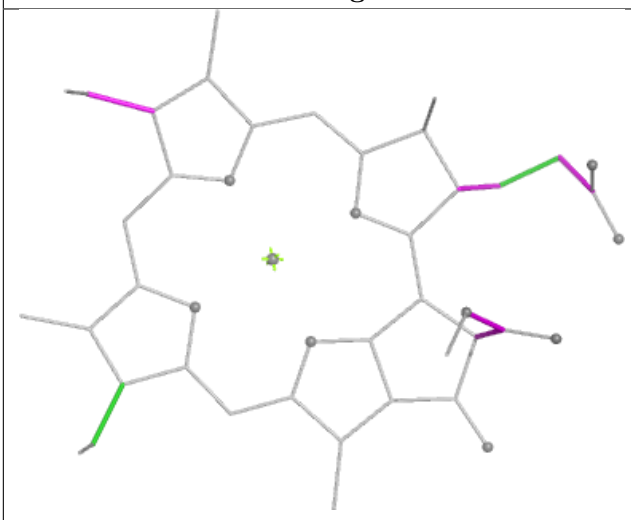
Ligand CLA 5 612



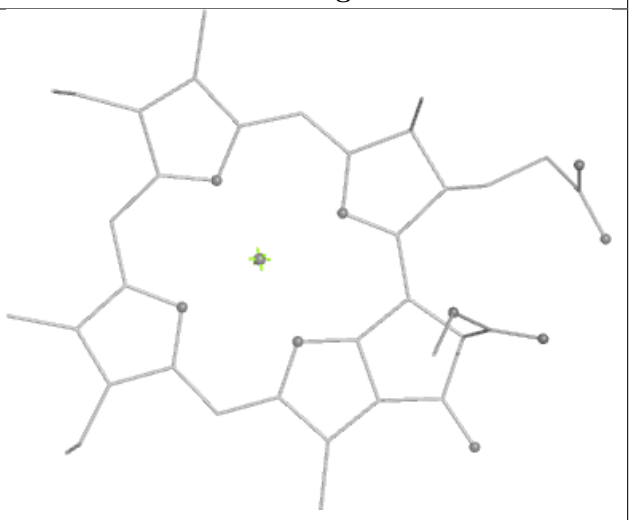
Bond lengths



Bond angles

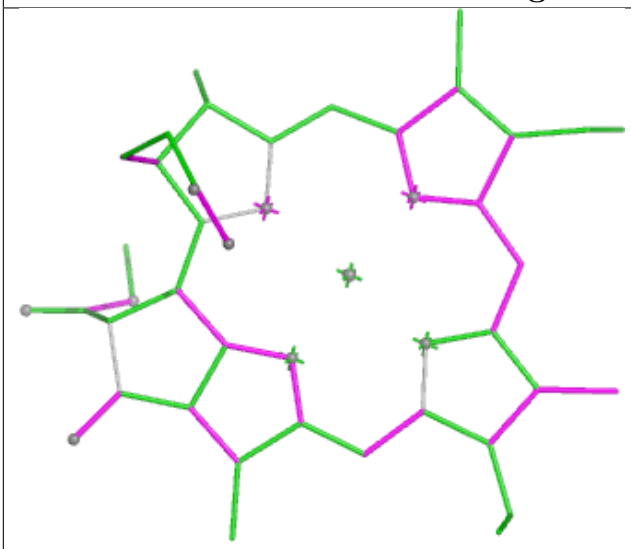


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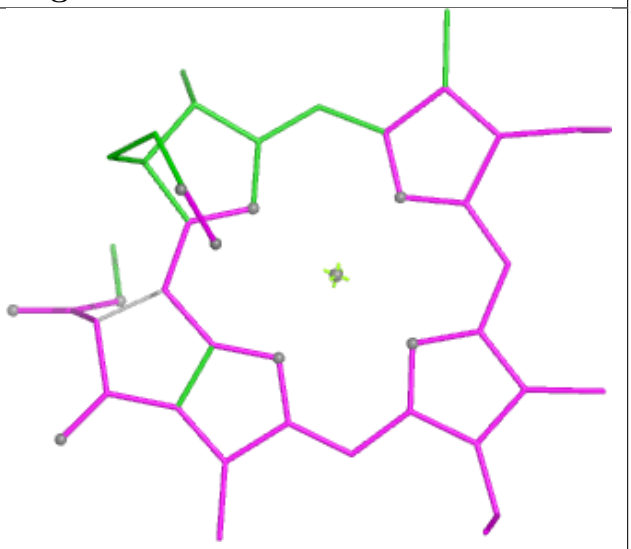


Rings

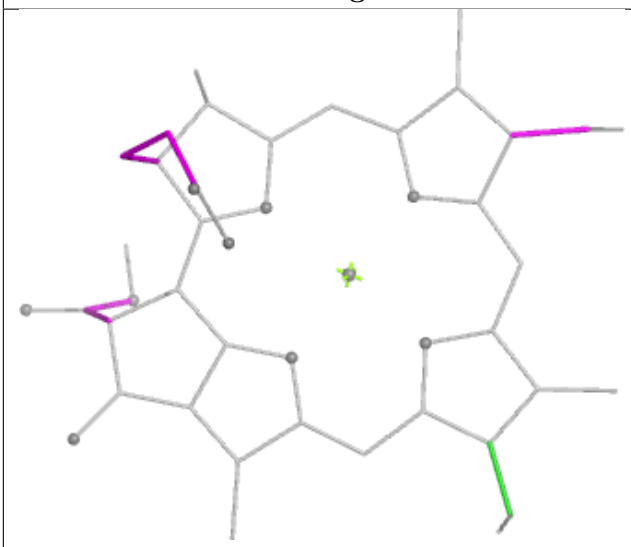
Ligand CLA g 602



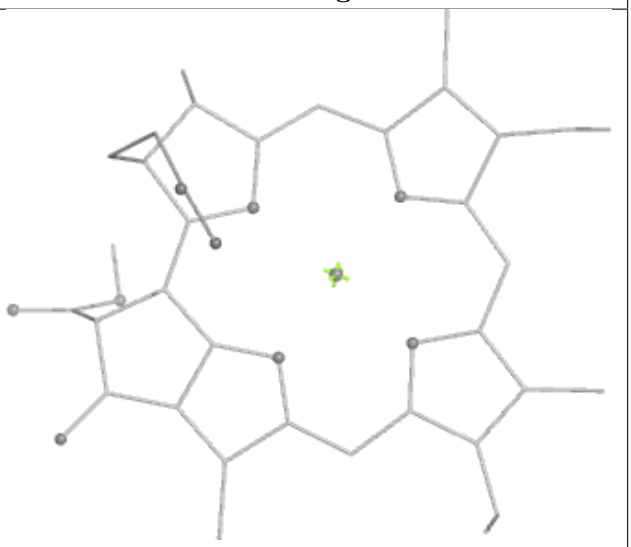
Bond lengths



Bond angles

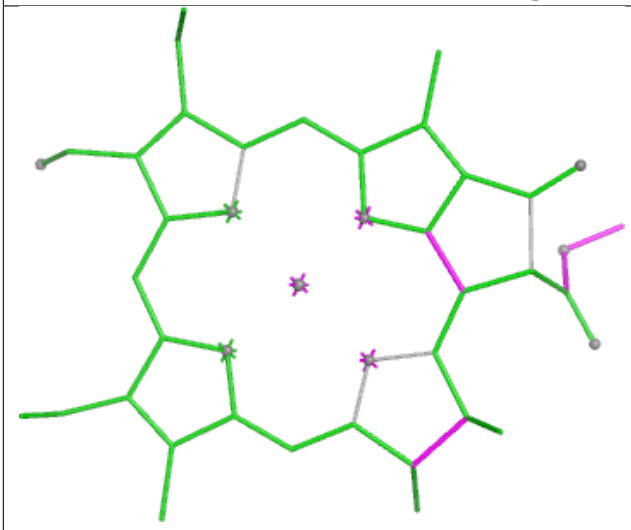


Torsions

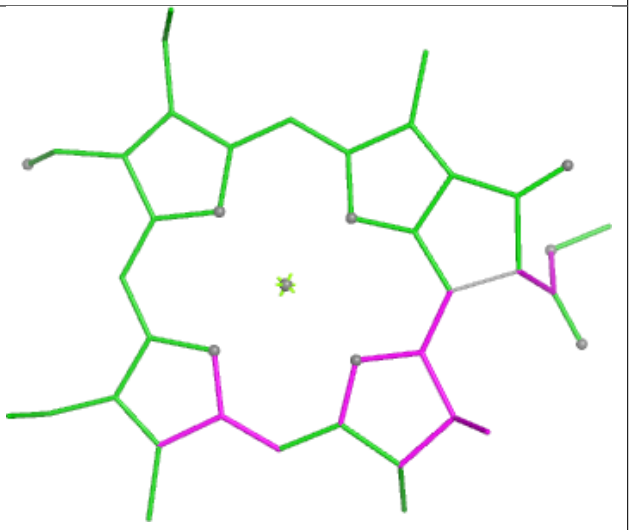


Rings

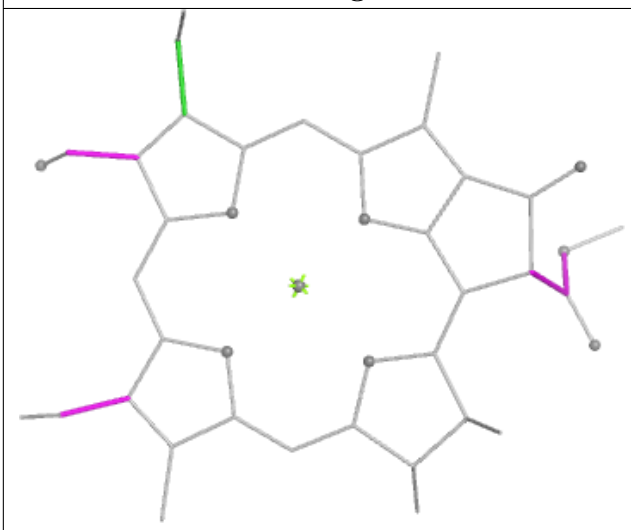
Ligand CHL n 605



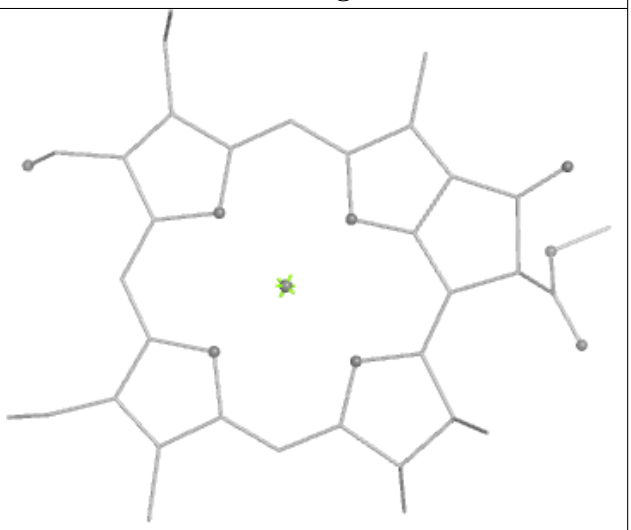
Bond lengths



Bond angles

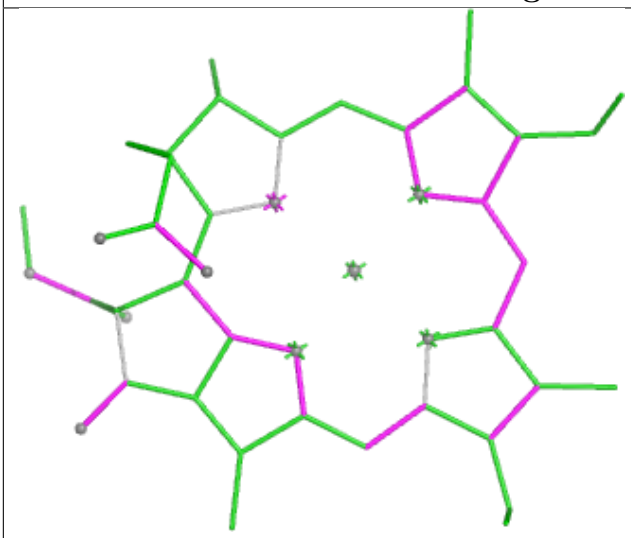


Torsions

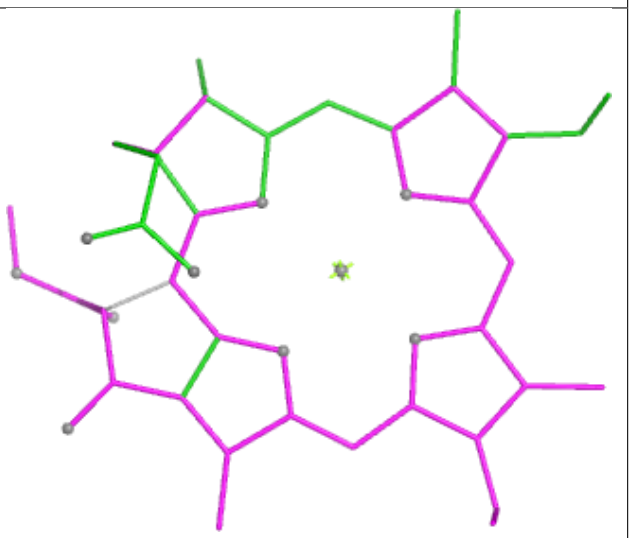


Rings

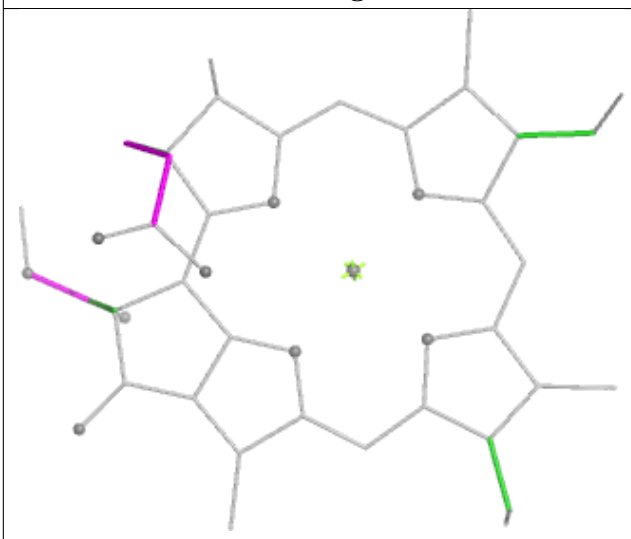
Ligand CLA G 611



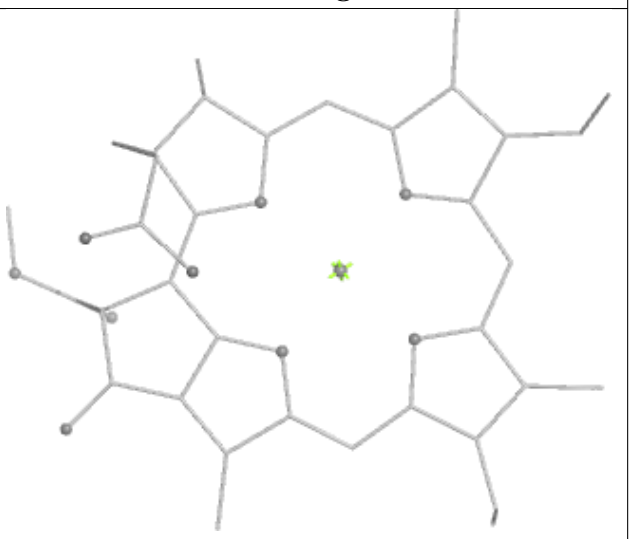
Bond lengths



Bond angles

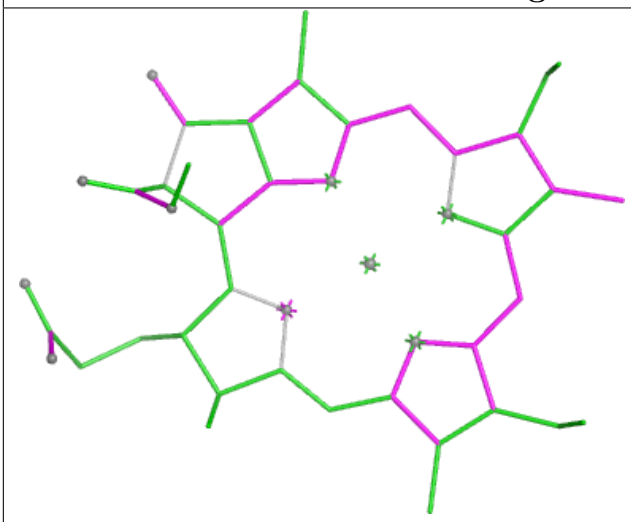


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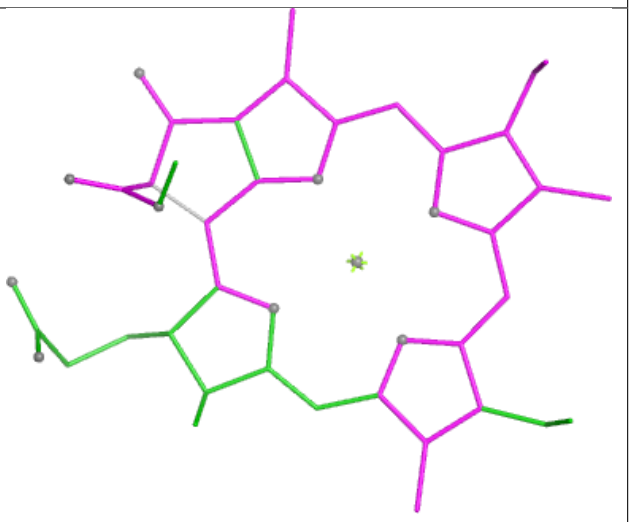


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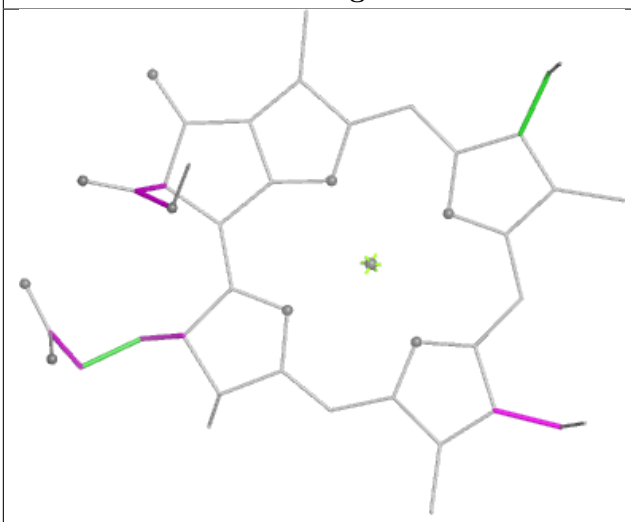
Ligand CLA 7 312



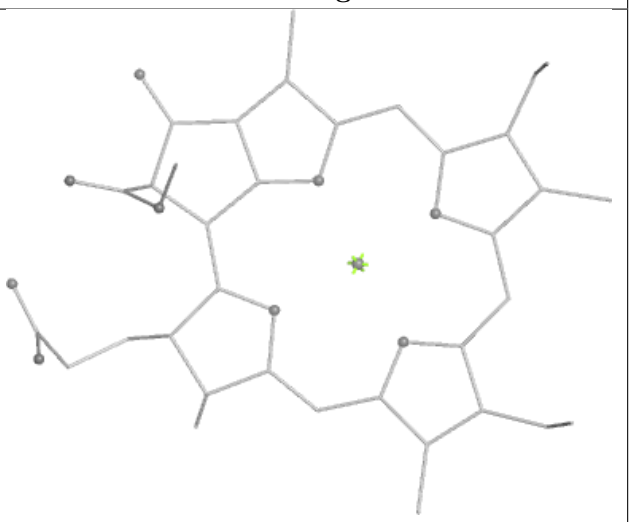
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Bond angles

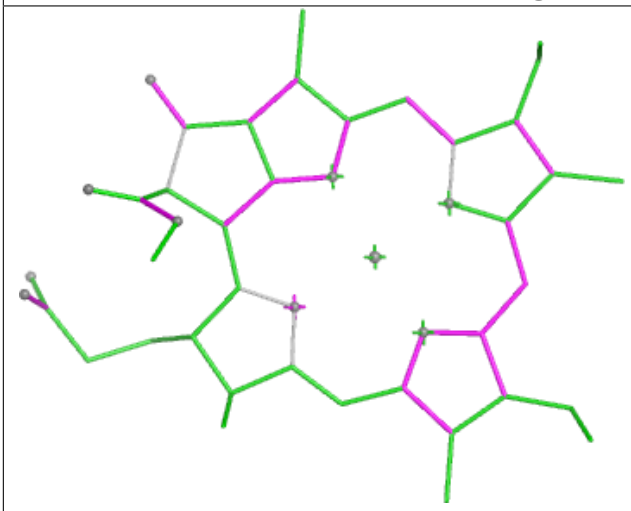


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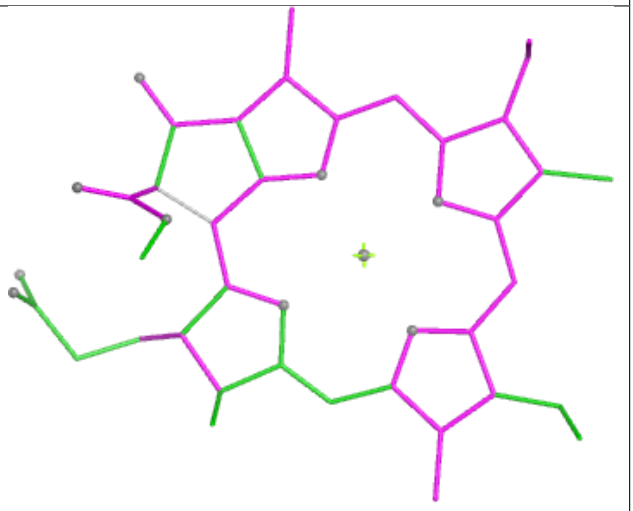


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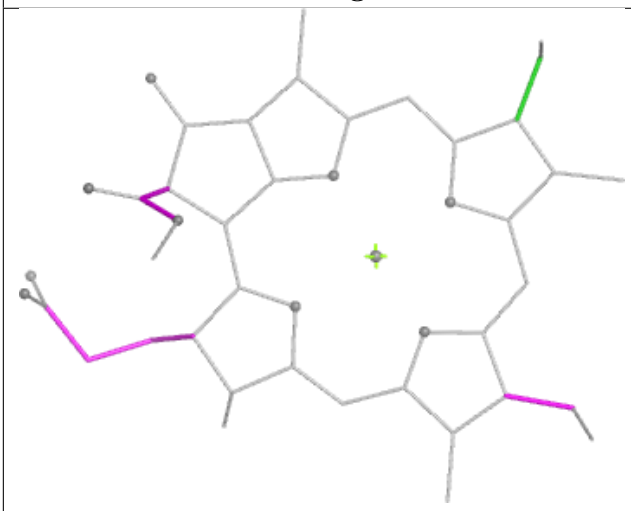
Ligand CLA r 302



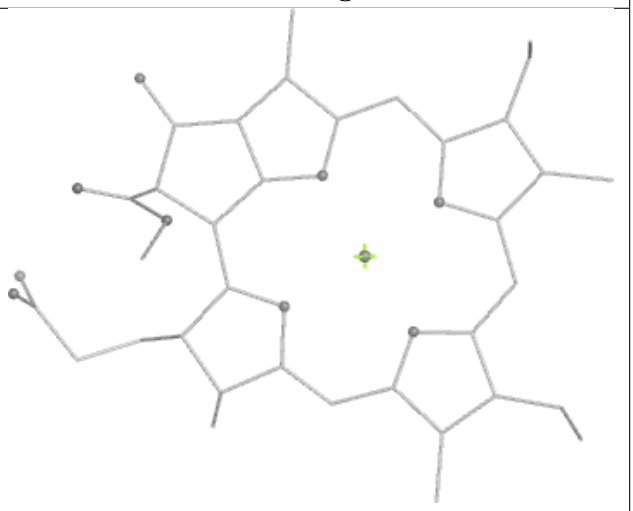
Bond lengths



Bond angles

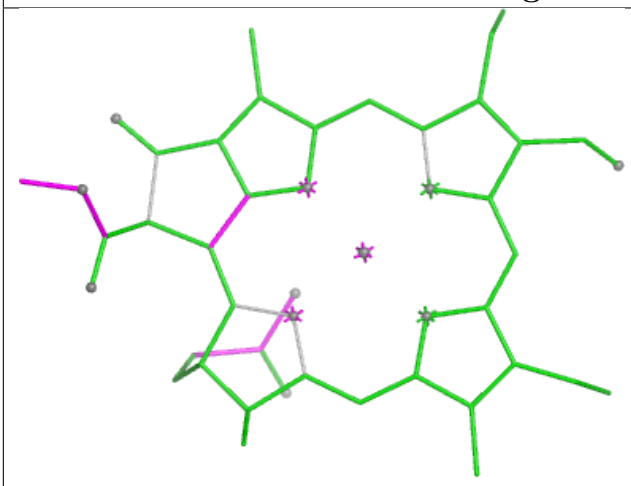


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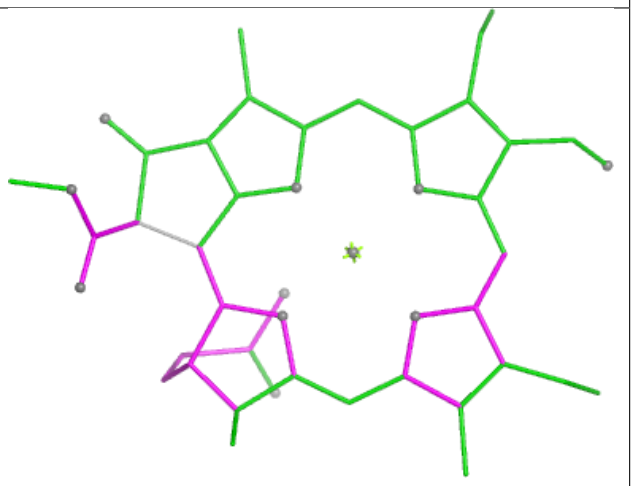


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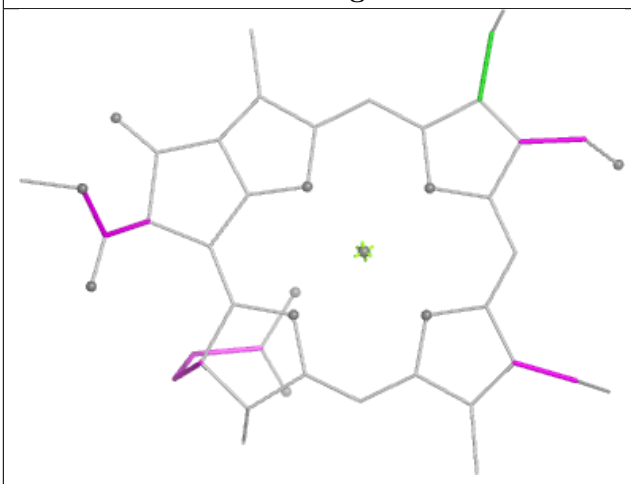
Ligand CHL G 609



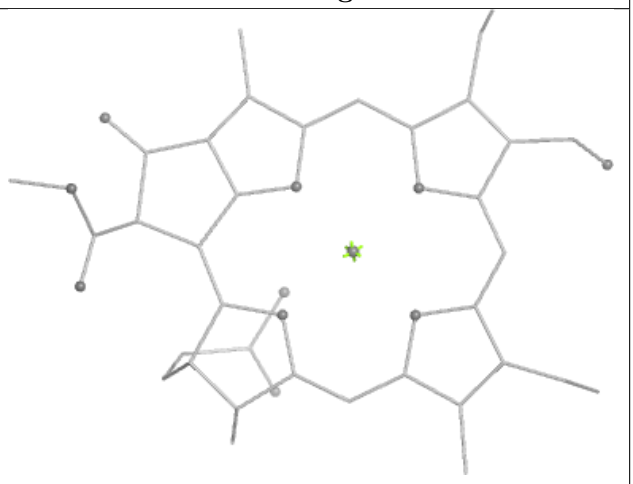
Bond lengths



Bond angles

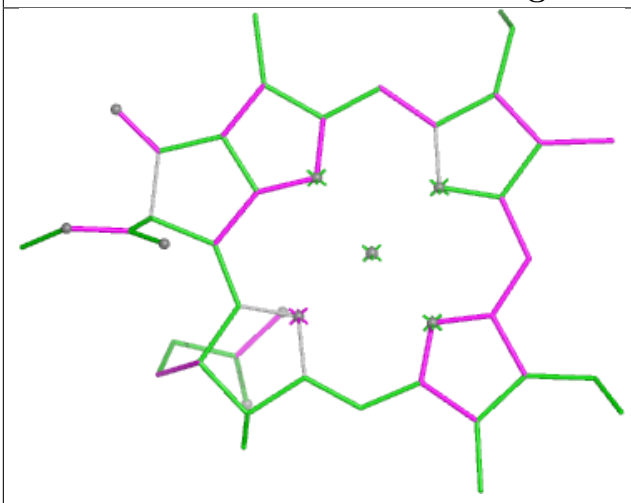


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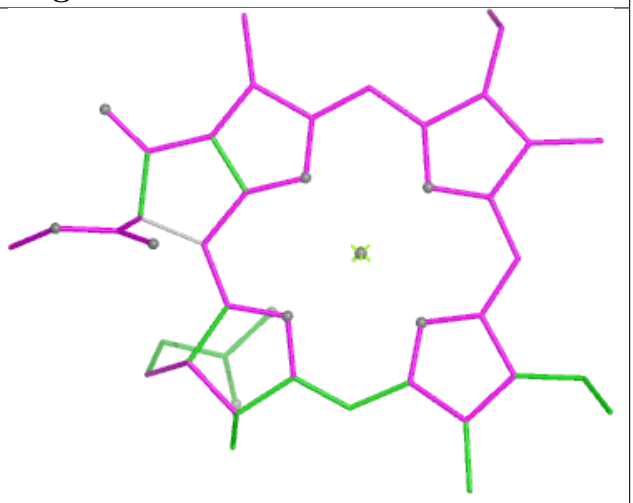


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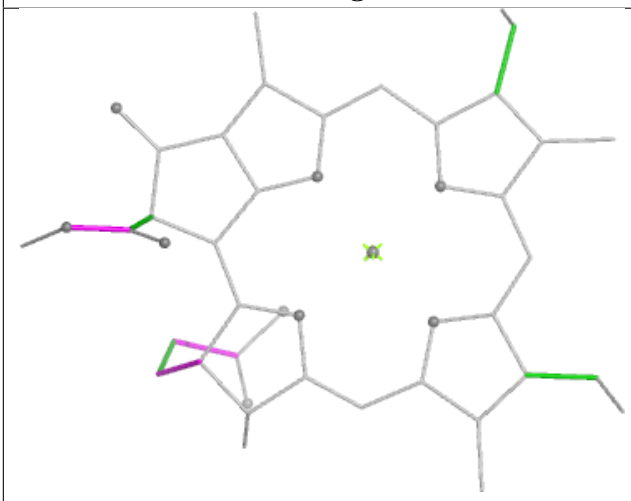
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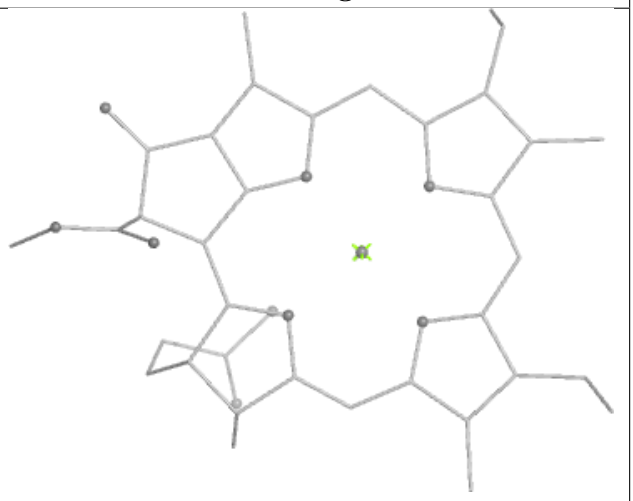
Bond lengths



Bond angles

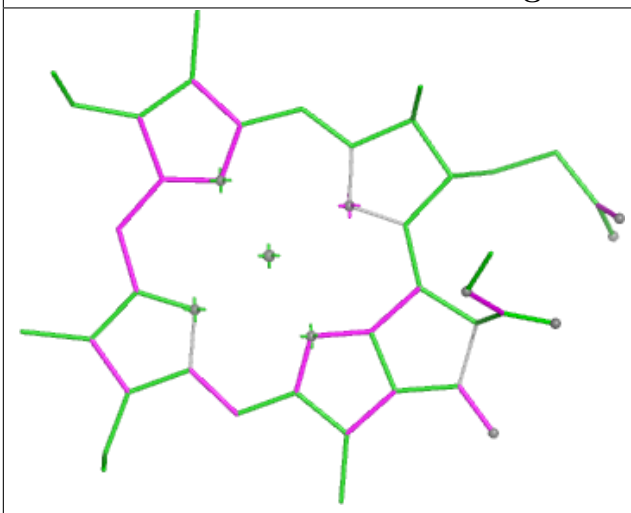


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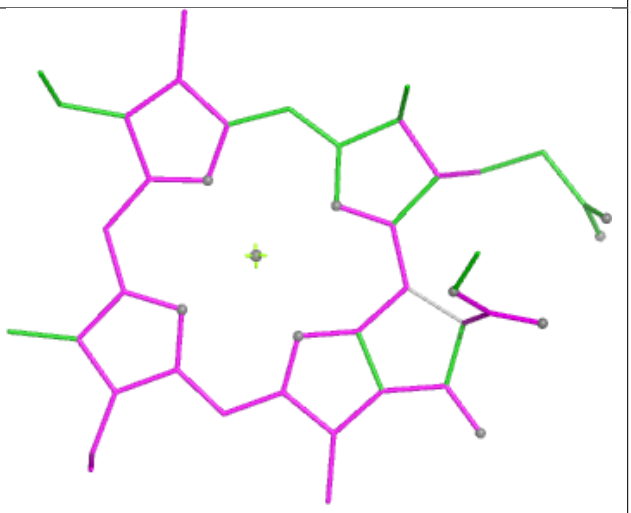


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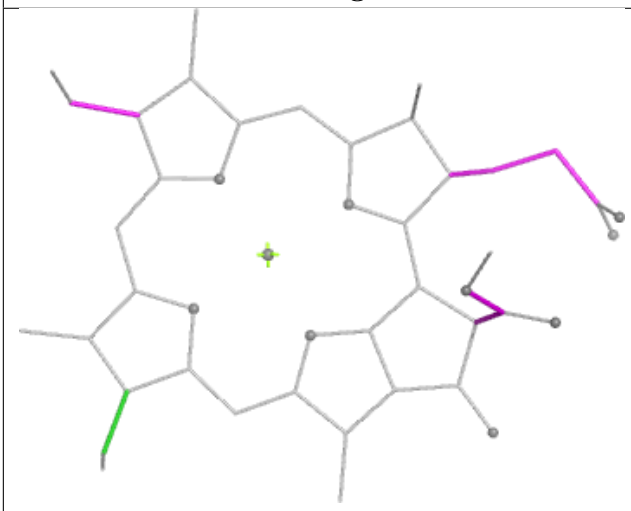
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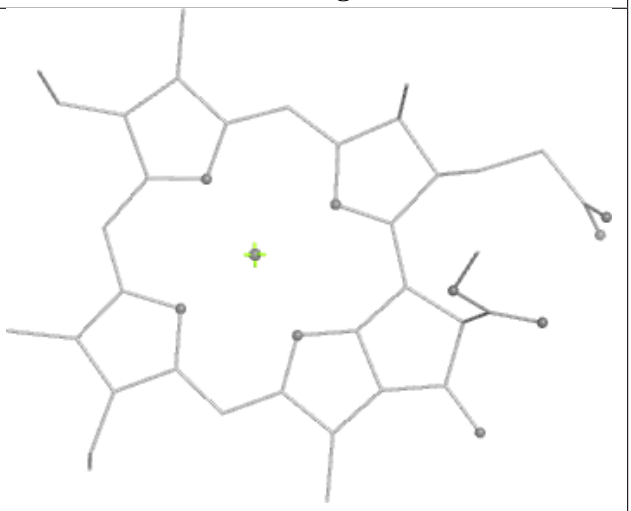
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Bond angles

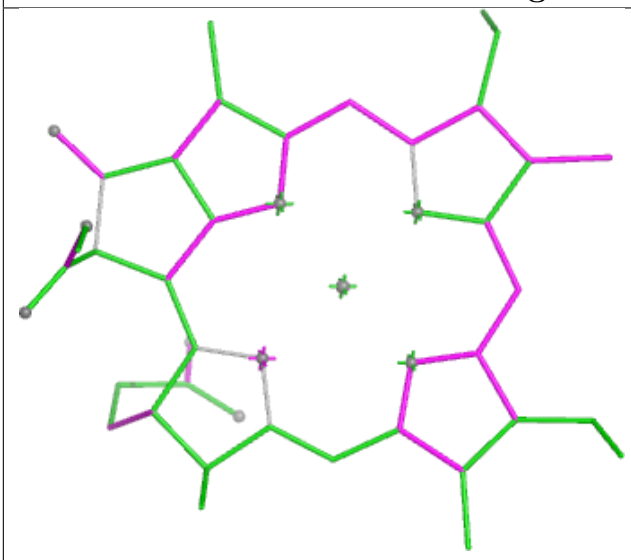


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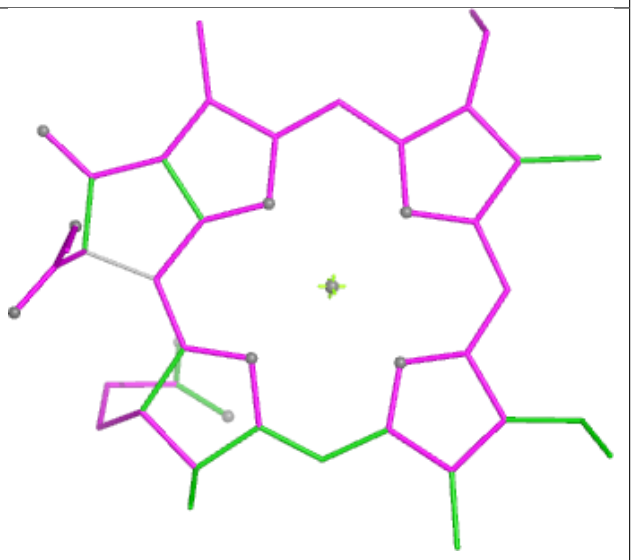


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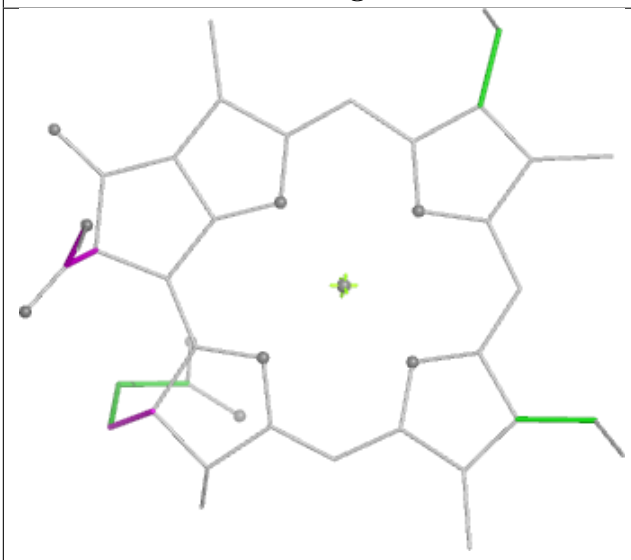
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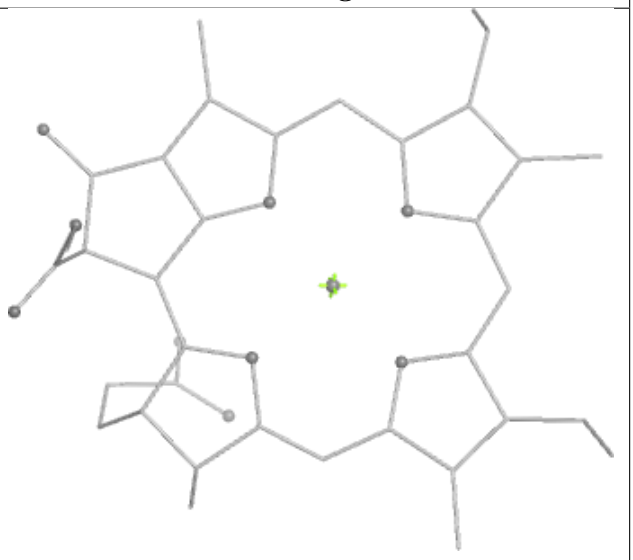
Bond lengths



Bond angles

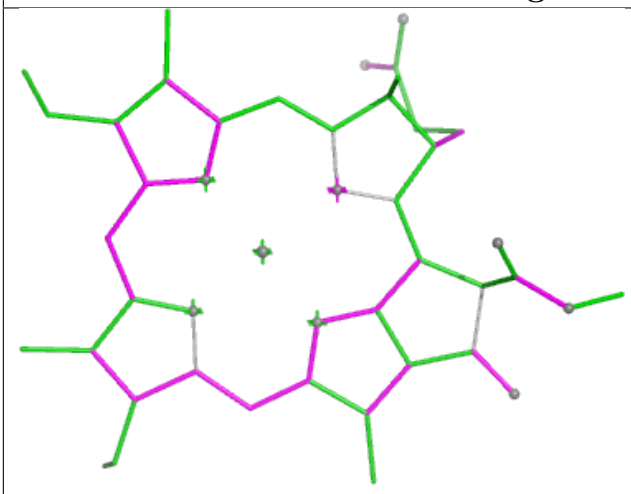


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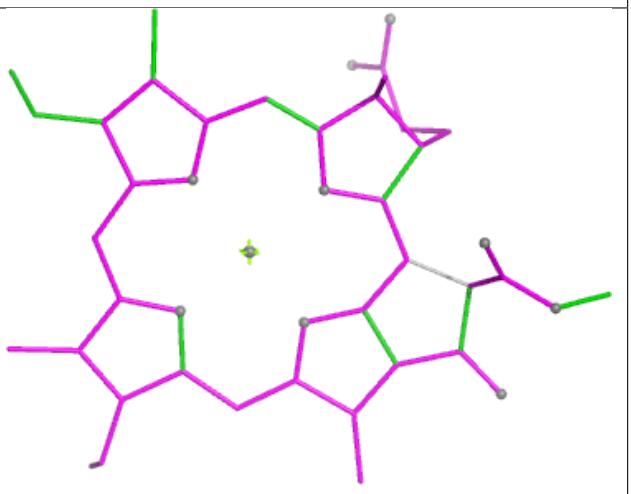


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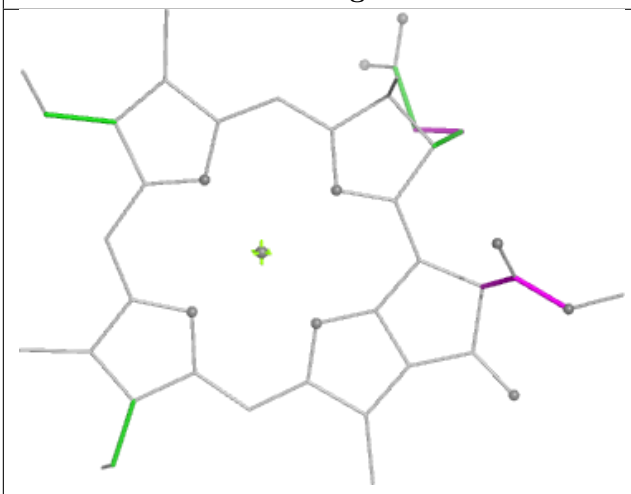
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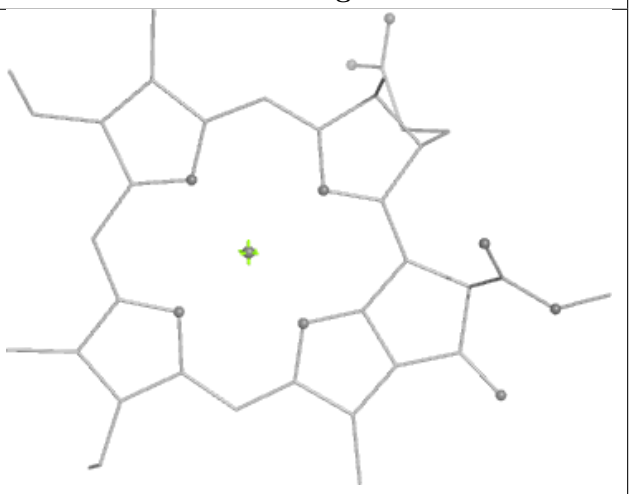
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Bond angles

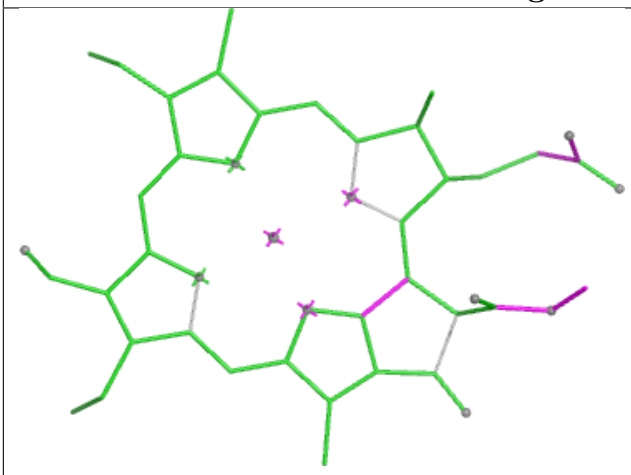


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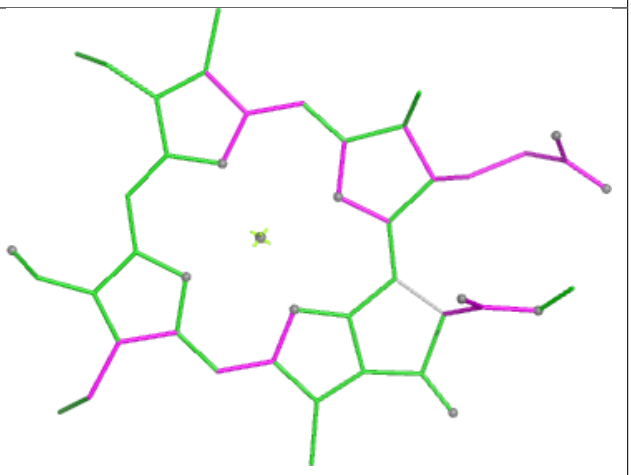


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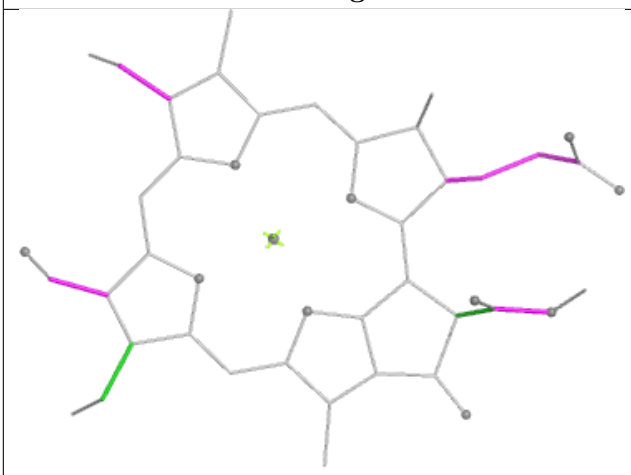
Ligand CHL 4 302



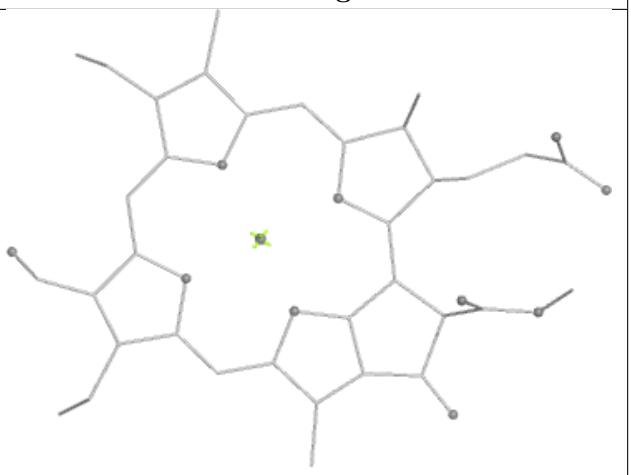
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Bond angles

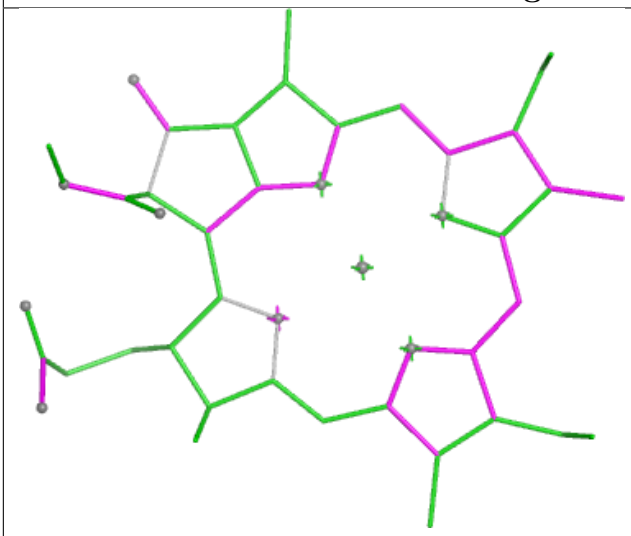


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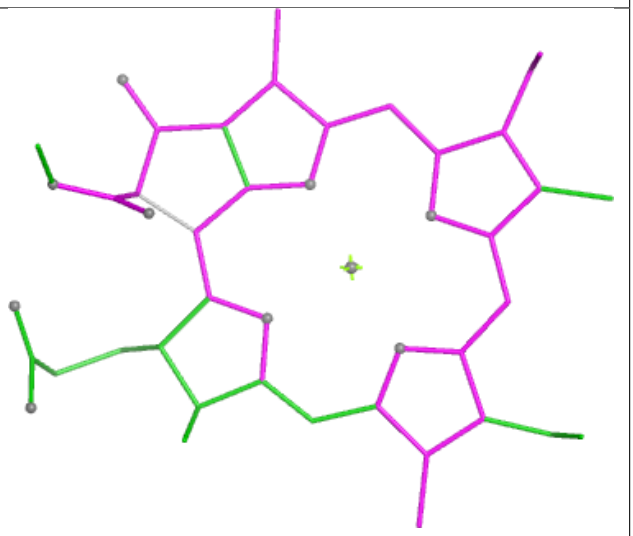


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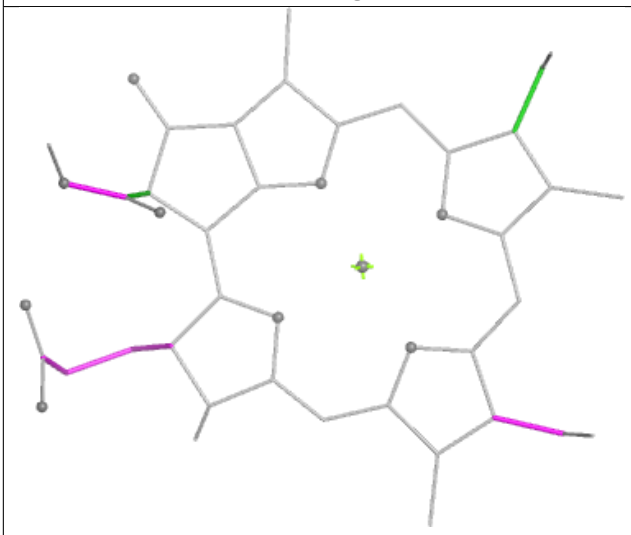
Ligand CLA R 310



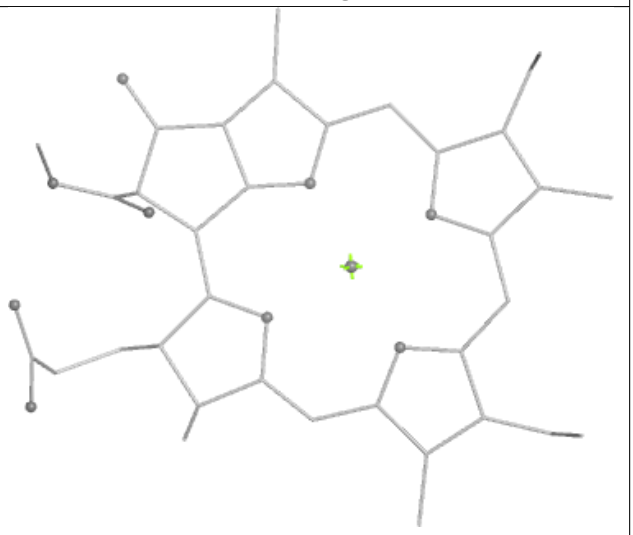
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Bond angles

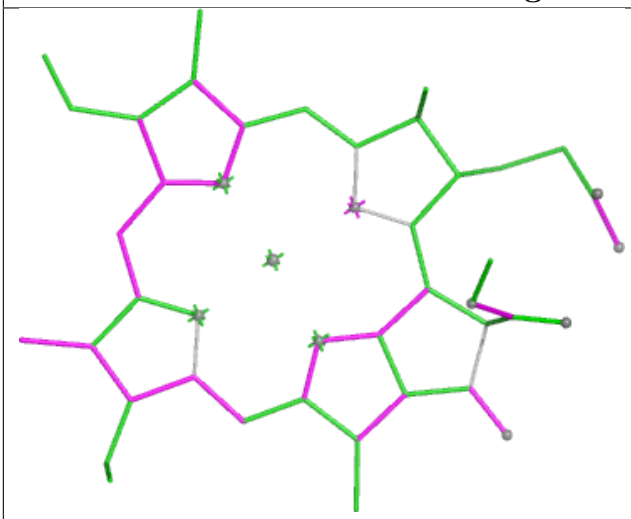


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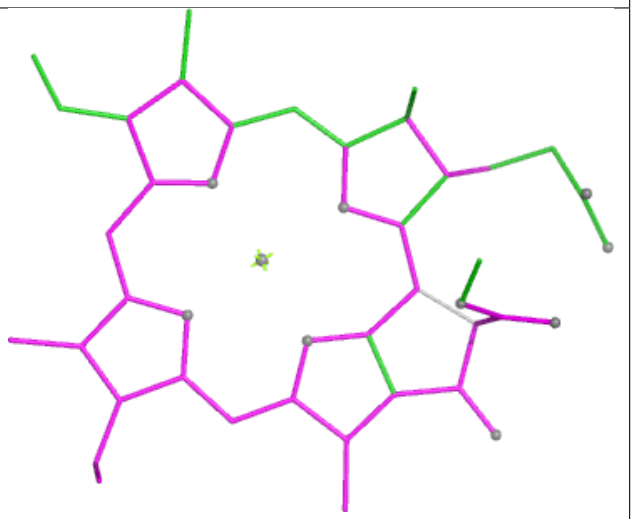


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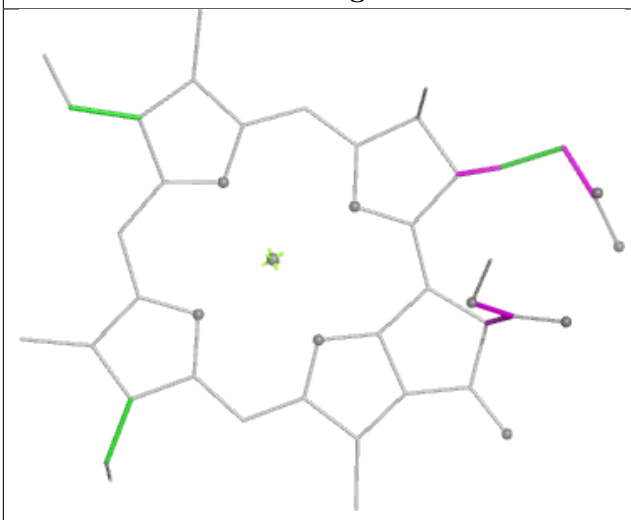
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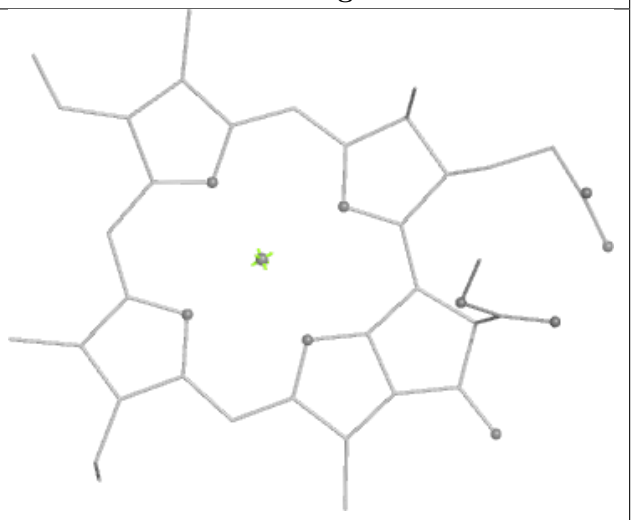
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Bond angles

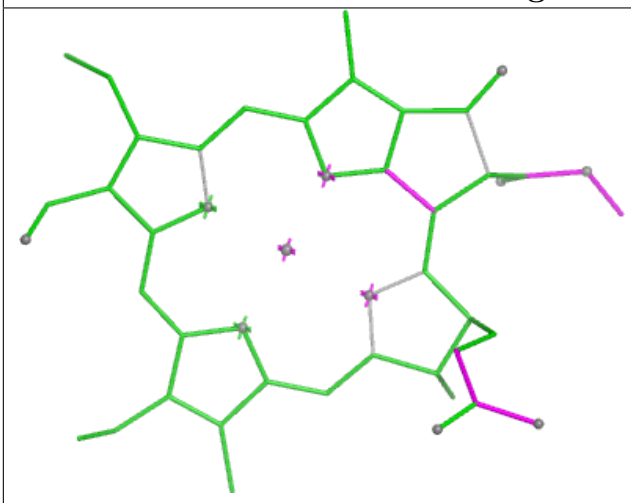


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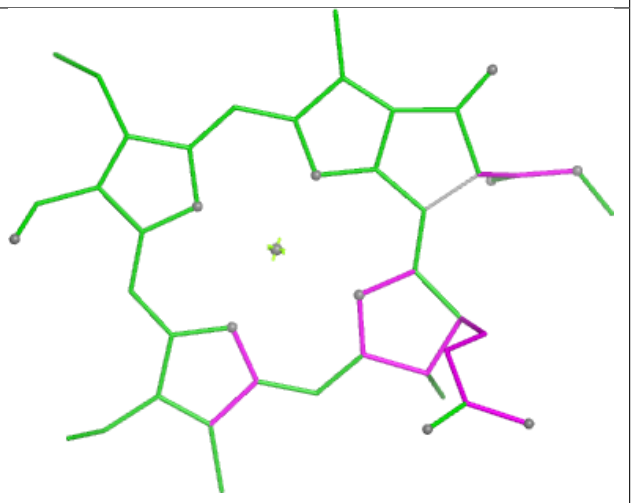


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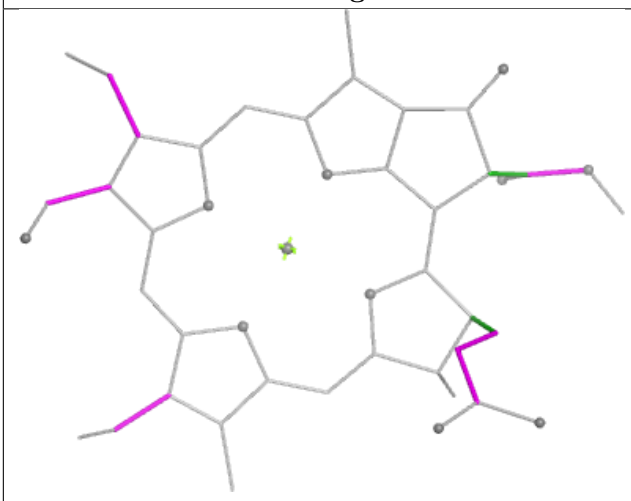
Ligand CHL 4 309



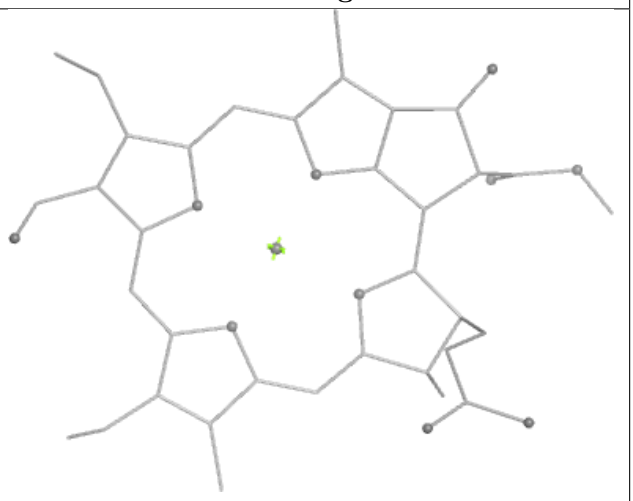
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Bond angles

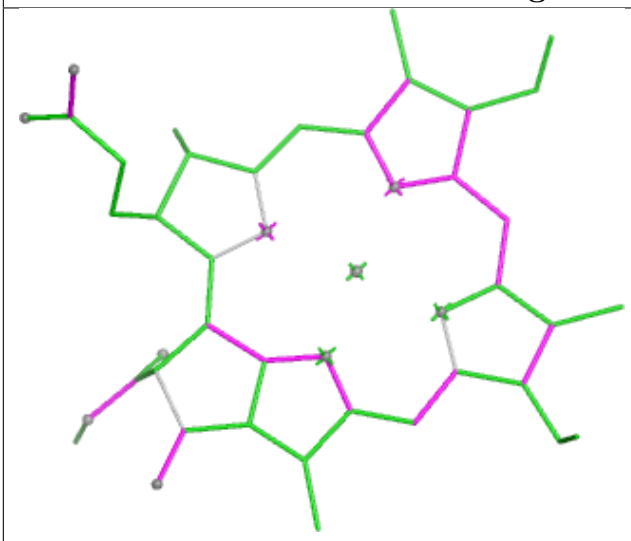


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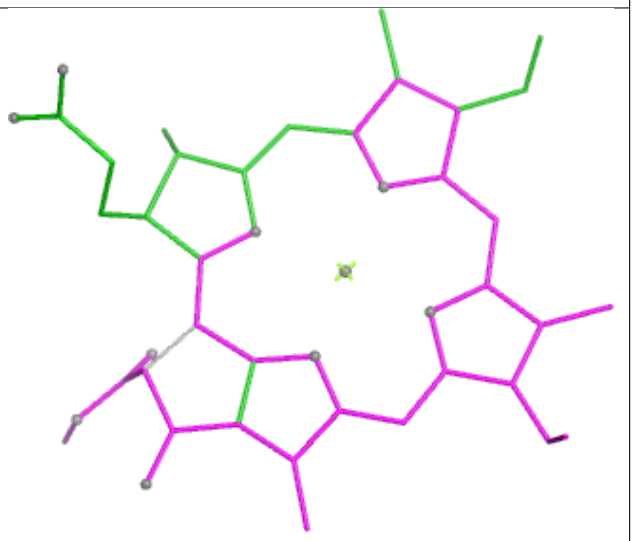


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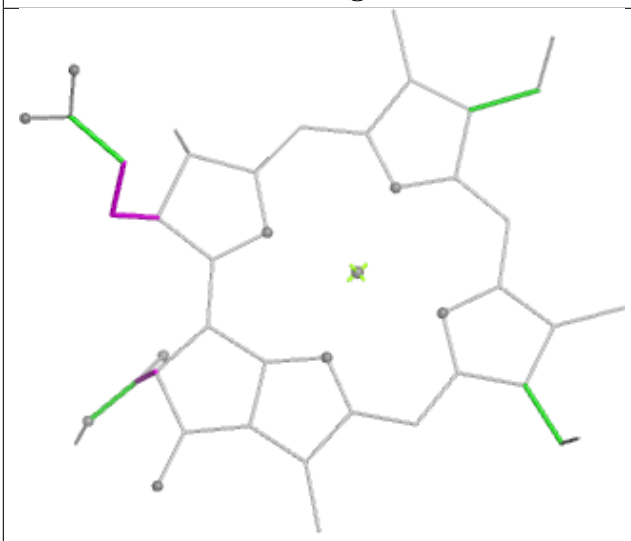
Ligand CLA a 405



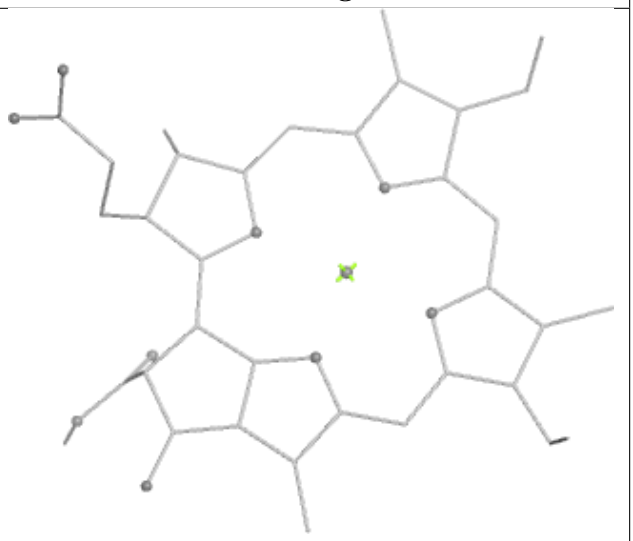
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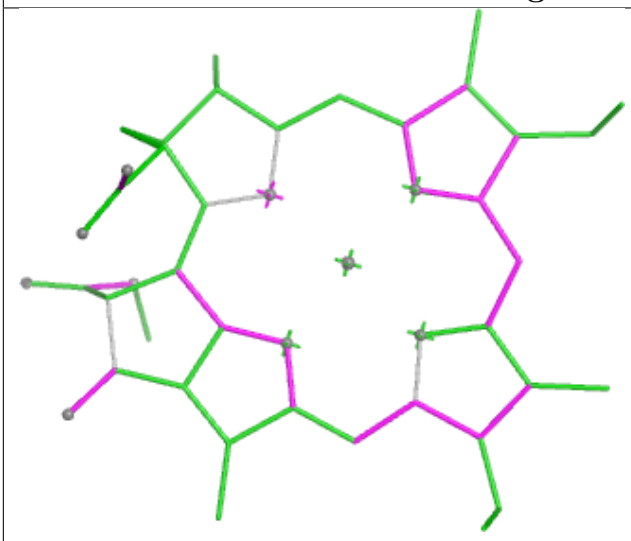


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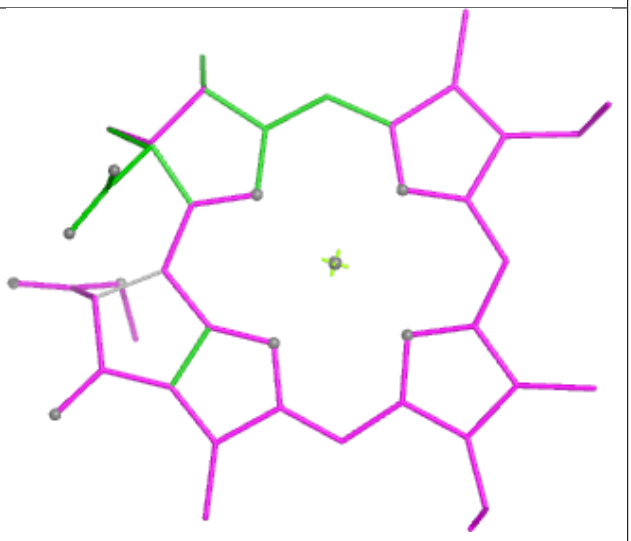


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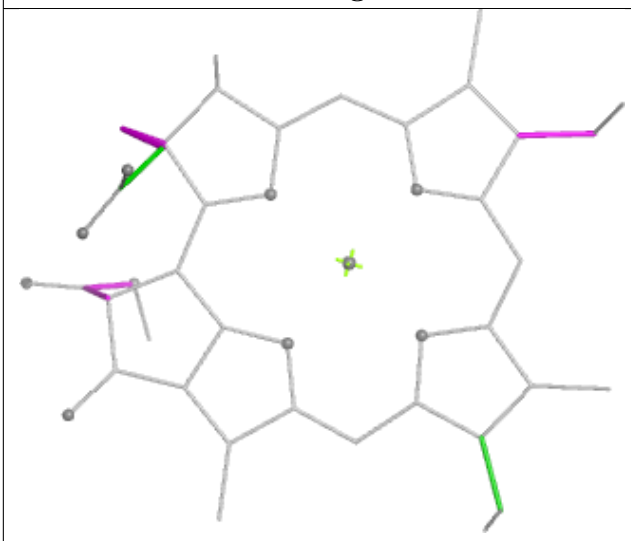
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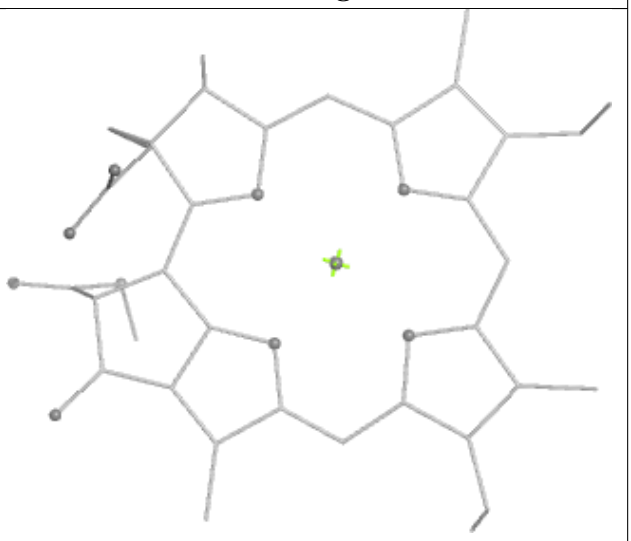
Bond lengths



Bond angles

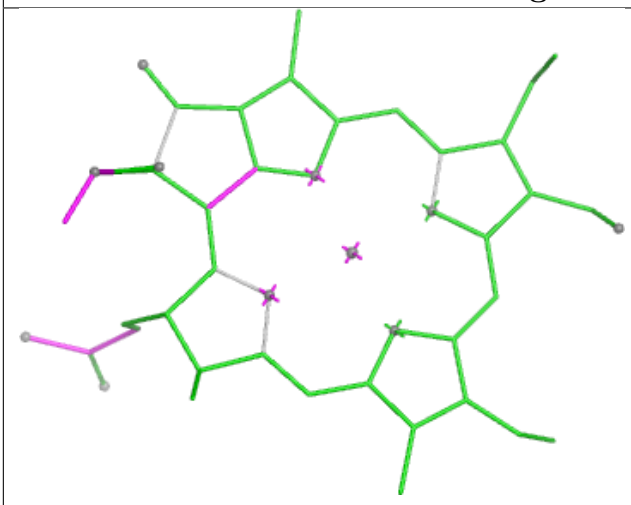


Torsions

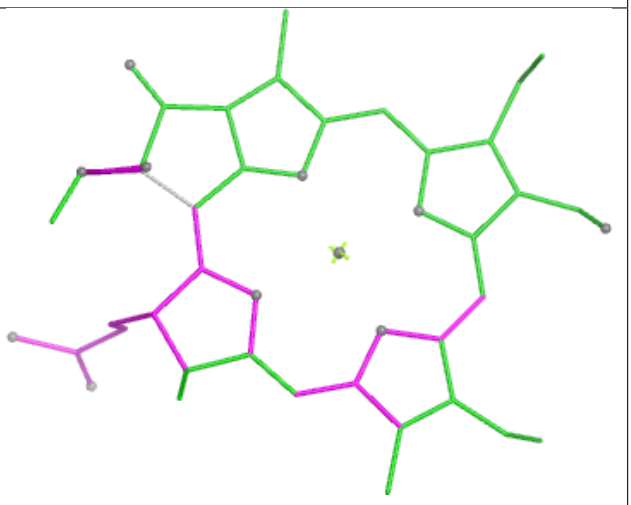


Rings

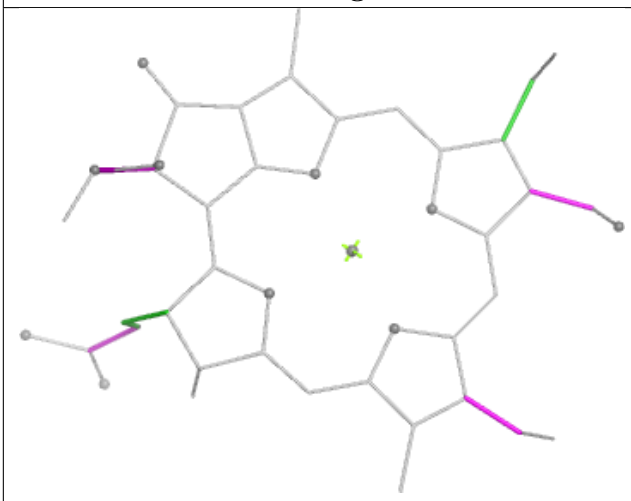
Ligand CHL s 307



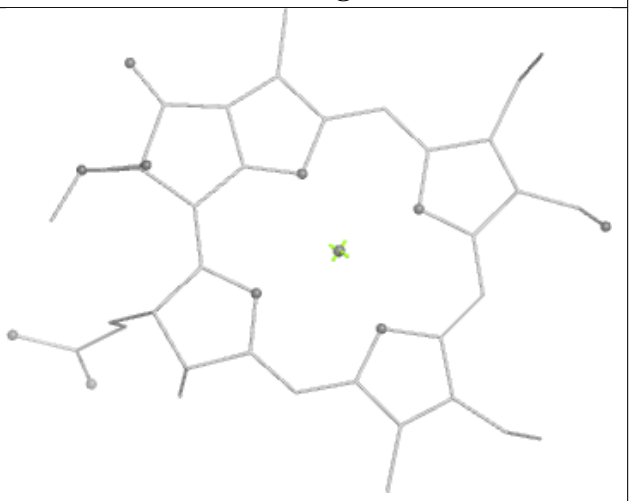
Bond lengths



Bond angles

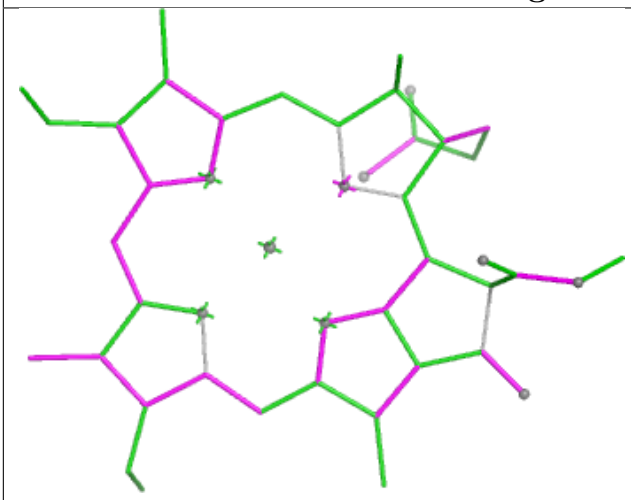


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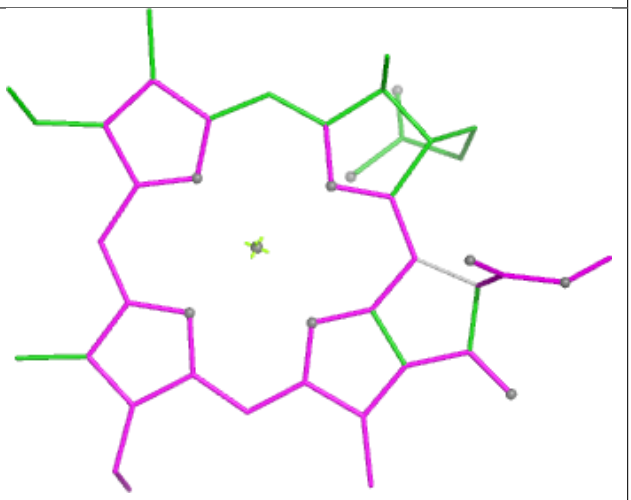


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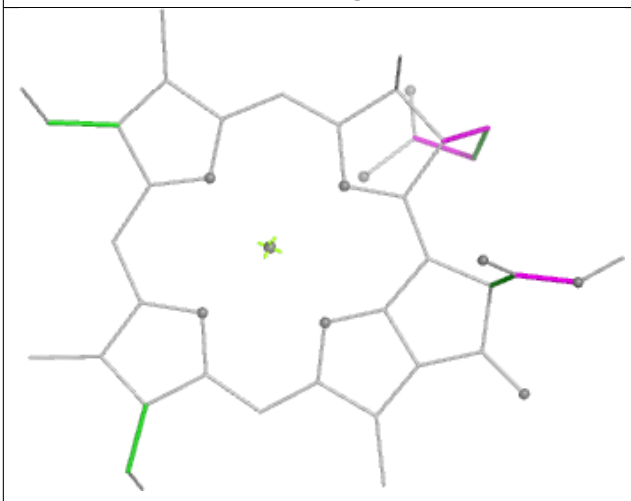
Ligand CLA 6 613



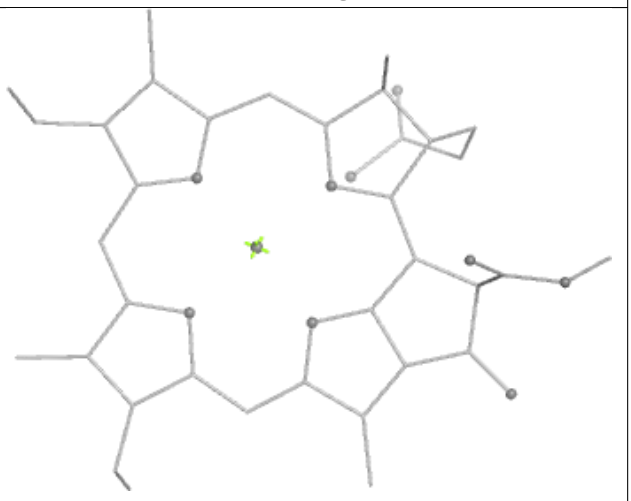
Bond lengths



Bond angles

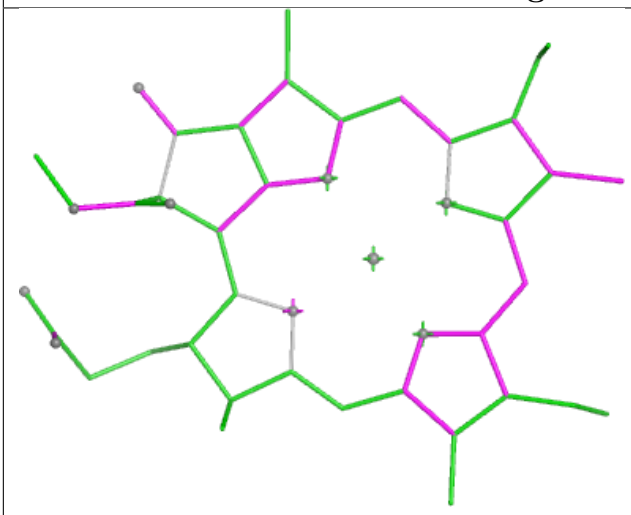


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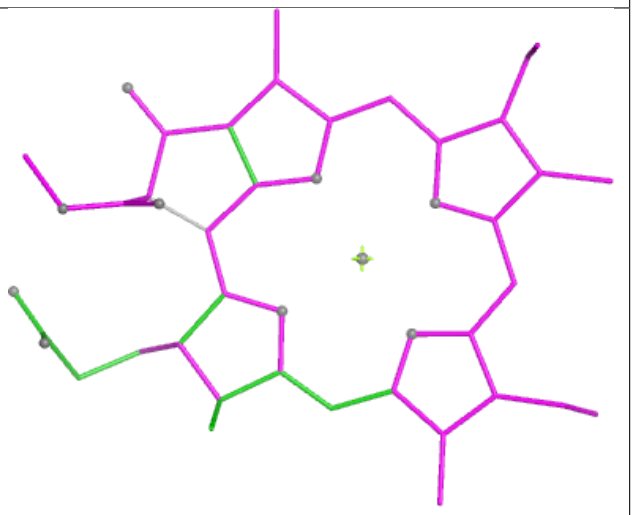


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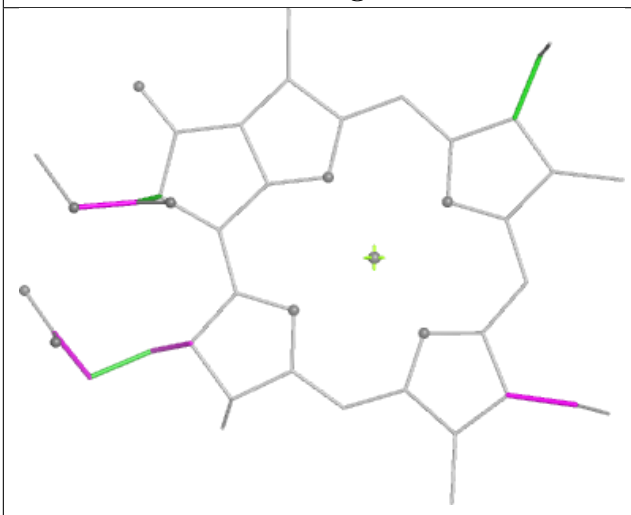
Ligand CLA S 312



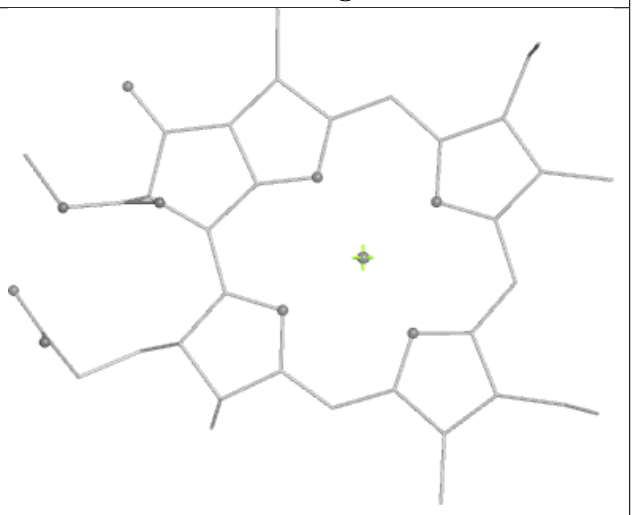
Bond lengths



Bond angles

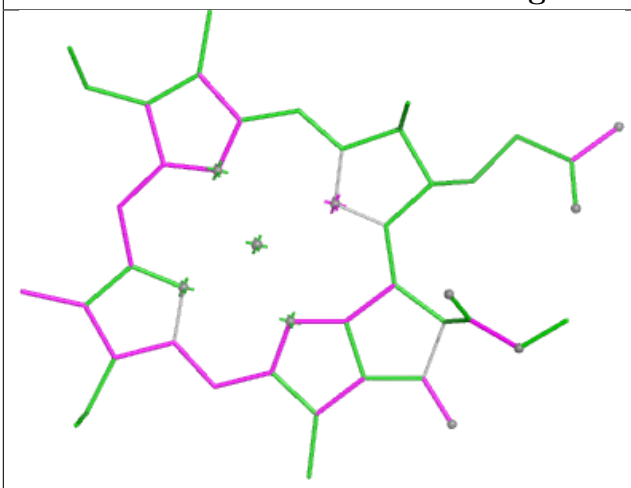


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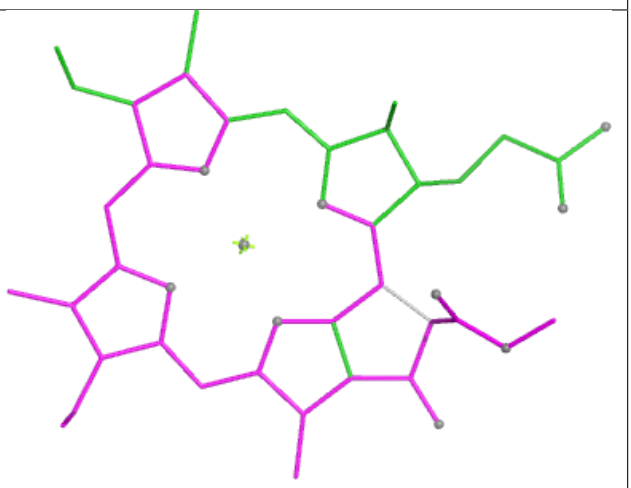


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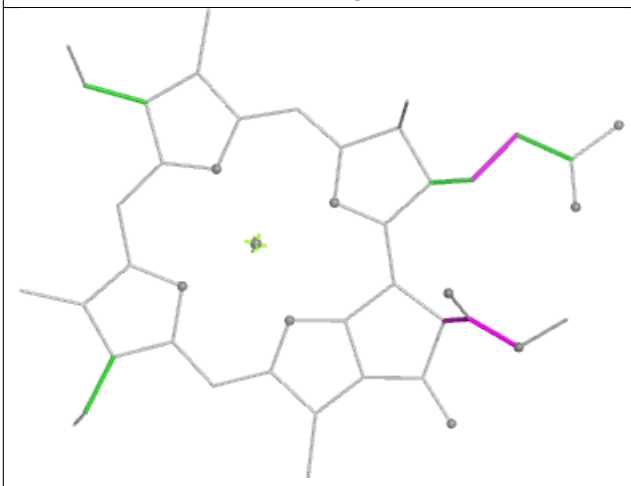
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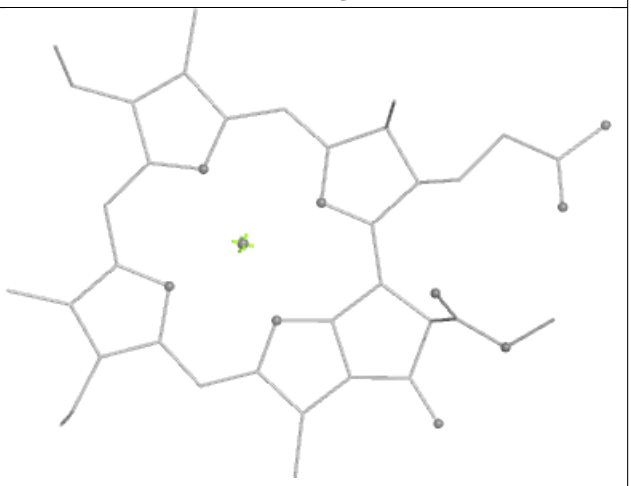
Bond lengths



Bond angles

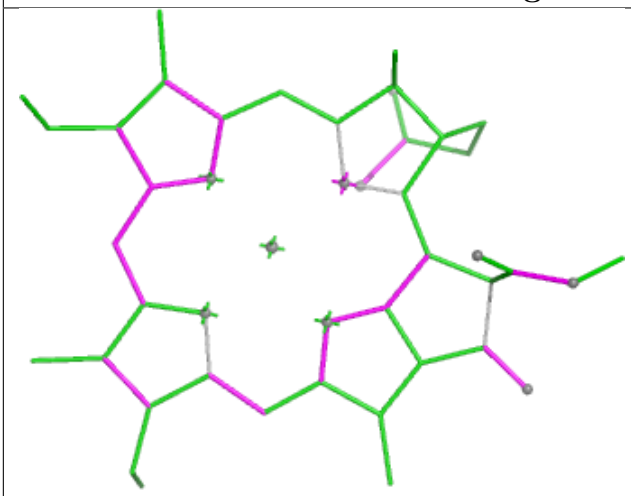


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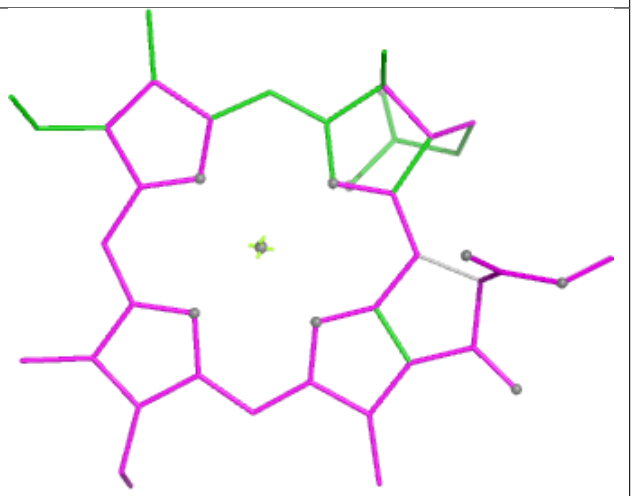


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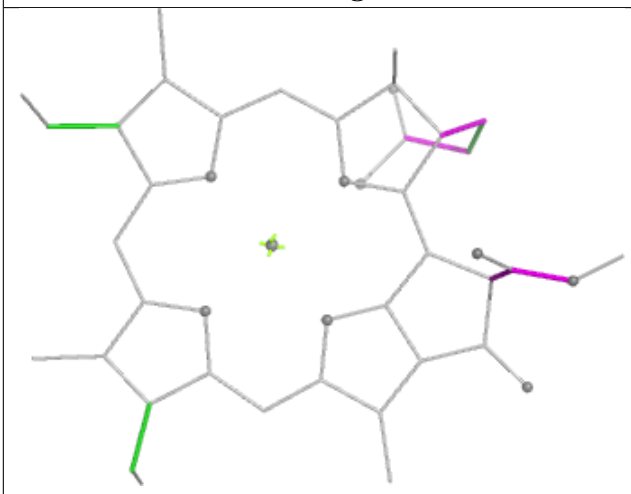
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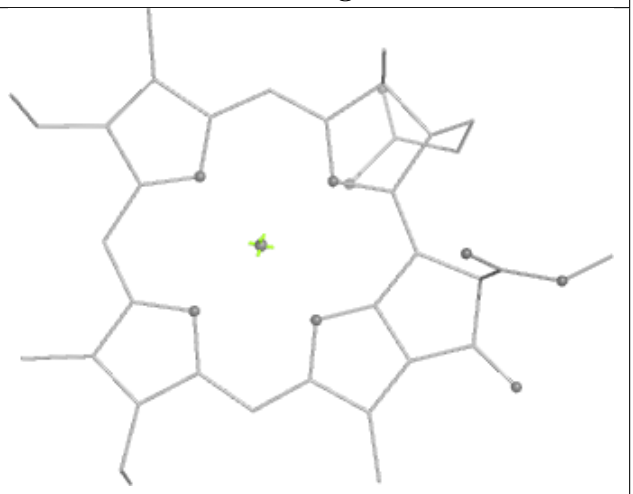
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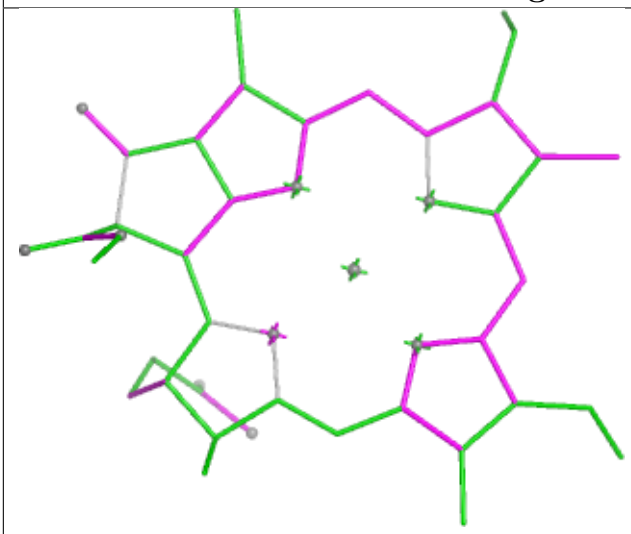


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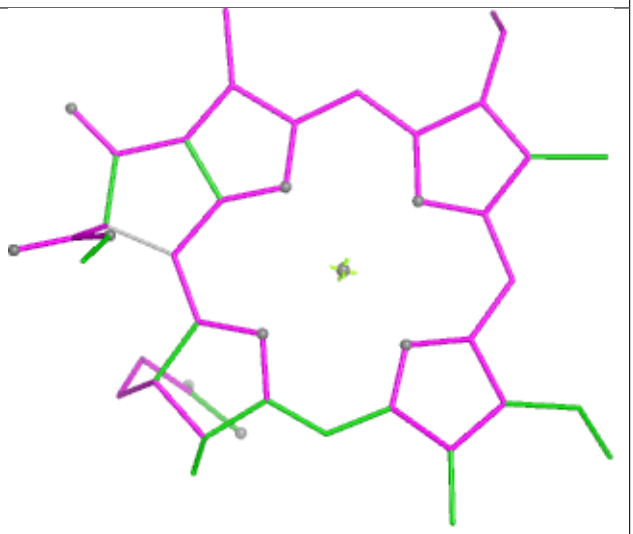


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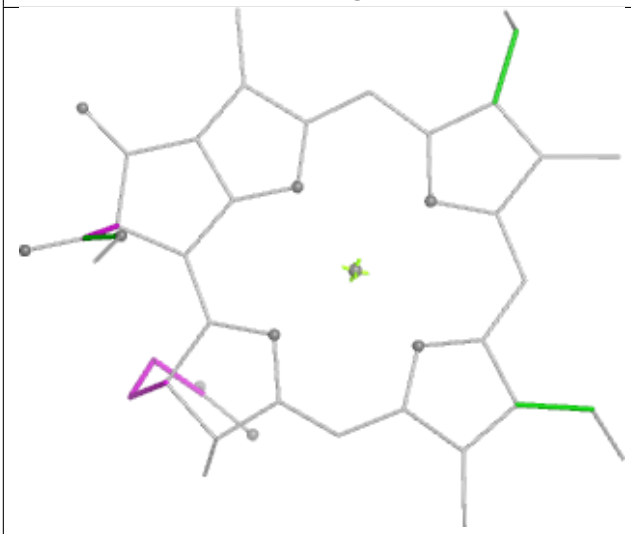
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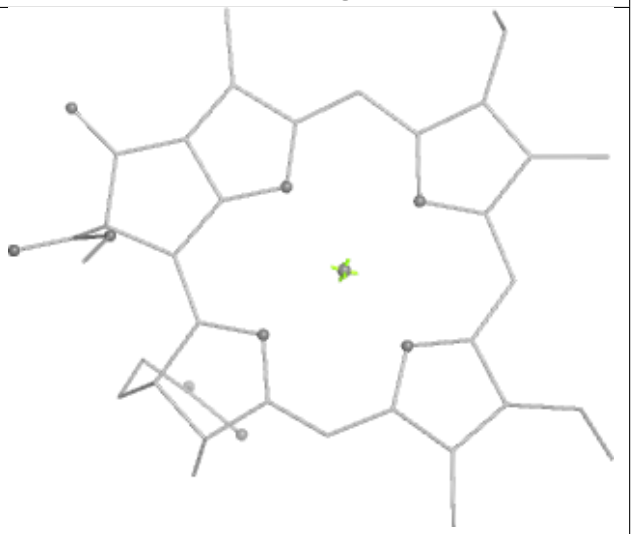
Bond lengths



Bond angles

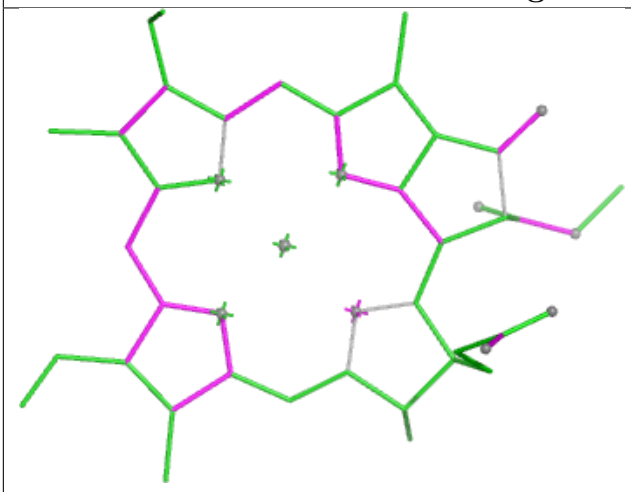


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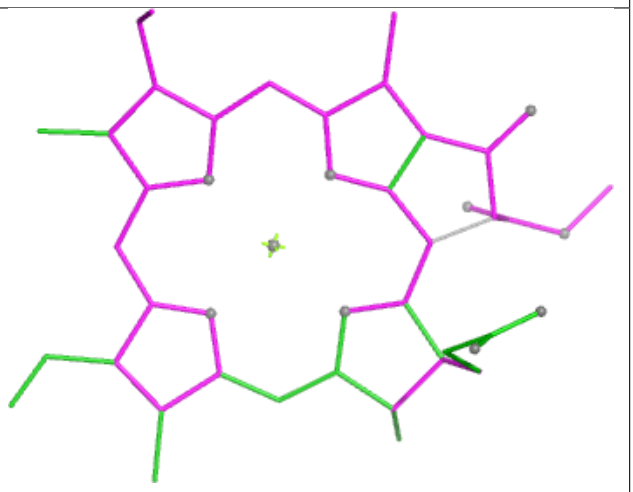


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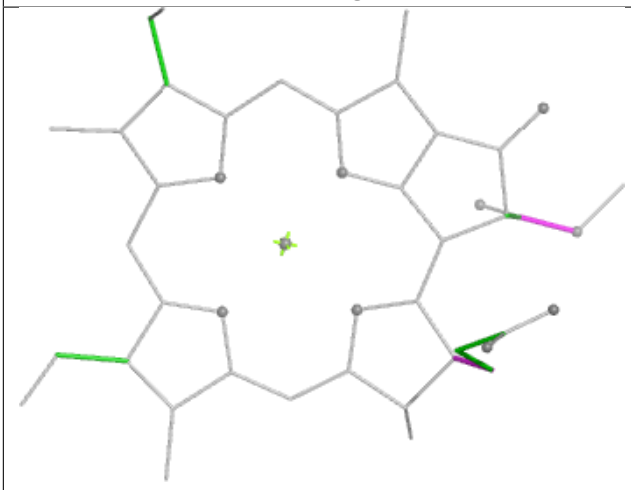
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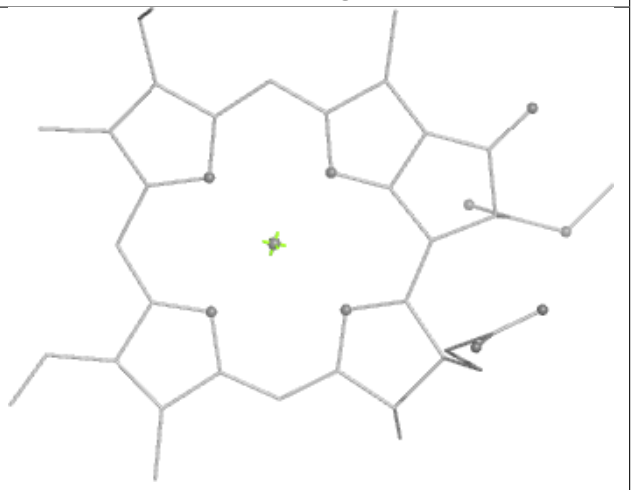
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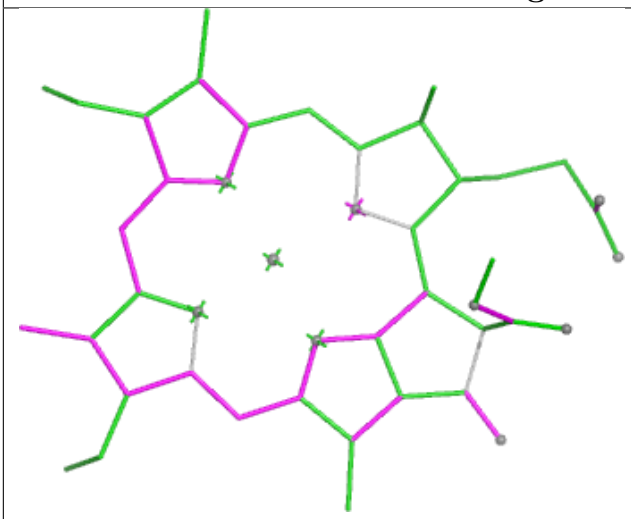


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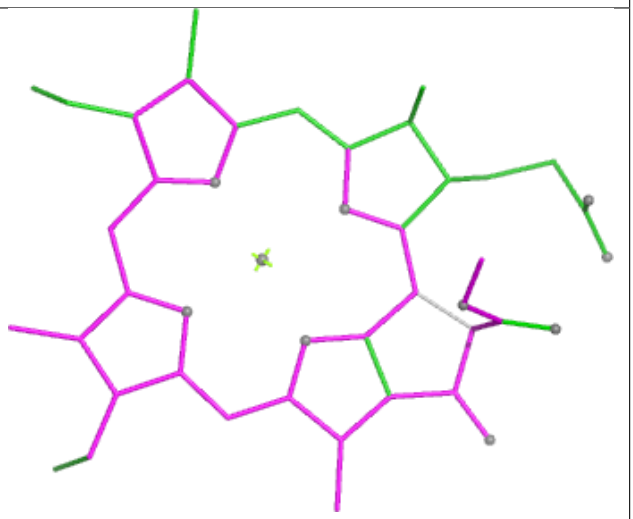


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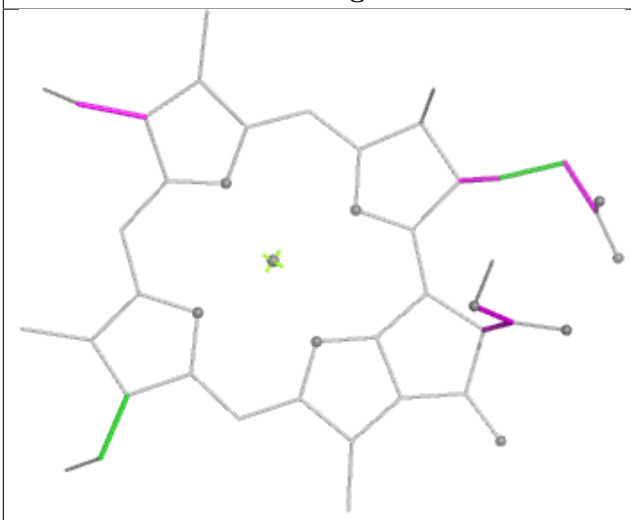
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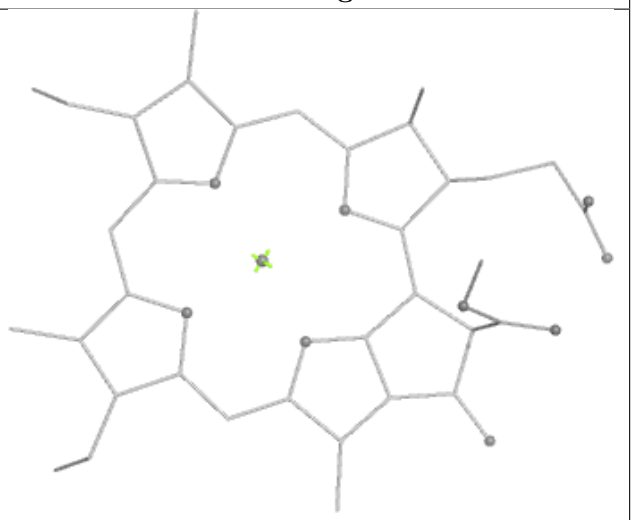
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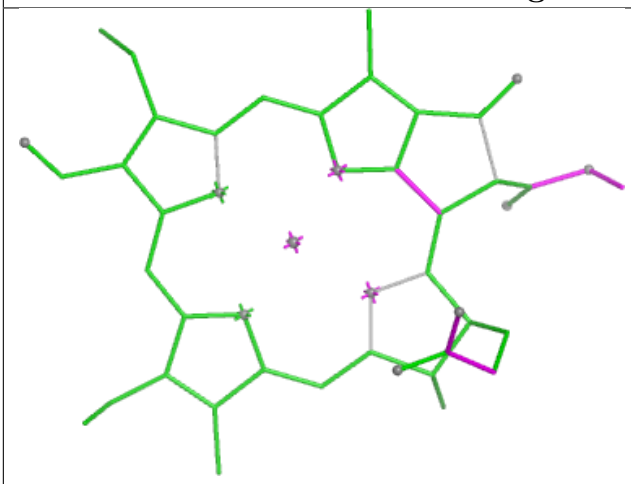


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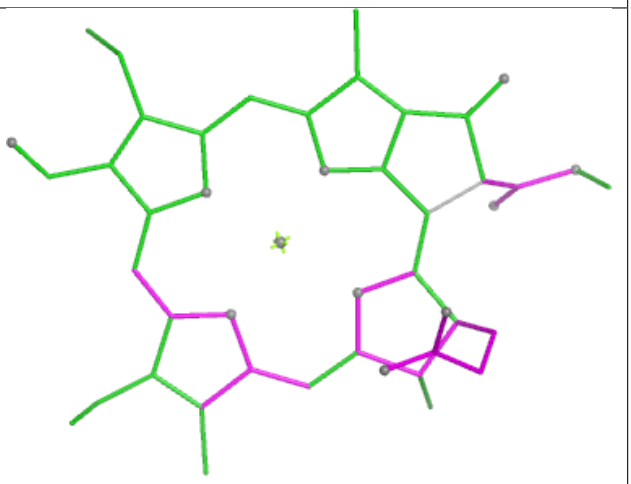


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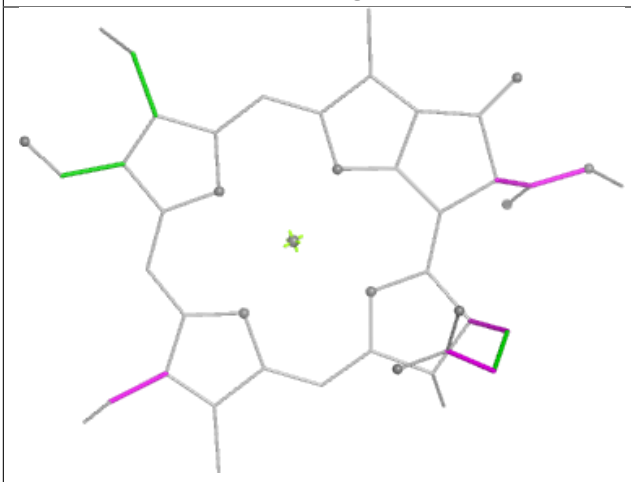
Ligand CHL 2 606



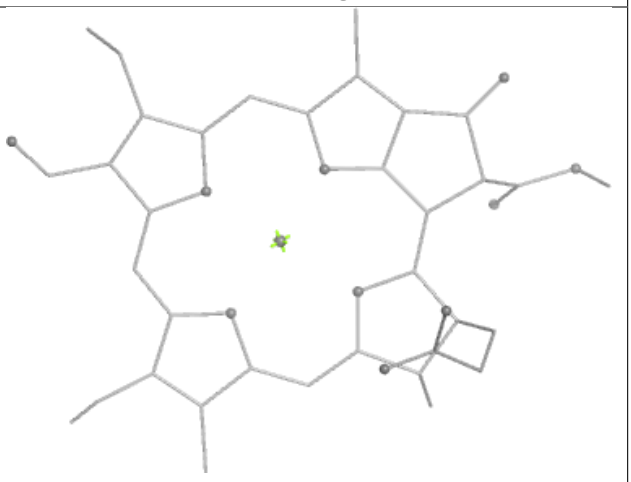
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Bond angles

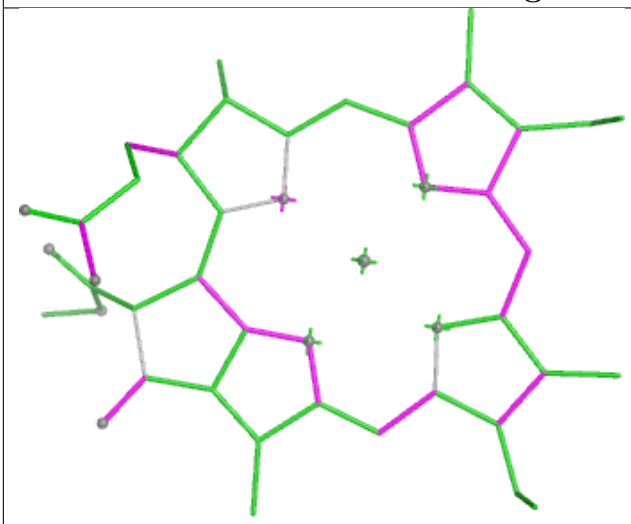


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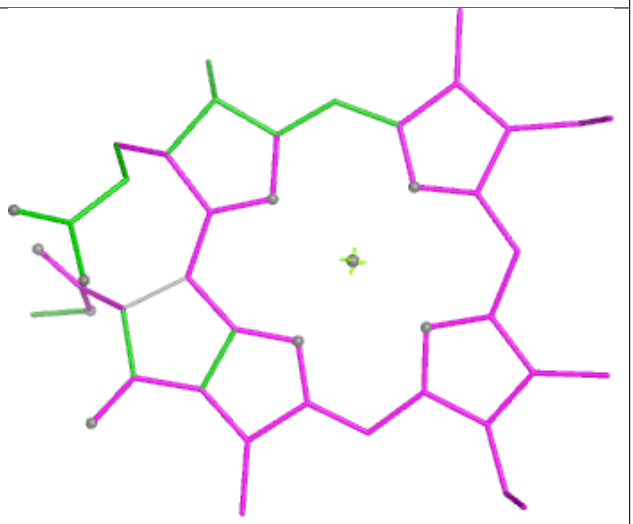


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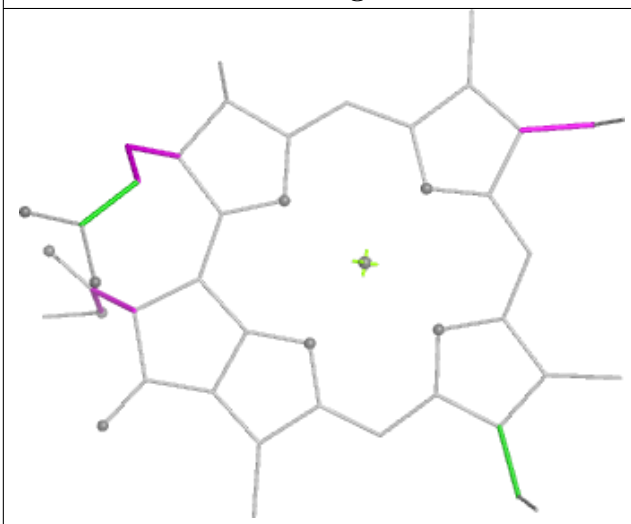
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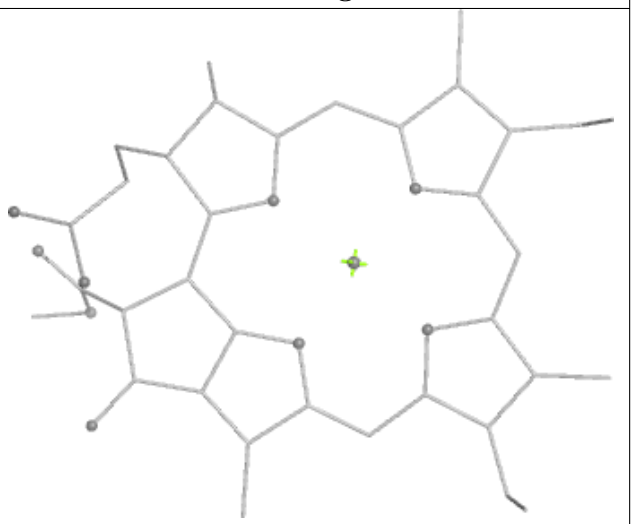
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Bond angles

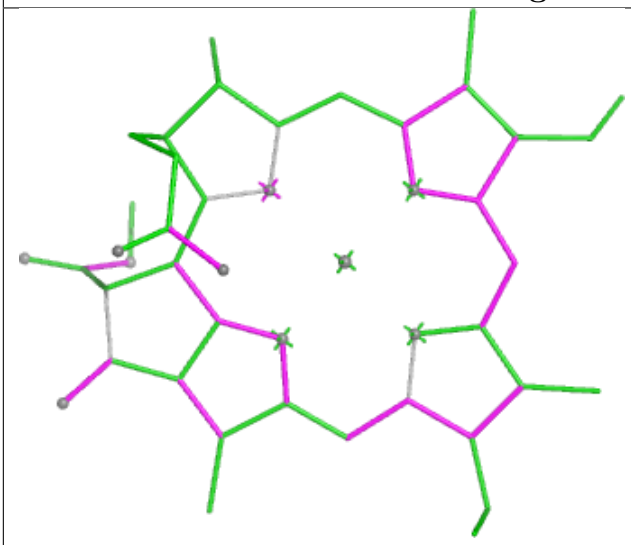


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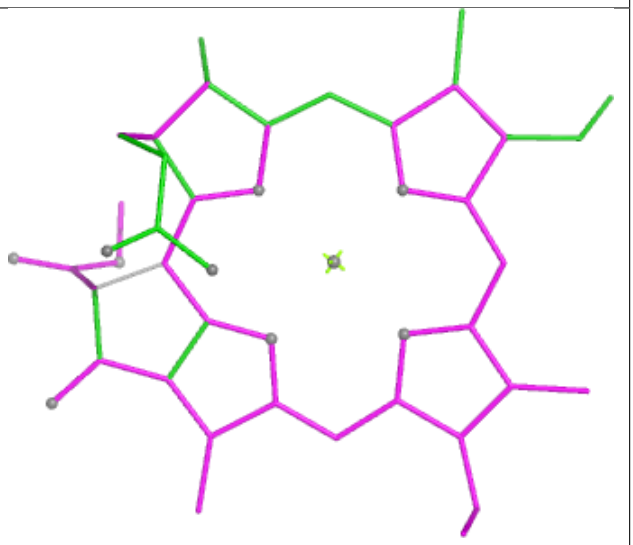


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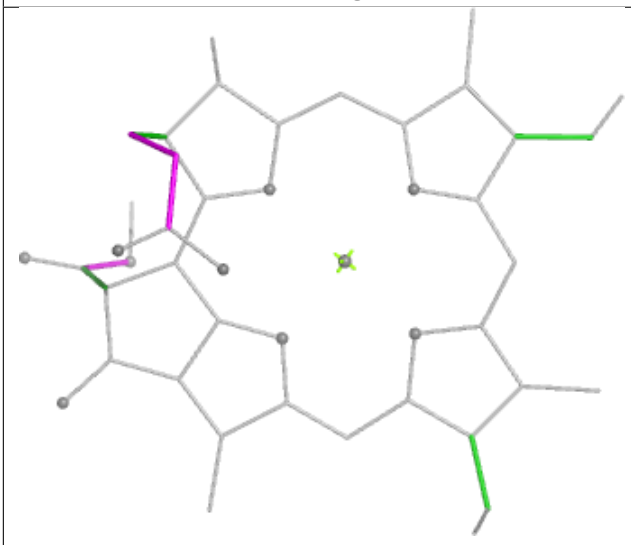
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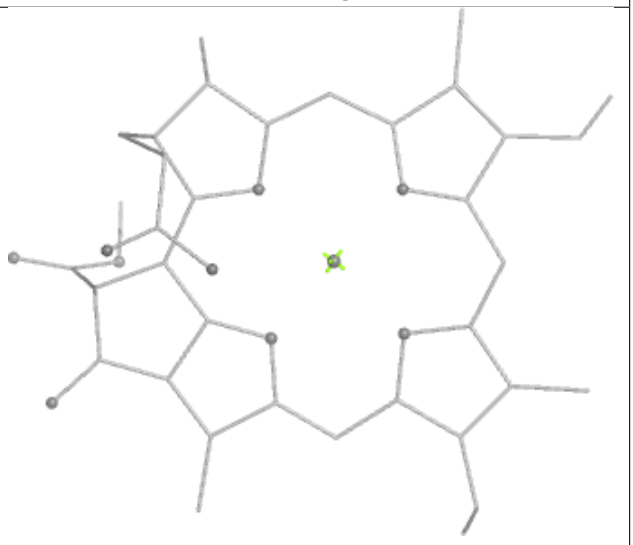
Bond lengths



Bond angles

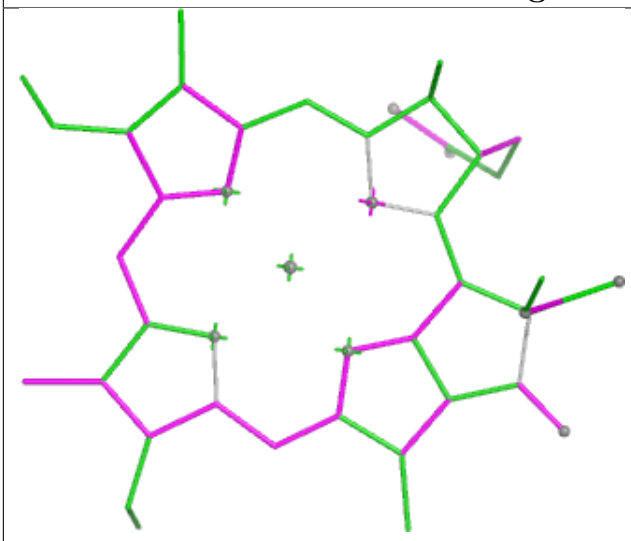


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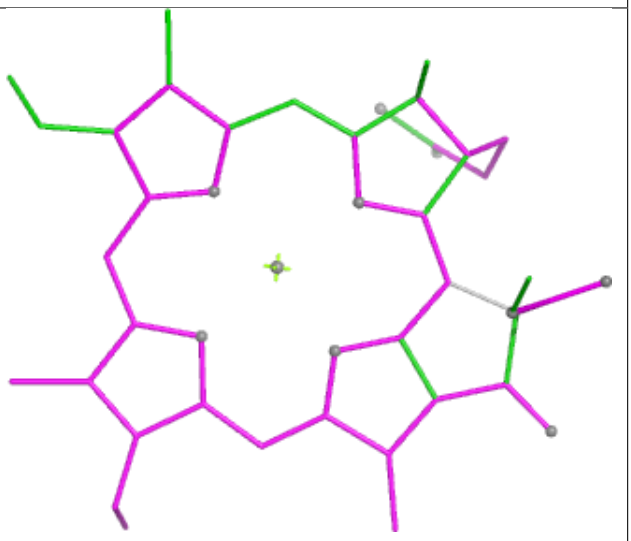


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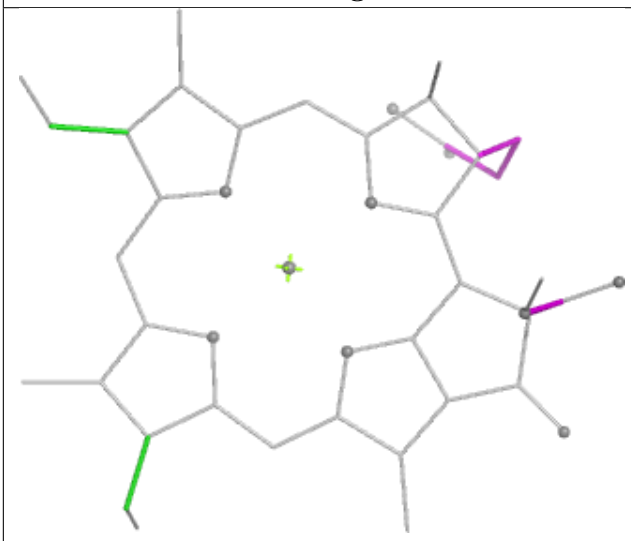
Ligand CLA 2 604



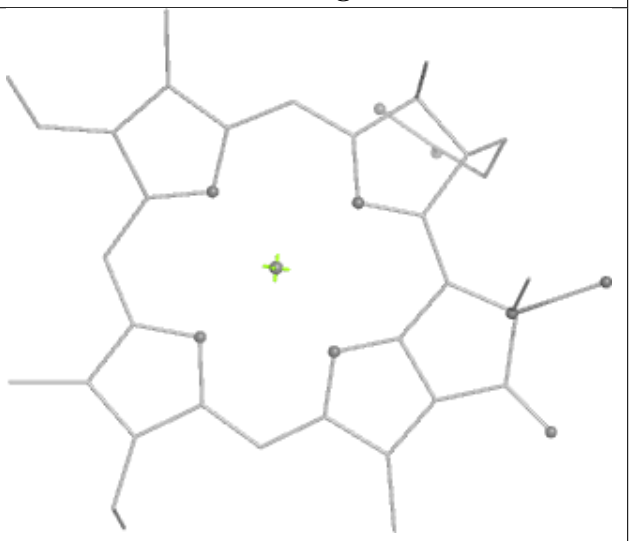
Bond lengths



Bond angles

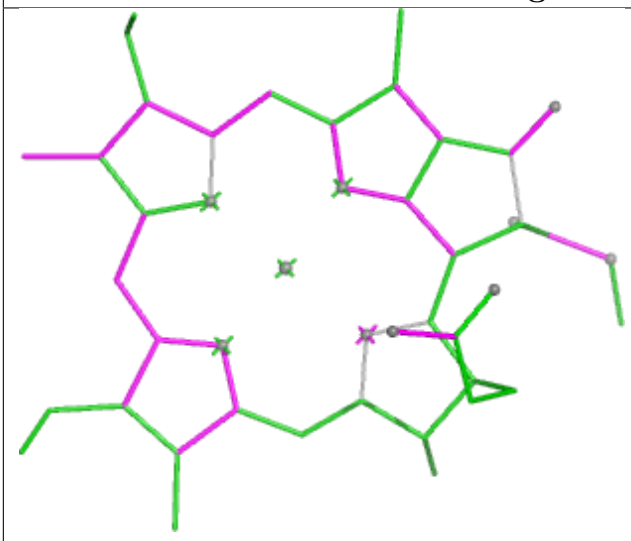


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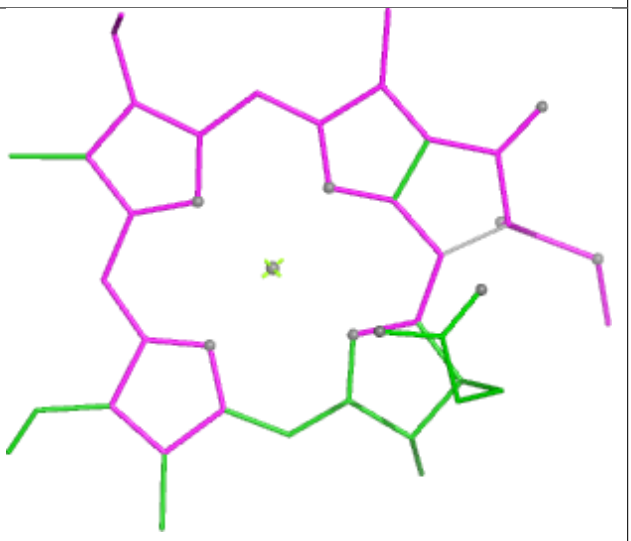


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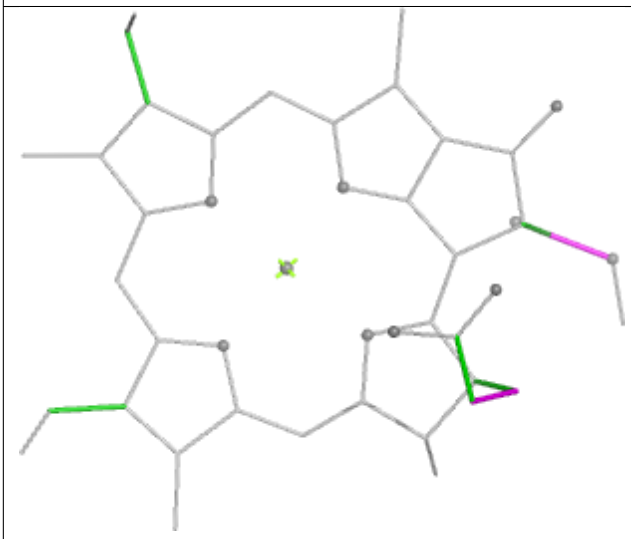
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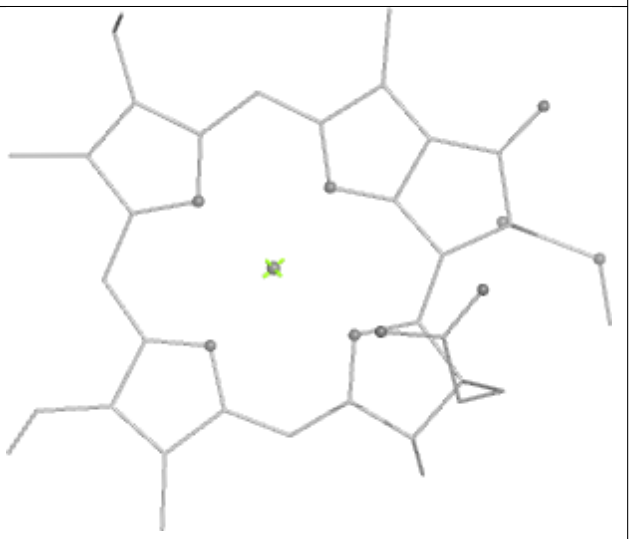
Bond lengths



Bond angles

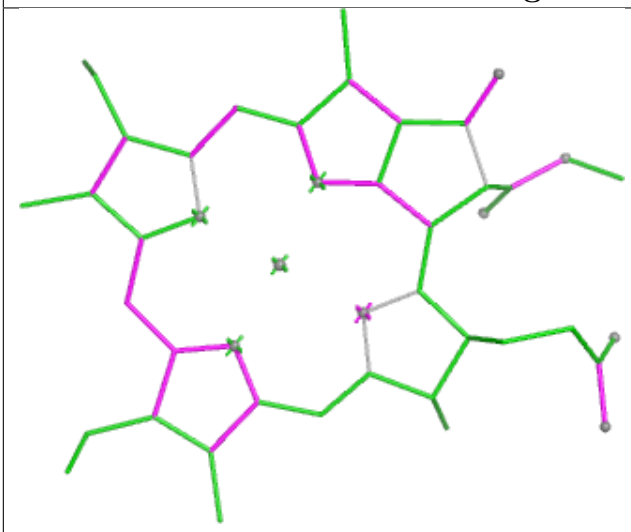


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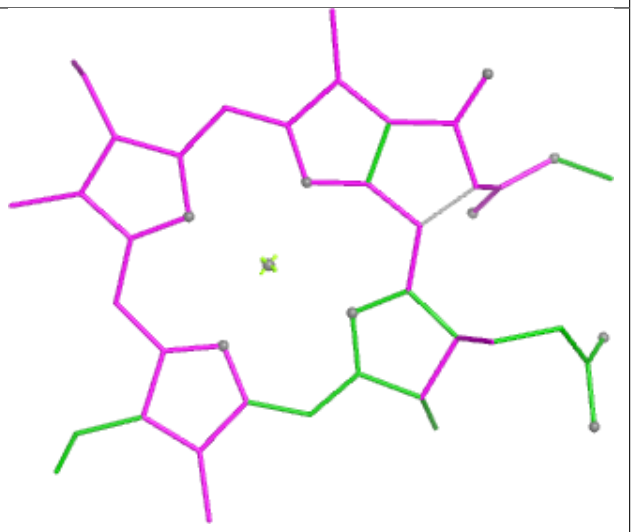


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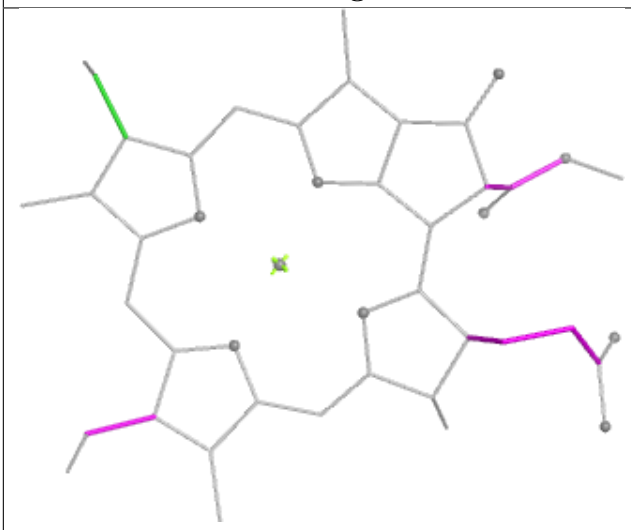
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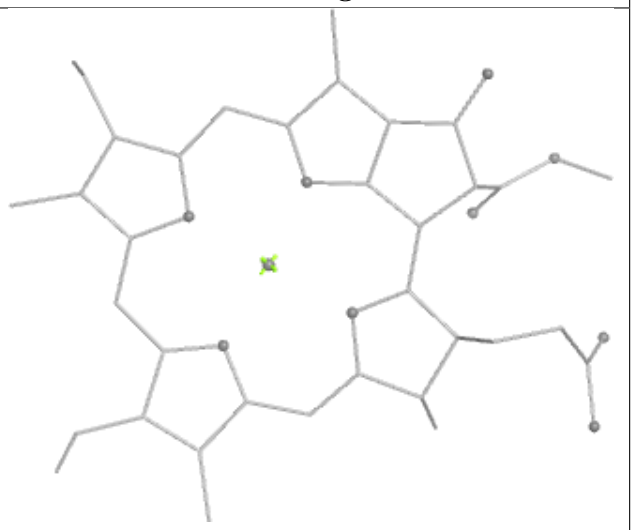
Bond lengths



Bond angles

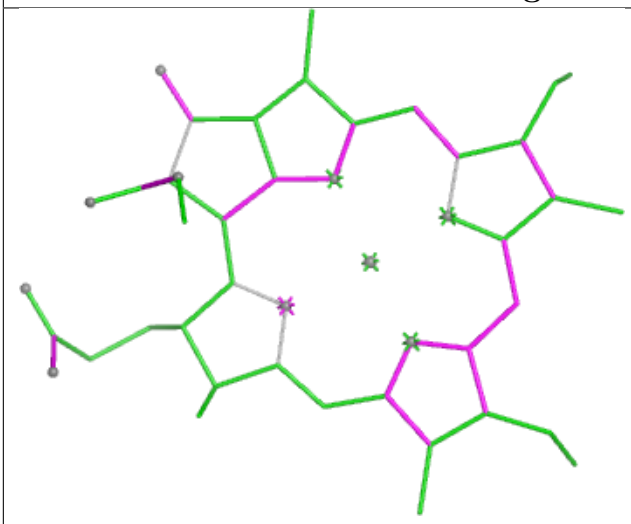


Torsions

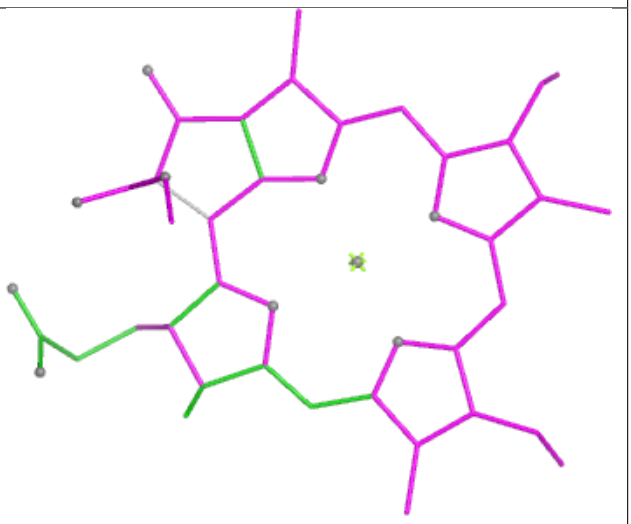


Rings

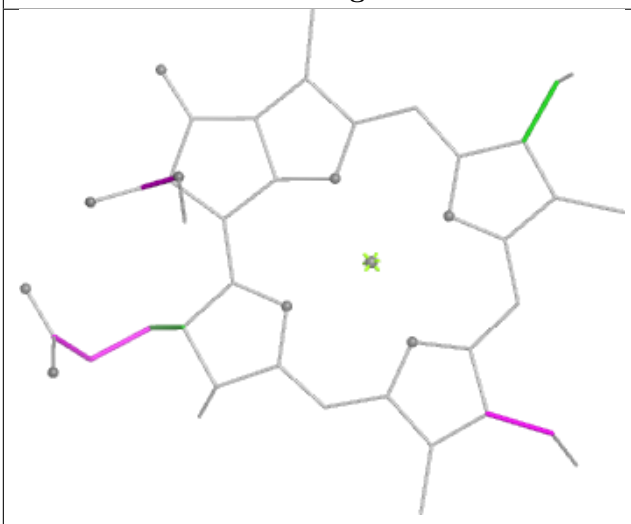
Ligand CLA N 603



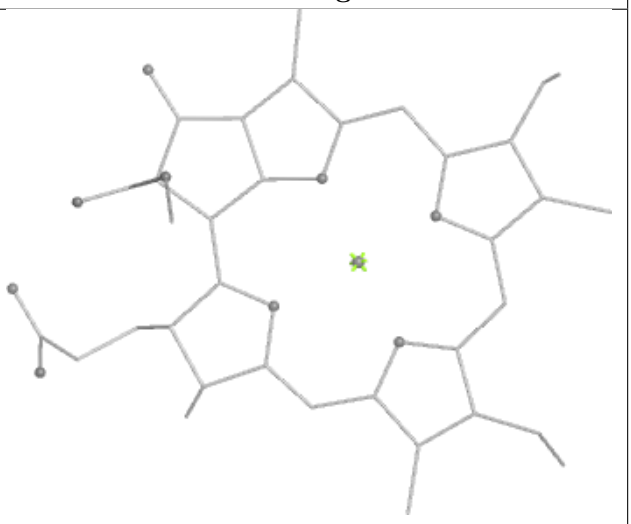
Bond lengths



Bond angles

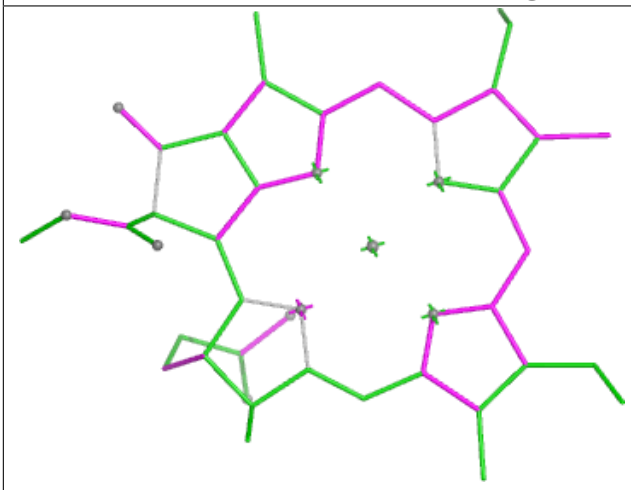


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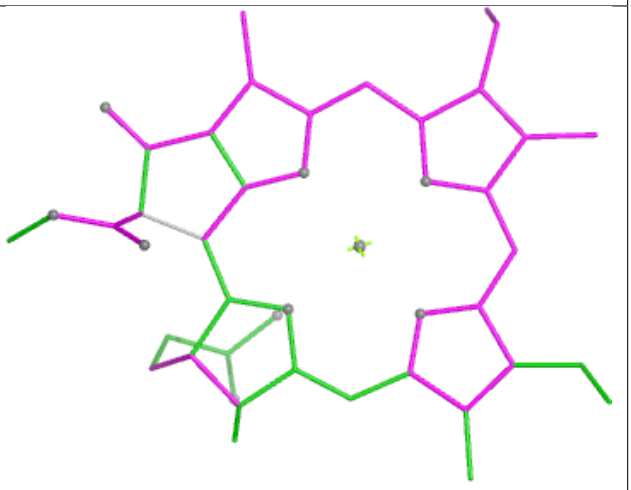


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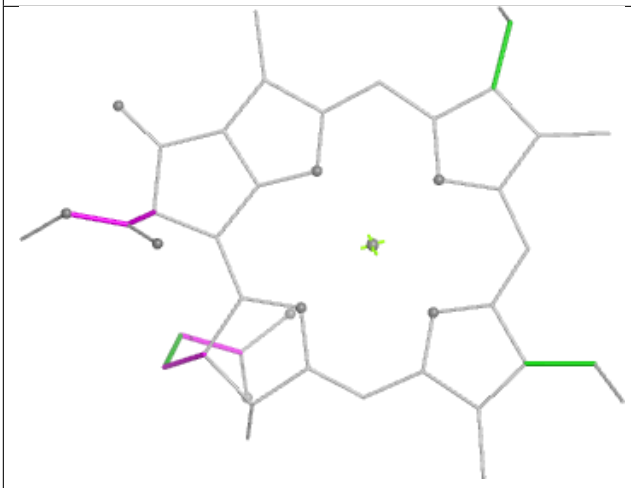
Ligand CLA N 614



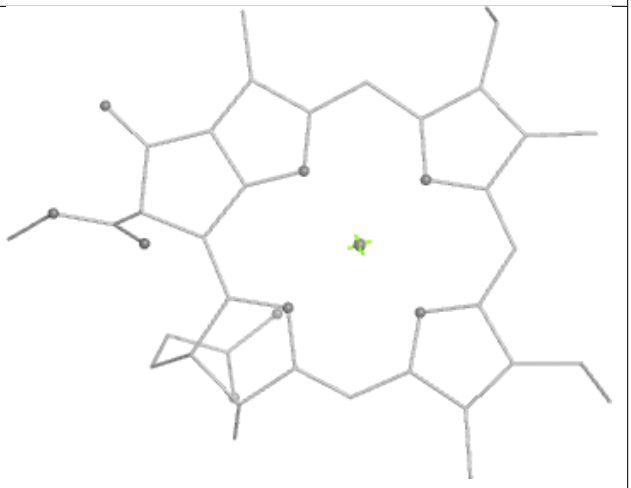
Bond lengths



Bond angles

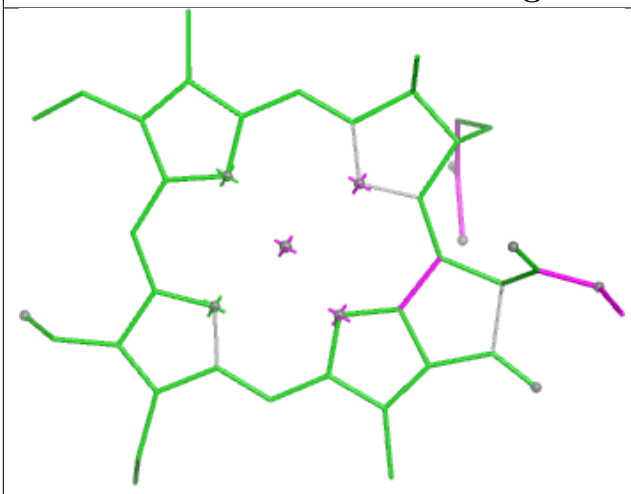


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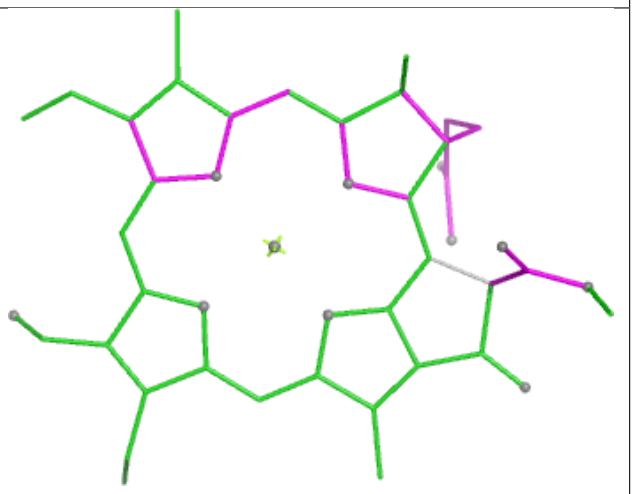


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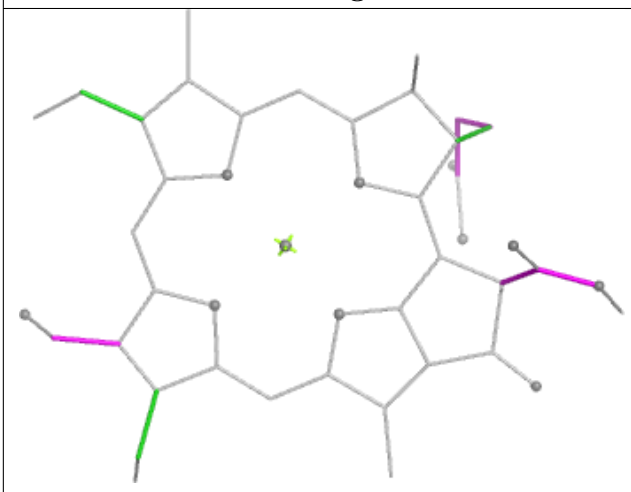
Ligand CHL Y 608



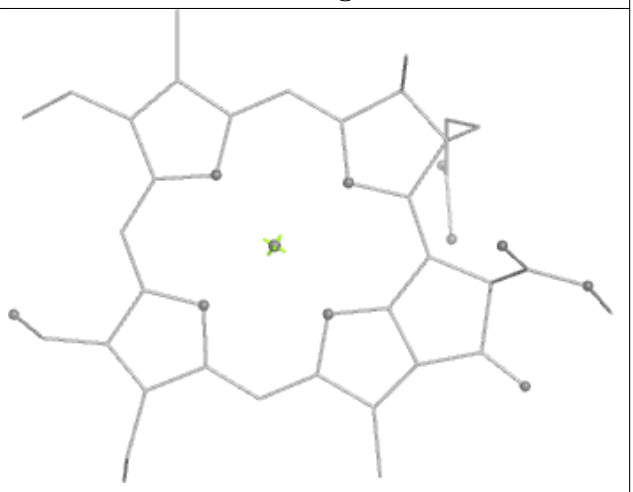
Bond lengths



Bond angles

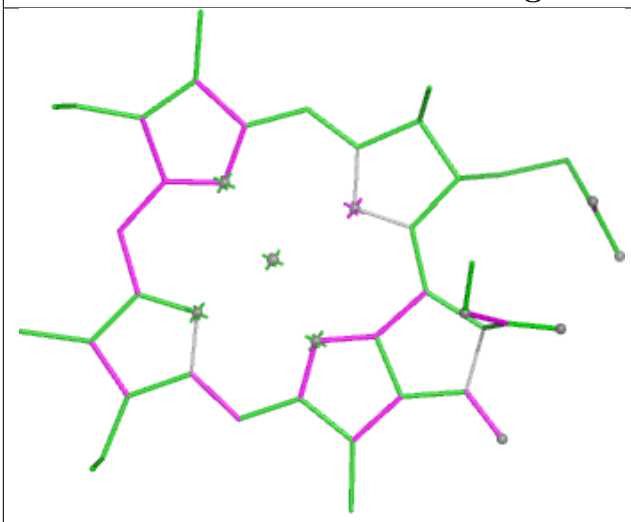


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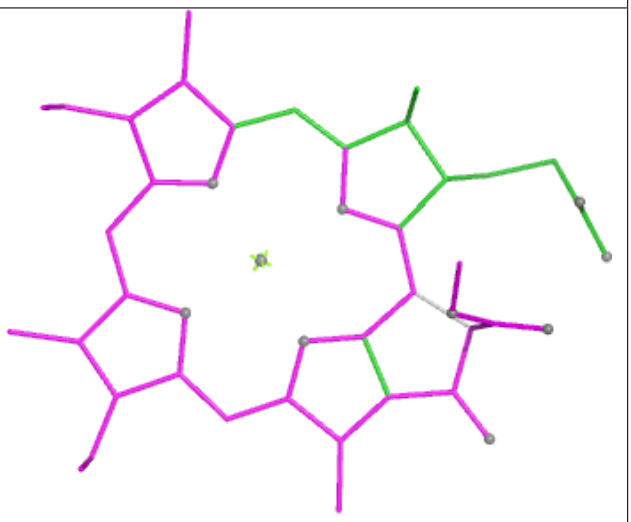


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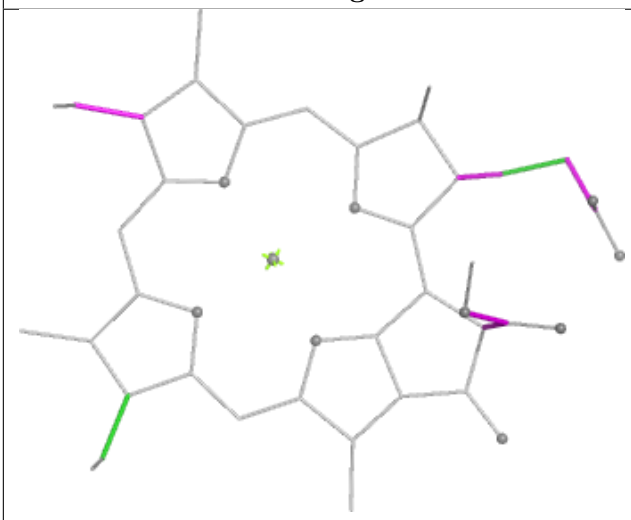
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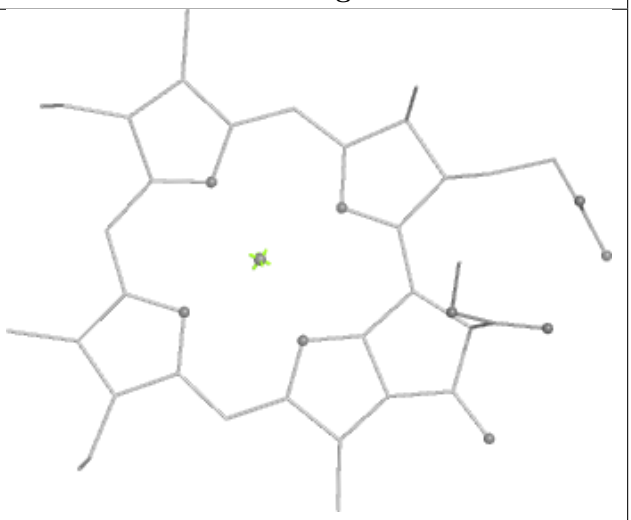
Bond lengths



Bond angles

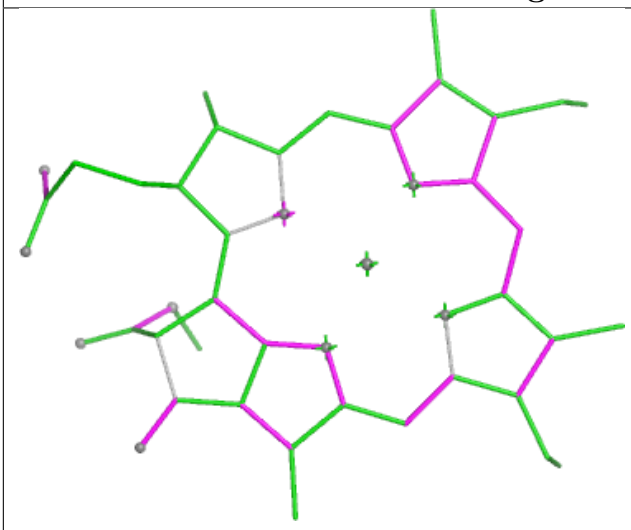


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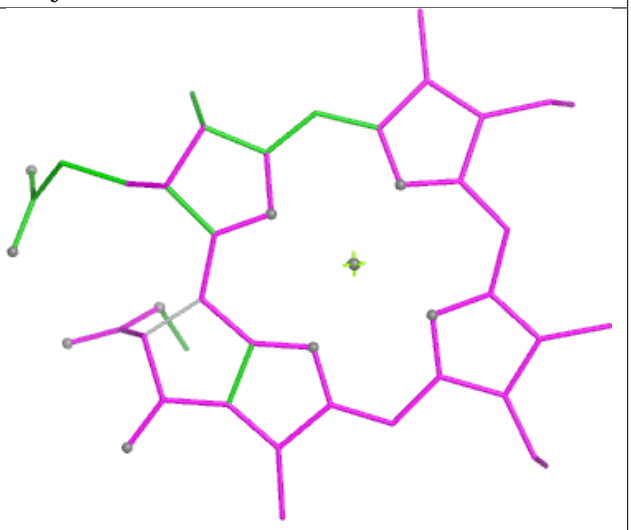


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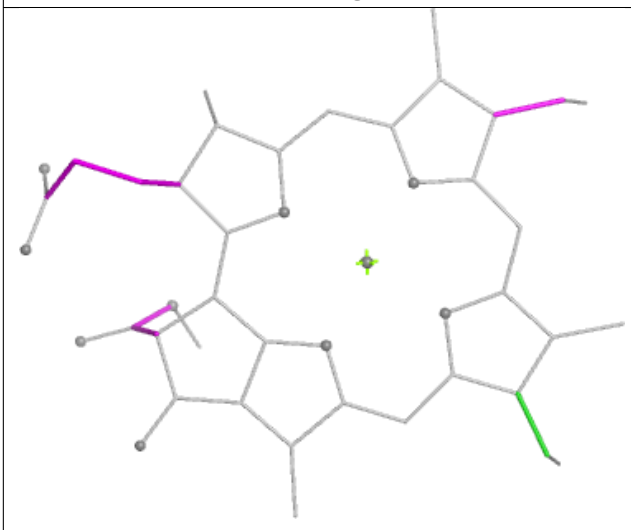
Ligand CLA y 612



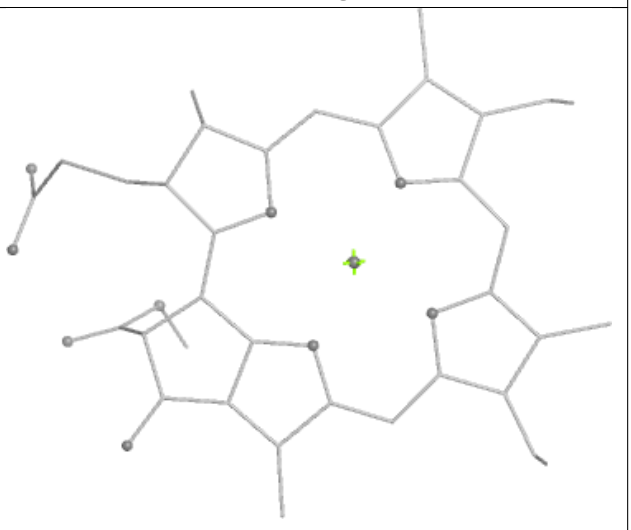
Bond lengths



Bond angles

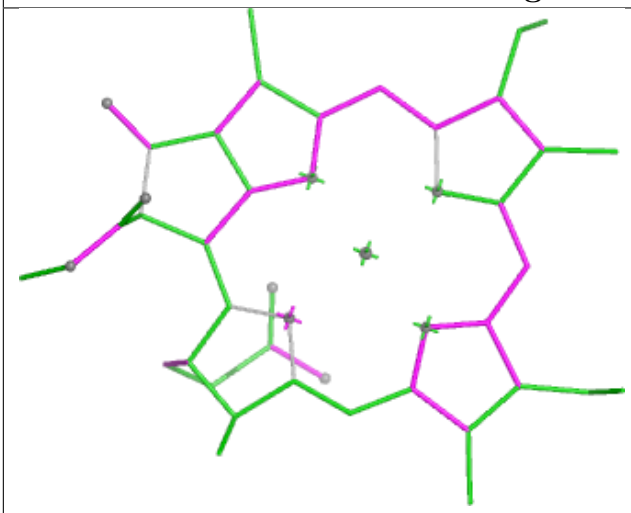


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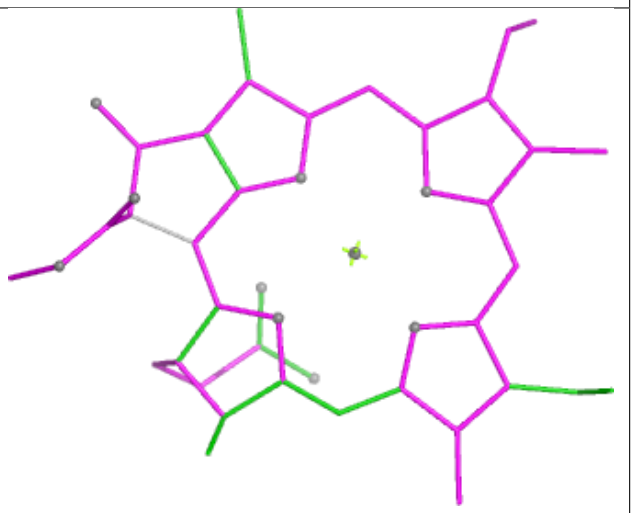


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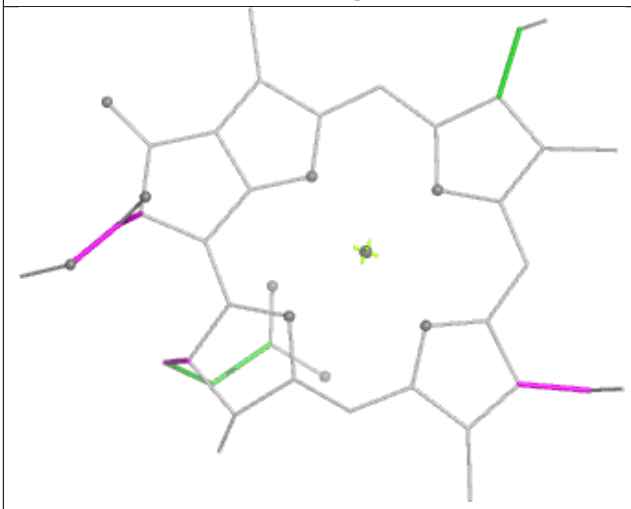
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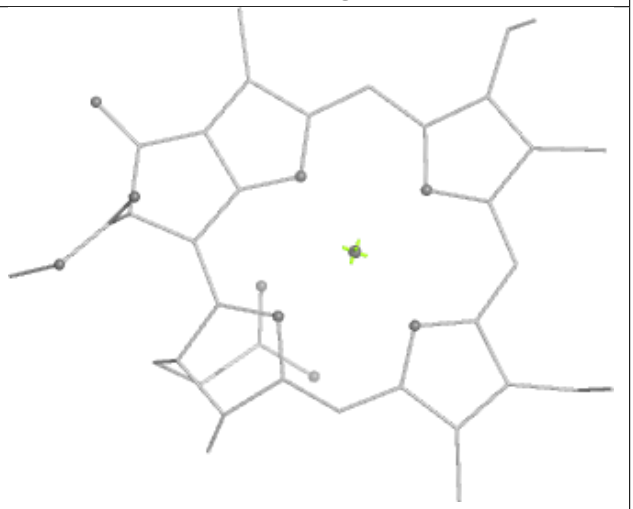
Bond lengths



Bond angles

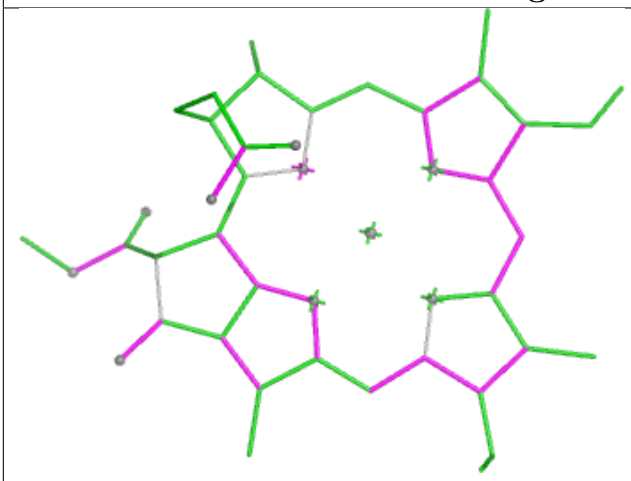


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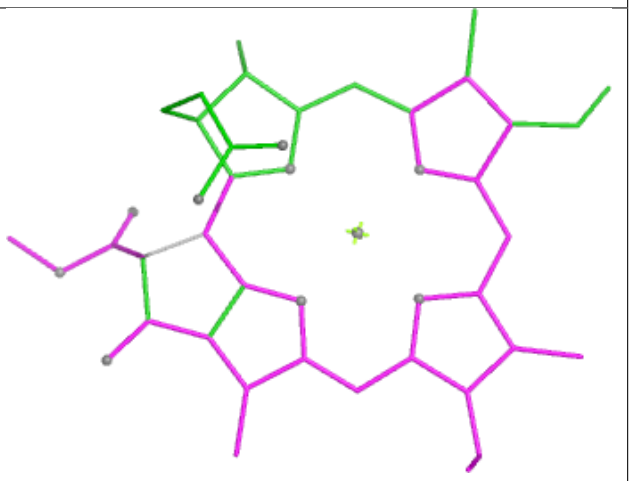


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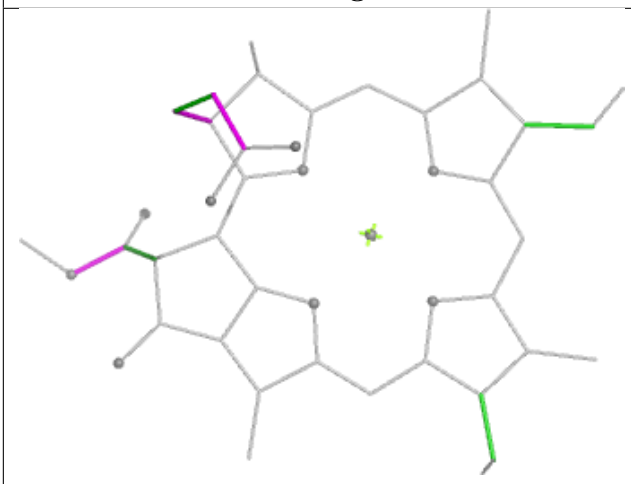
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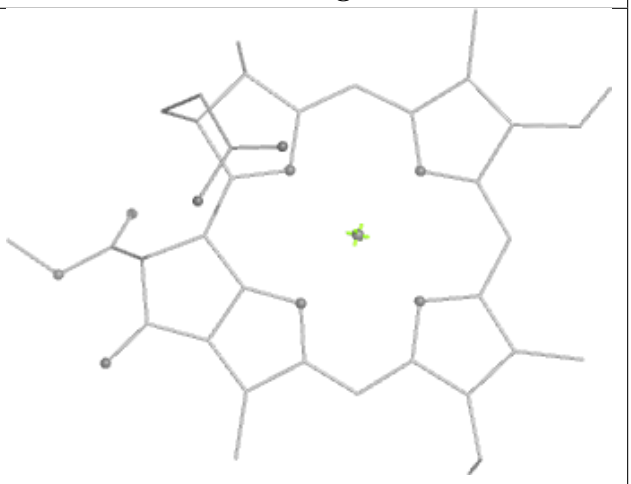
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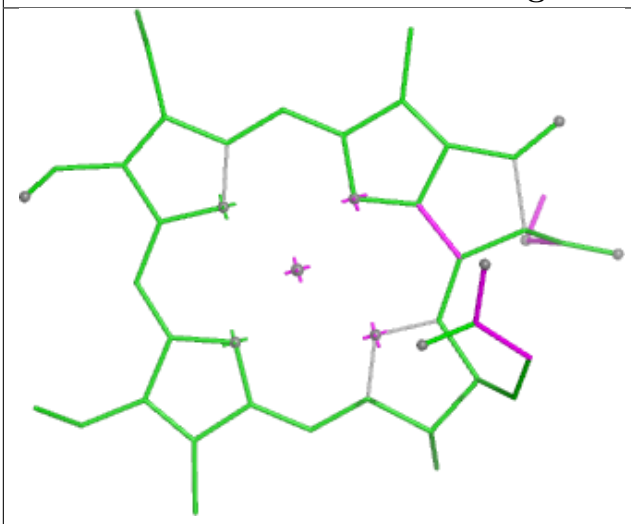


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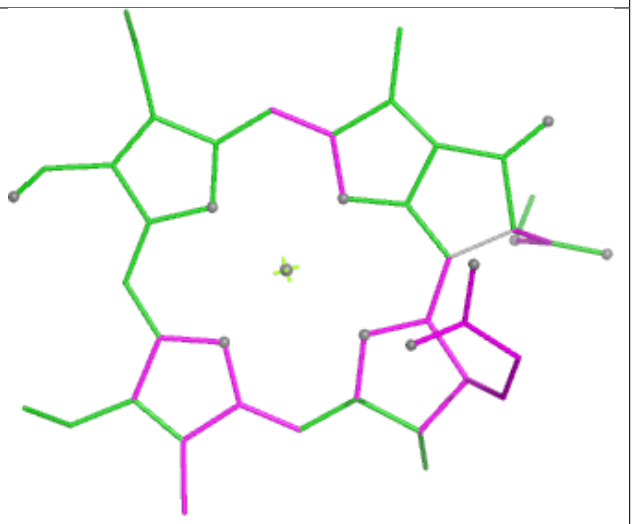


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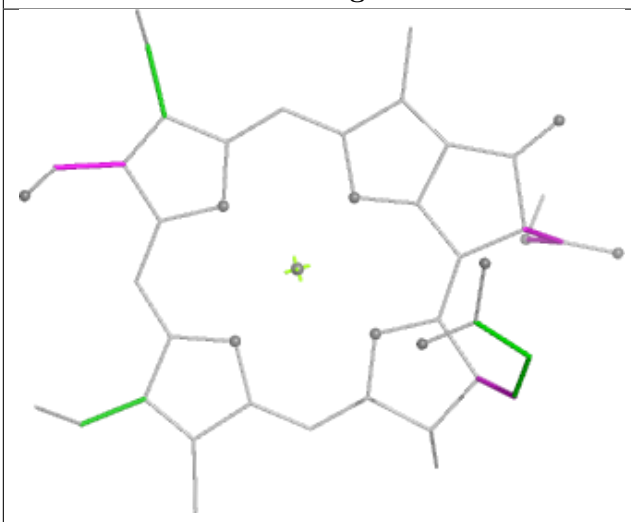
Ligand CHL 4 306



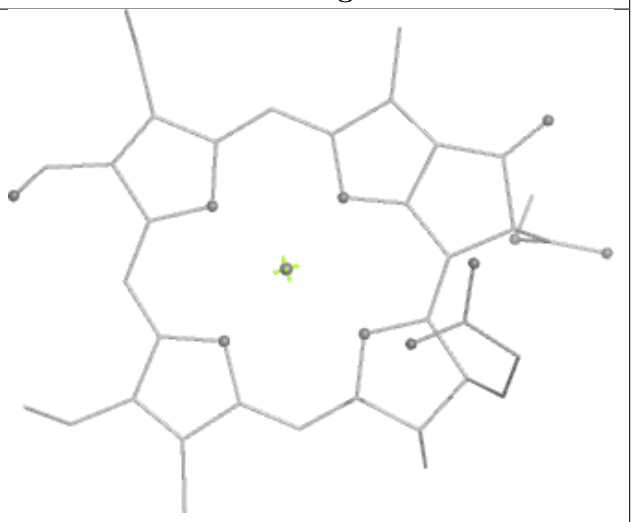
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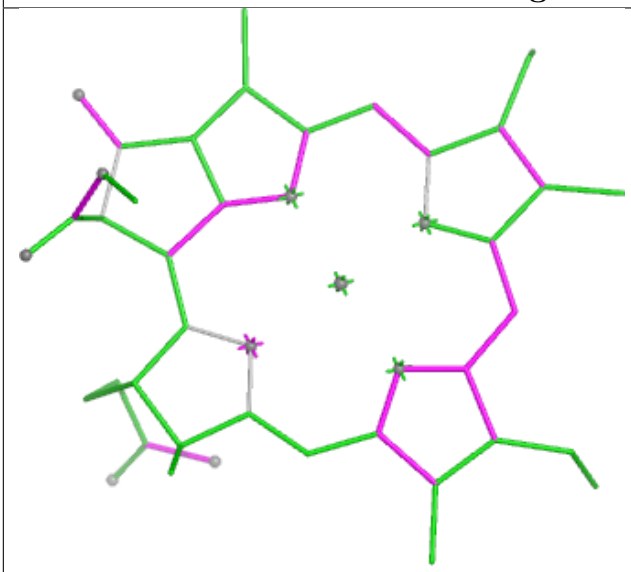


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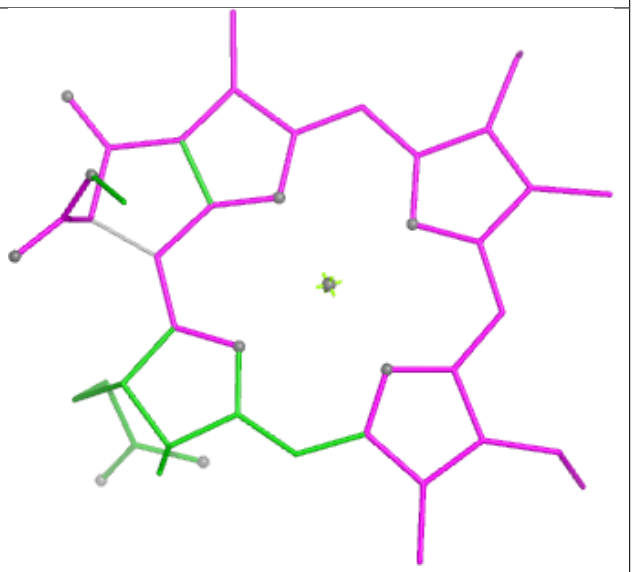


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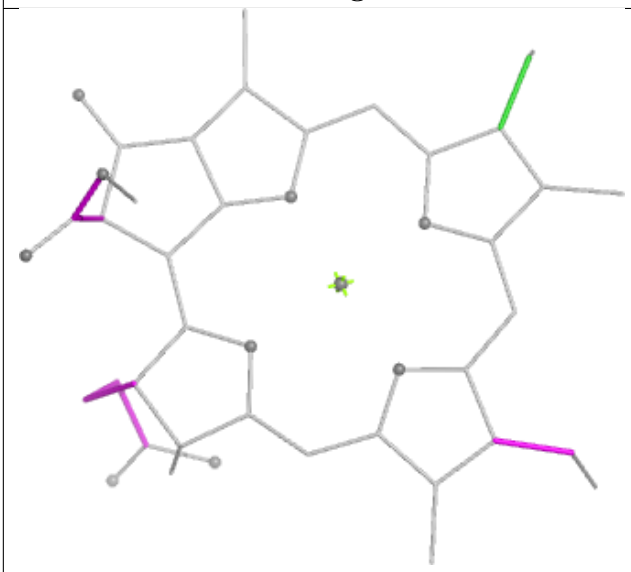
Ligand CLA c 503



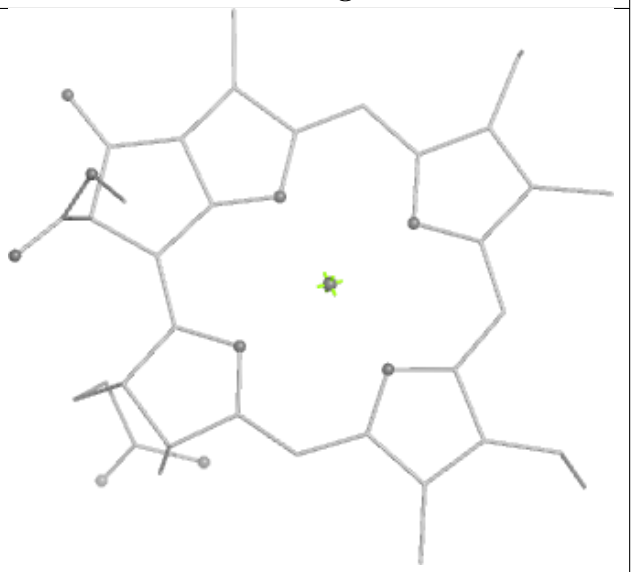
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Bond angles

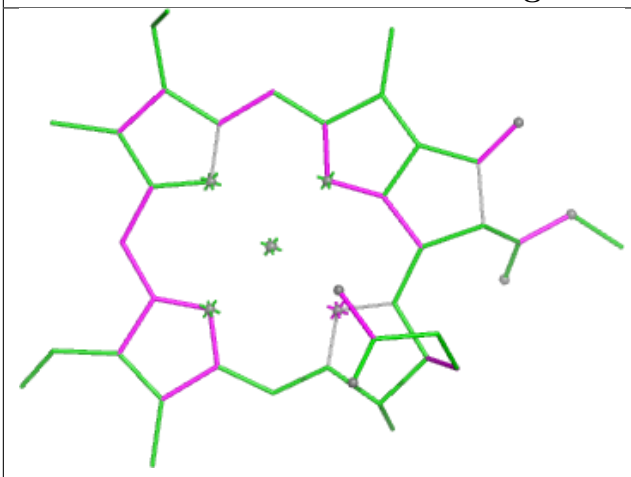


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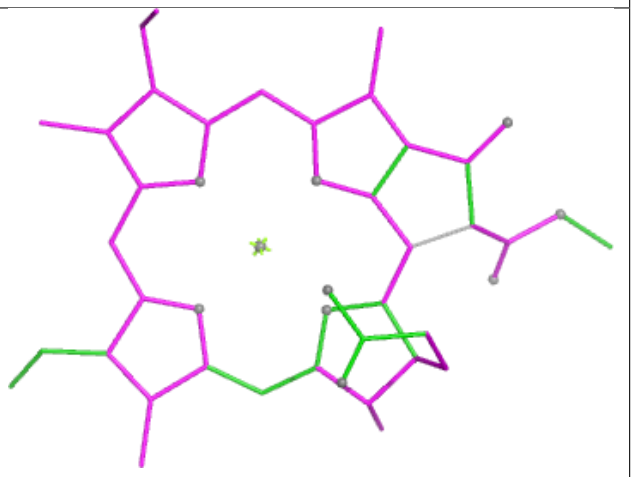


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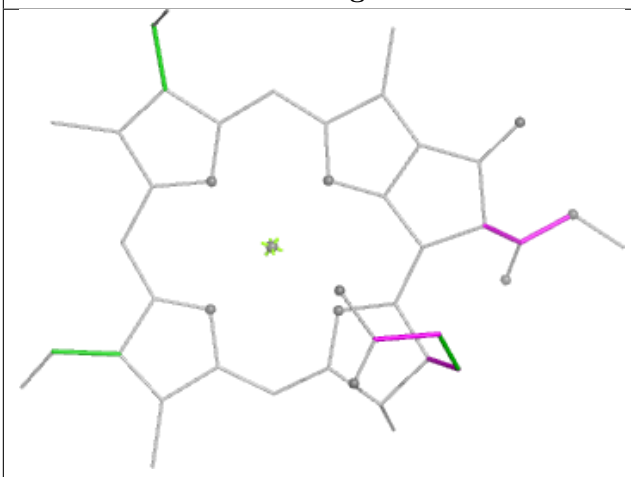
Ligand CLA R 308



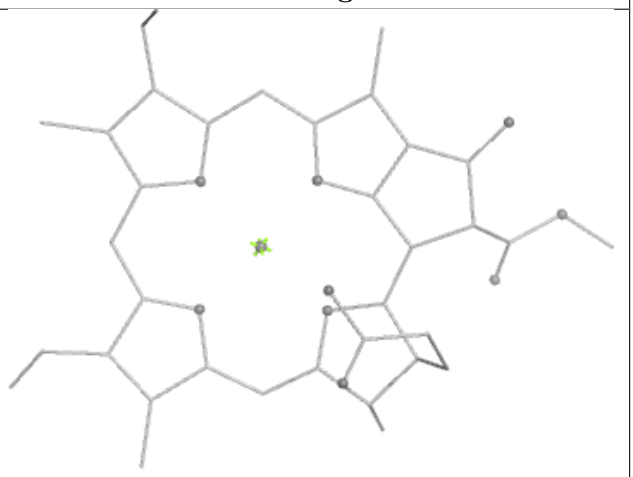
Bond lengths



Bond angles

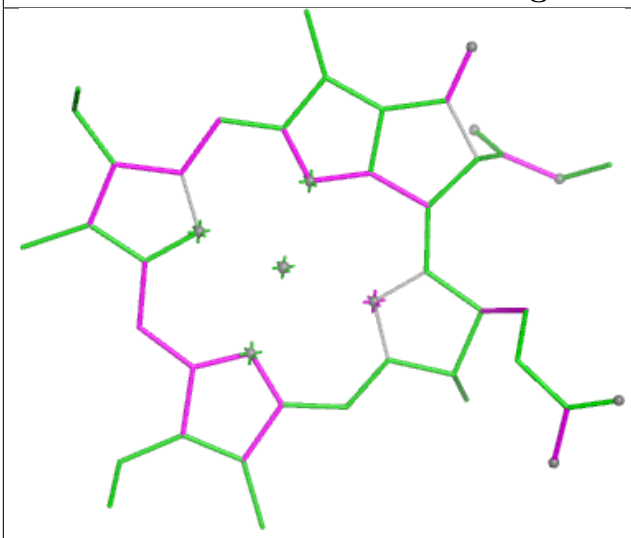


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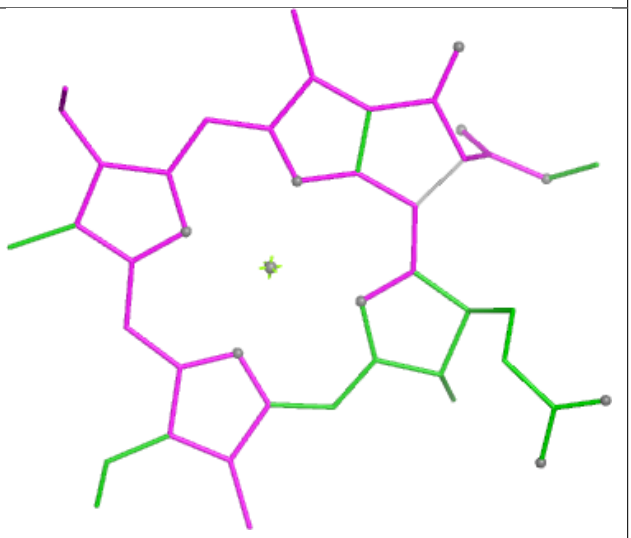


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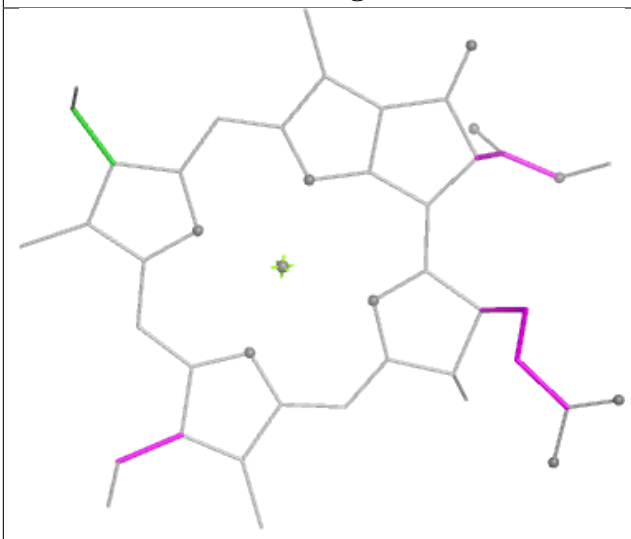
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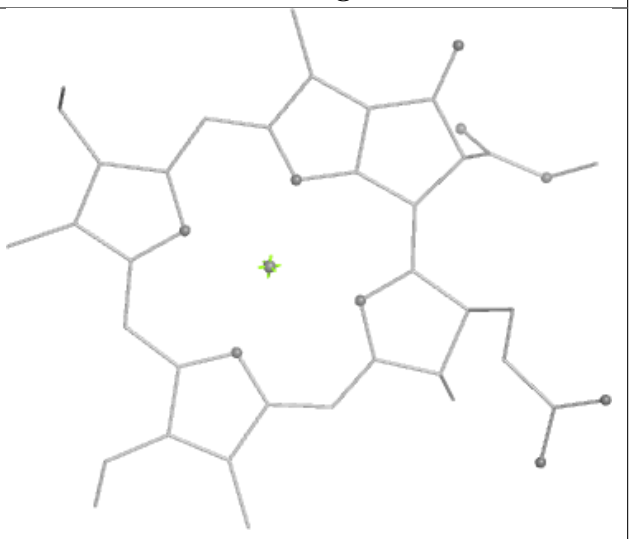
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Bond angles

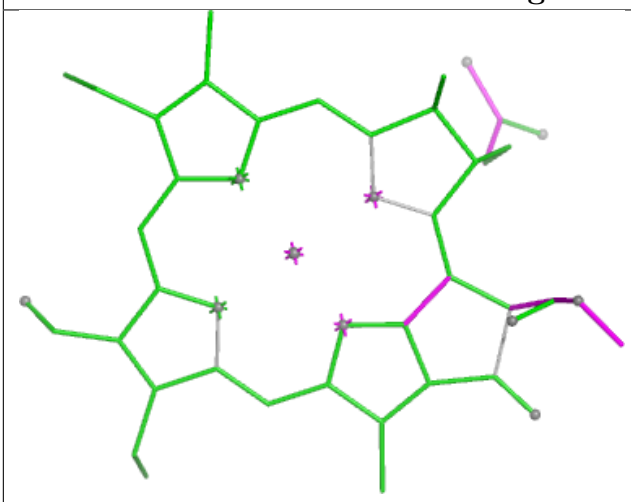


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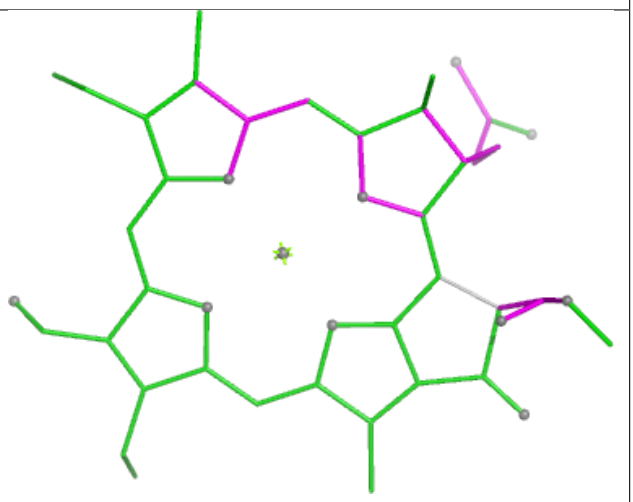


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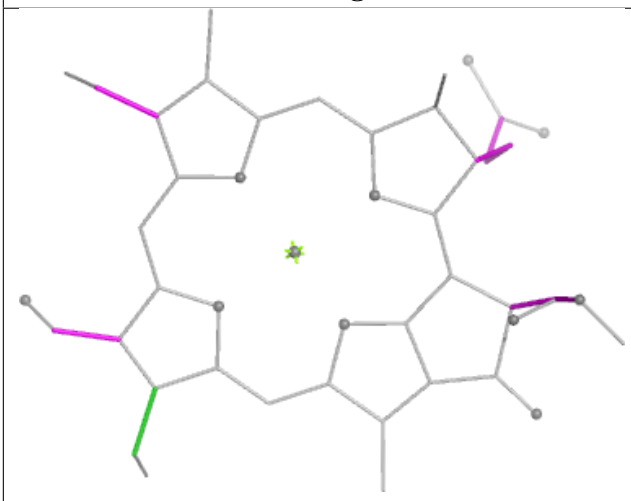
Ligand CHL 4 308



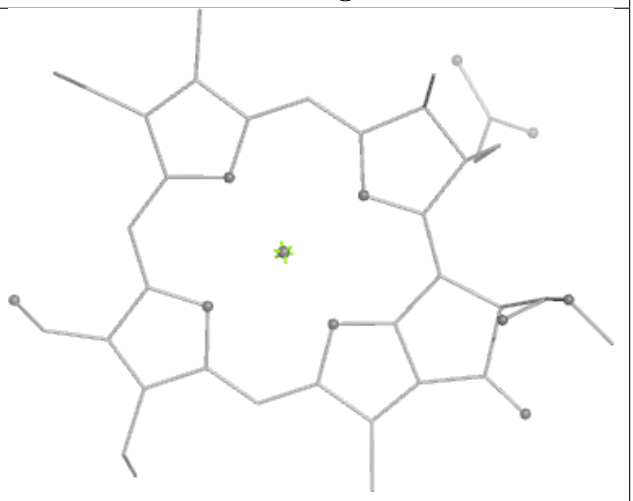
Bond lengths



Bond angles

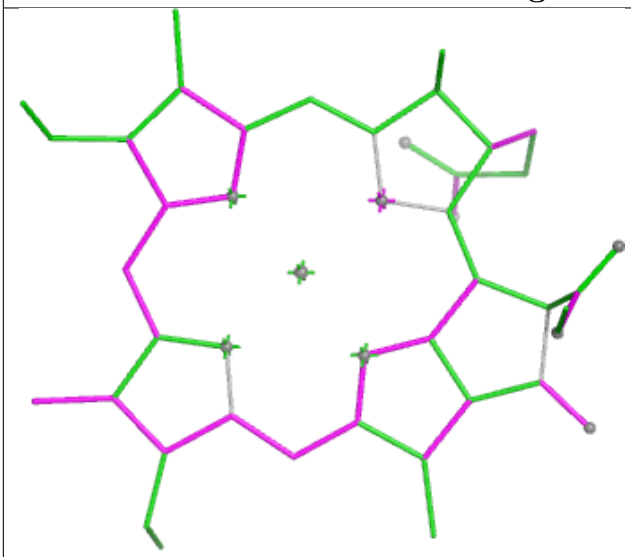


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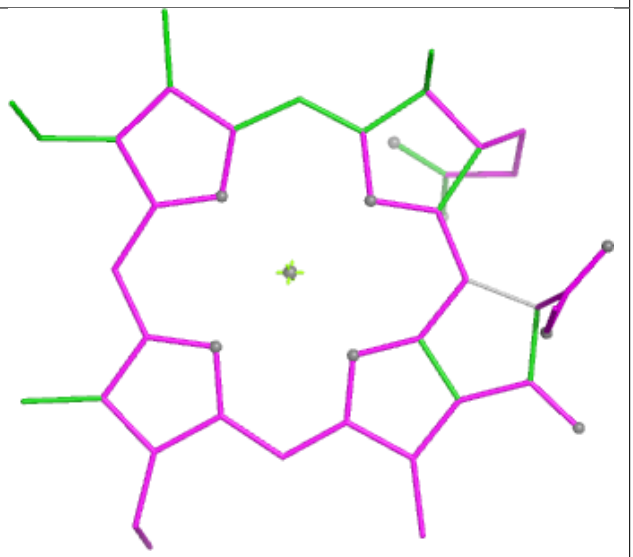


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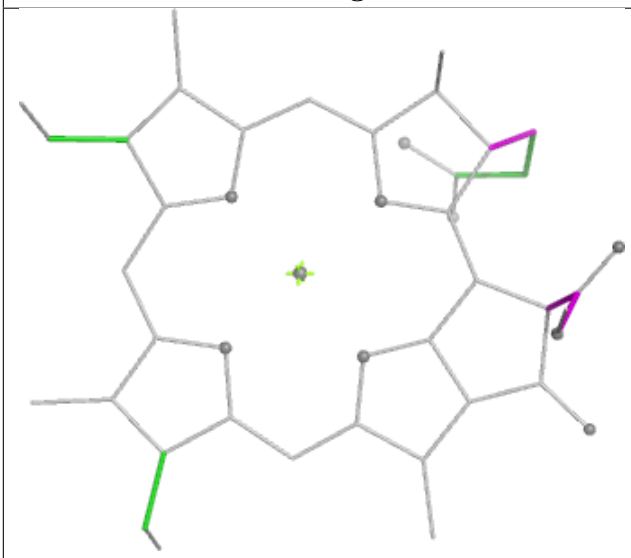
Ligand CLA 8 305



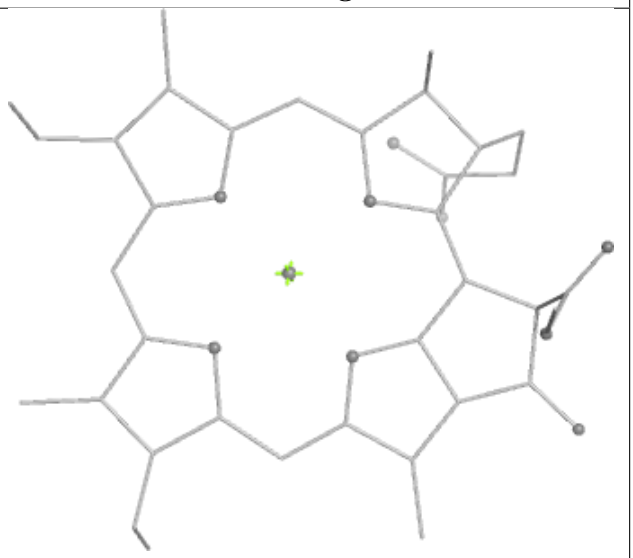
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Bond angles

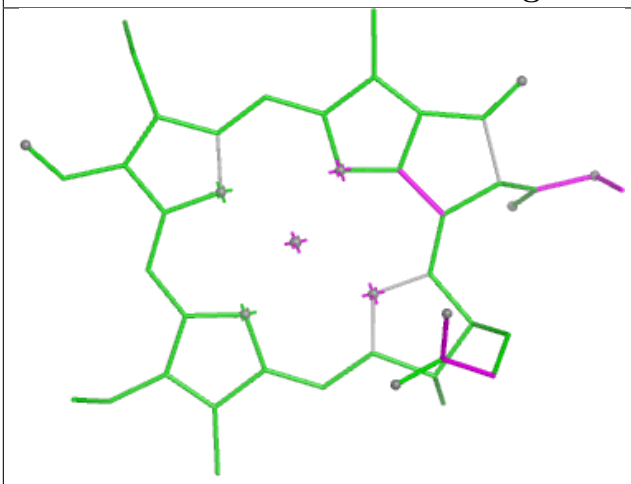


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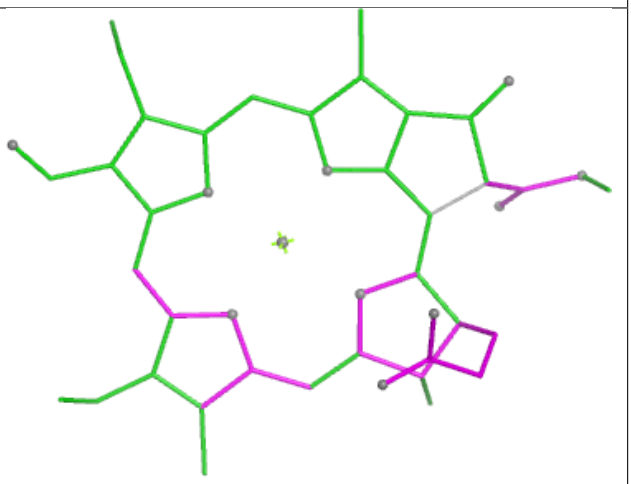


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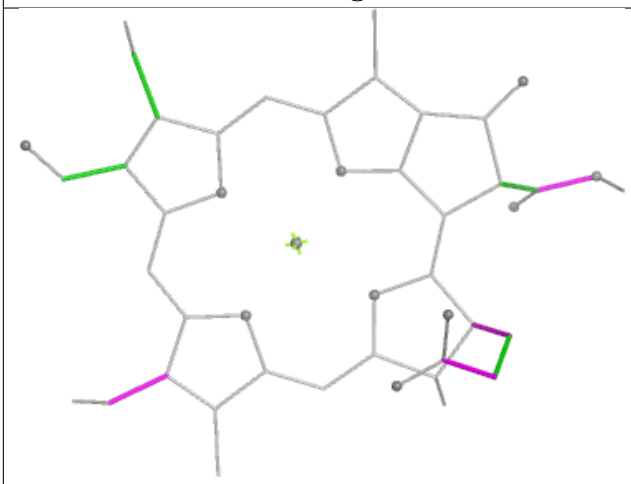
Ligand CHL N 606



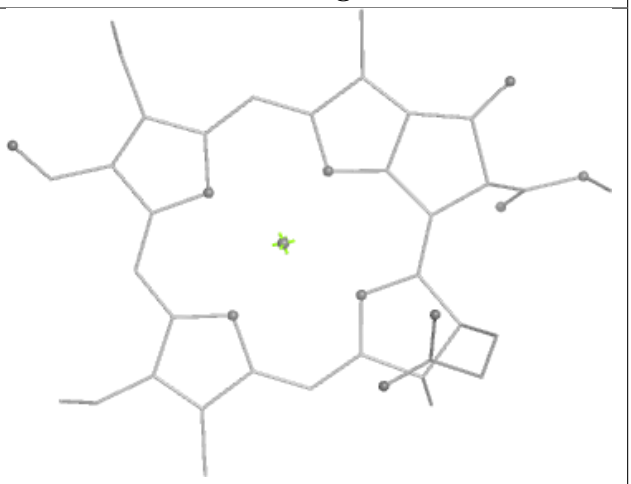
Bond lengths



Bond angles

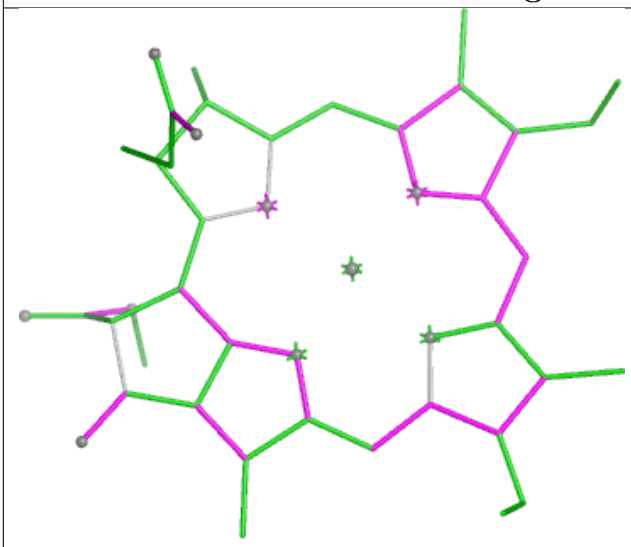


Torsions

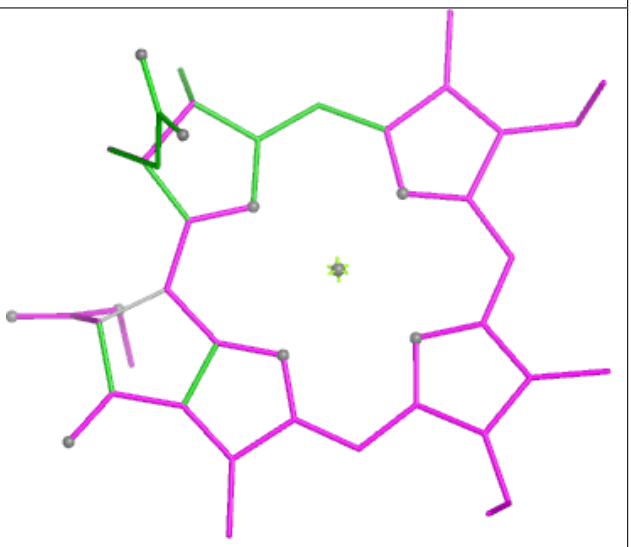


Rings

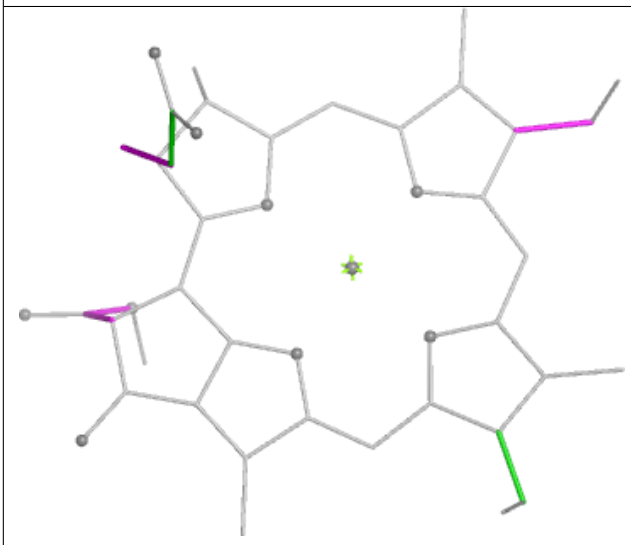
Ligand CLA C 506



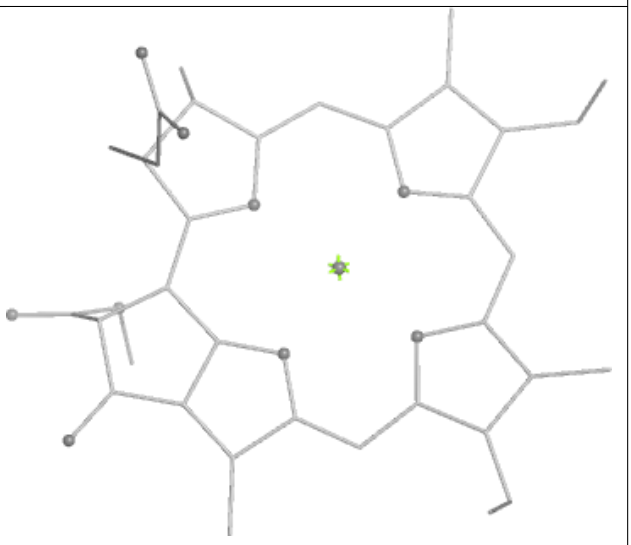
Bond lengths



Bond angles

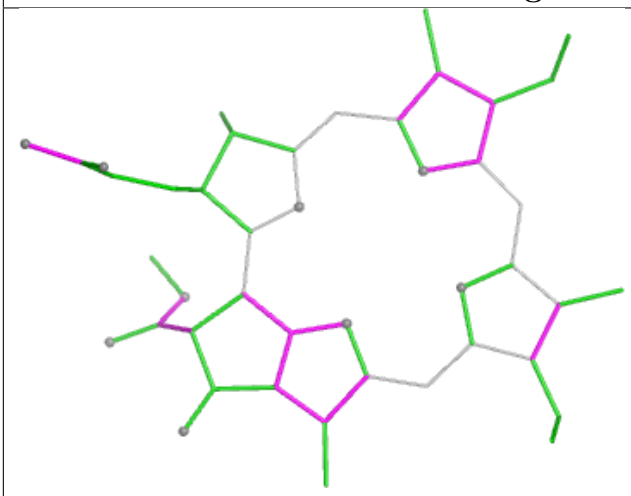


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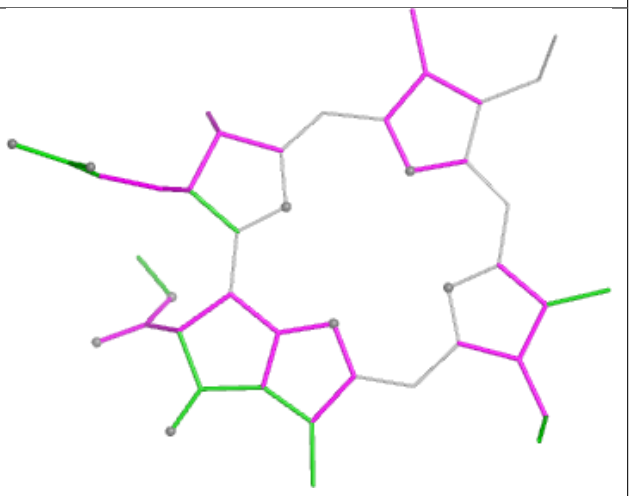


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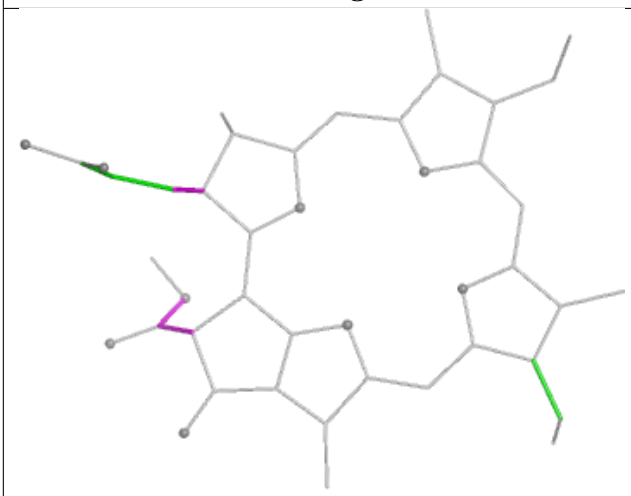
Ligand PHO d 402



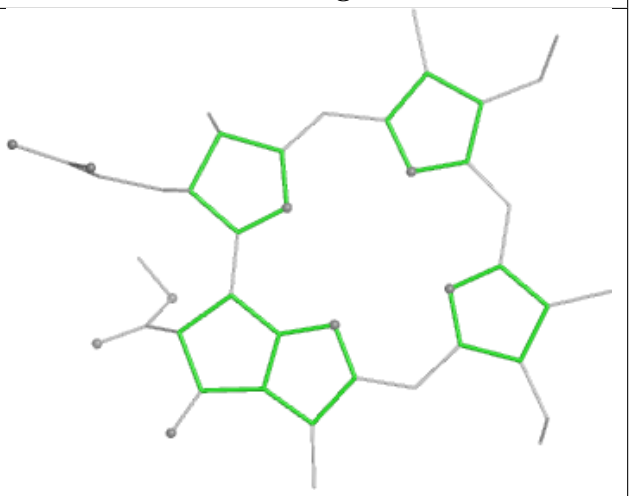
Bond lengths



Bond angles

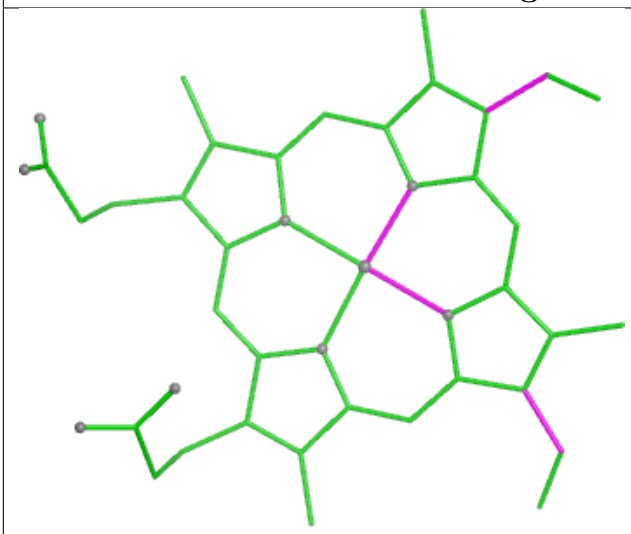


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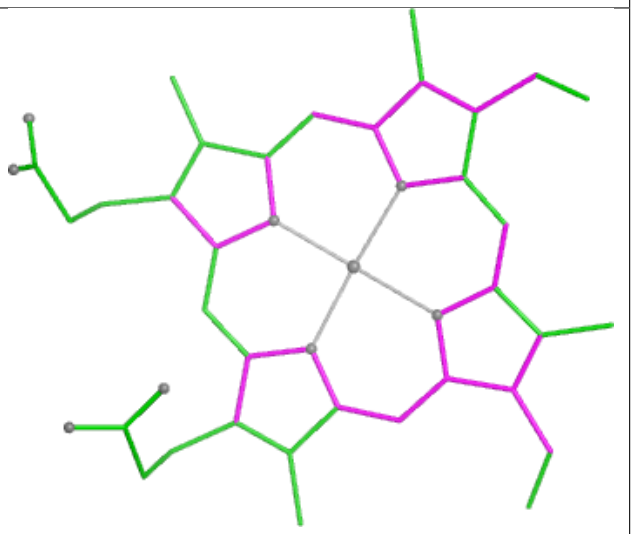


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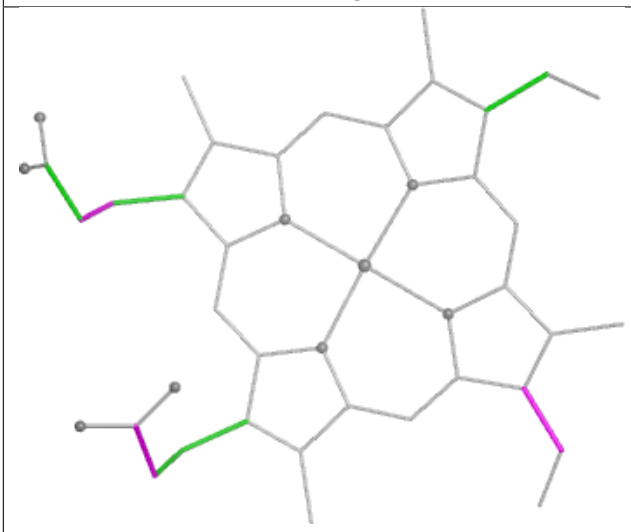
Ligand HEM F 101



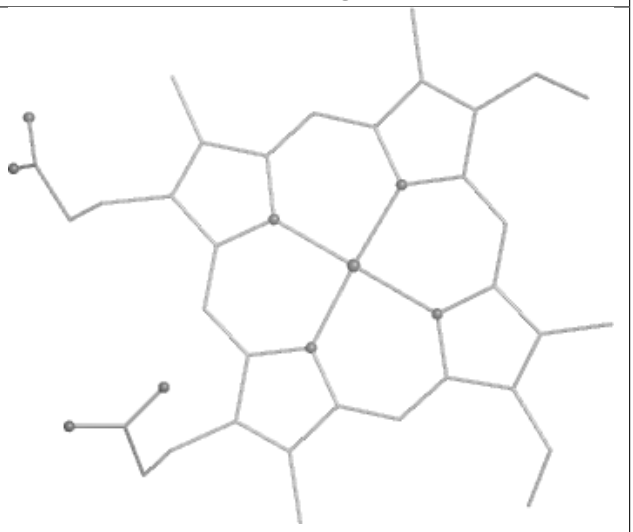
Bond lengths



Bond angles

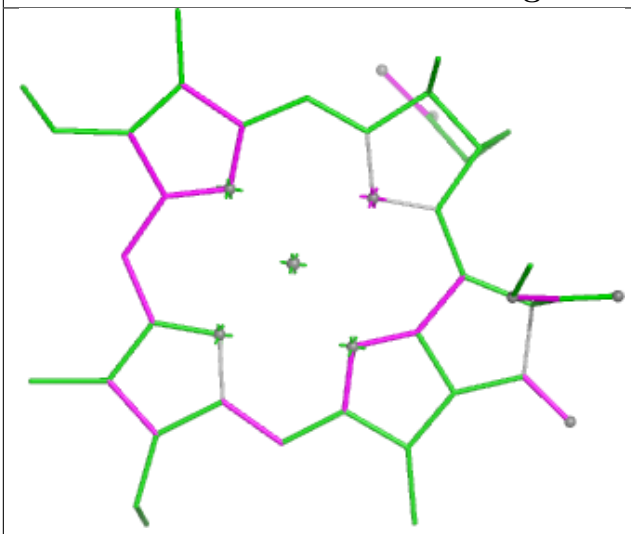


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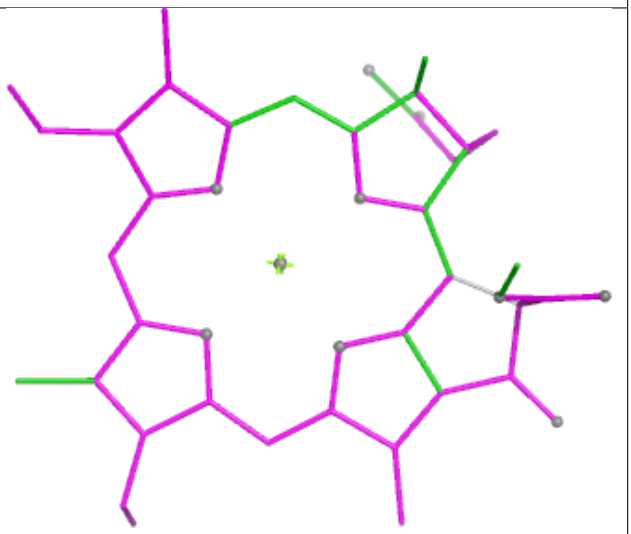


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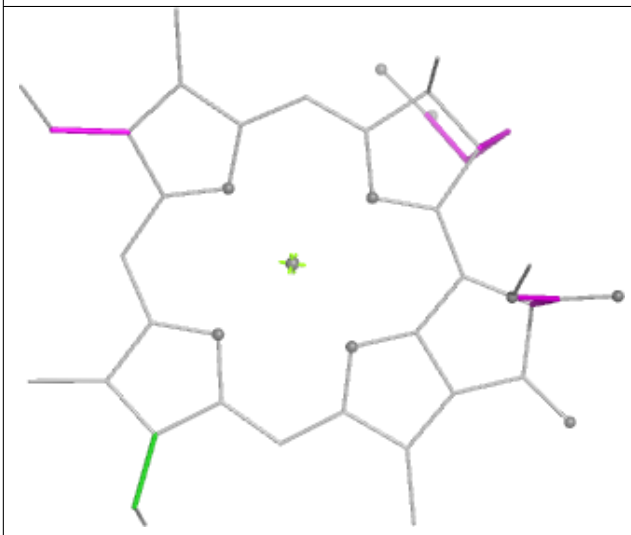
Ligand CLA N 604



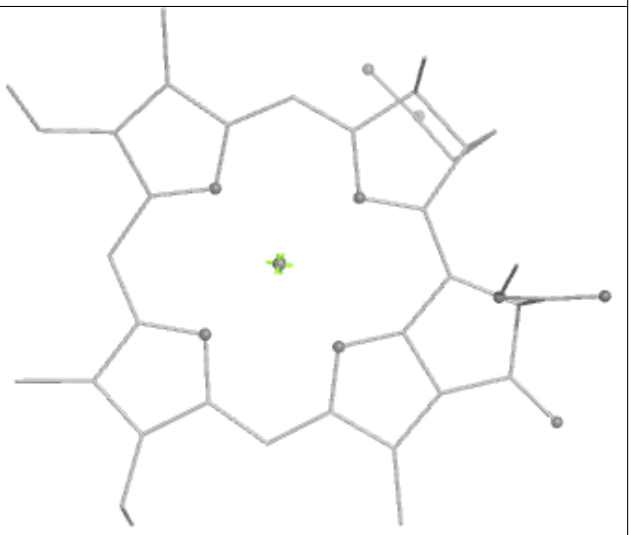
Bond lengths



Bond angles

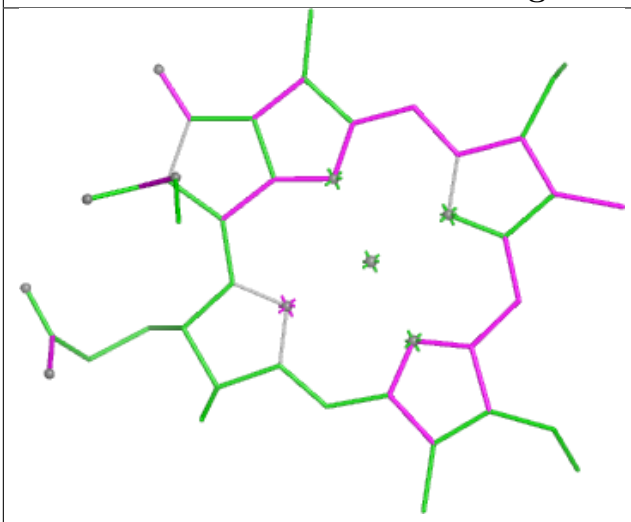


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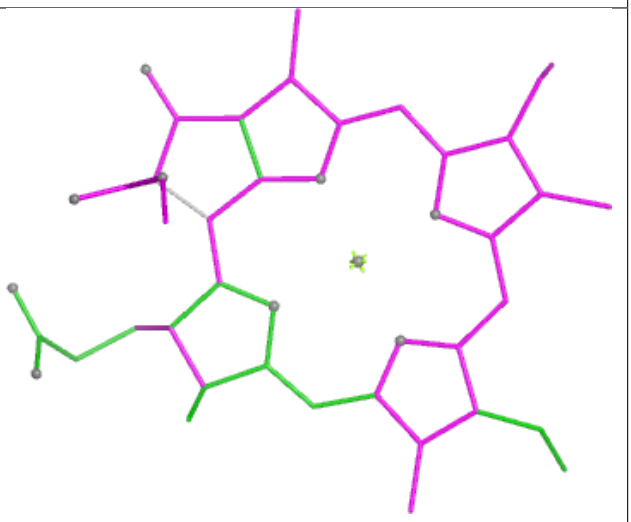


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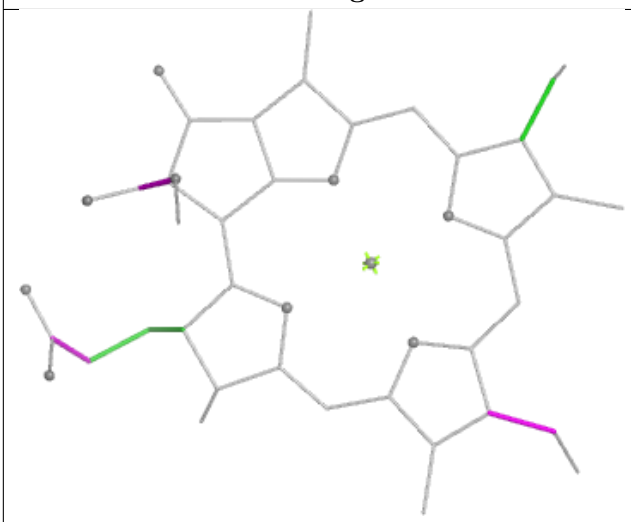
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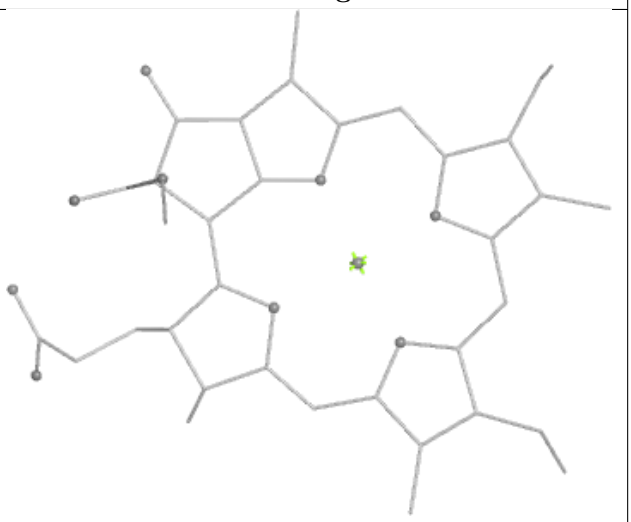
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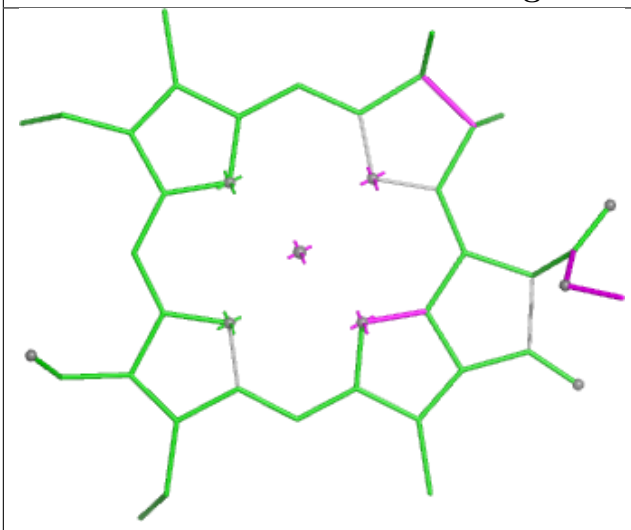


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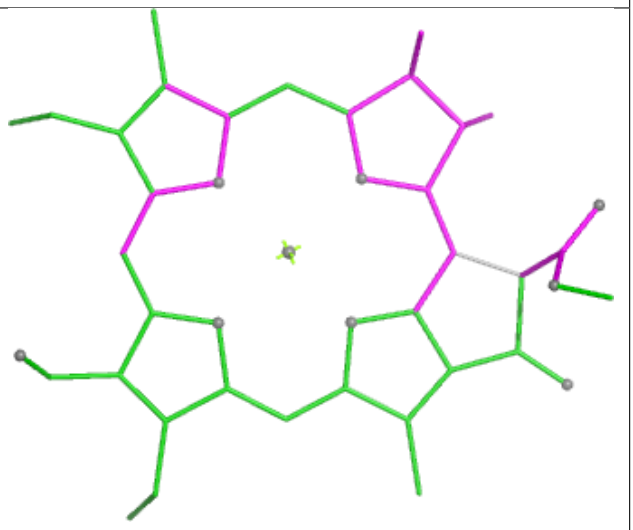


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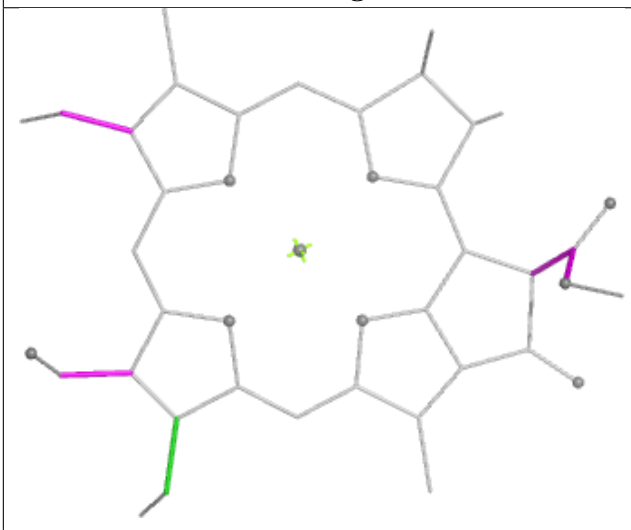
Ligand CHL Y 605



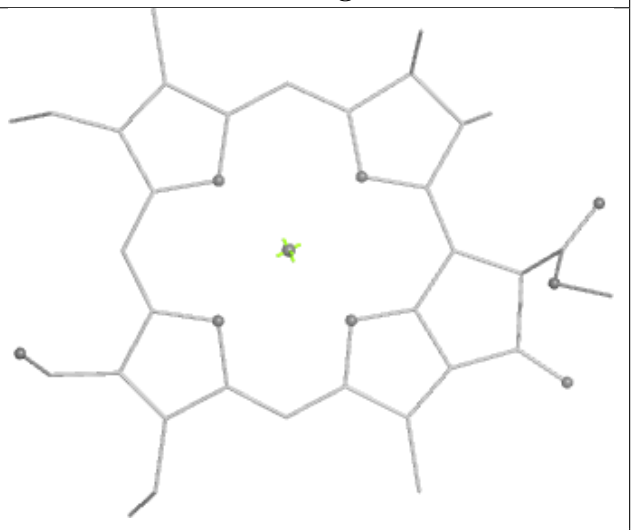
Bond lengths



Bond angles

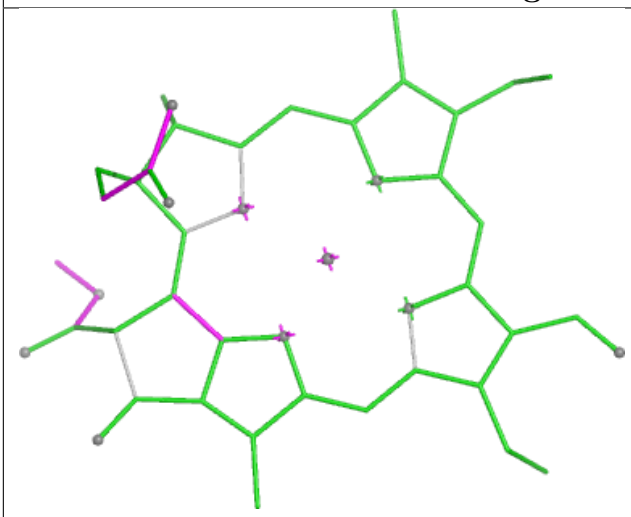


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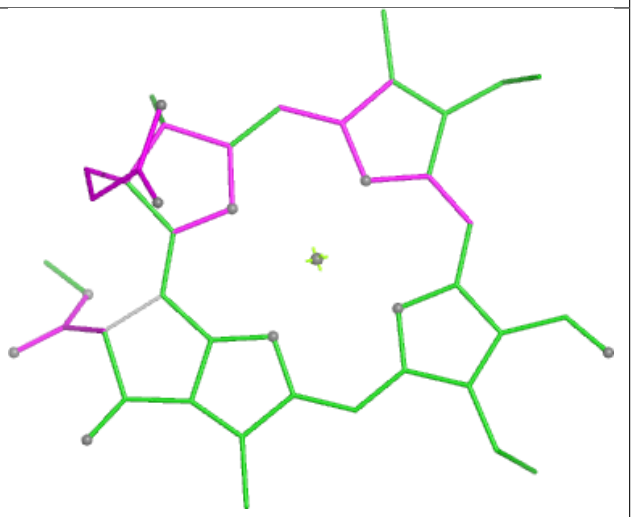


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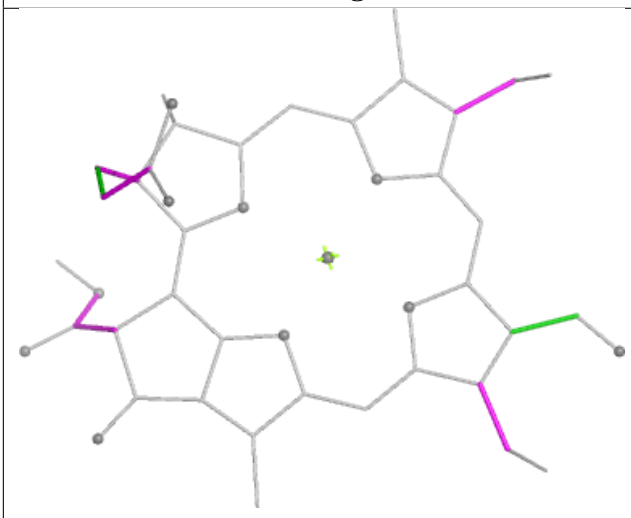
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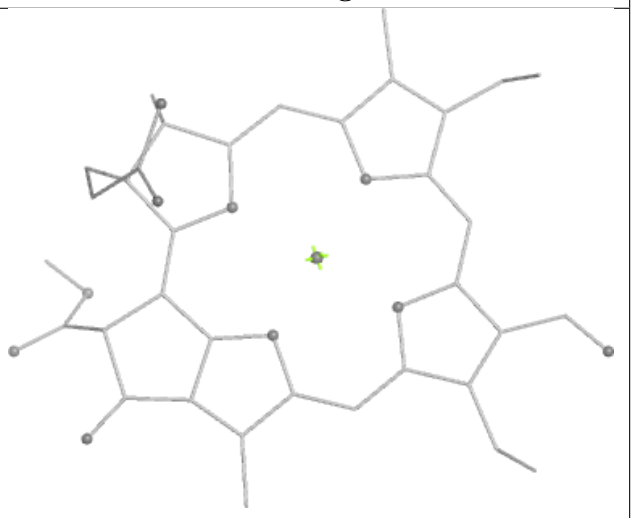
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Bond angles

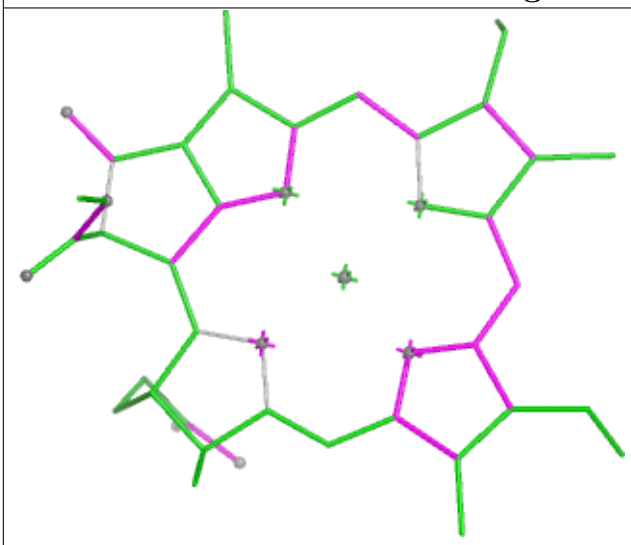


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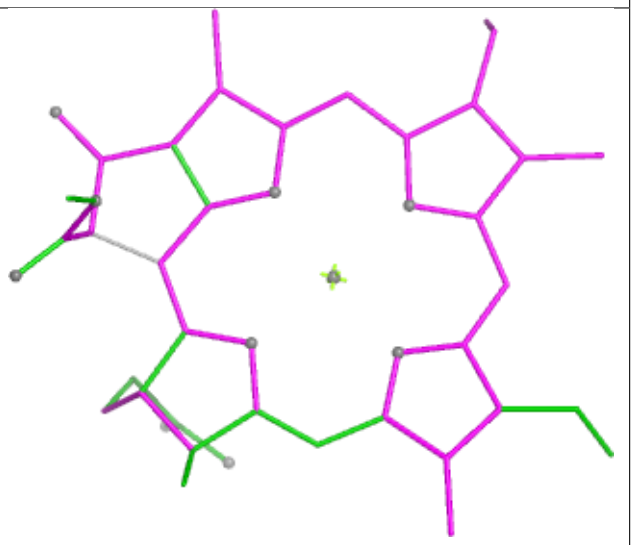


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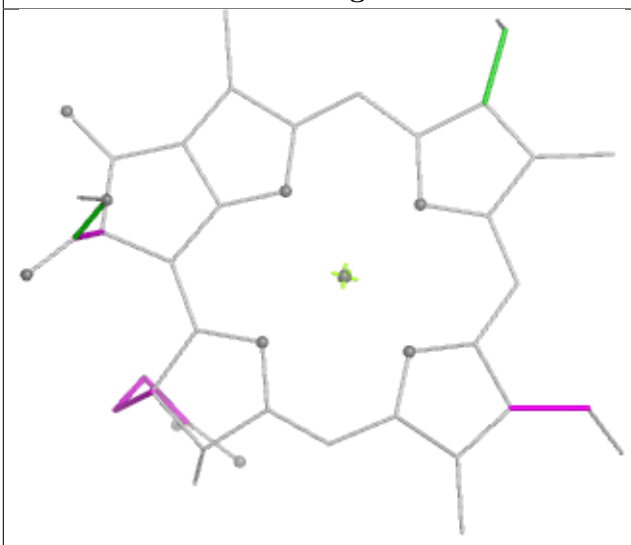
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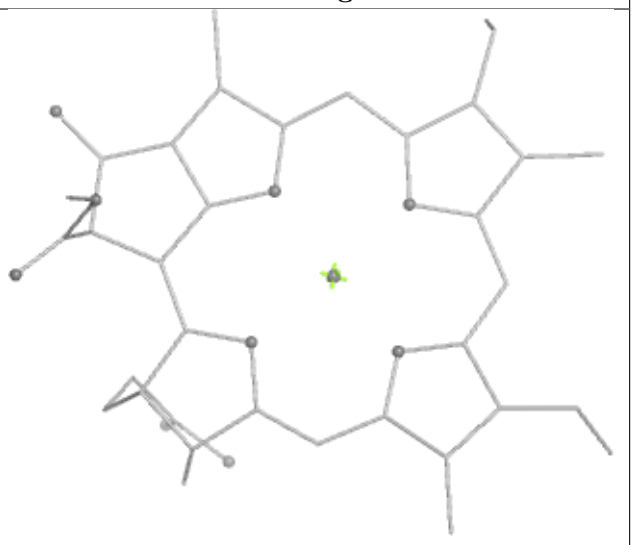
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Bond angles

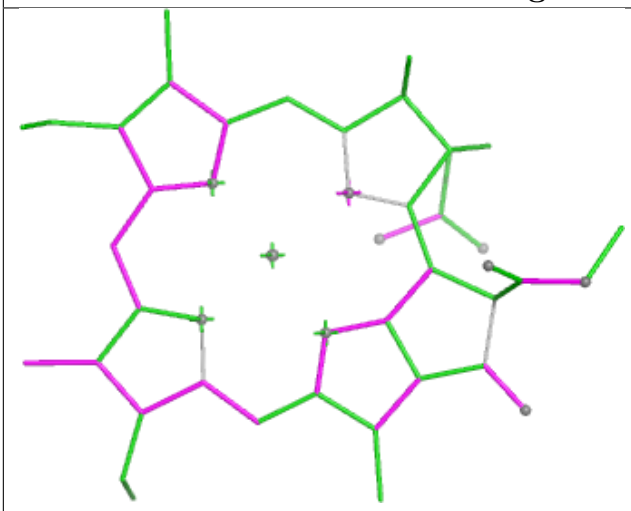


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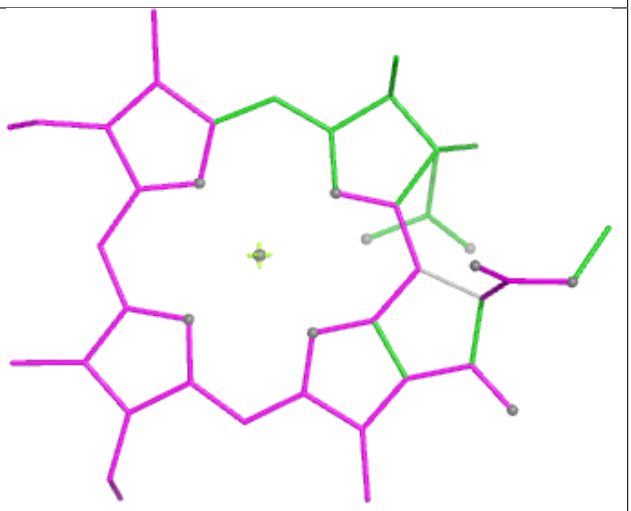


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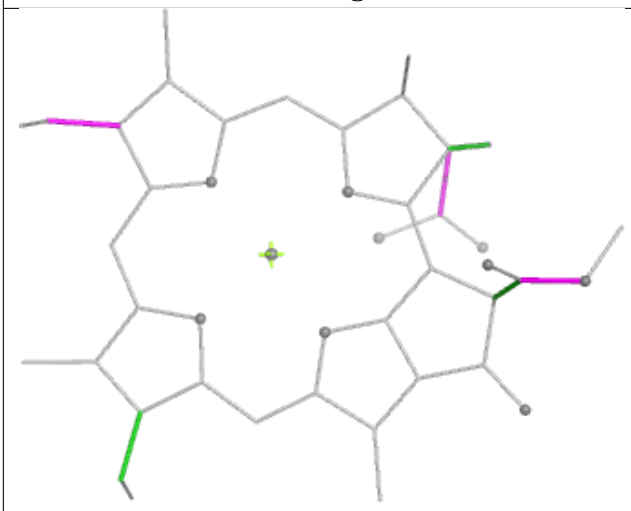
Ligand CLA 6 612



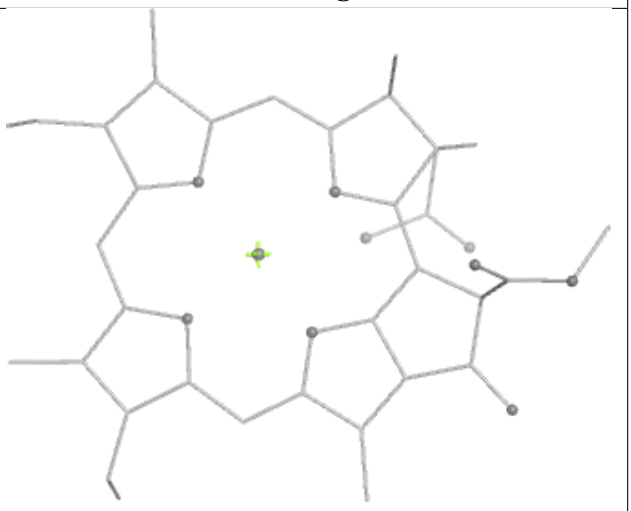
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Bond angles

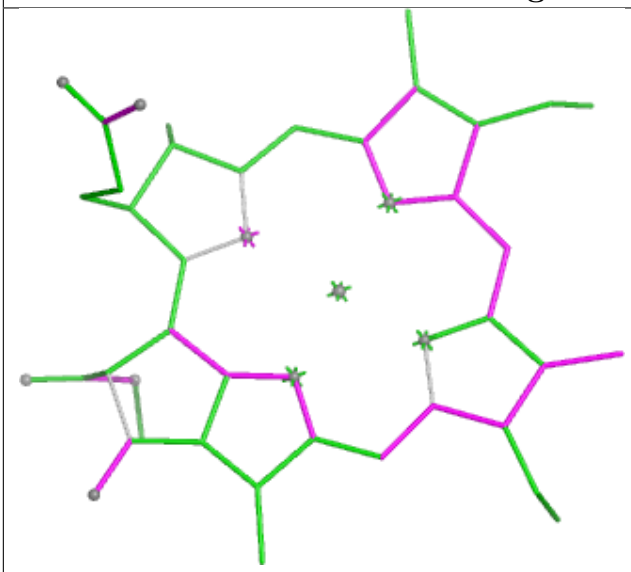


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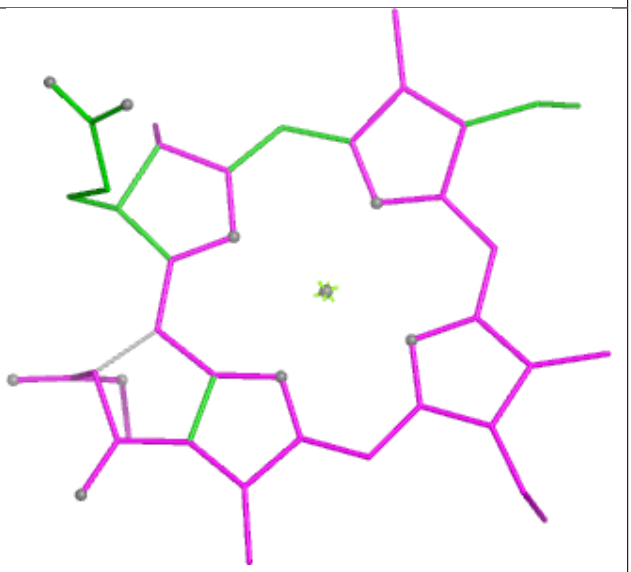


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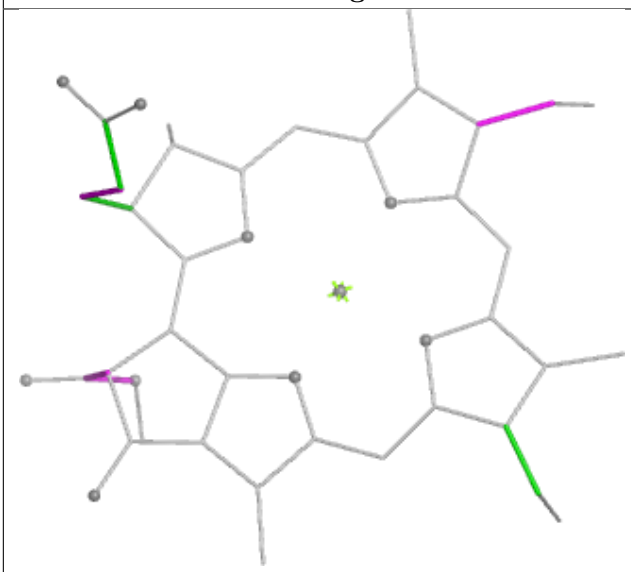
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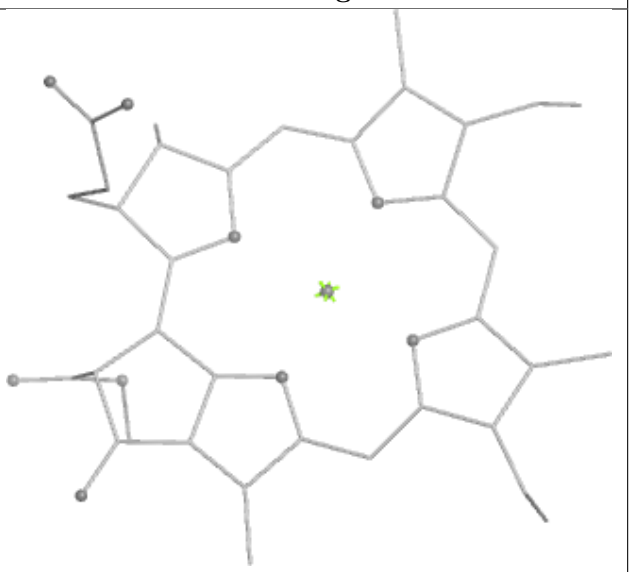
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Bond angles

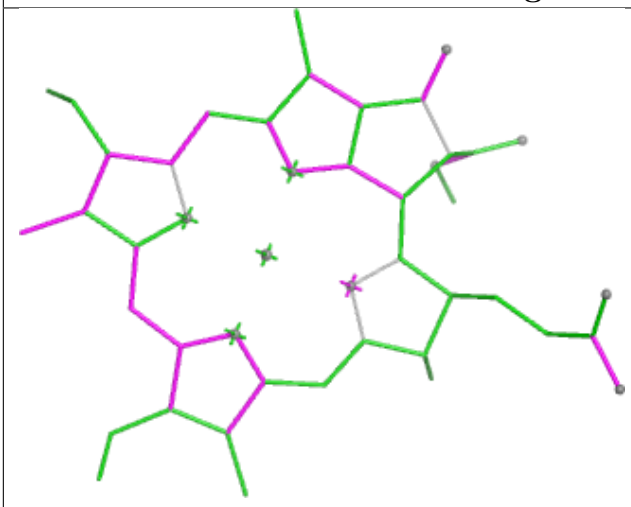


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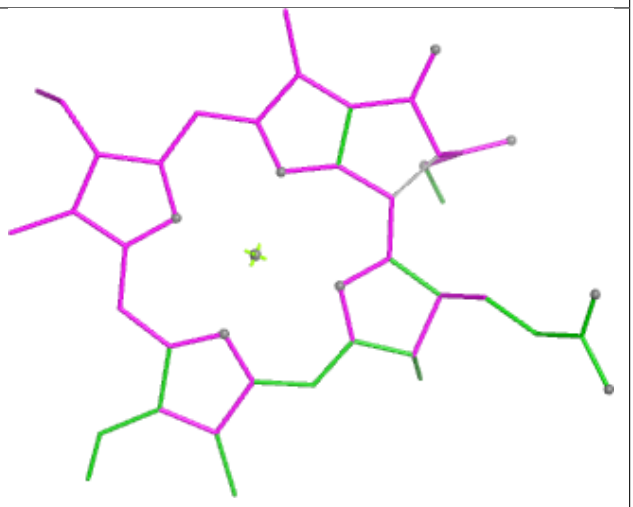


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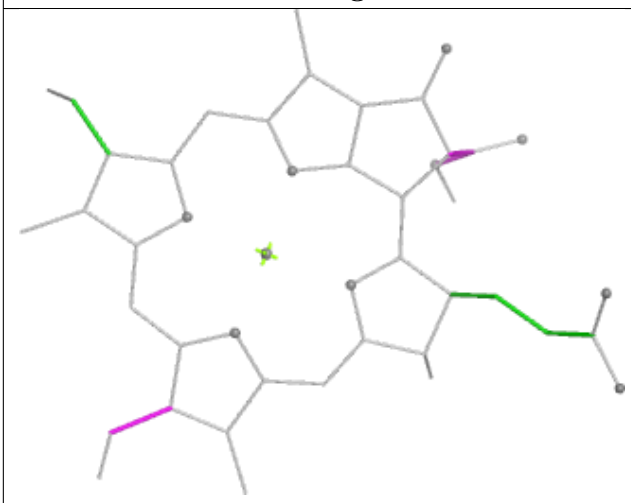
Ligand CLA C 512



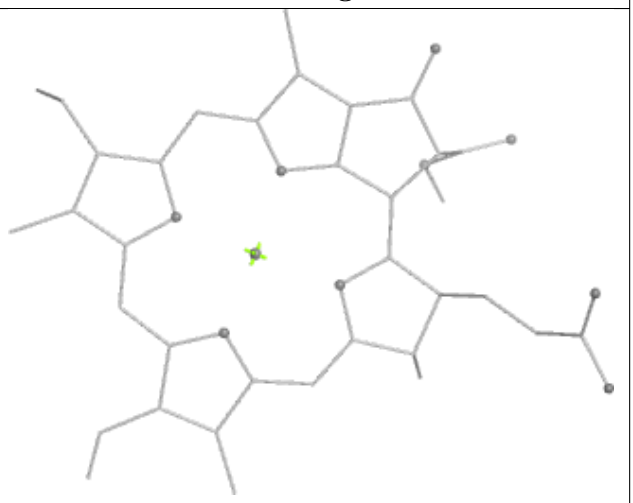
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Bond angles

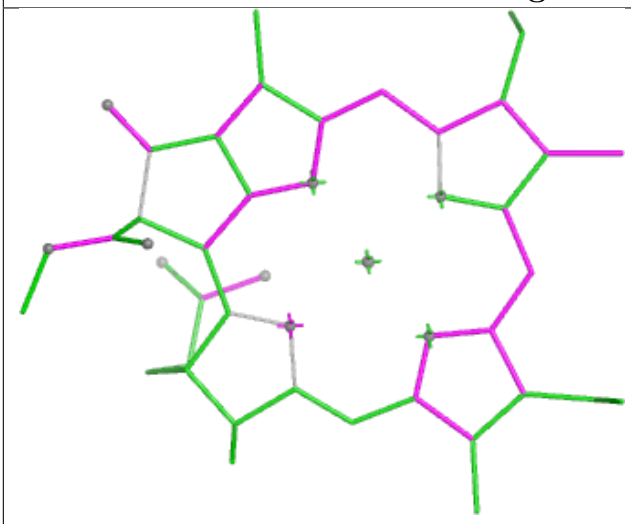


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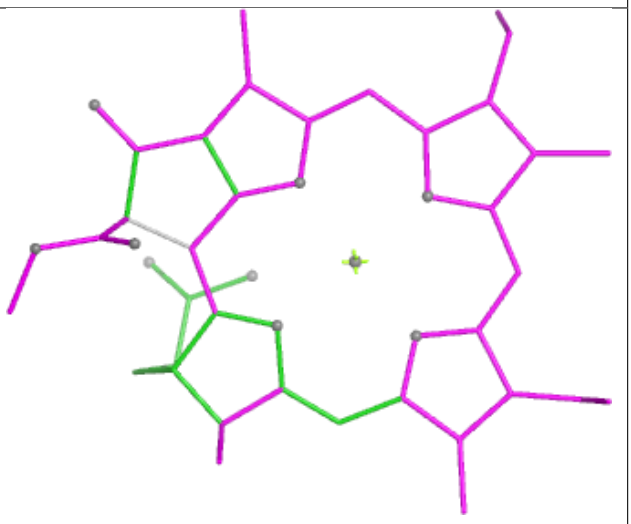


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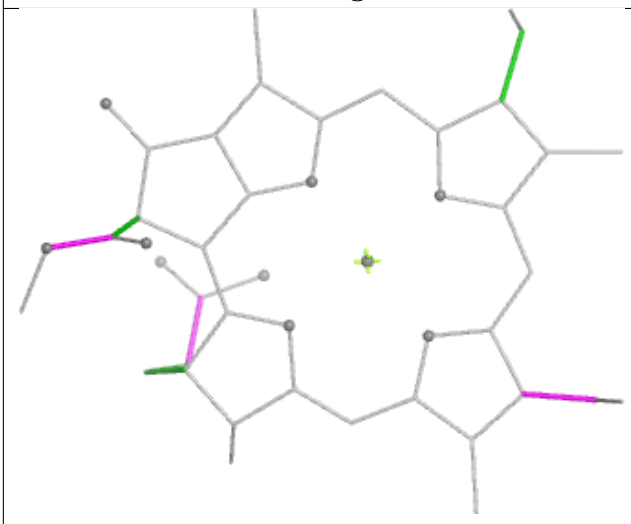
Ligand CLA 5 613



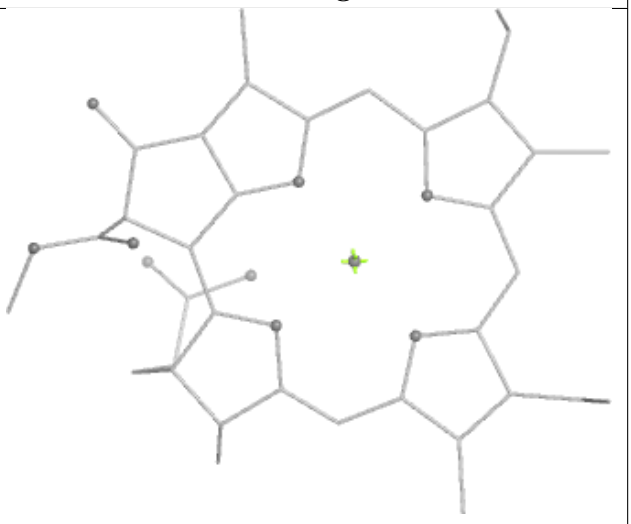
Bond lengths



Bond angles

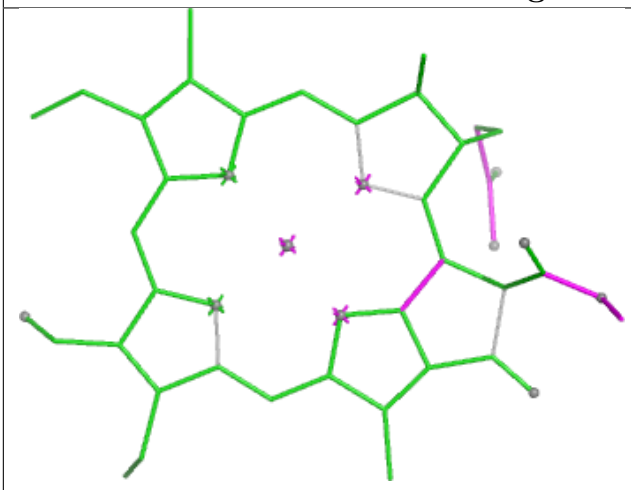


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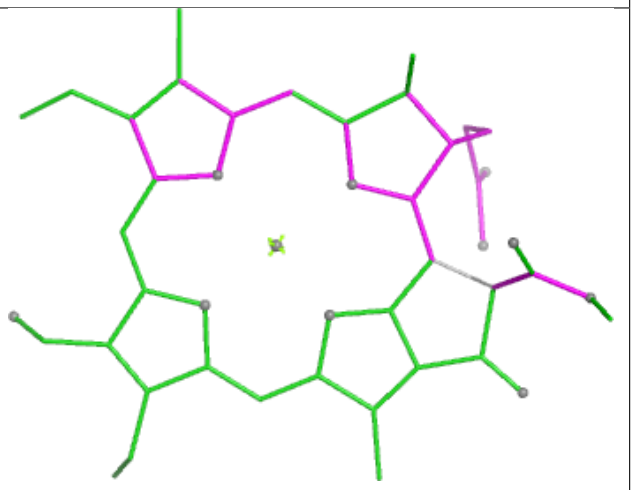


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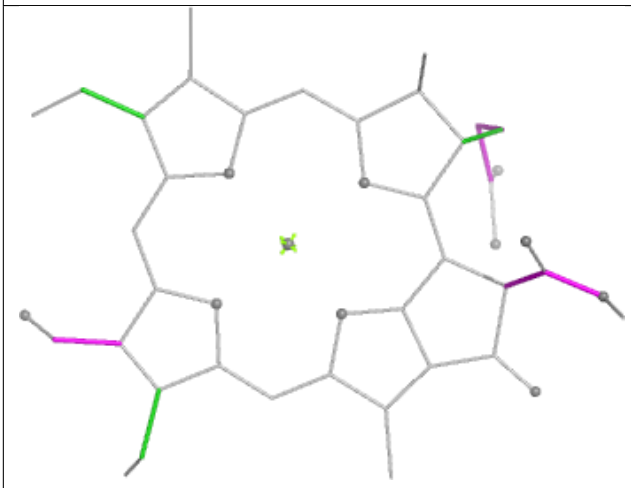
Ligand CHL 3 308



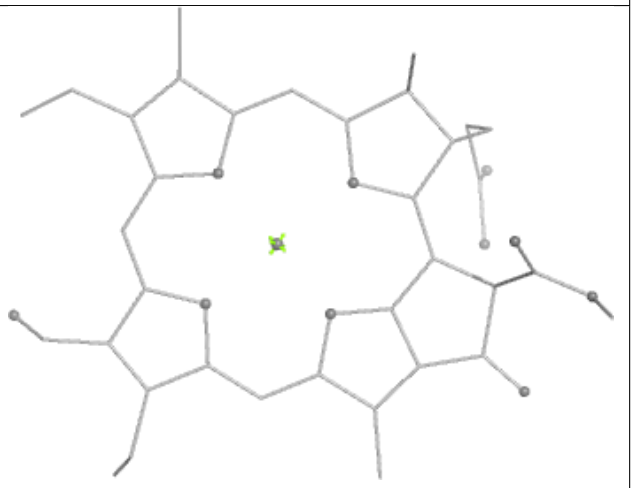
Bond lengths



Bond angles

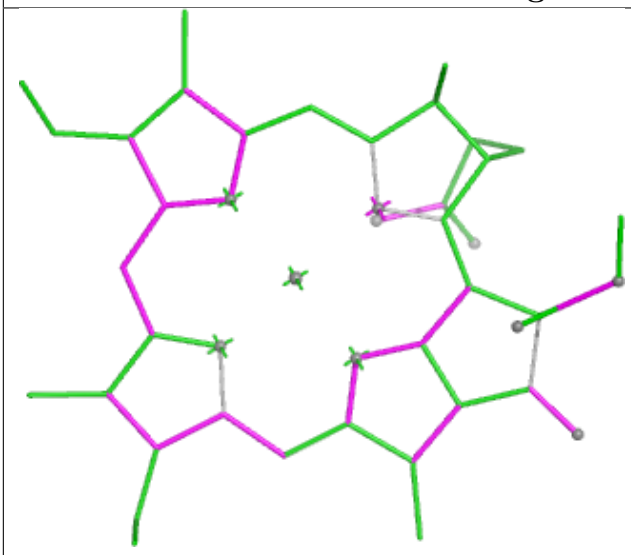


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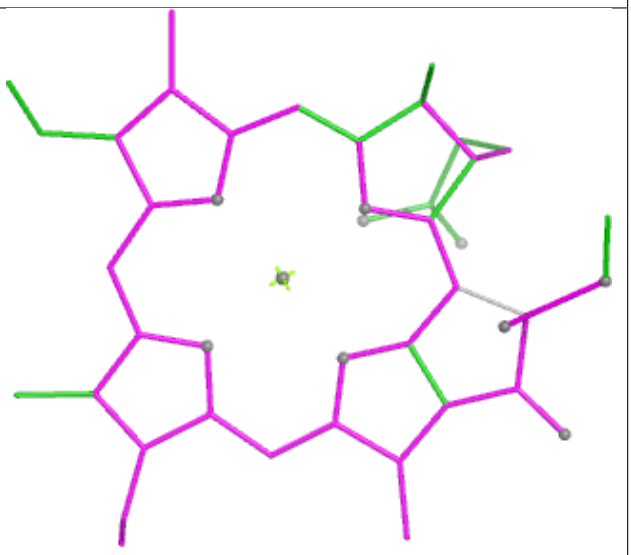


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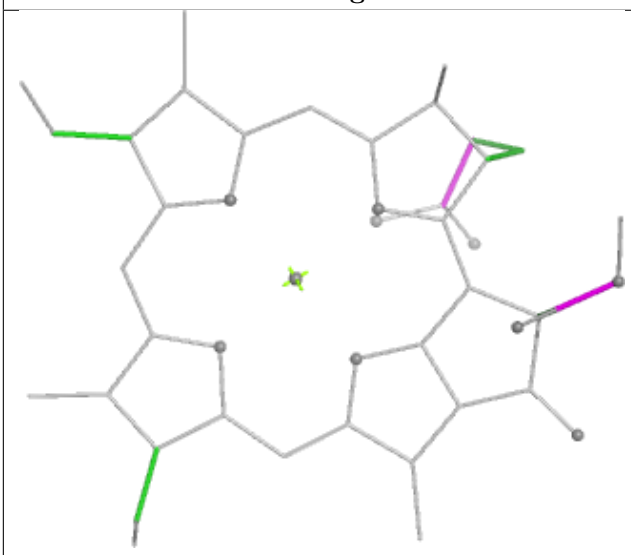
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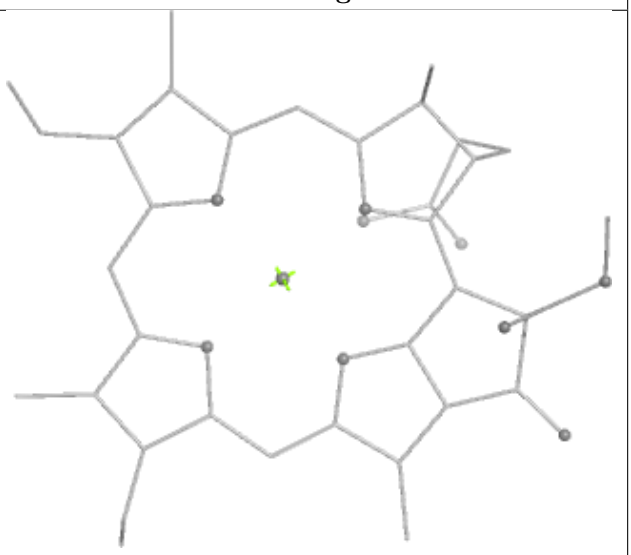
Bond lengths



Bond angles

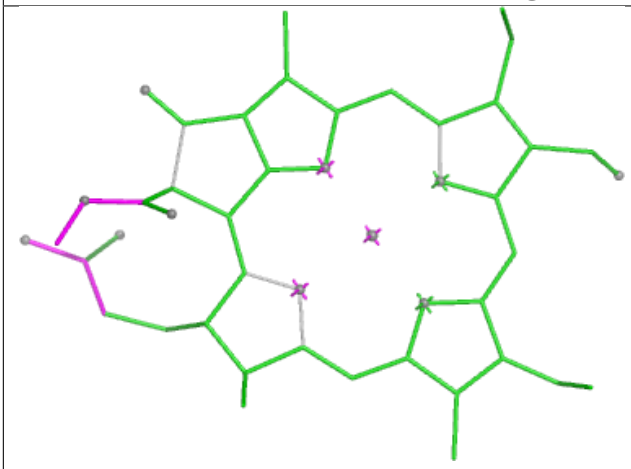


Torsions

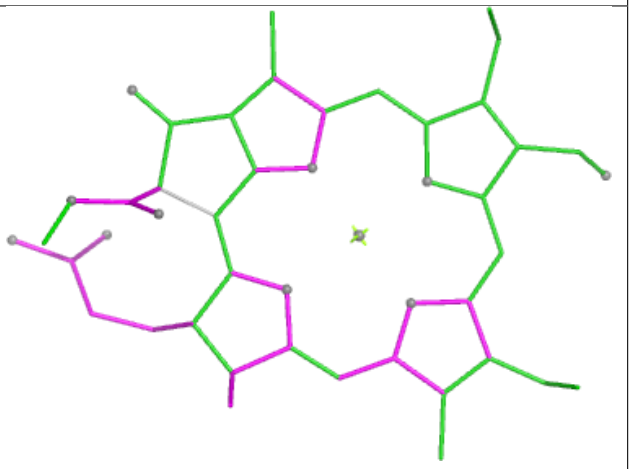


Rings

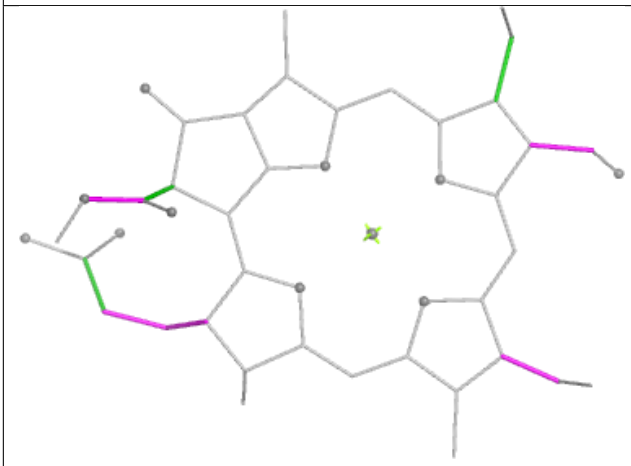
Ligand CHL Y 601



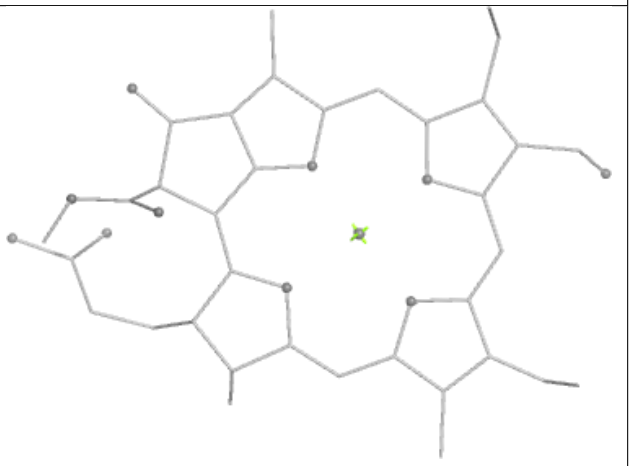
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Bond angles

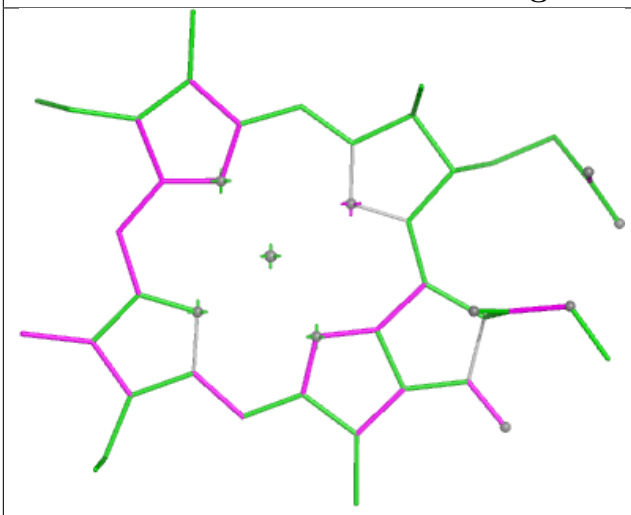


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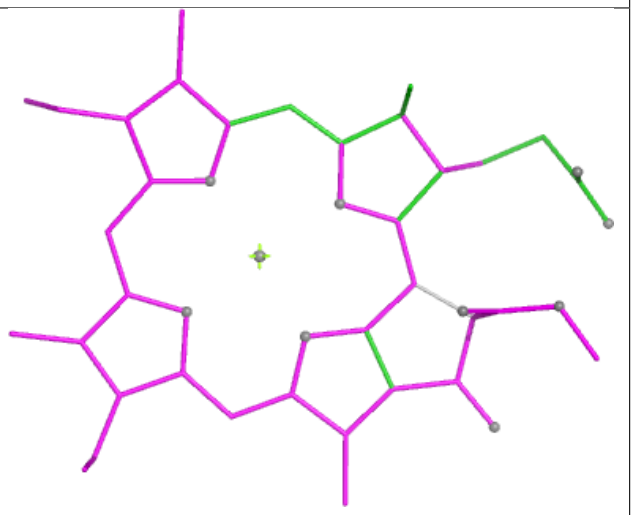


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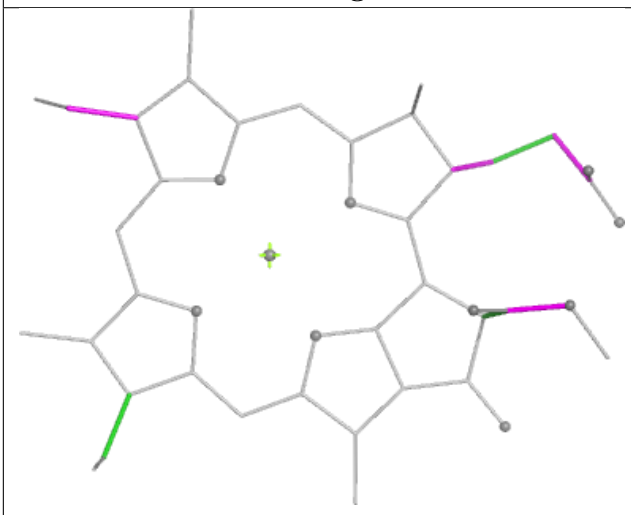
Ligand CLA s 312



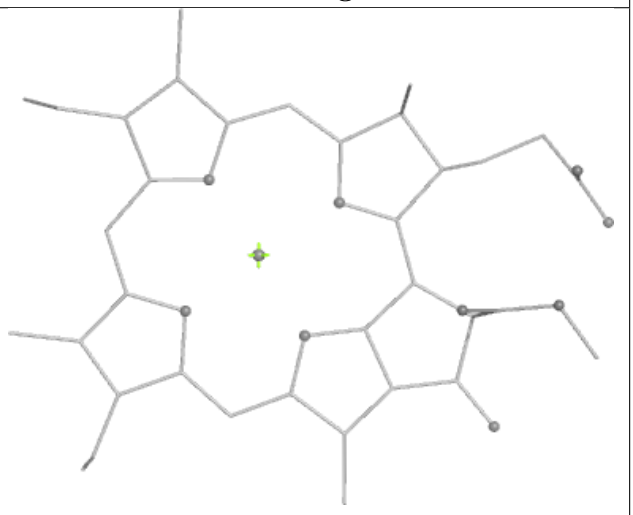
Bond lengths



Bond angles

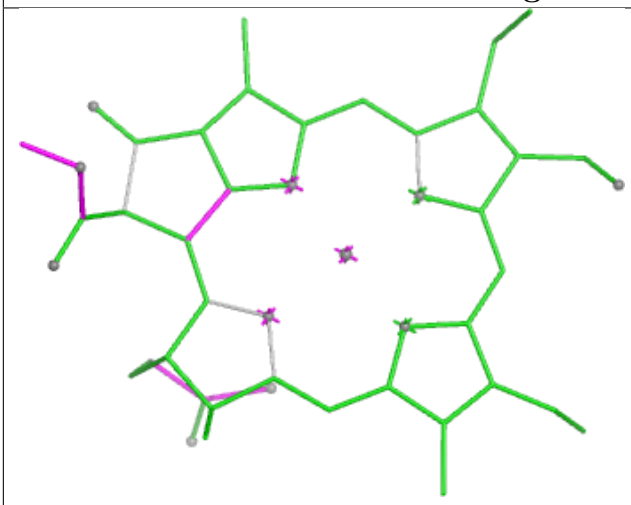


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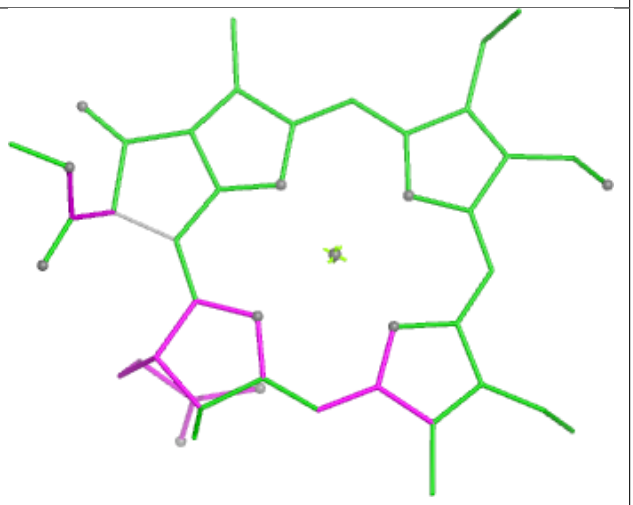


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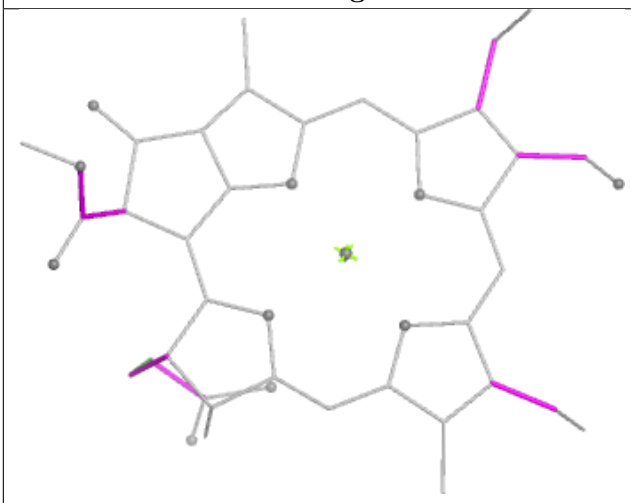
Ligand CHL R 306



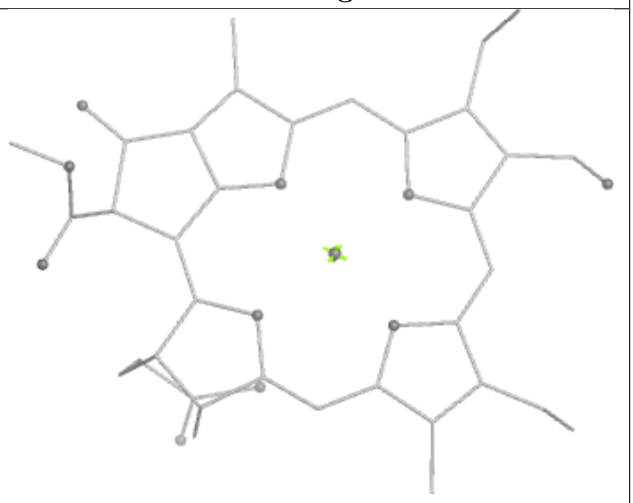
Bond lengths



Bond angles

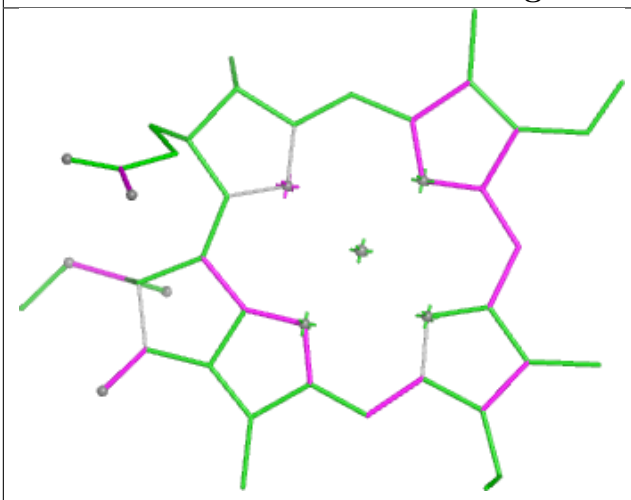


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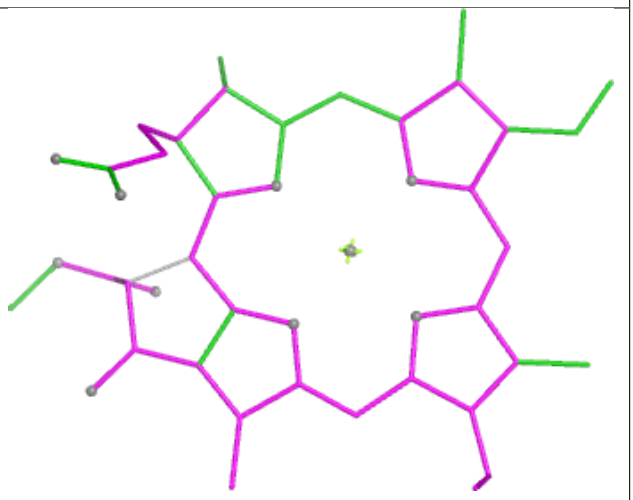


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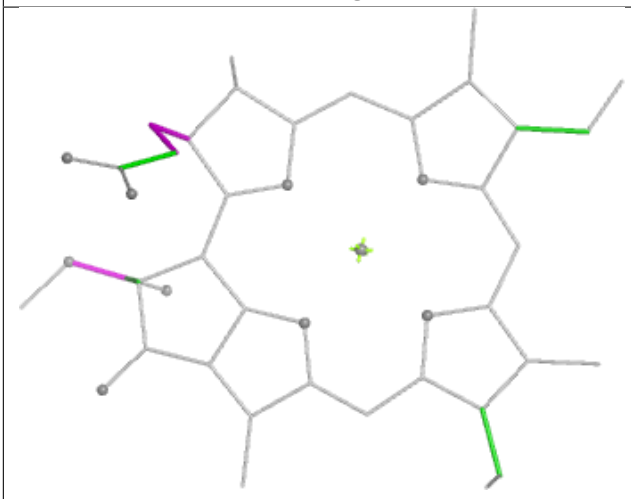
Ligand CLA B 611



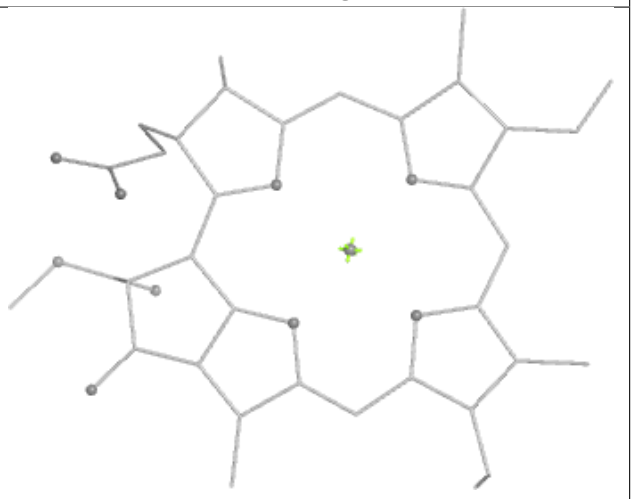
Bond lengths



Bond angles

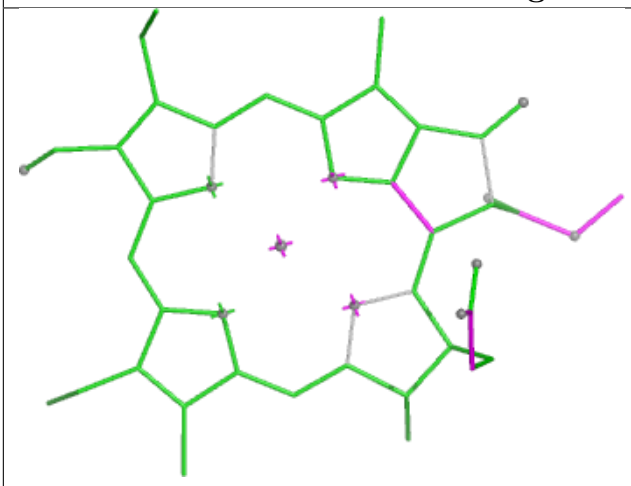


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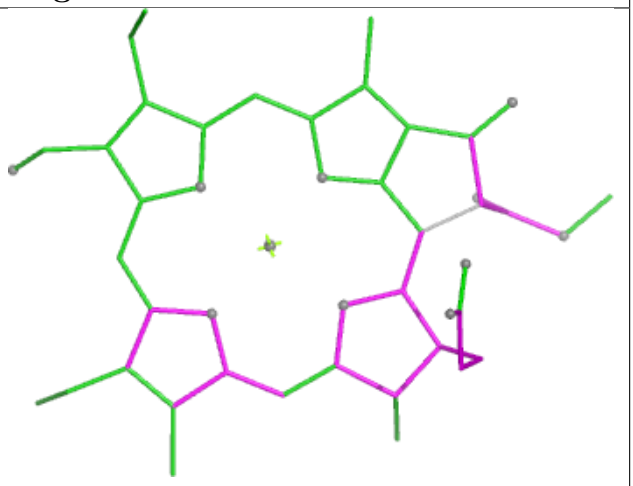


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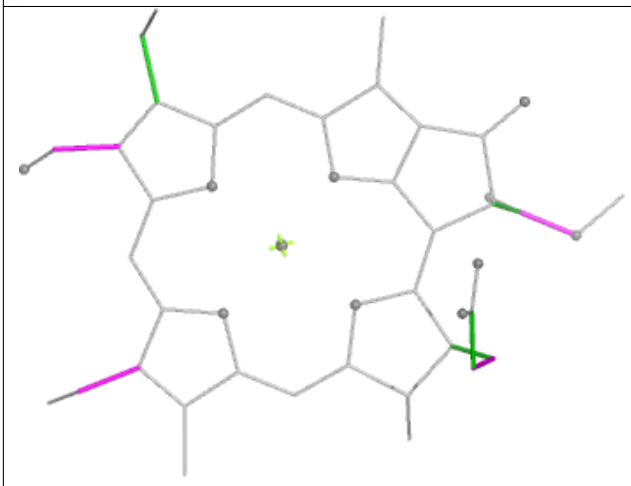
Ligand CHL g 607



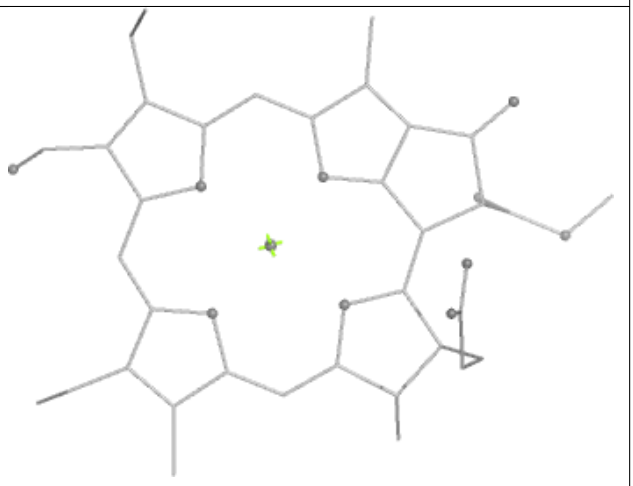
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Bond angles

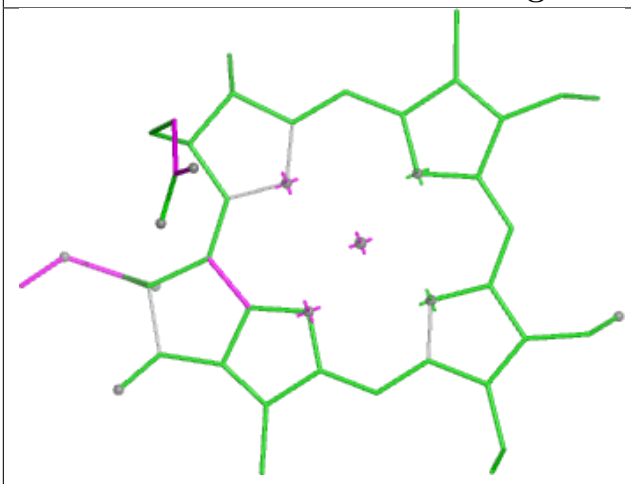


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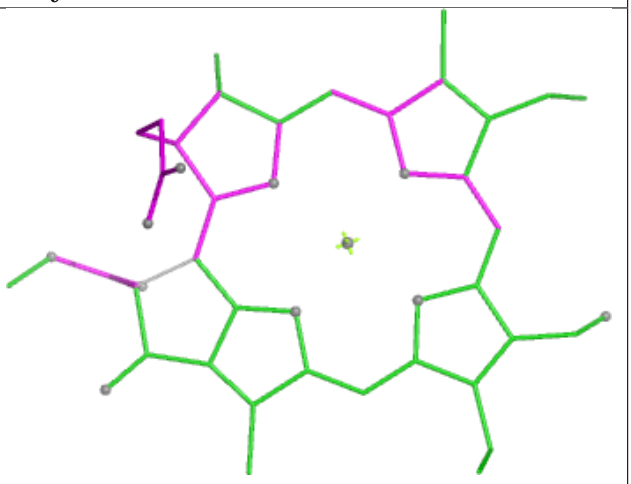


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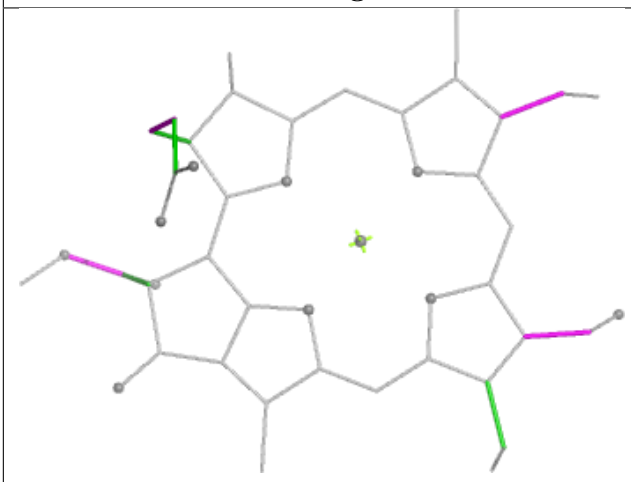
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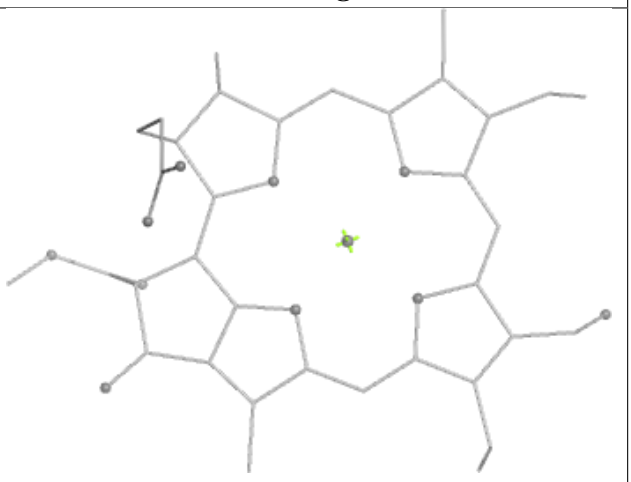
Bond lengths



Bond angles

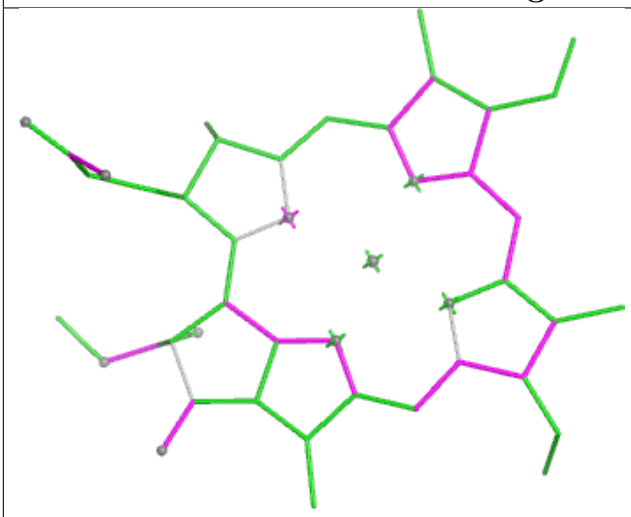


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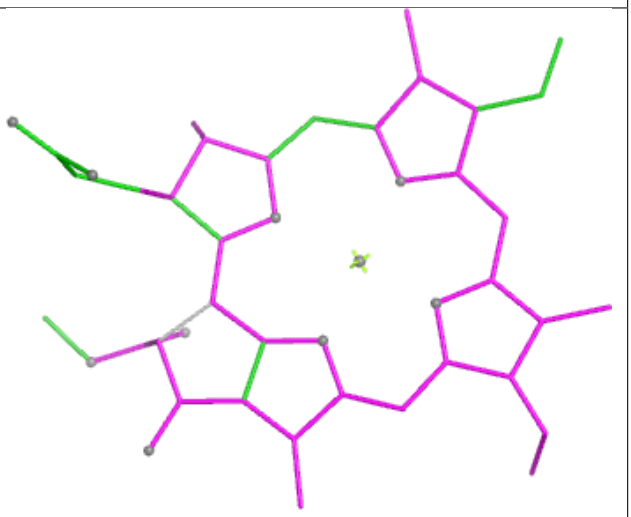


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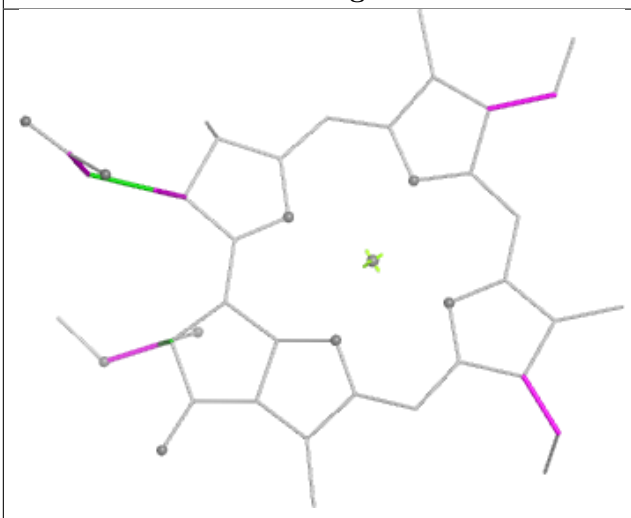
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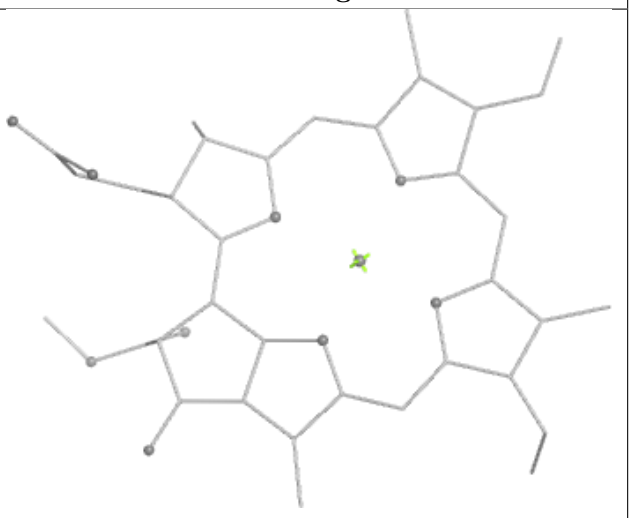
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Bond angles

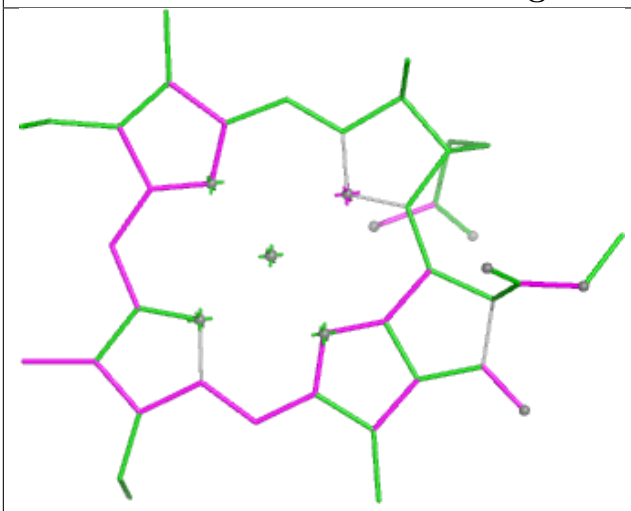


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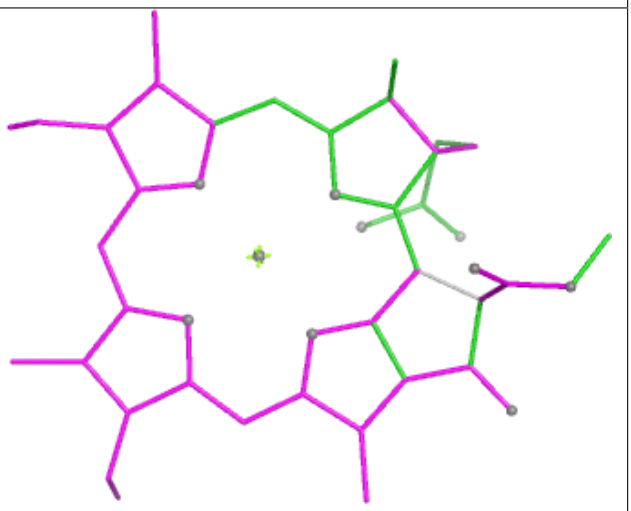


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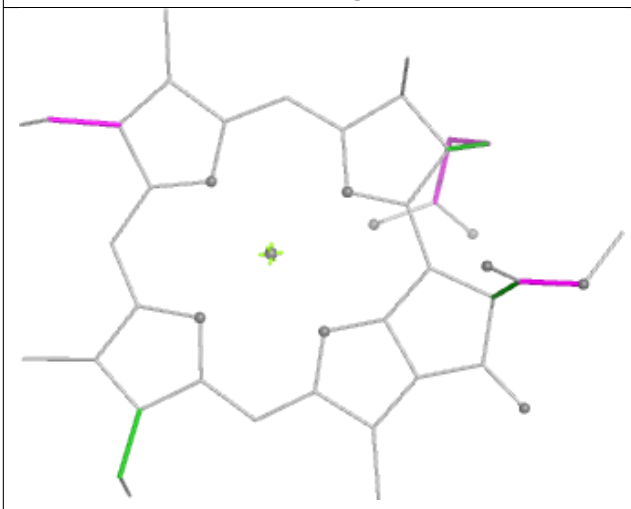
Ligand CLA 3 313



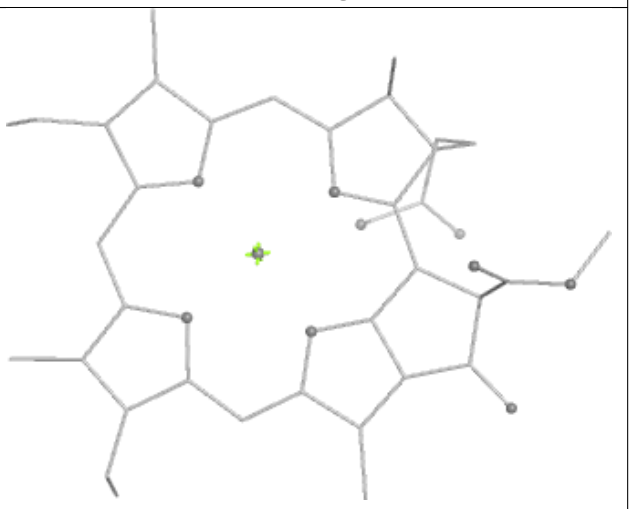
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Bond angles

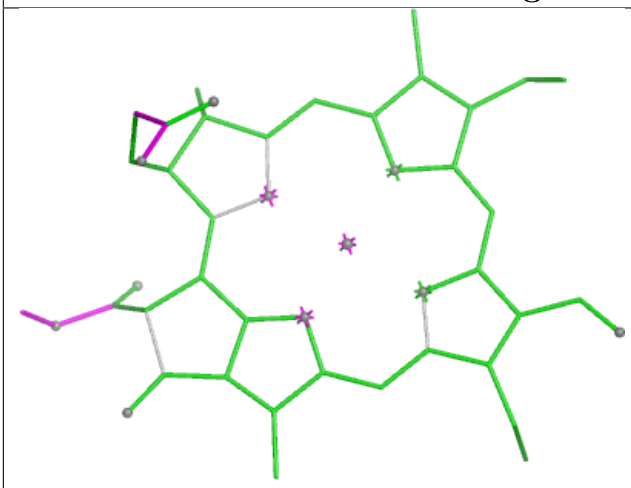


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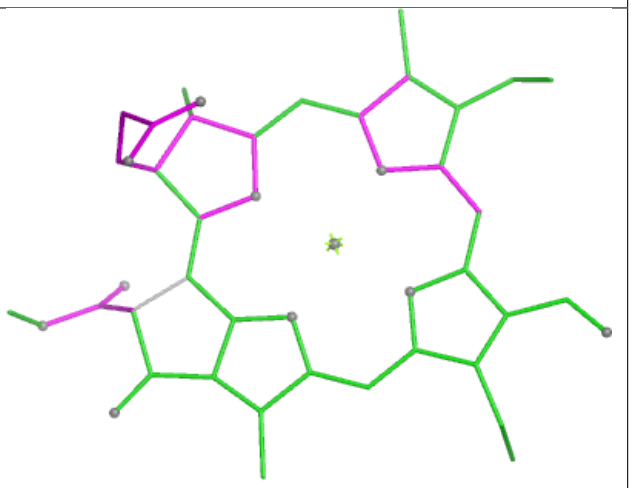


Rings

Ligand CHL Y 606



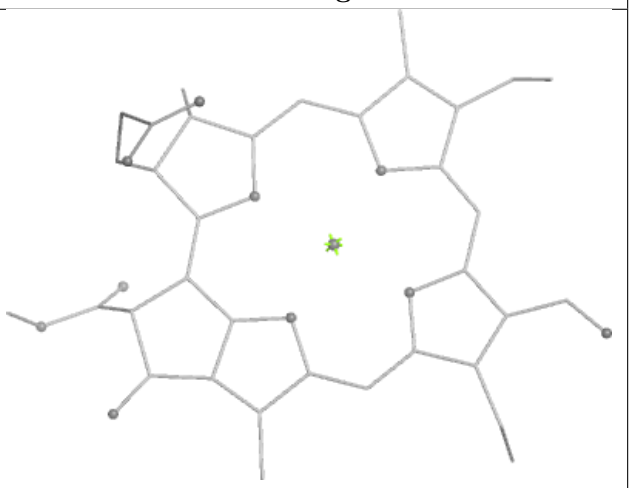
Bond lengths



Bond angles

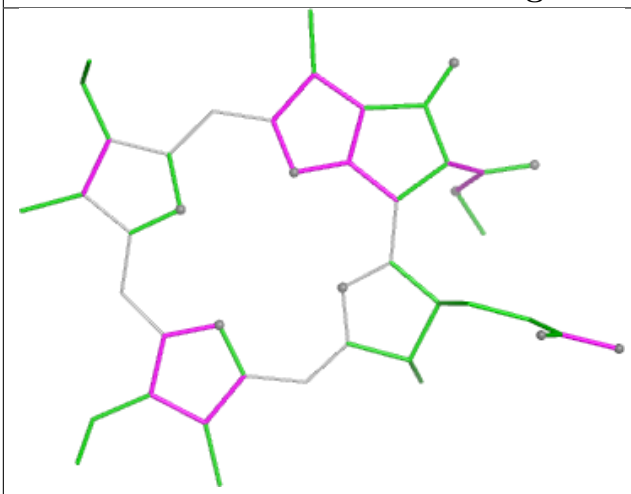


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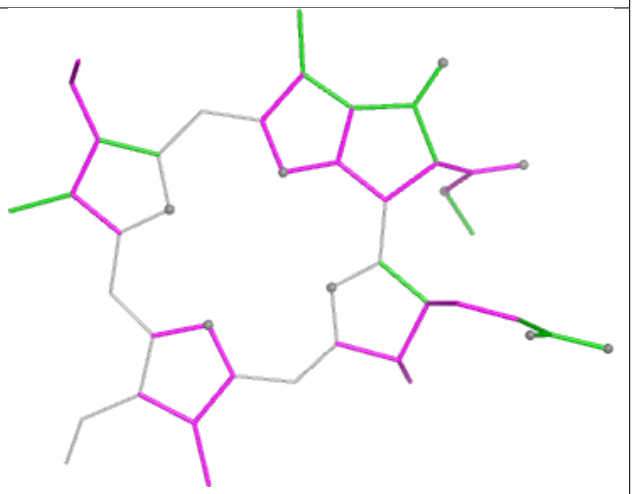


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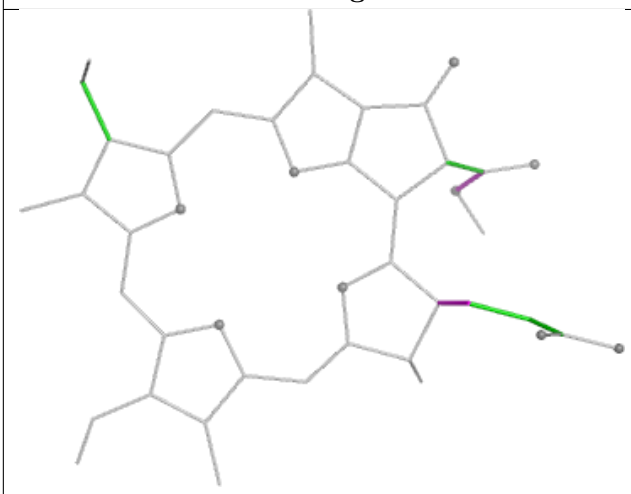
Ligand PHO a 404



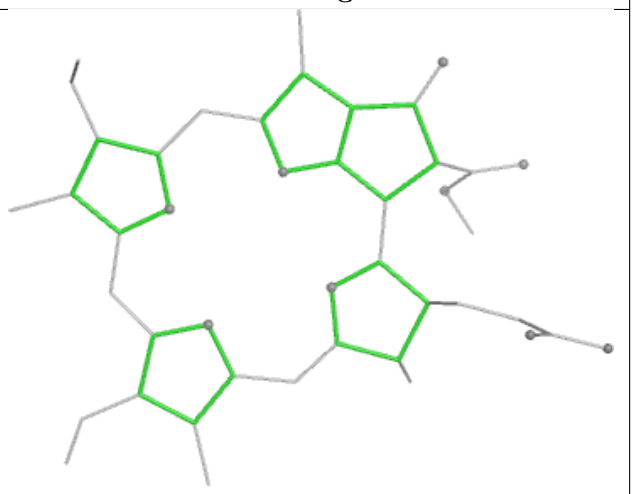
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Bond angles

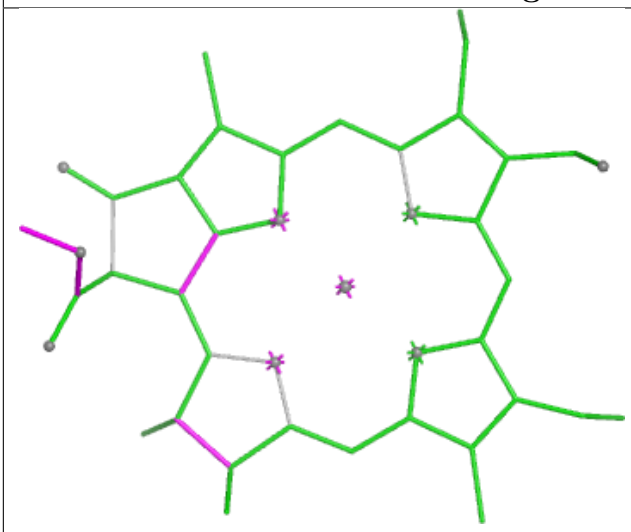


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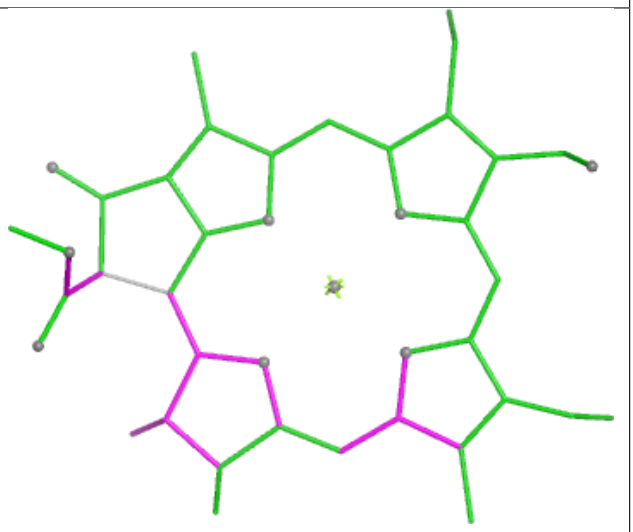


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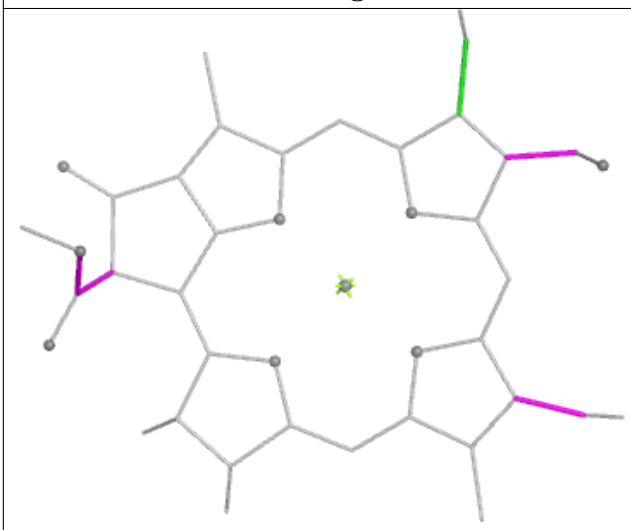
Ligand CHL N 605



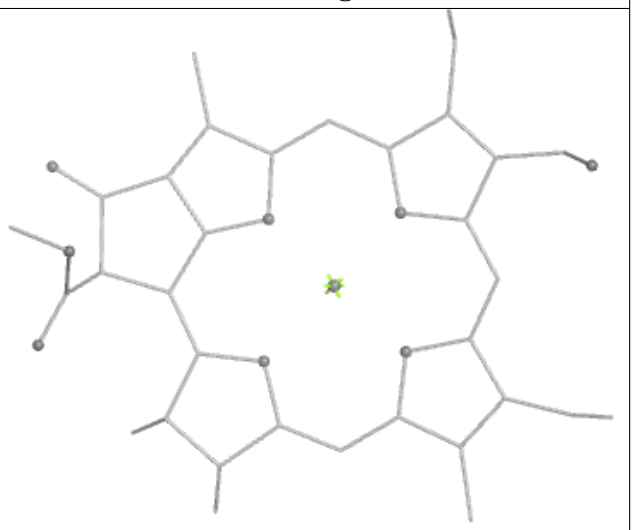
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Bond angles

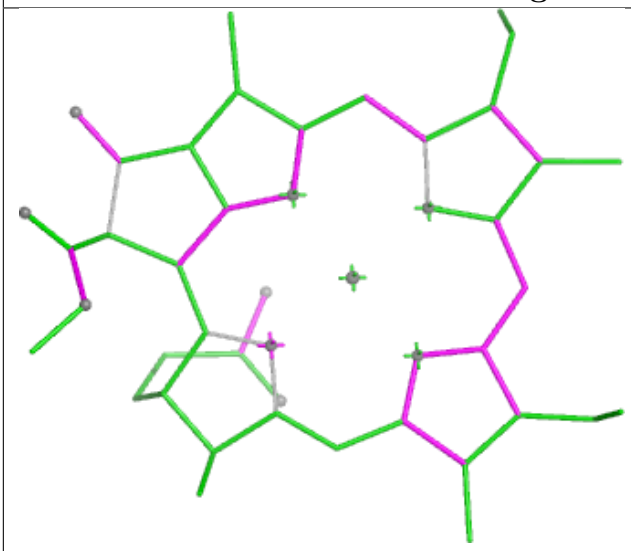


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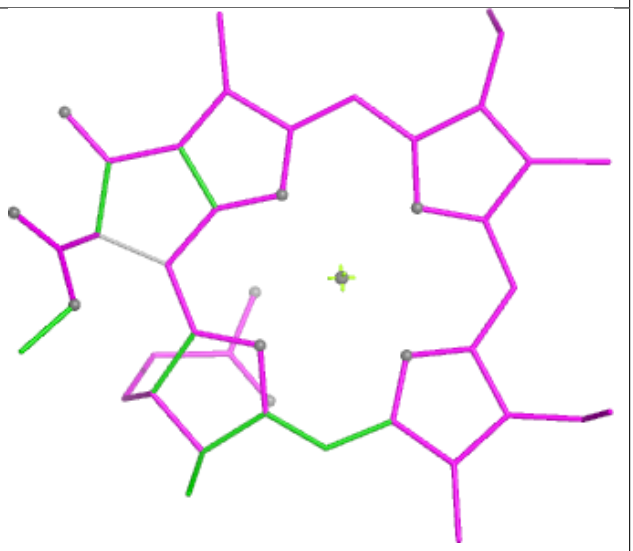


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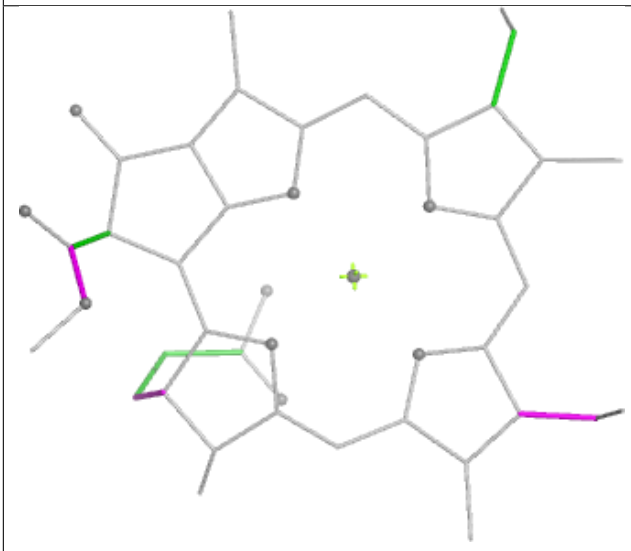
Ligand CLA r 303



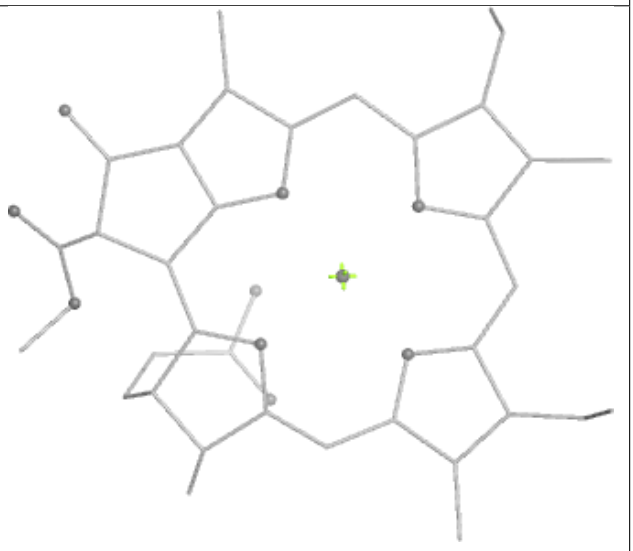
Bond lengths



Bond angles

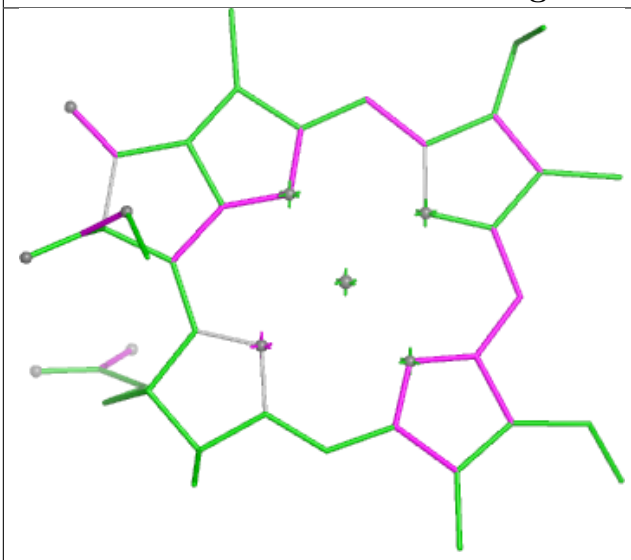


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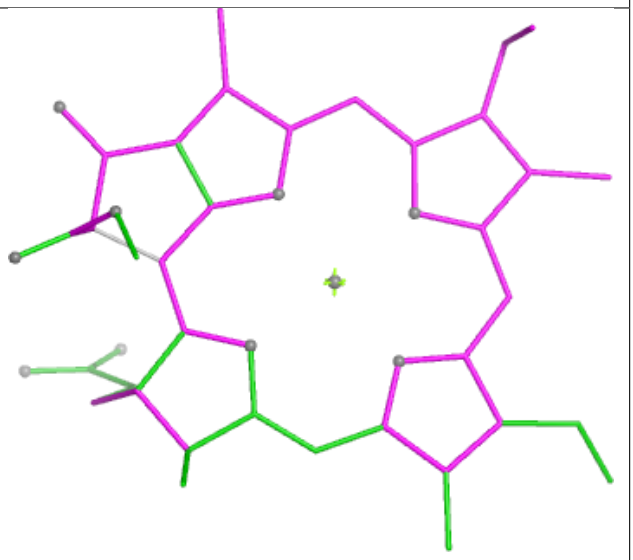


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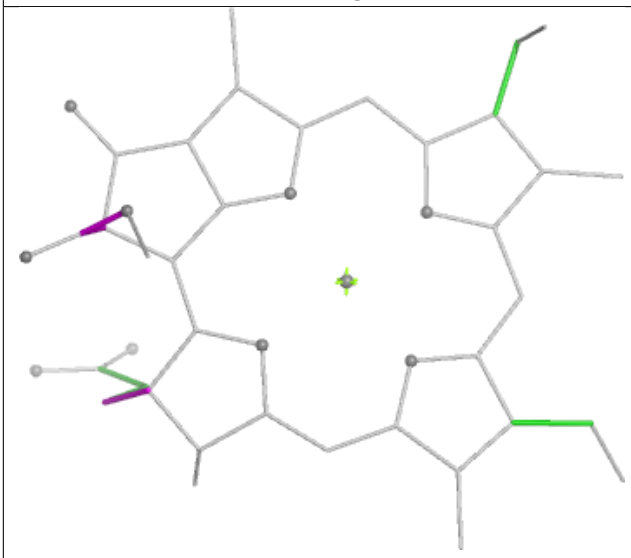
Ligand CLA c 501



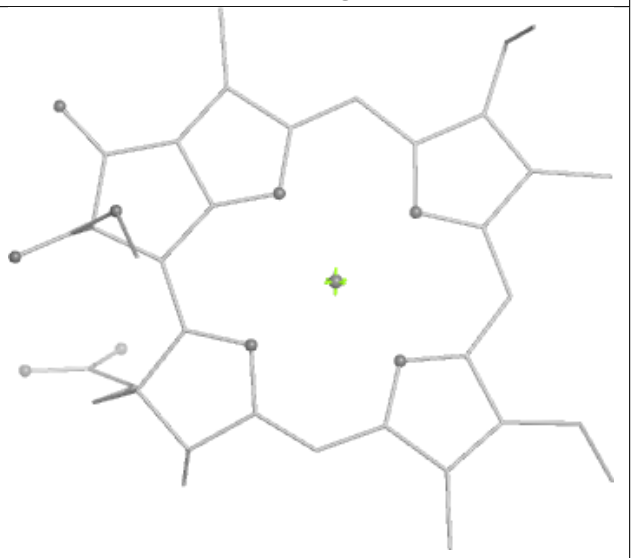
Bond lengths



Bond angles

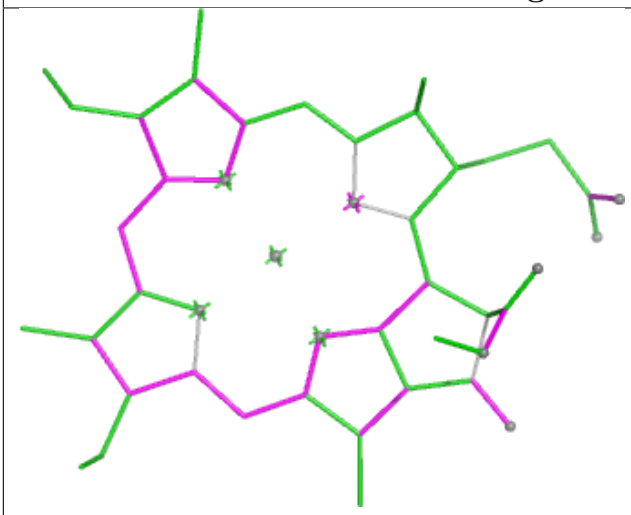


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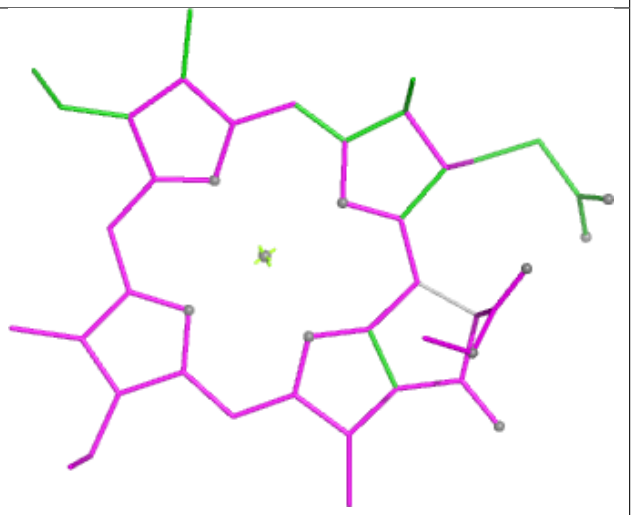


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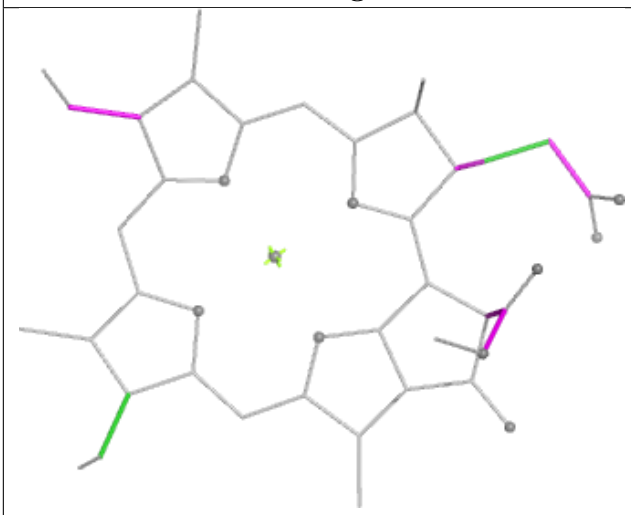
Ligand CLA b 616



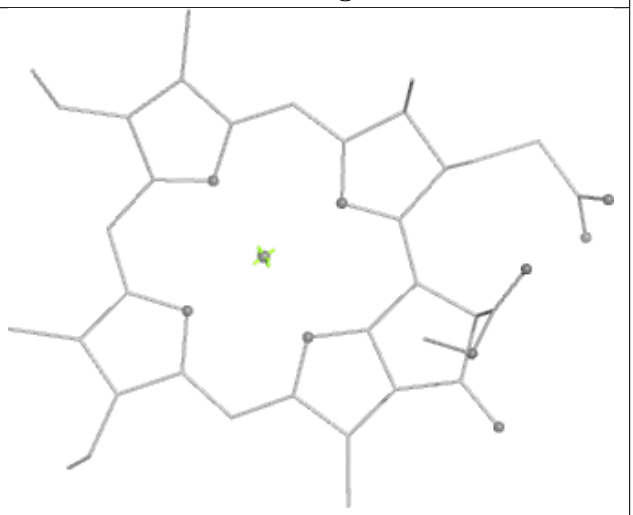
Bond lengths



Bond angles

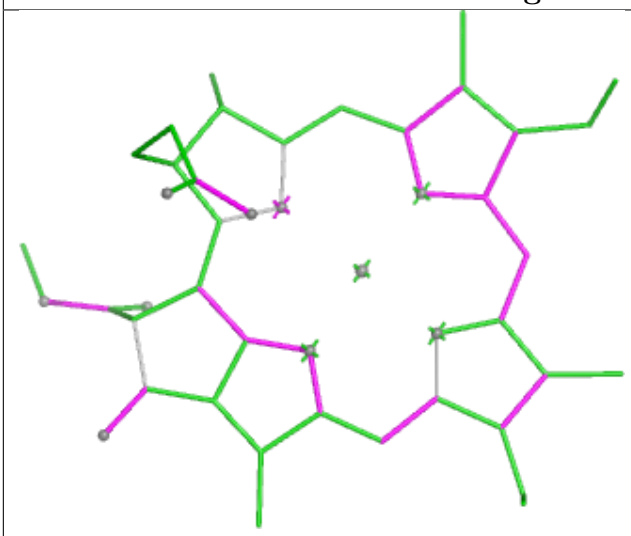


Torsions

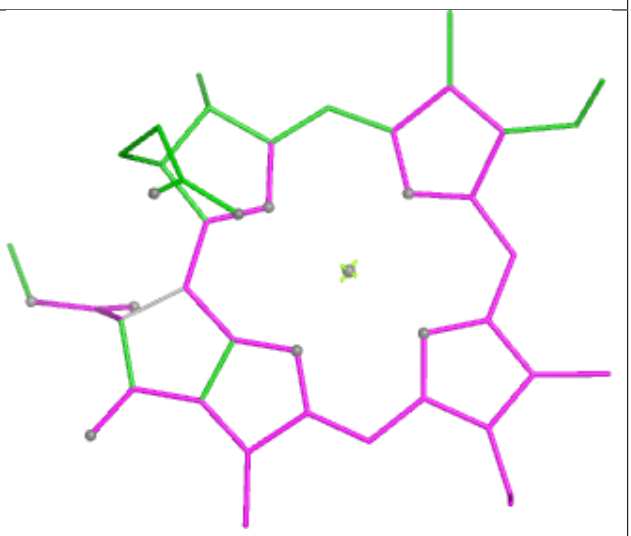


Rings

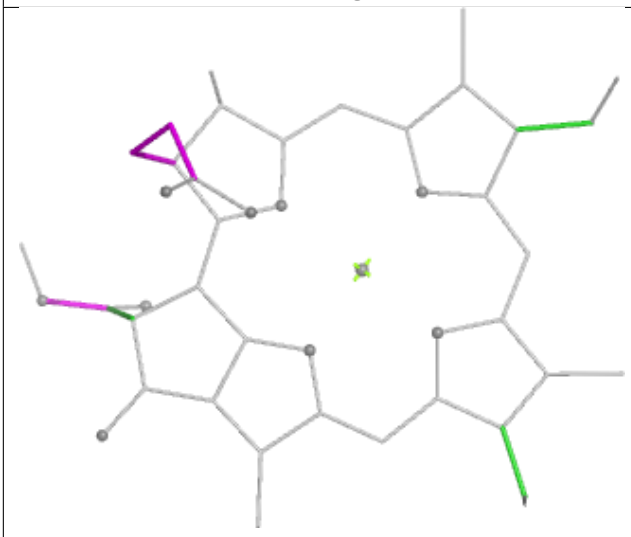
Ligand CLA Y 611



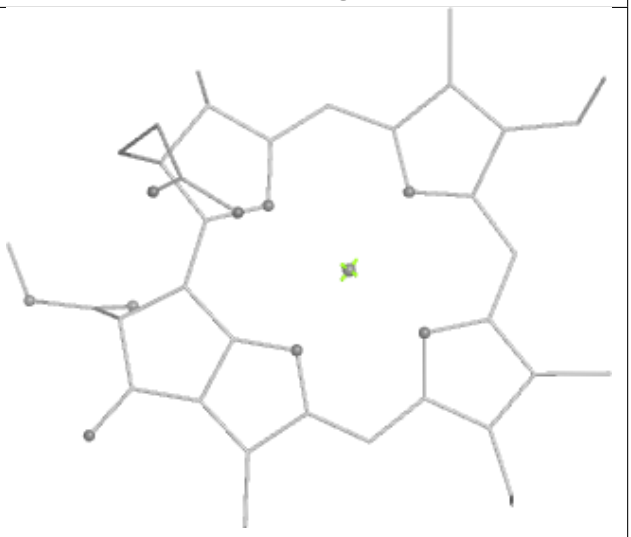
Bond lengths



Bond angles

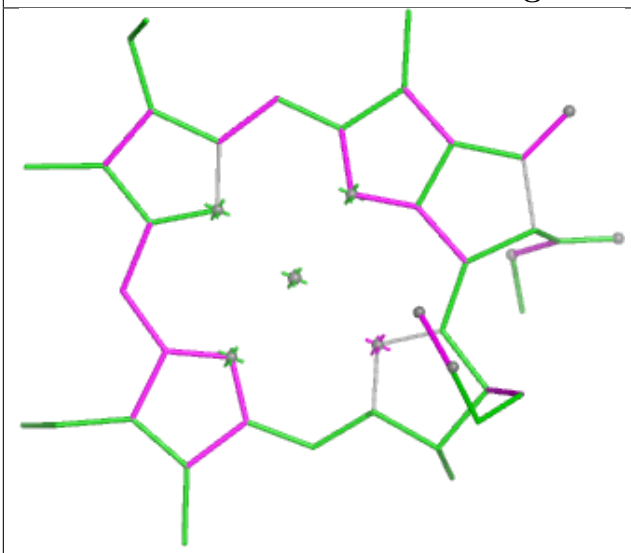


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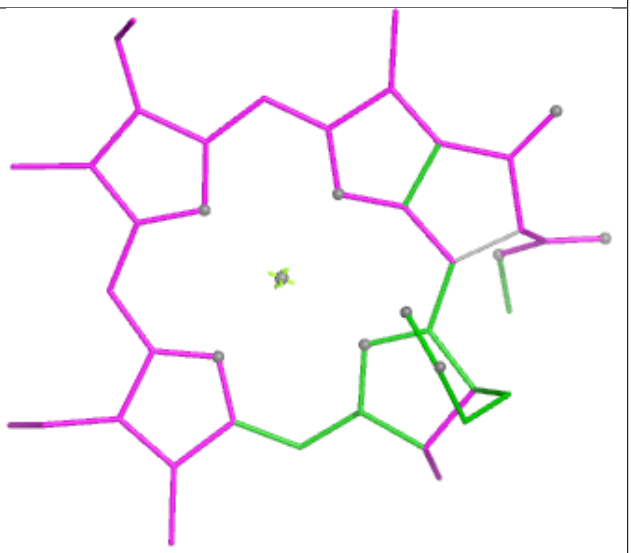


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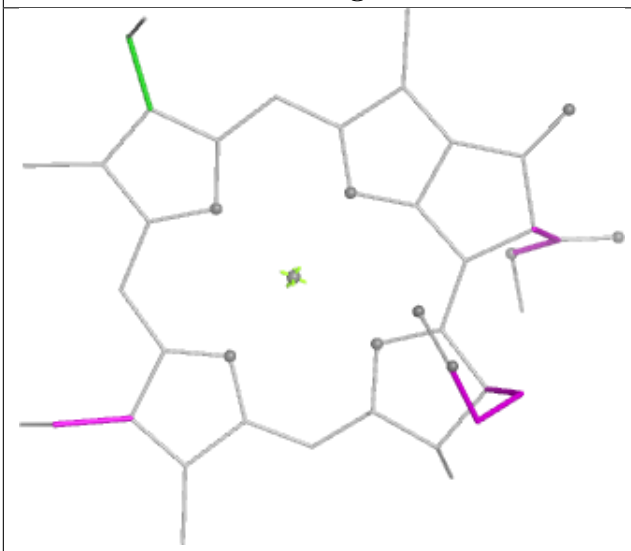
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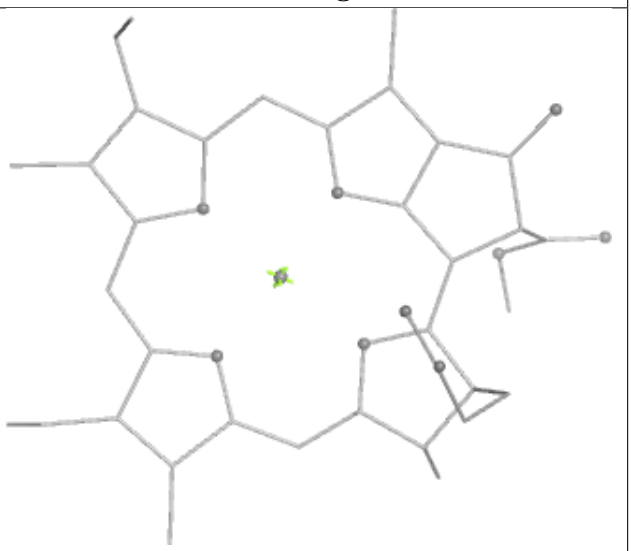
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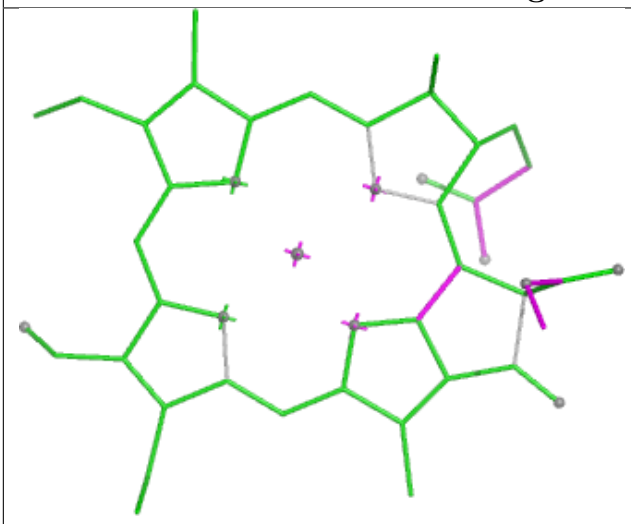


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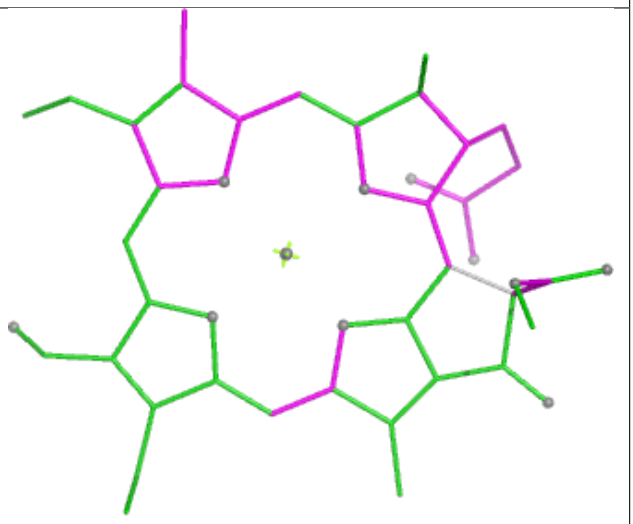


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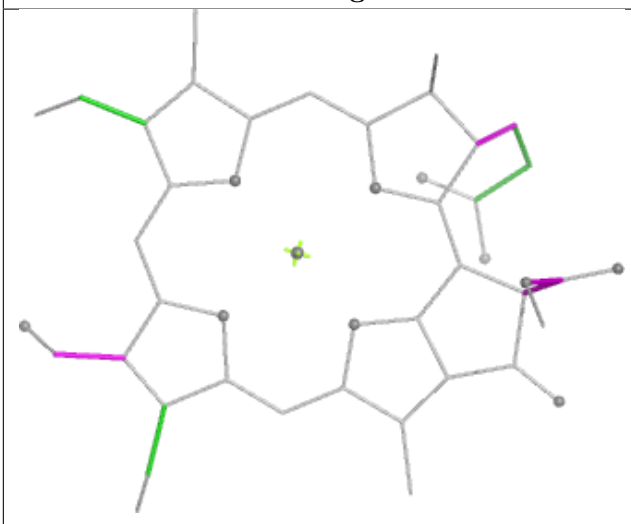
Ligand CHL 8 306



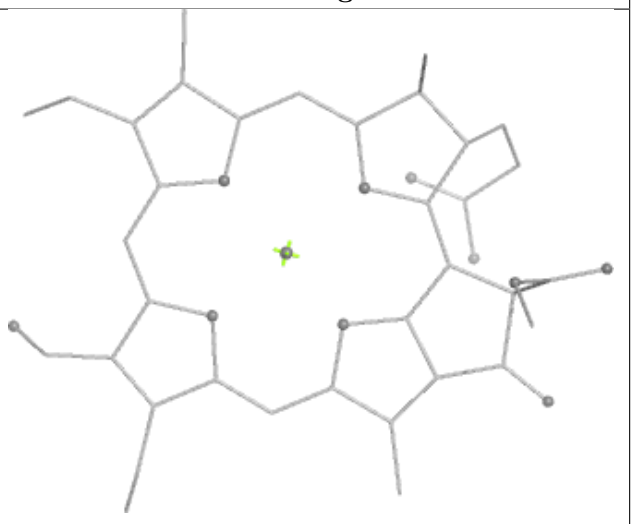
Bond lengths



Bond angles

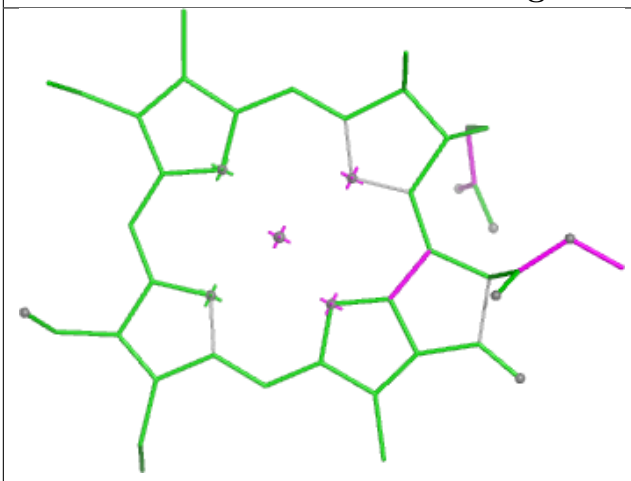


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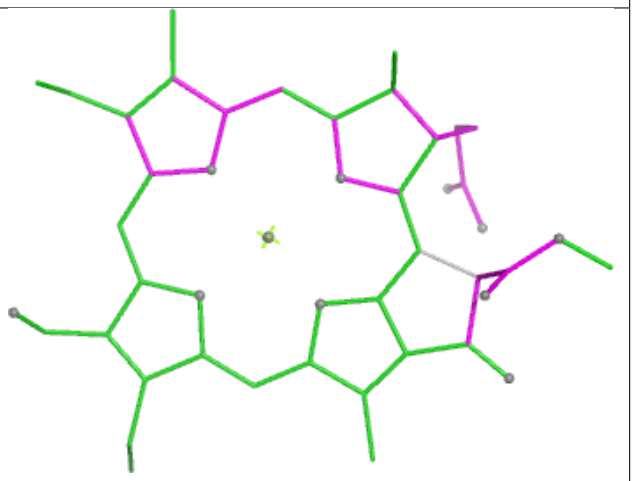


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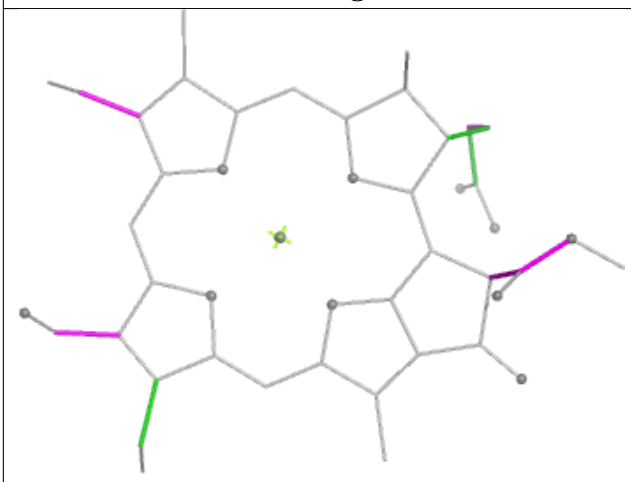
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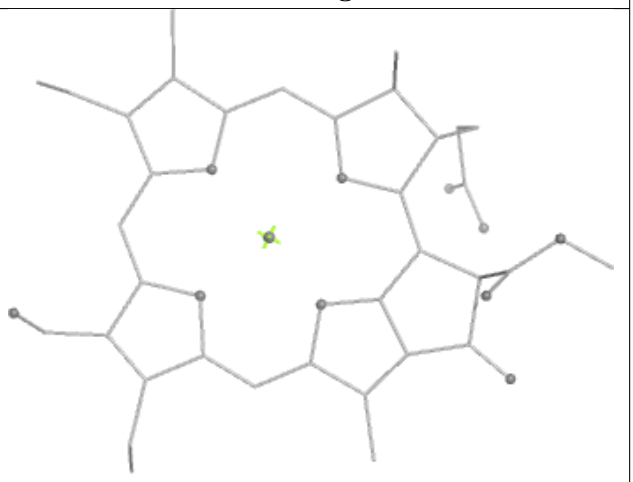
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Bond angles

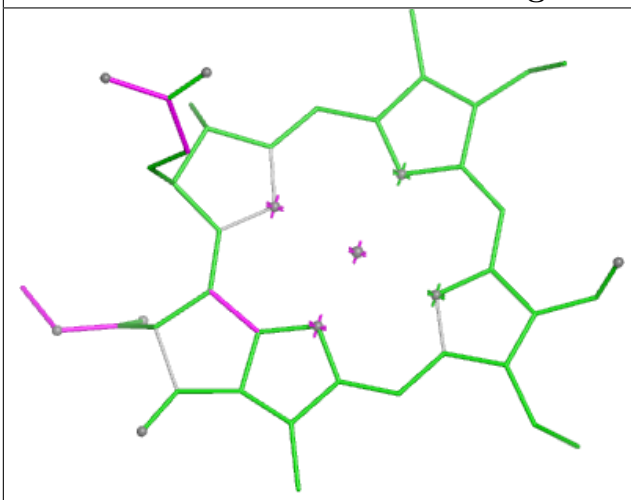


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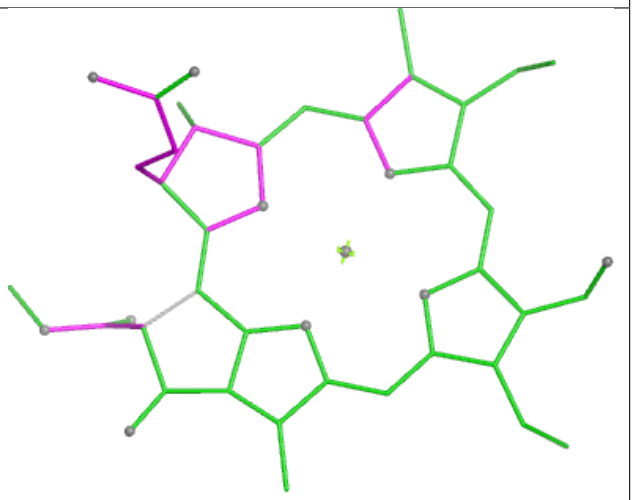


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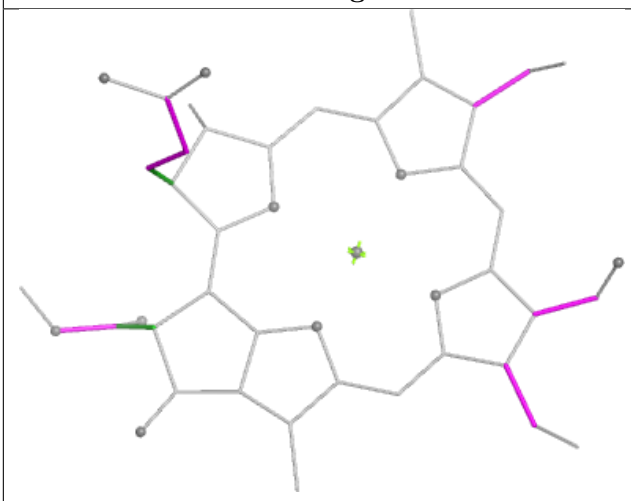
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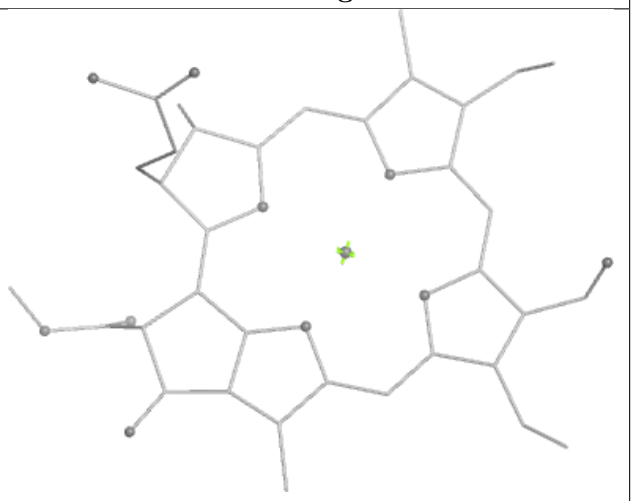
Bond lengths



Bond angles

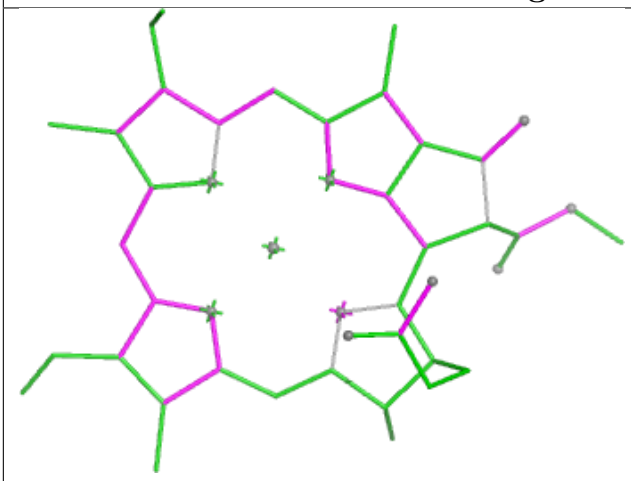


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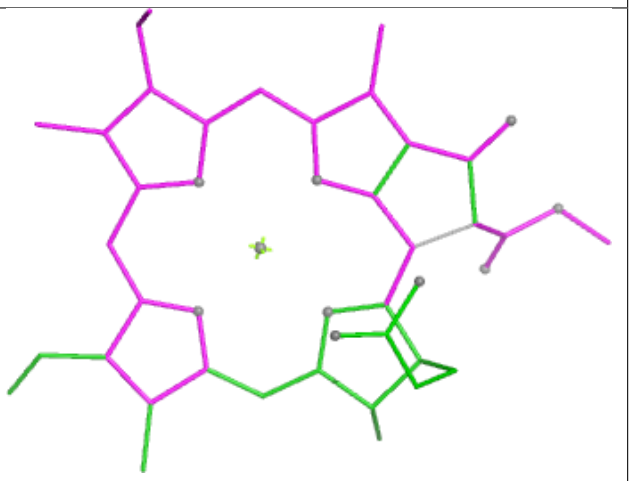


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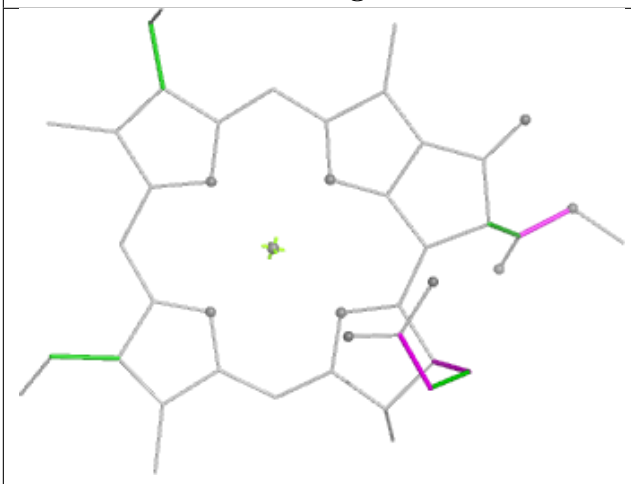
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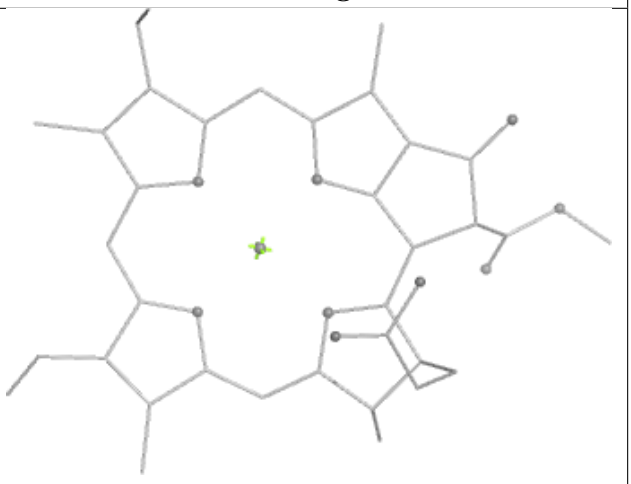
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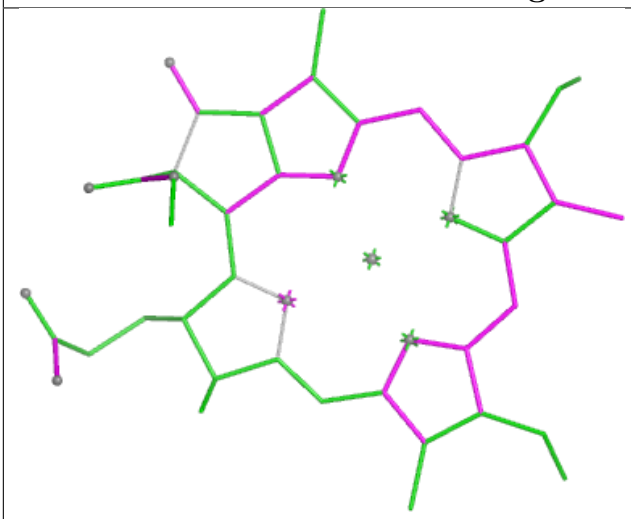


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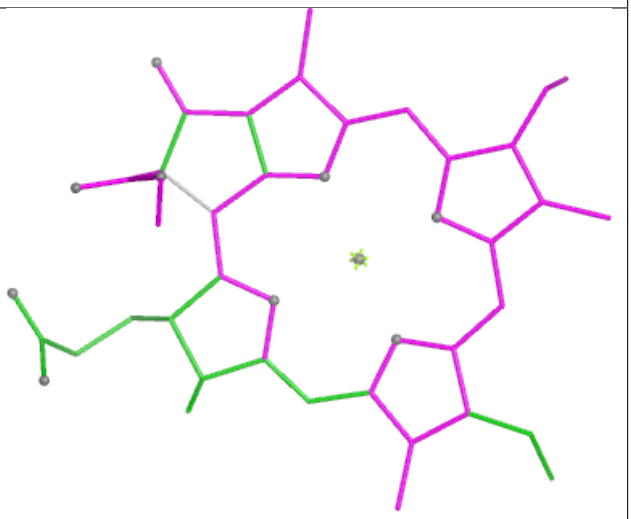


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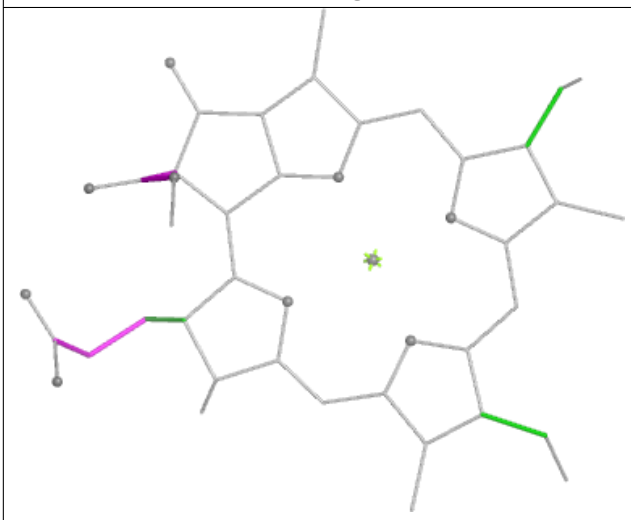
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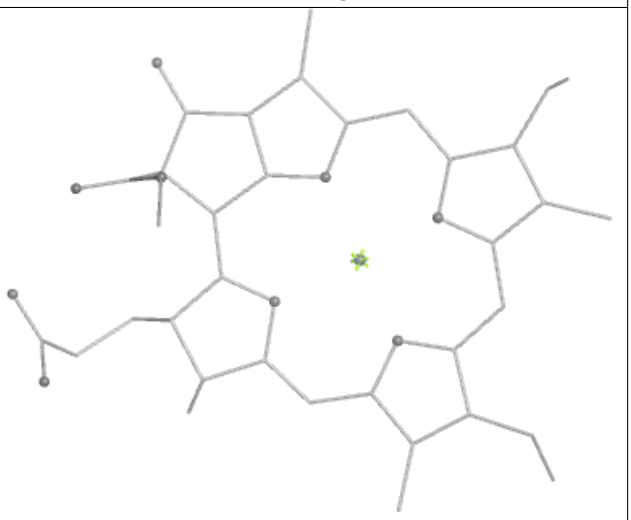
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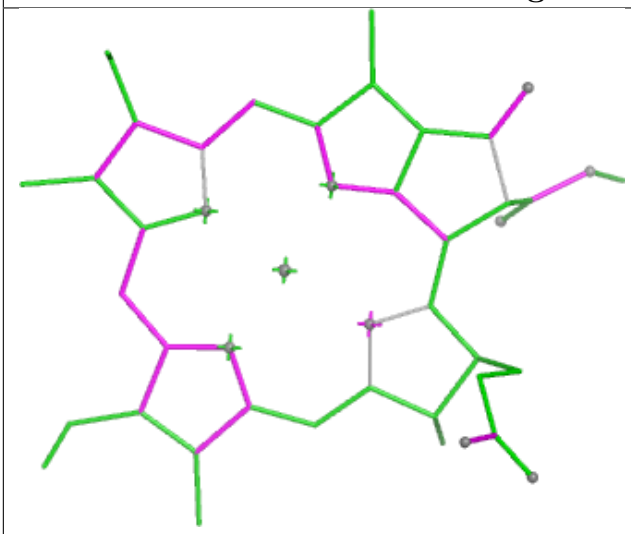


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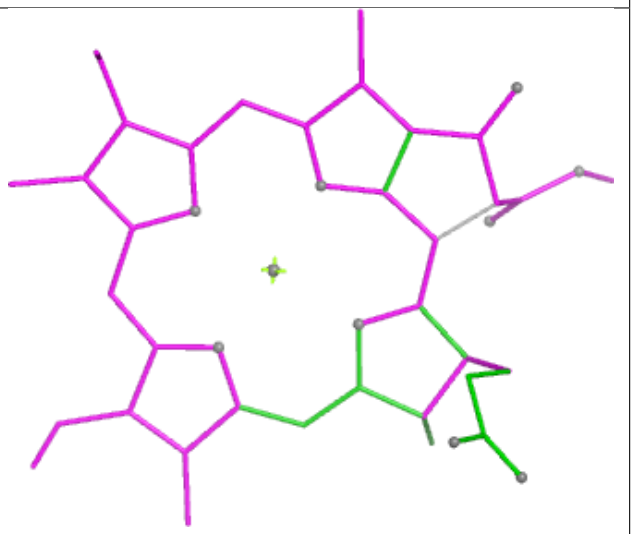


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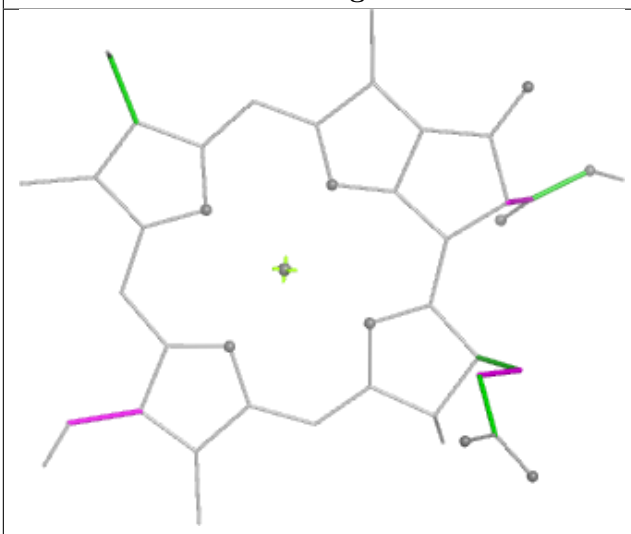
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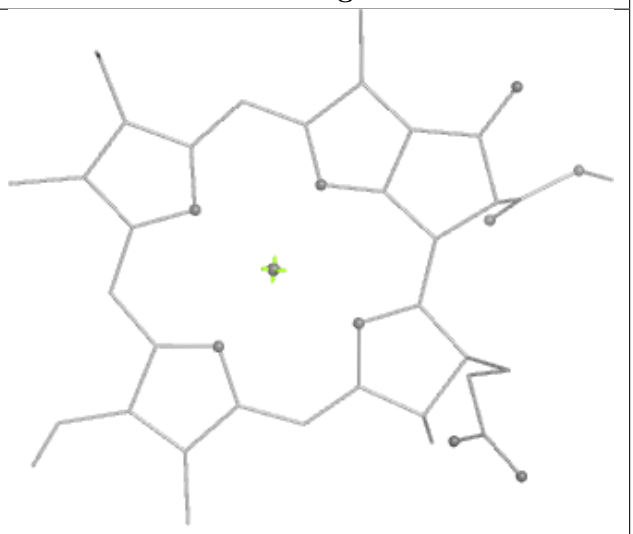
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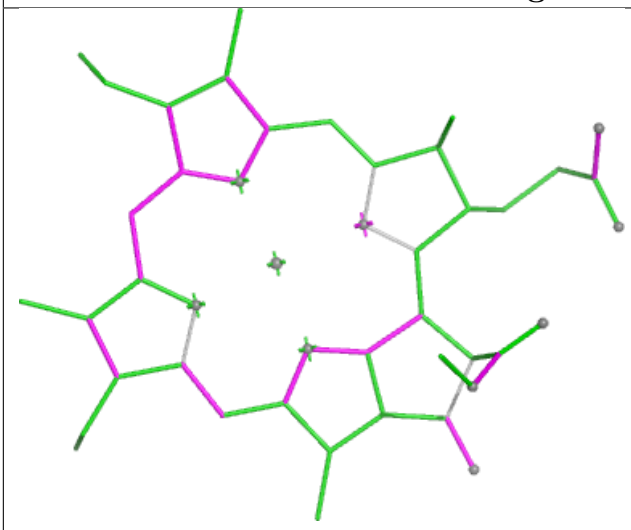


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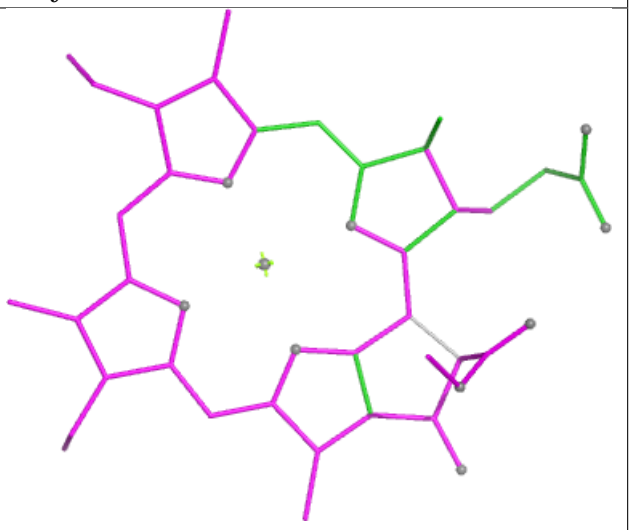


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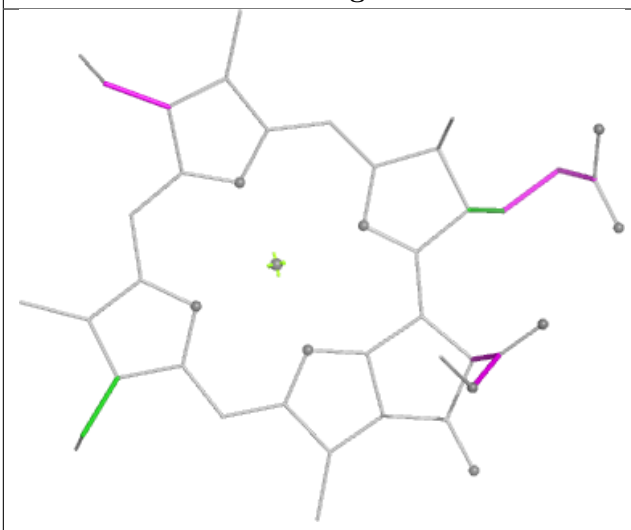
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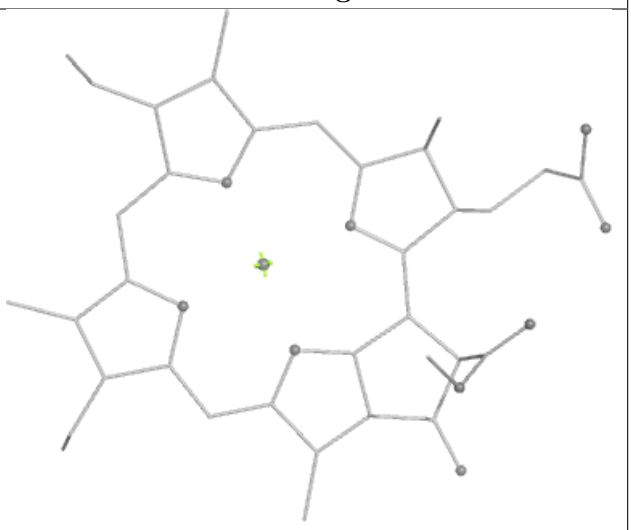
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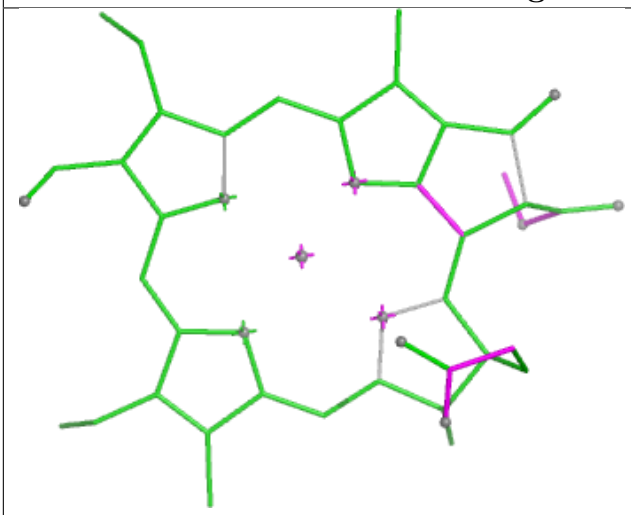


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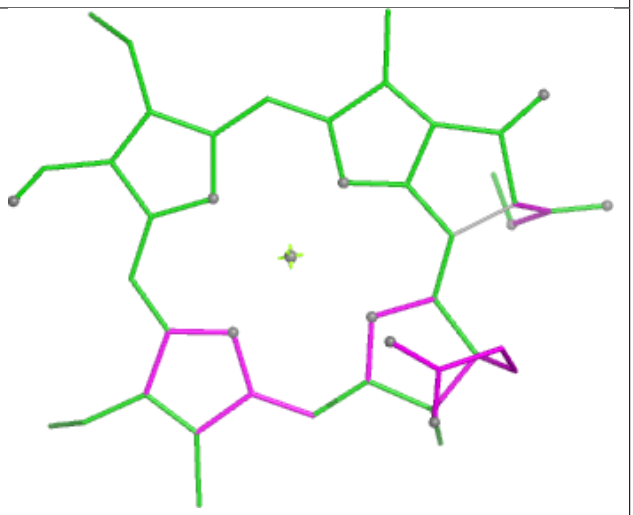


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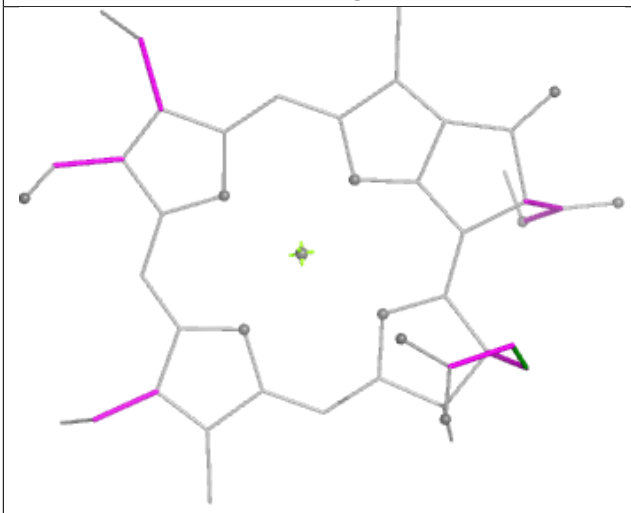
Ligand CHL 4 307



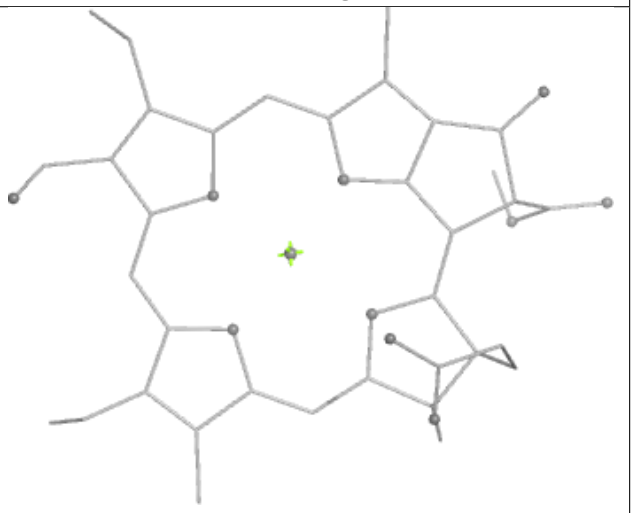
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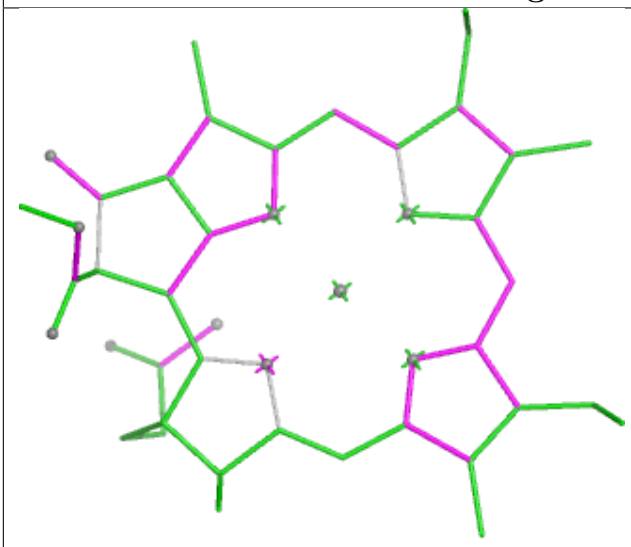
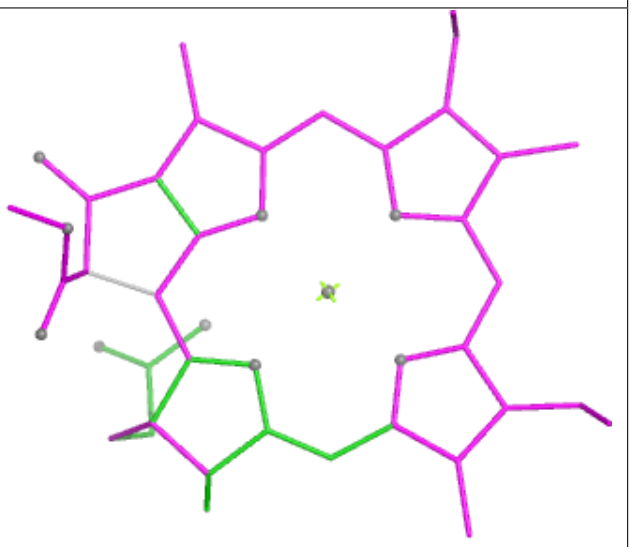
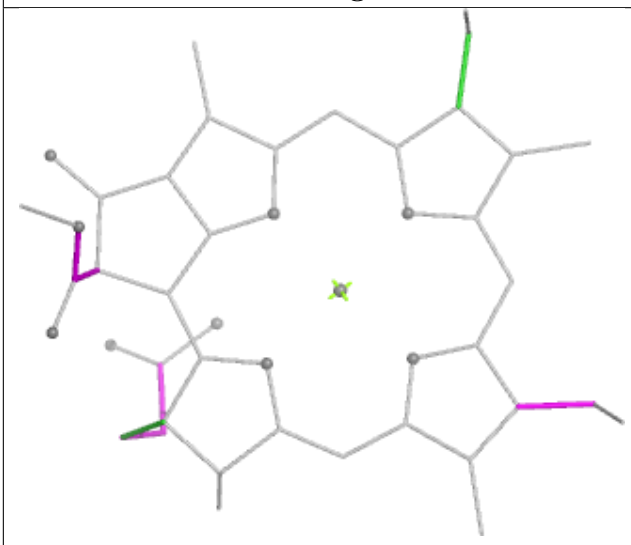
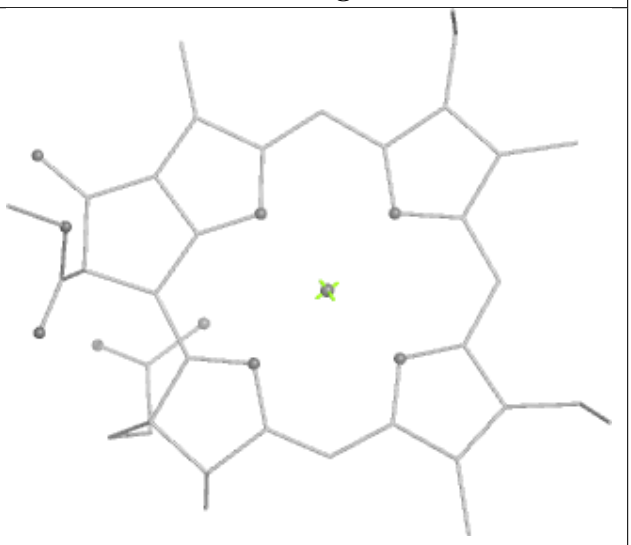
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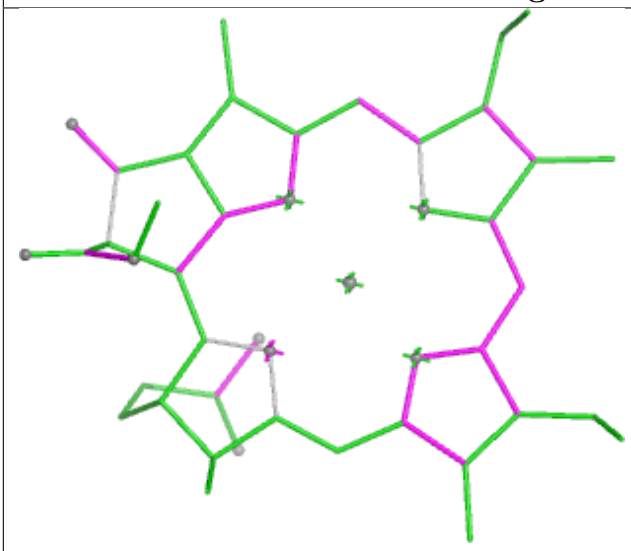
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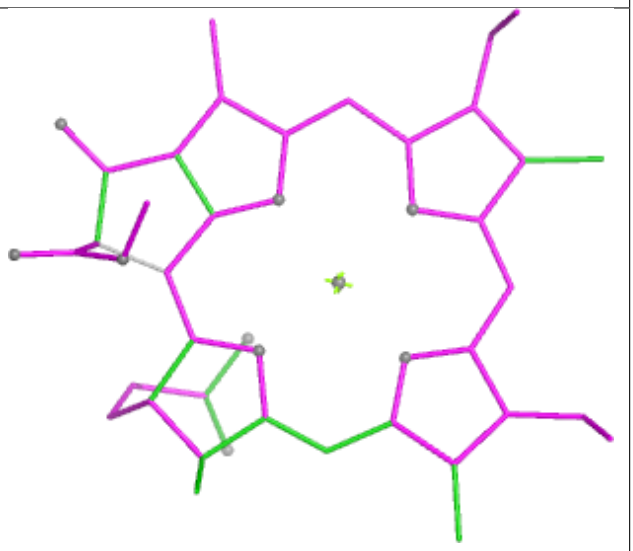
Rings

Ligand CLA b 601	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

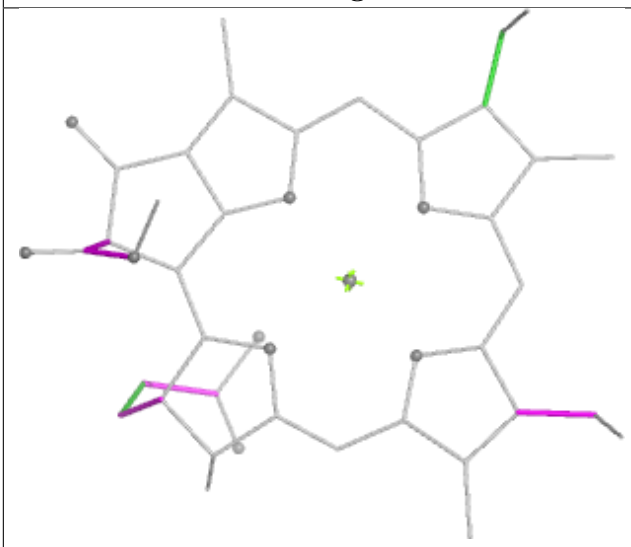
Ligand CLA a 403



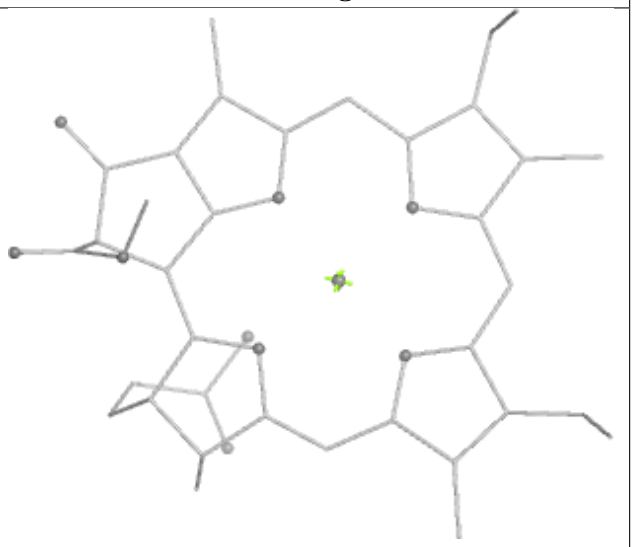
Bond lengths



Bond angles

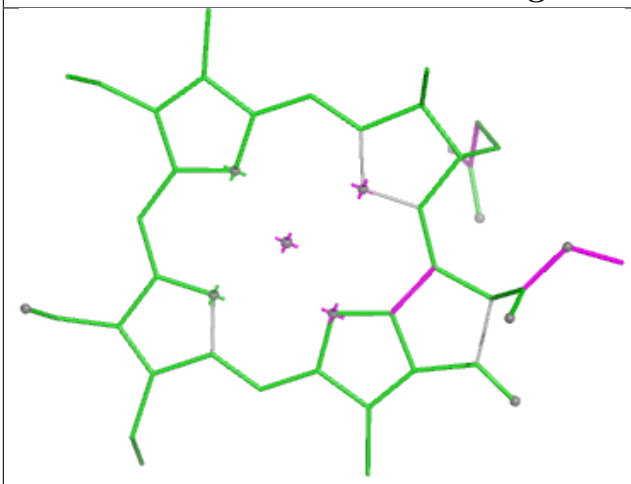


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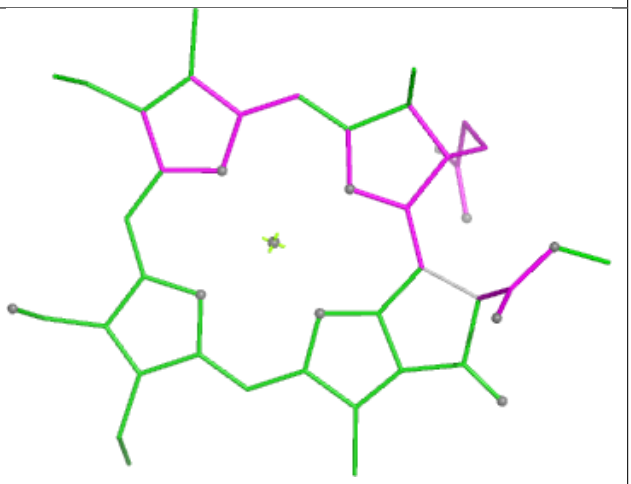


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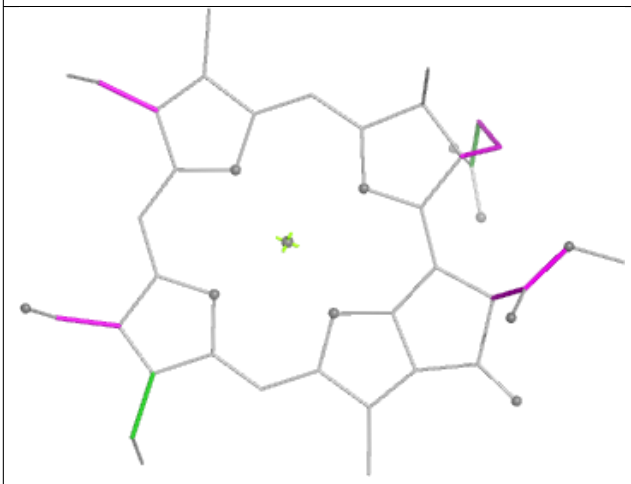
Ligand CHL 5 615



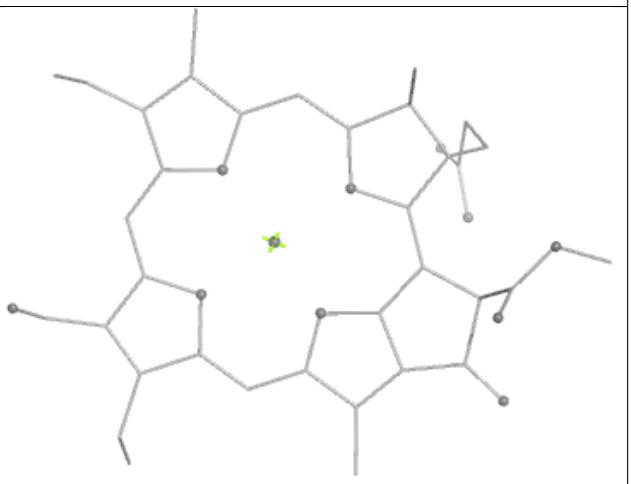
Bond lengths



Bond angles

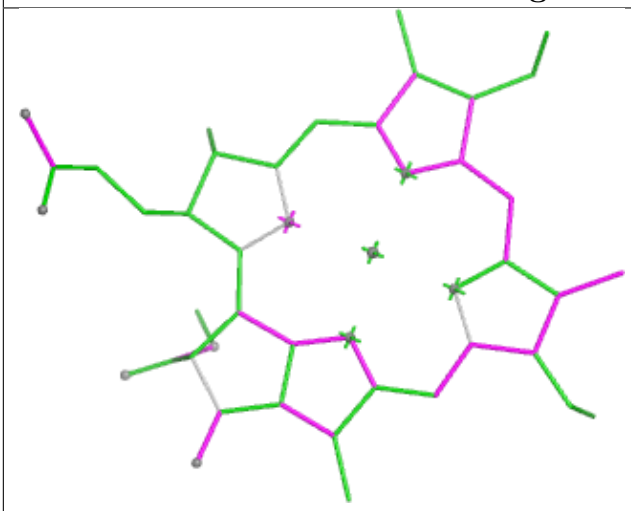


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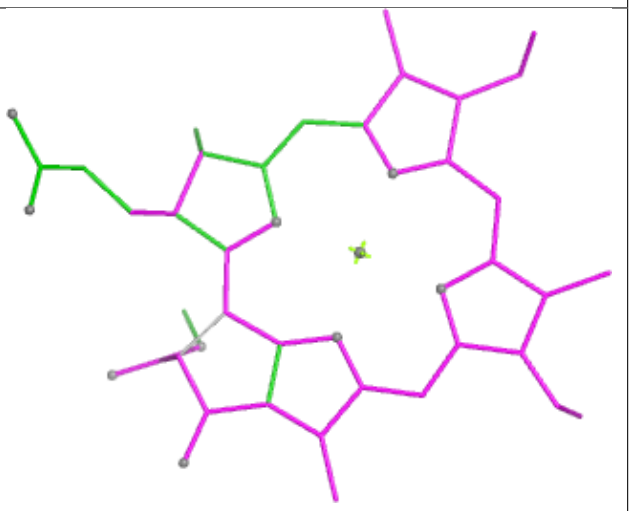


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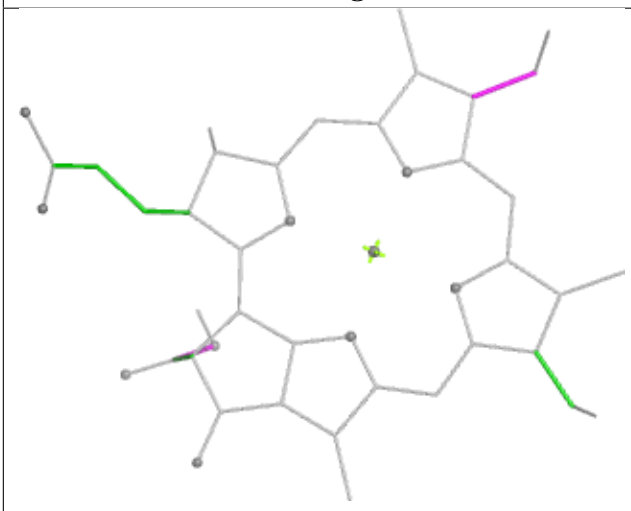
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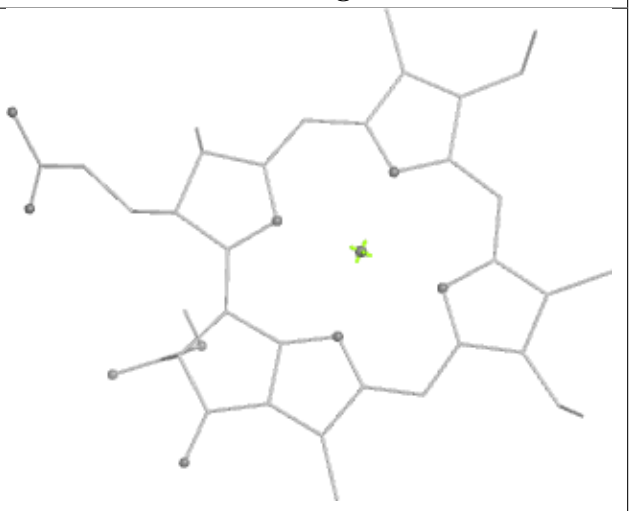
Bond lengths



Bond angles

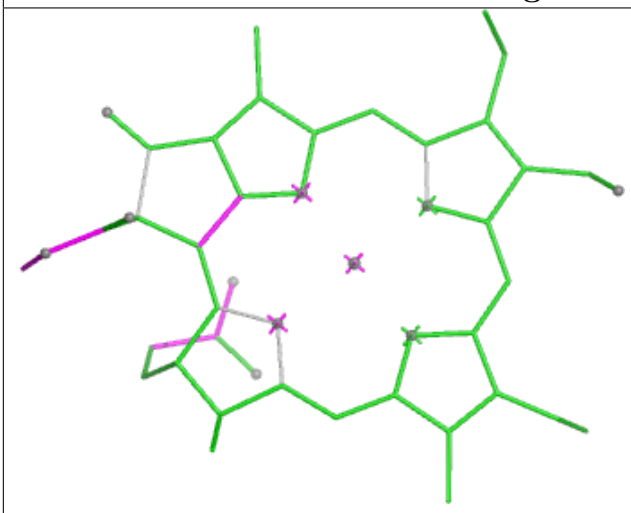


Torsions

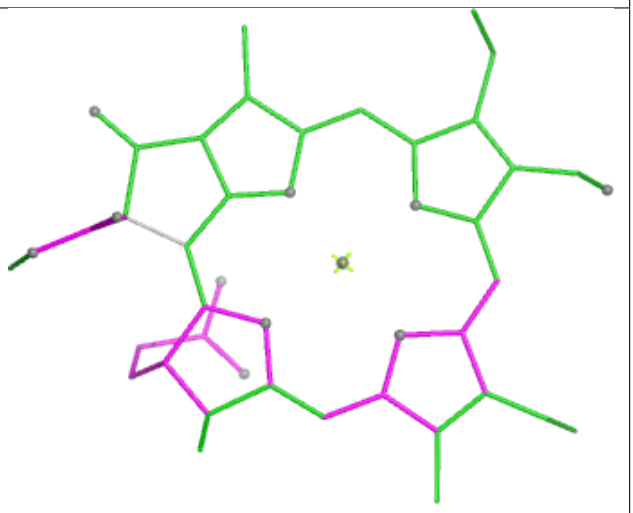


Rings

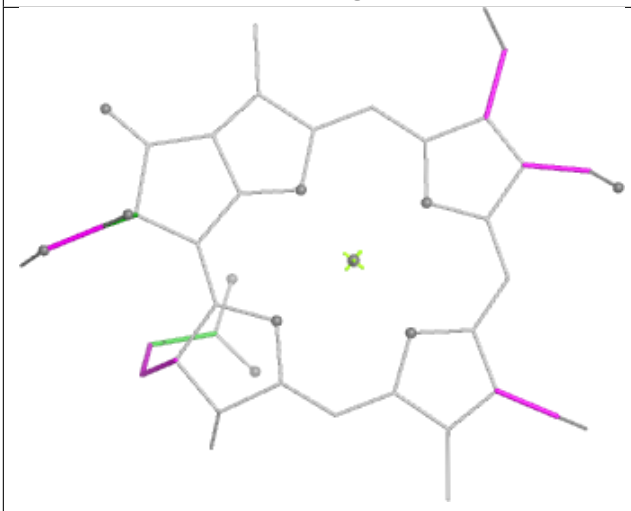
Ligand CHL R 305



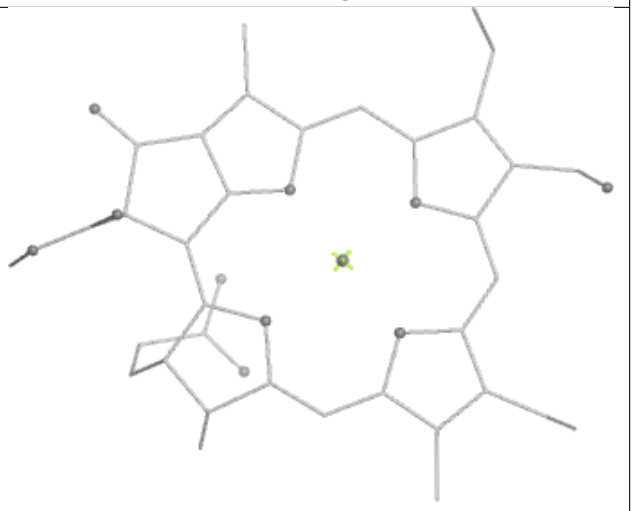
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Bond angles

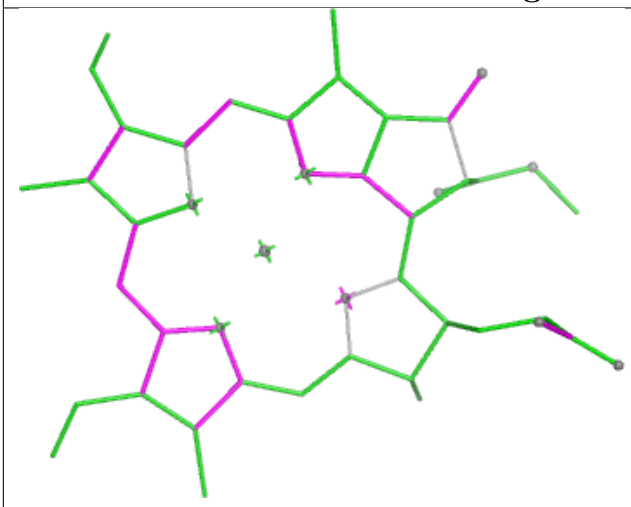


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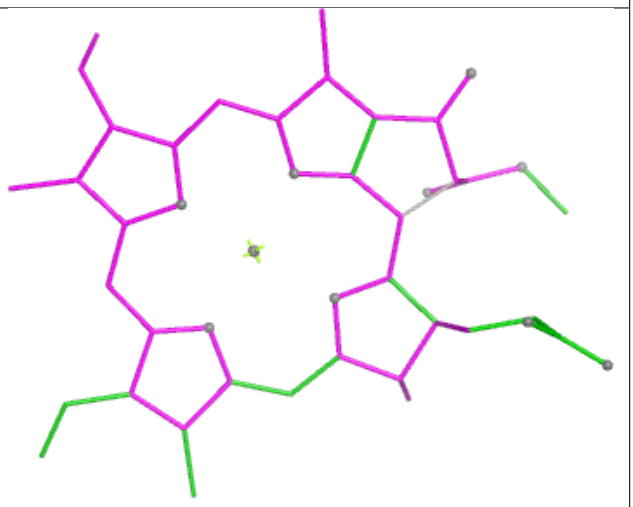


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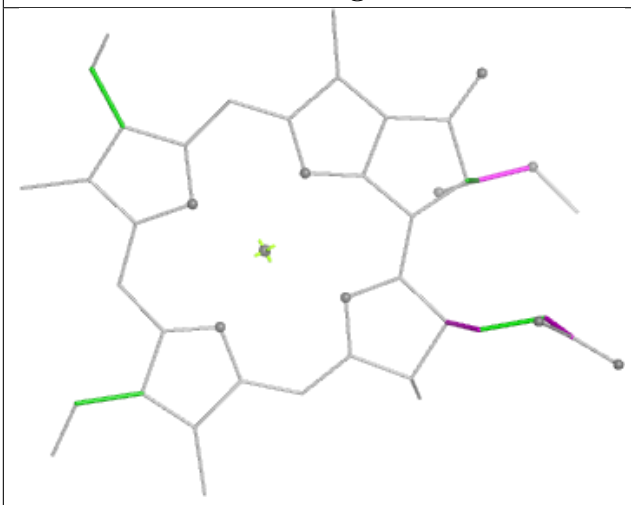
Ligand CLA D 403



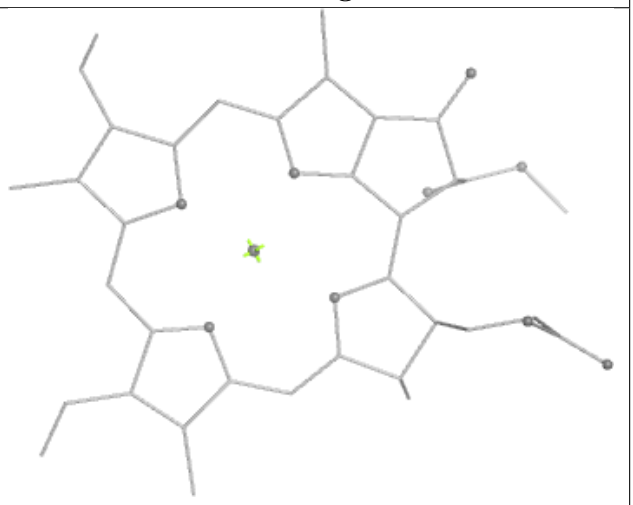
Bond lengths



Bond angles

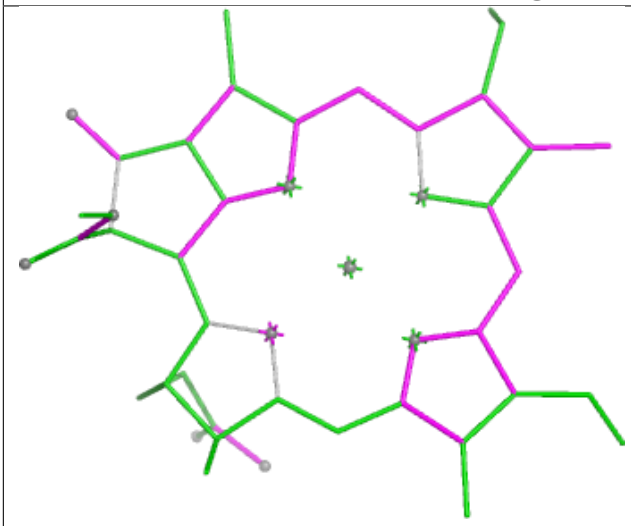


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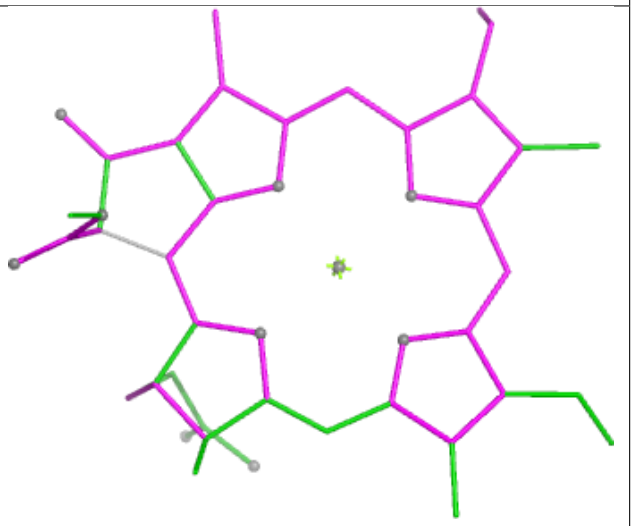


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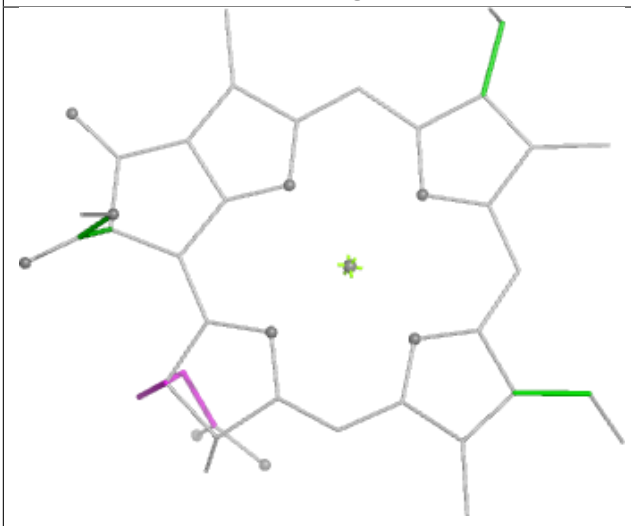
Ligand CLA 1 604



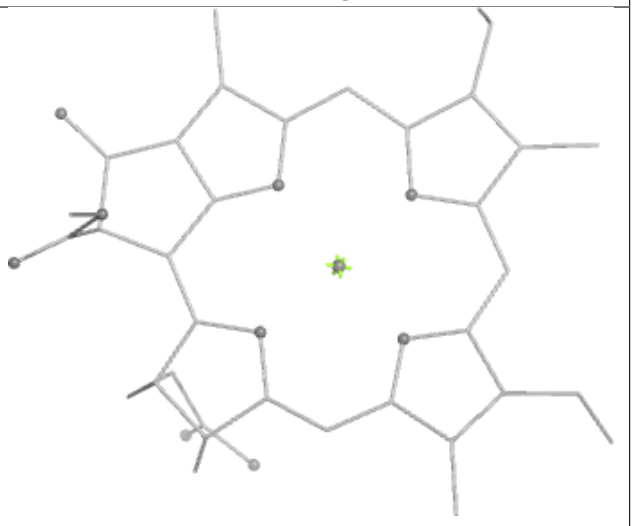
Bond lengths



Bond angles

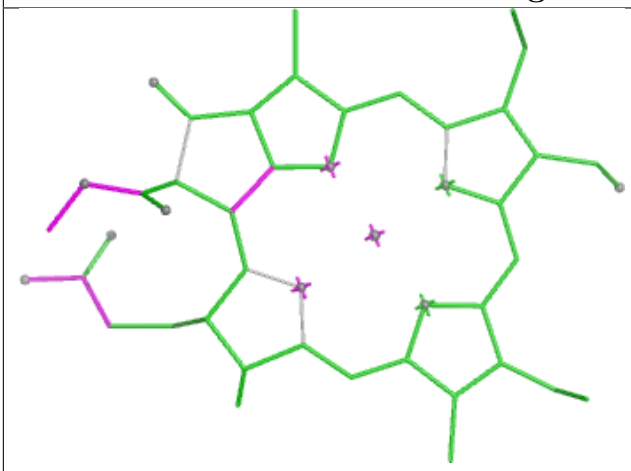


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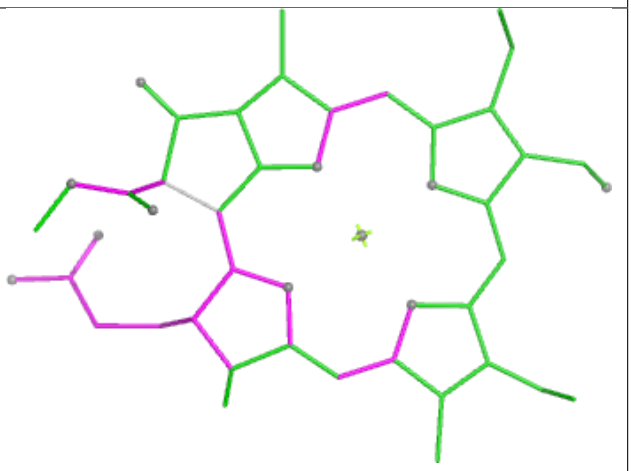


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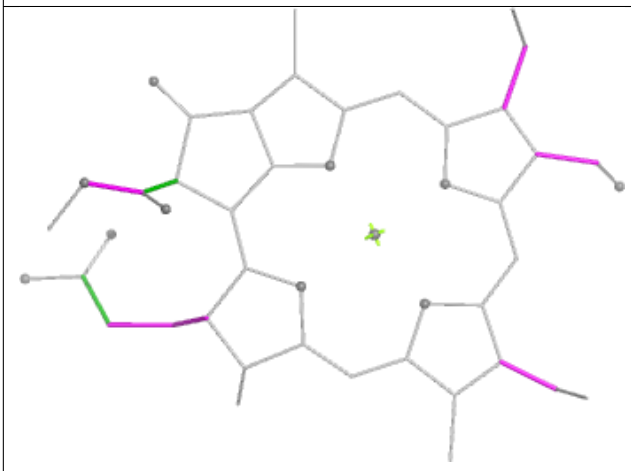
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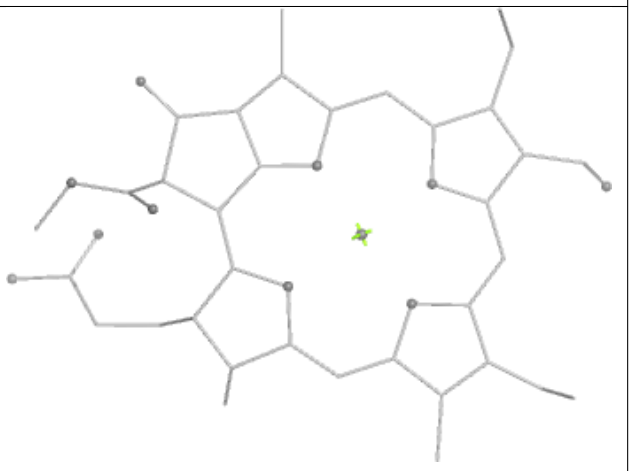
Bond lengths



Bond angles

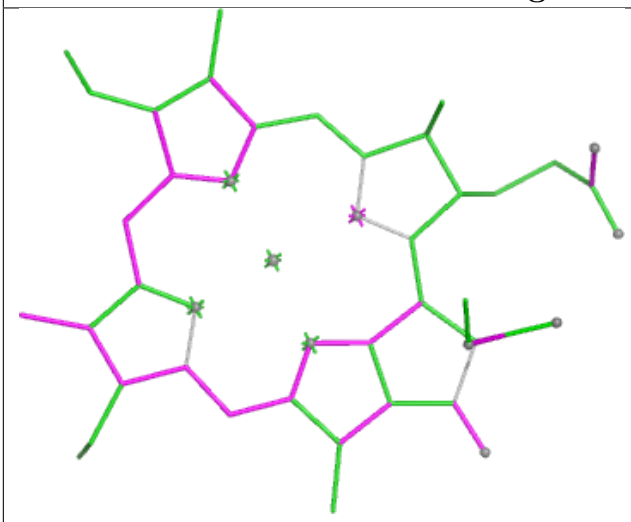


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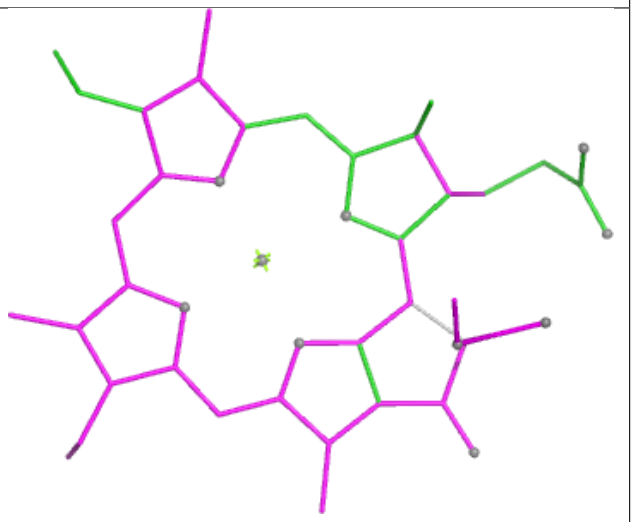


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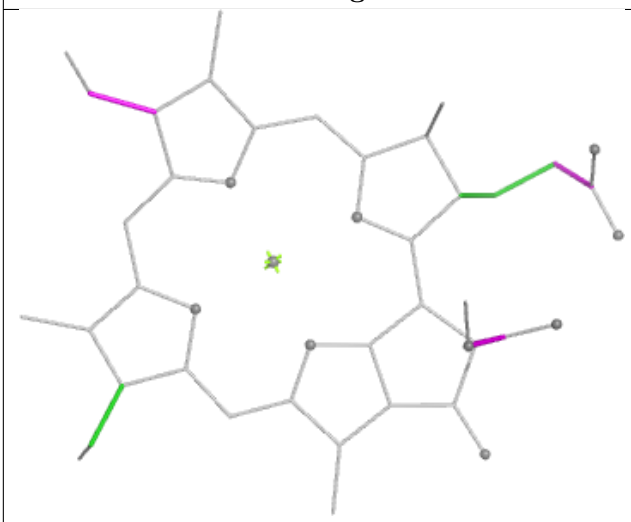
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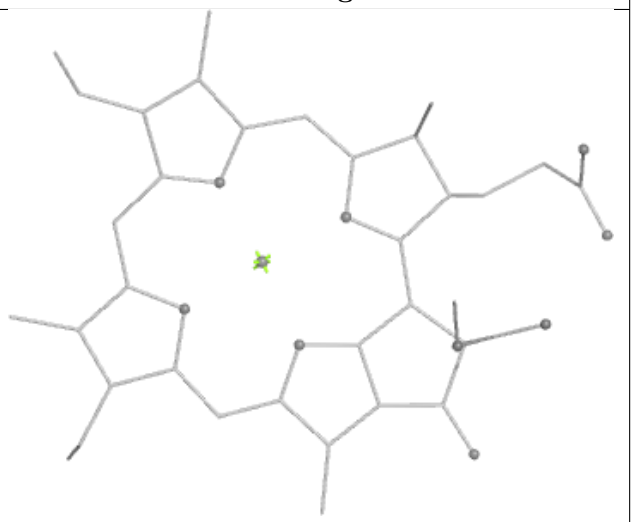
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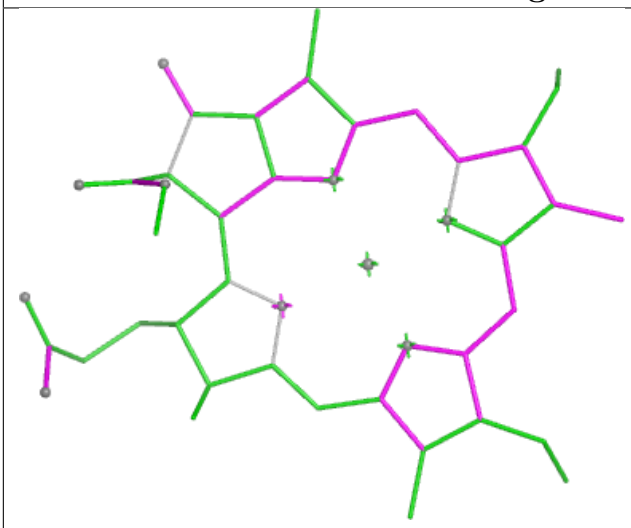


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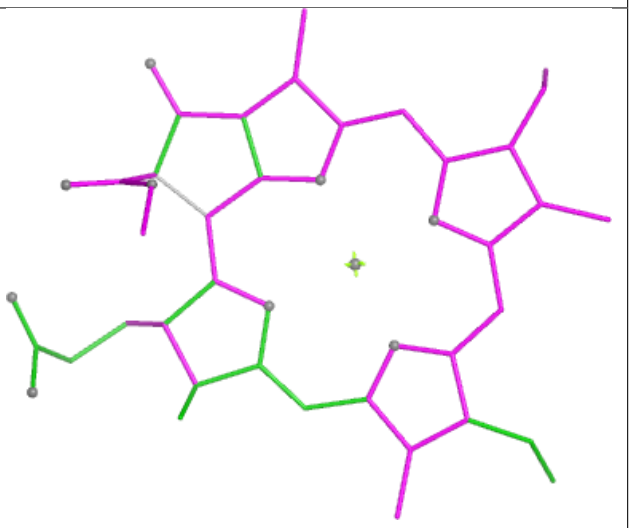


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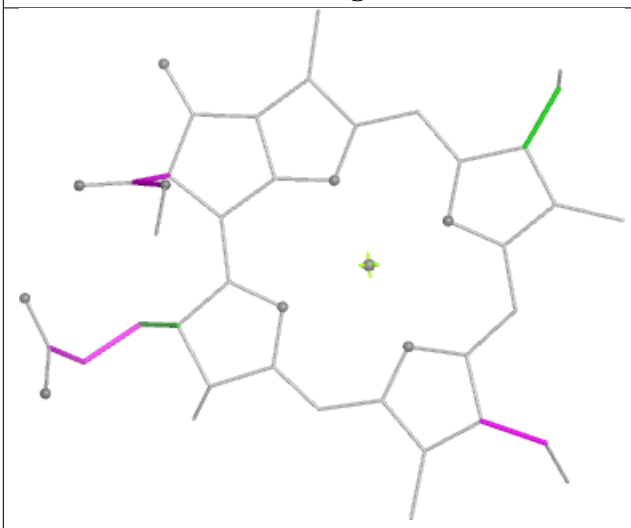
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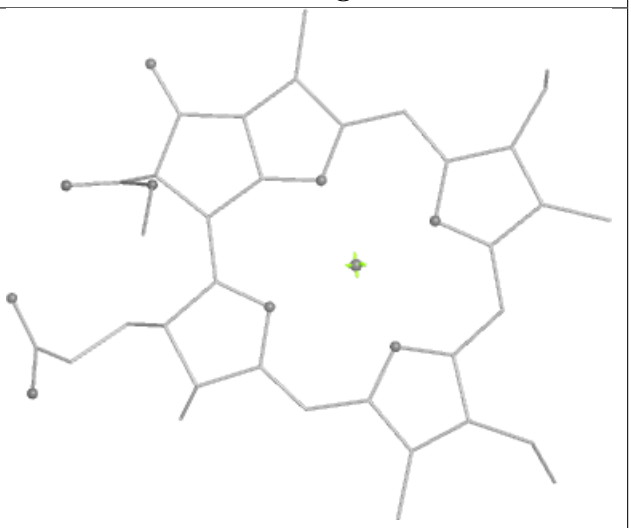
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Bond angles

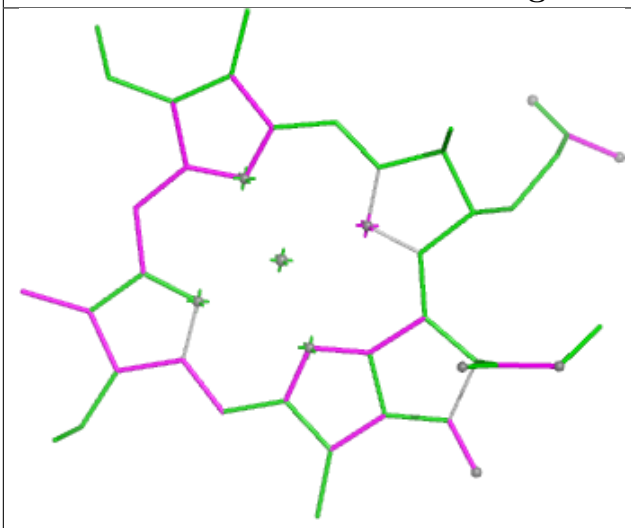


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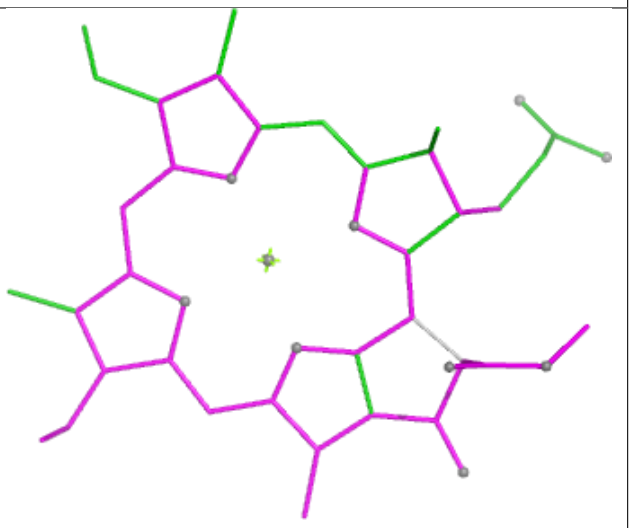


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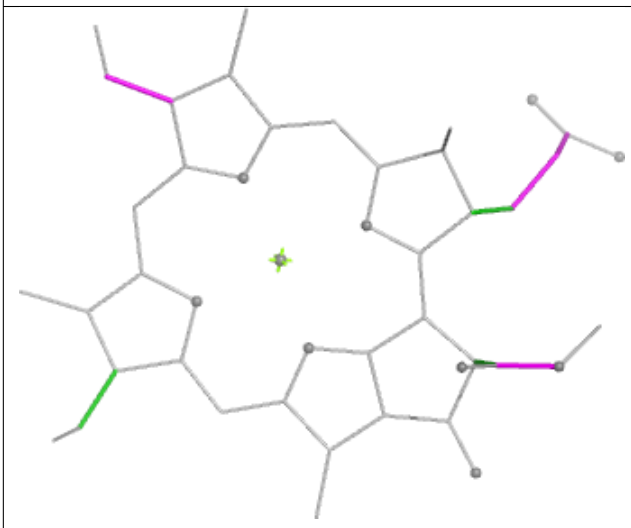
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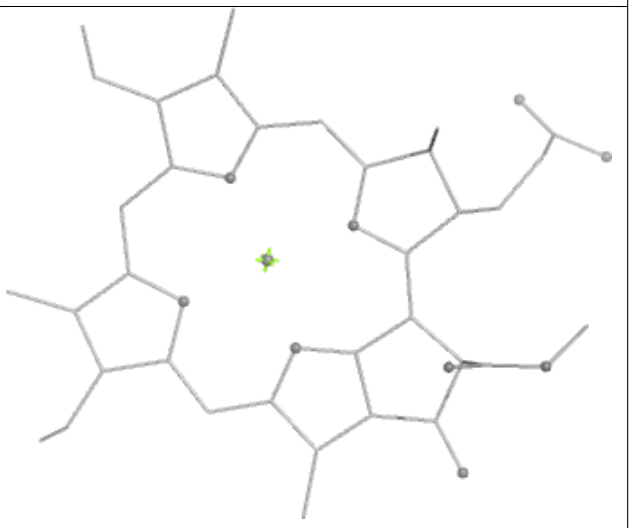
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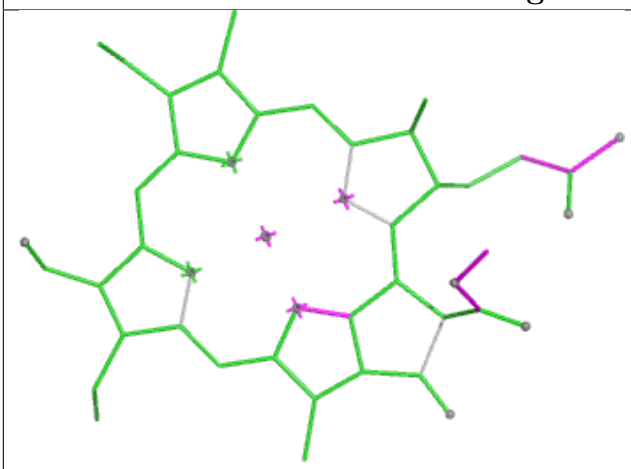


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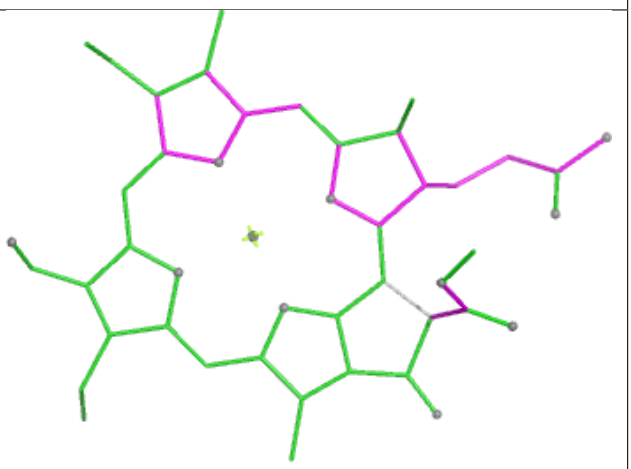


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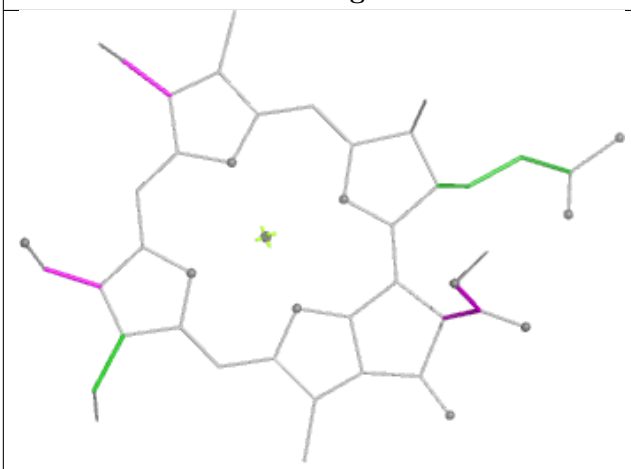
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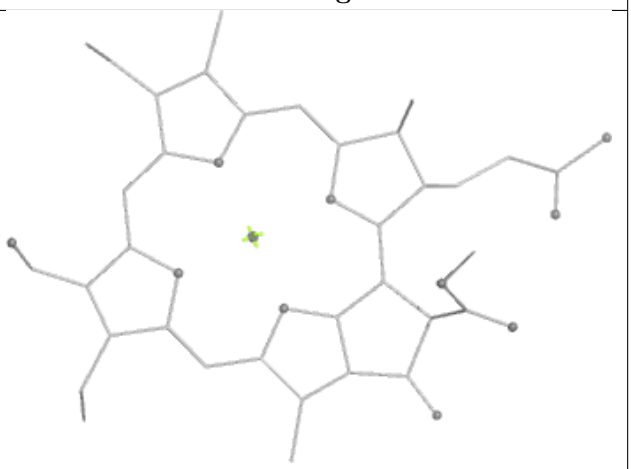
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Bond angles

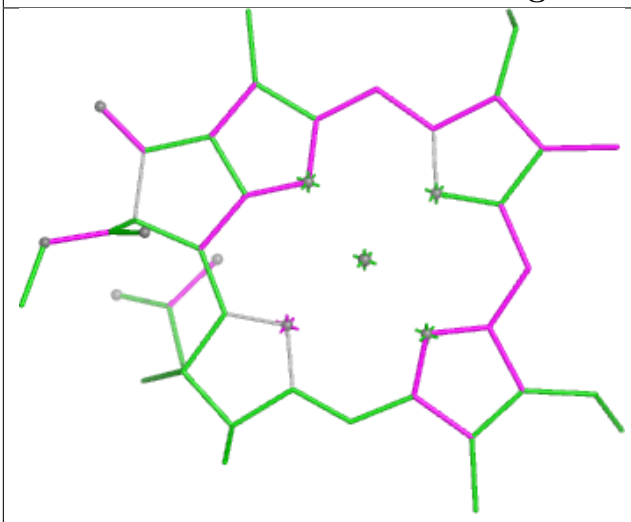


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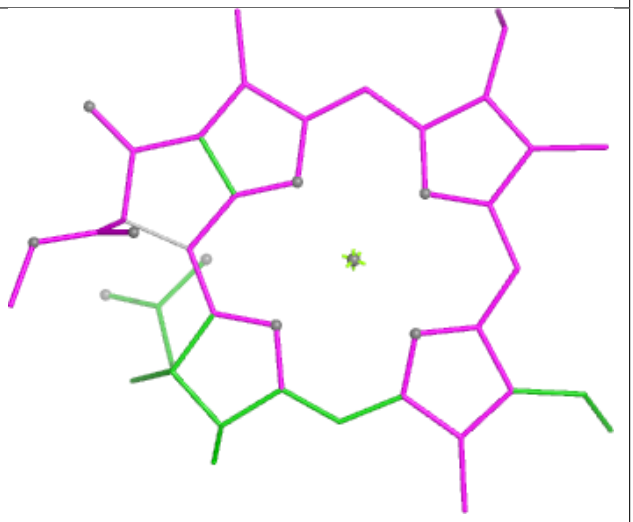


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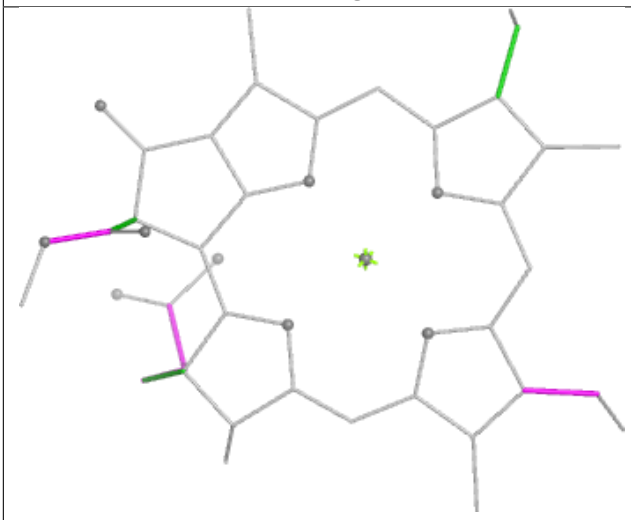
Ligand CLA 3 311



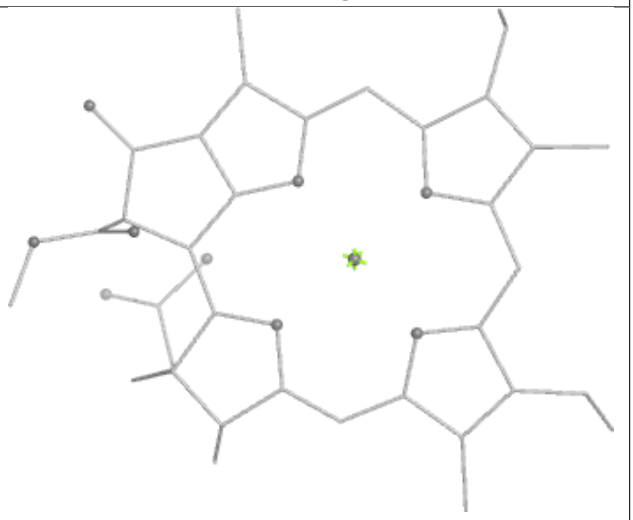
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Bond angles

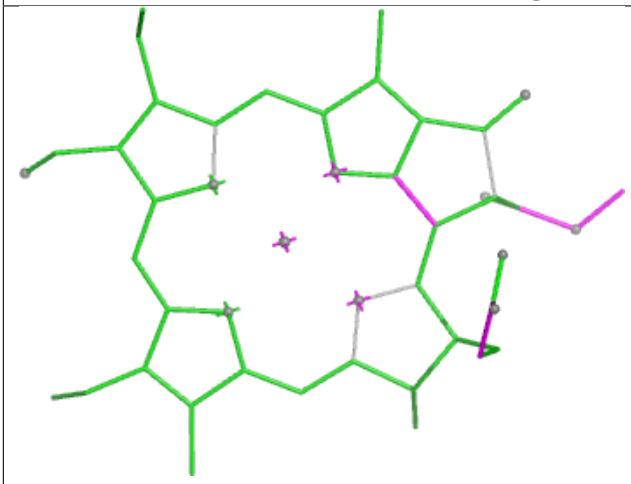


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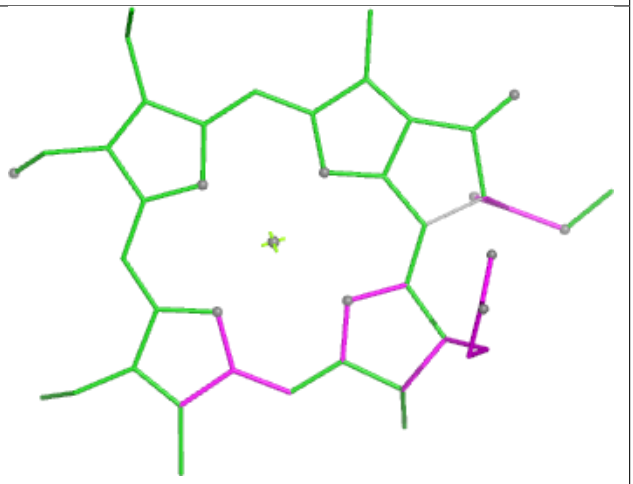


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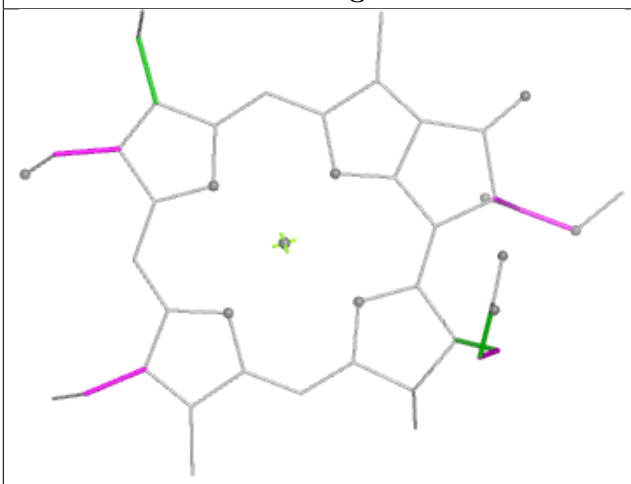
Ligand CHL 5 607



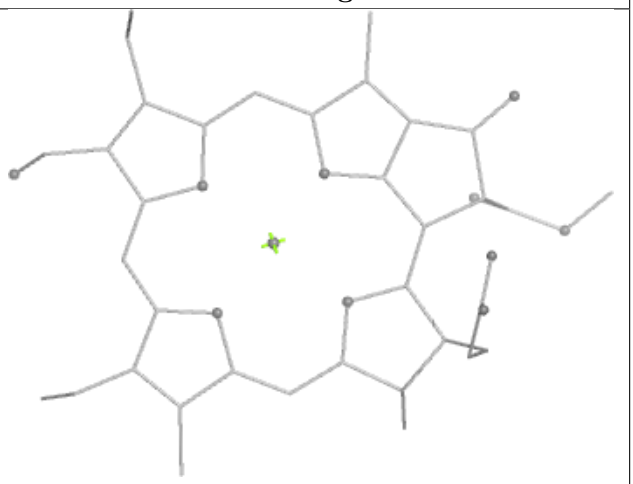
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Bond angles

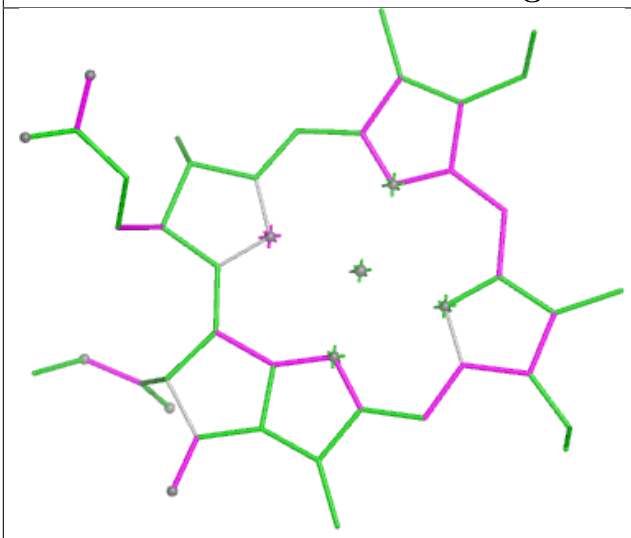


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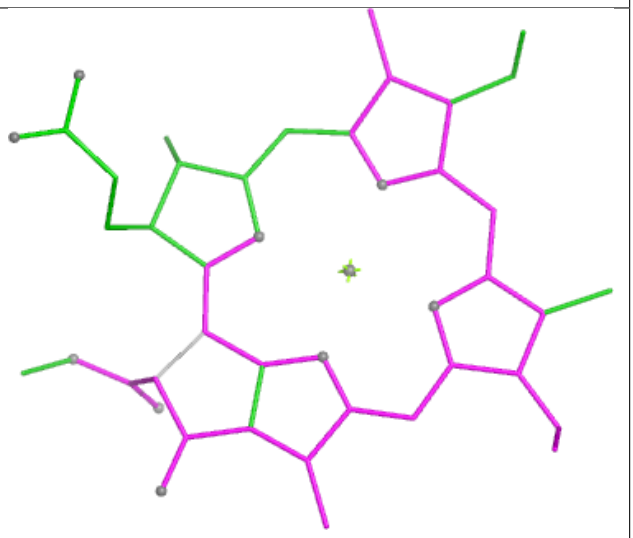


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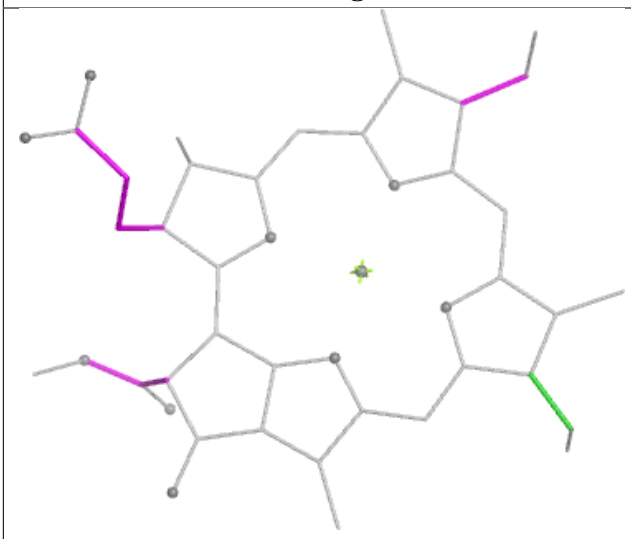
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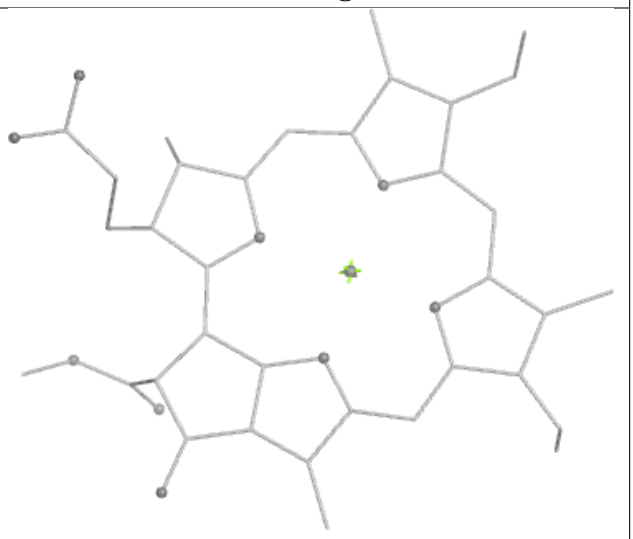
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Bond angles

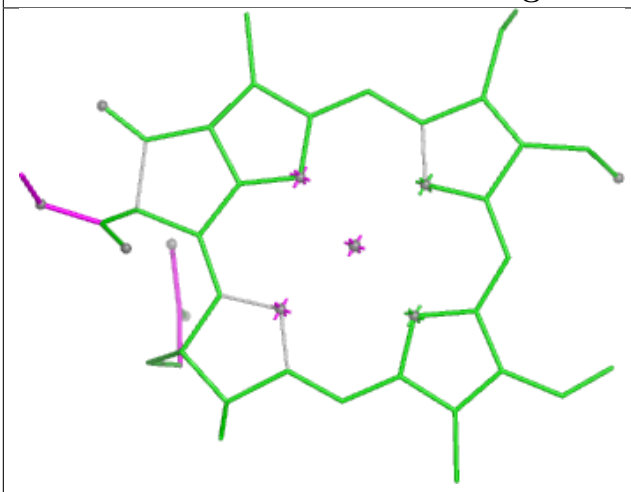


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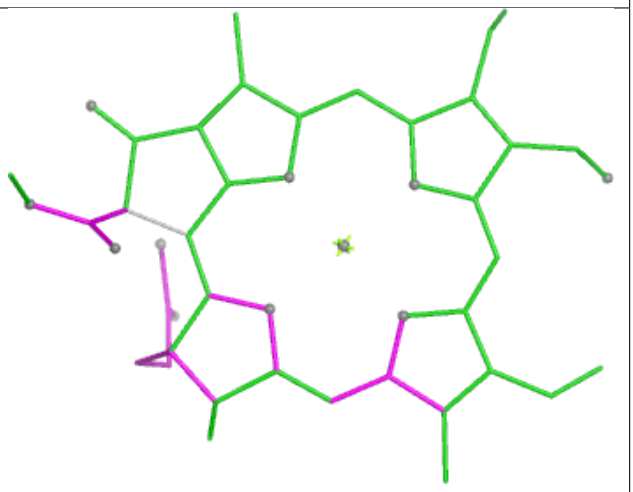


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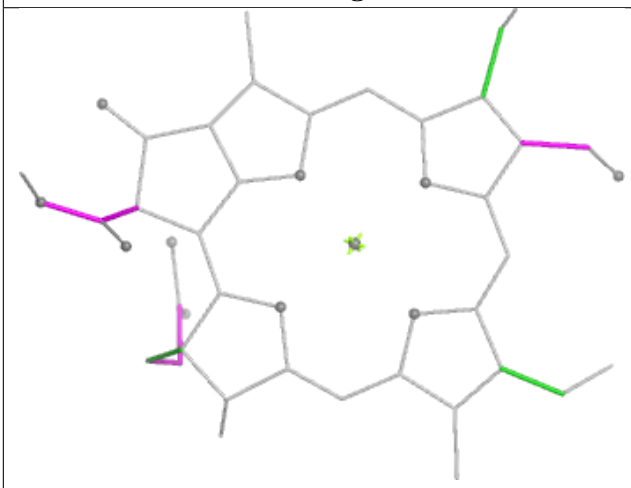
Ligand CHL N 608



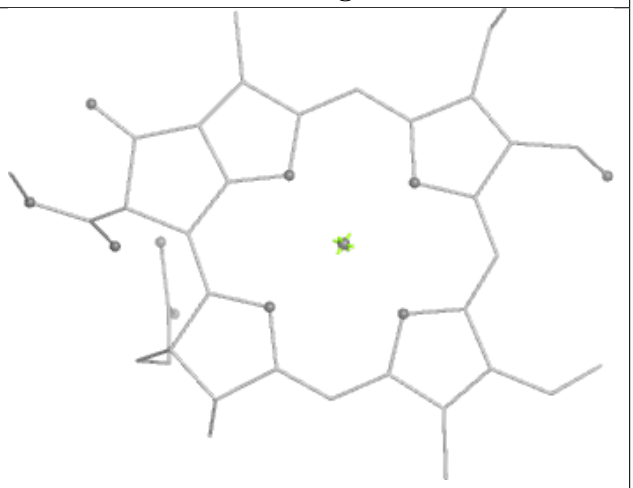
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Bond angles

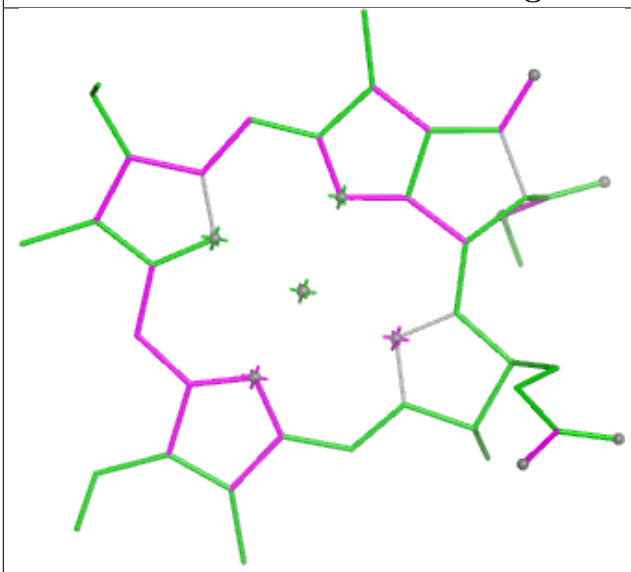


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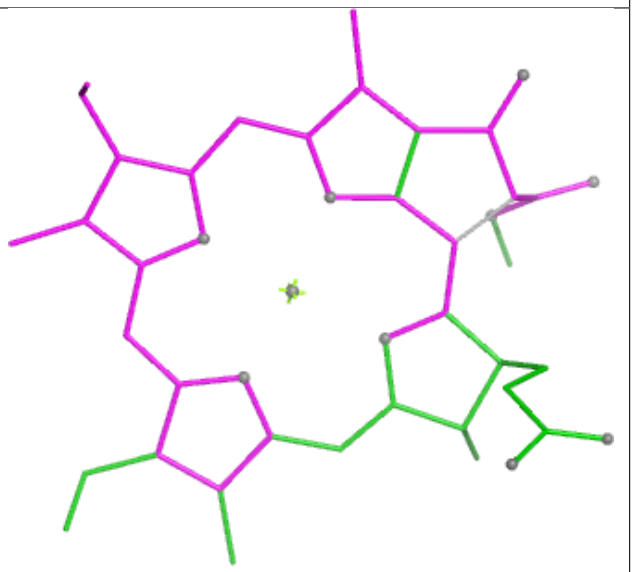


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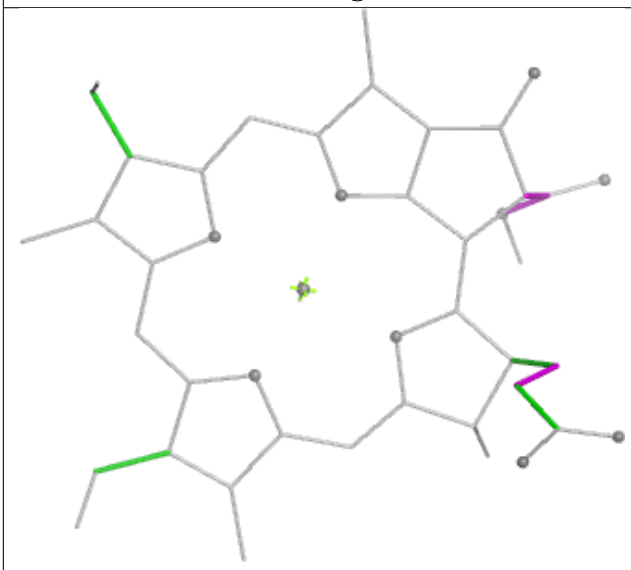
Ligand CLA C 508



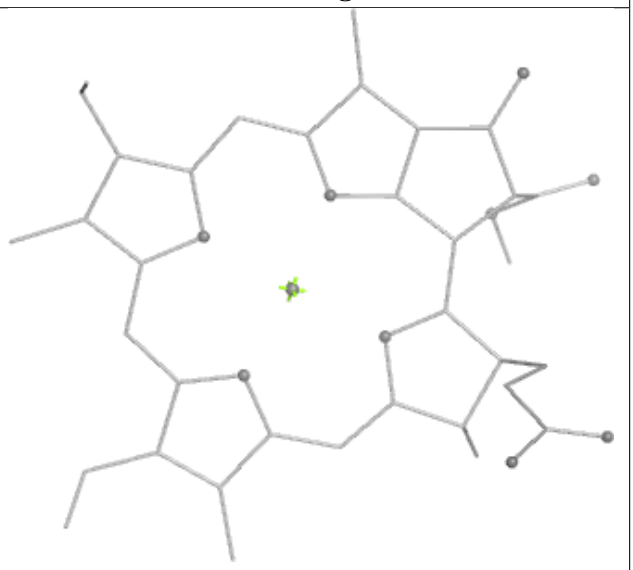
Bond lengths



Bond angles

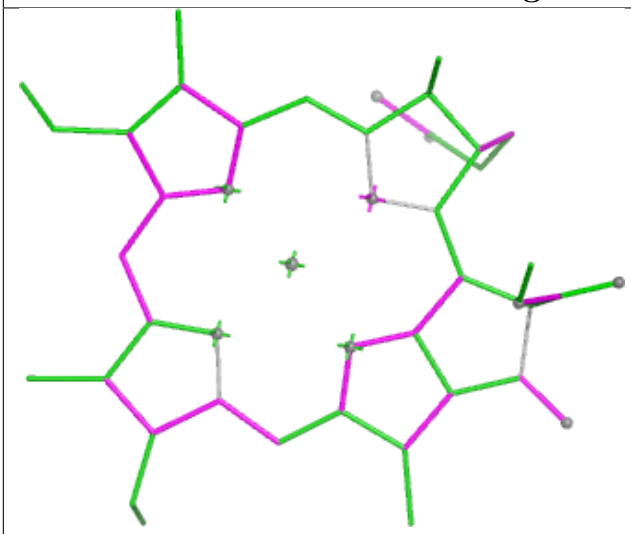


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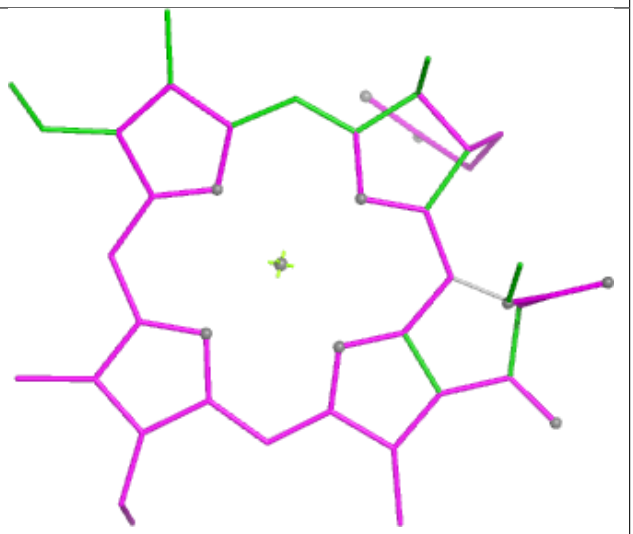


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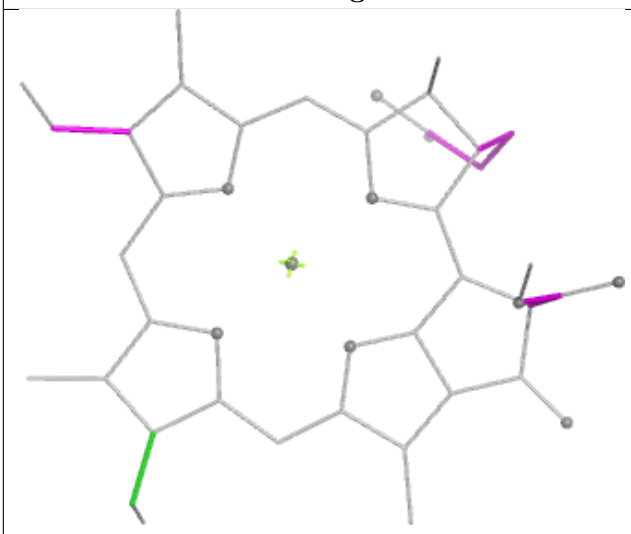
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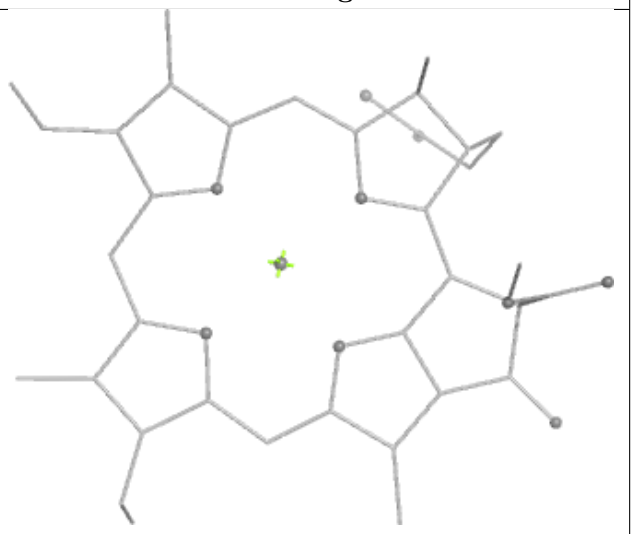
Bond lengths



Bond angles

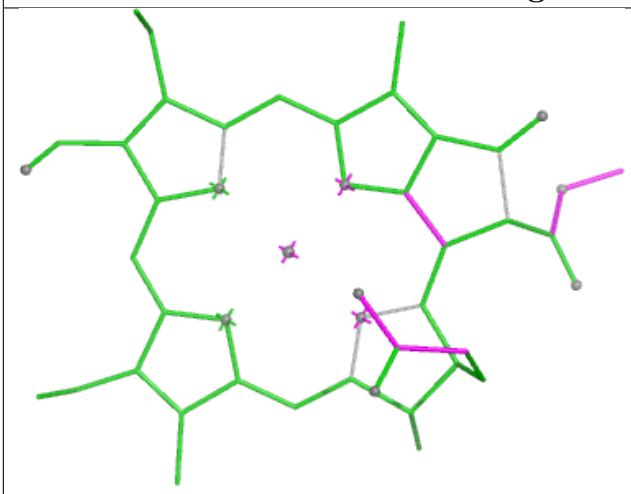


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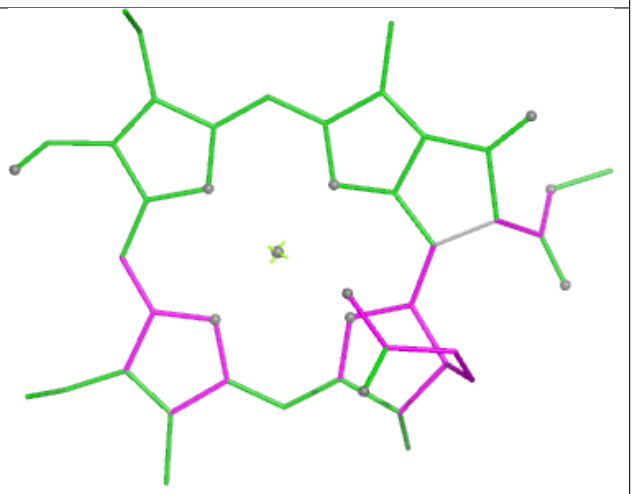


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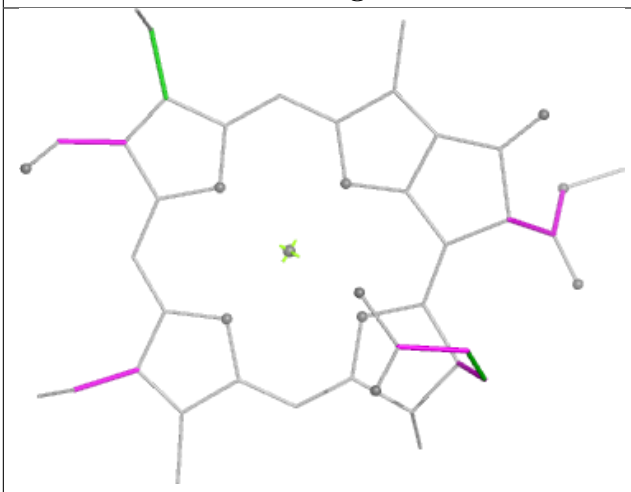
Ligand CHL 1 609



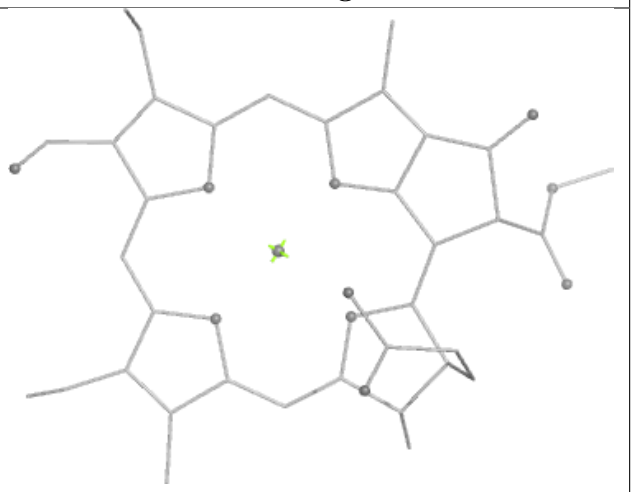
Bond lengths



Bond angles

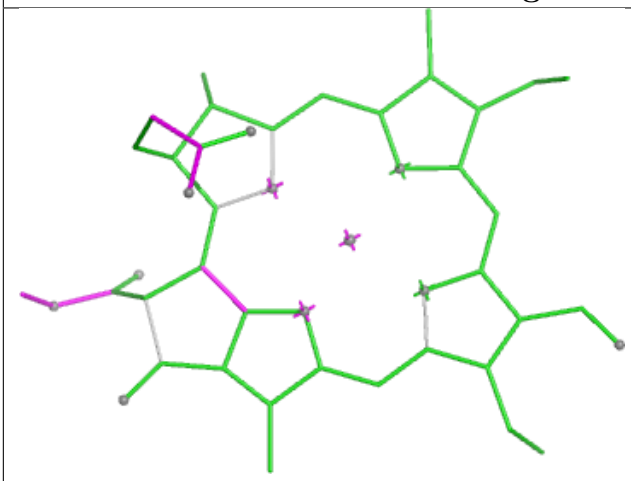


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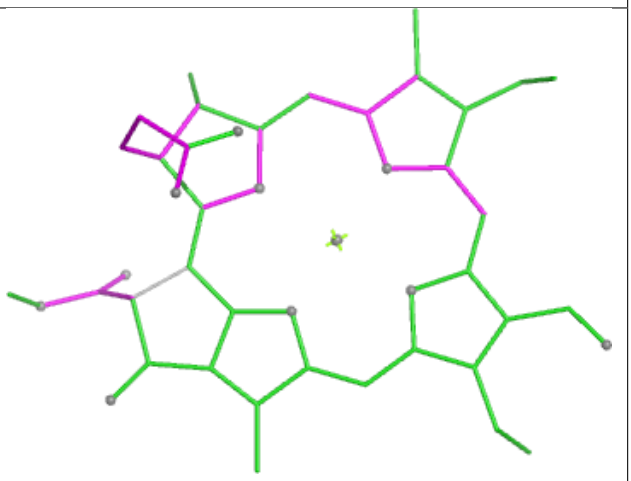


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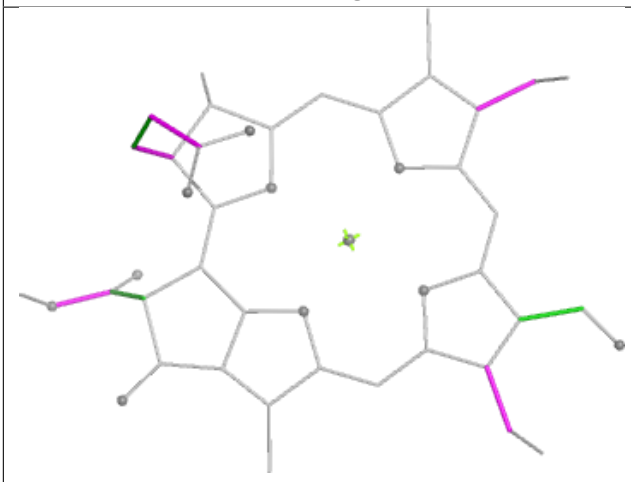
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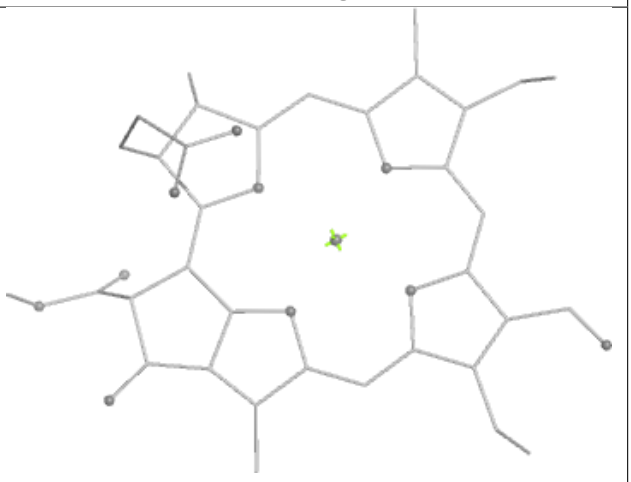
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Bond angles

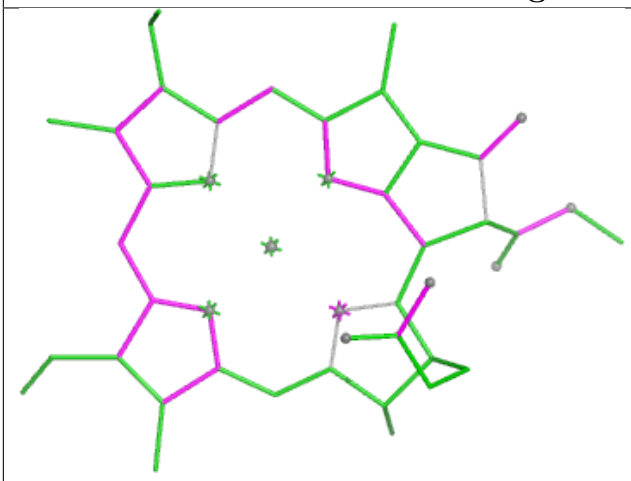


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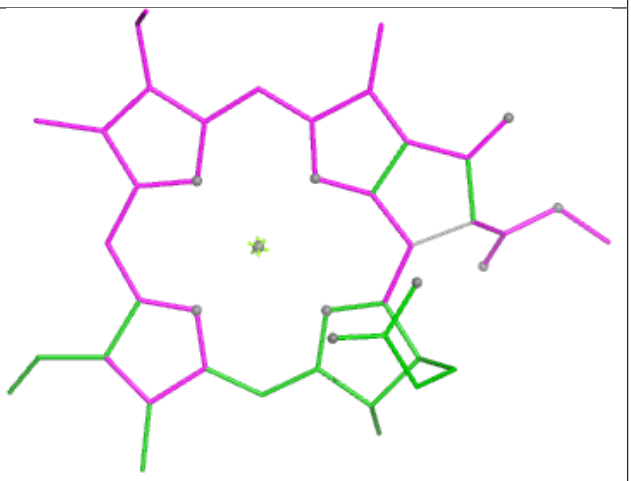


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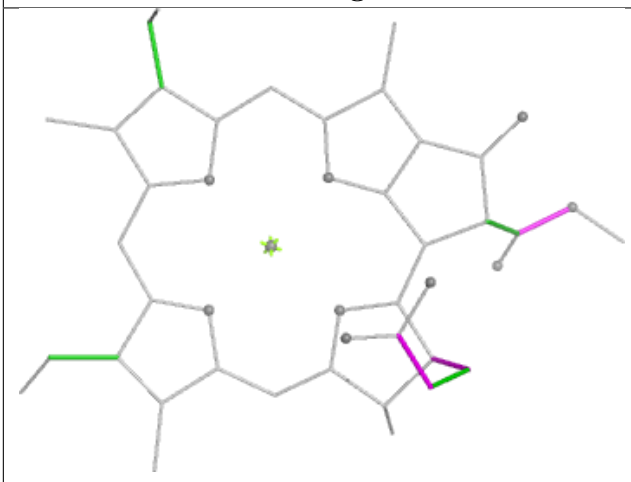
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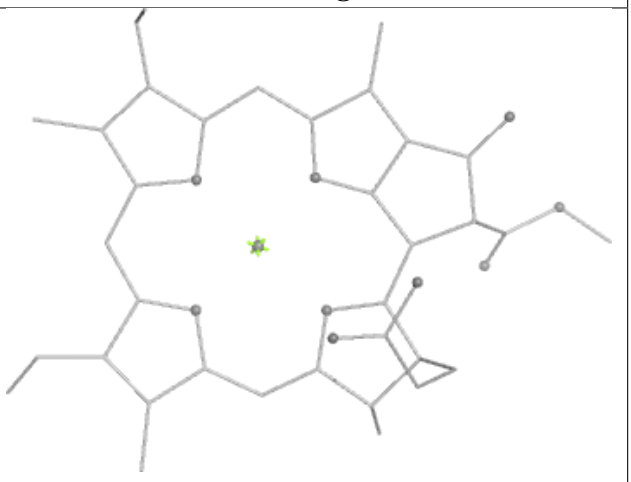
Bond lengths



Bond angles

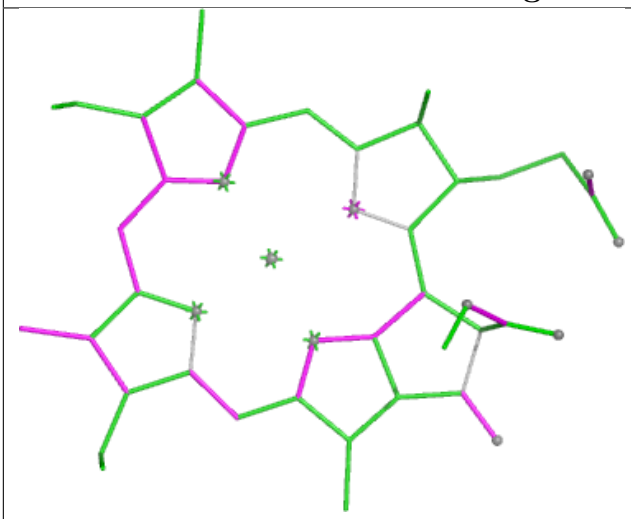


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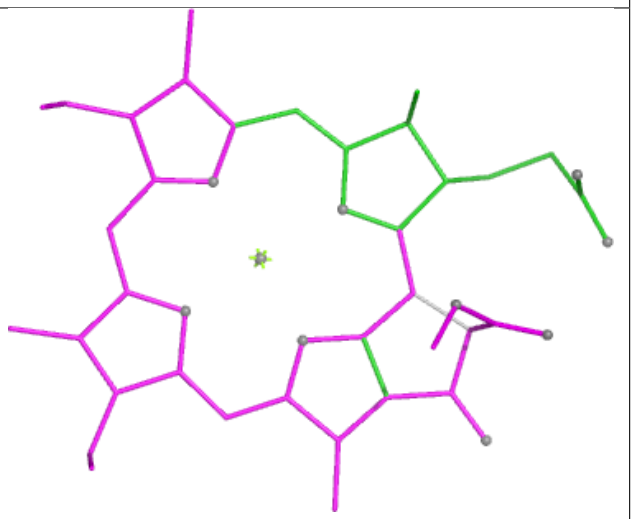


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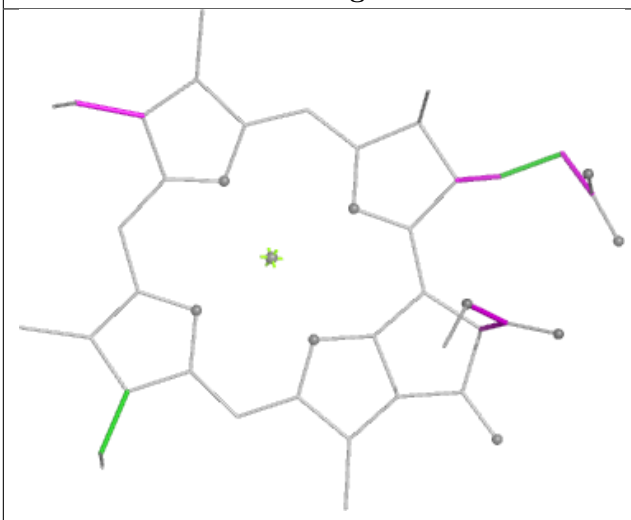
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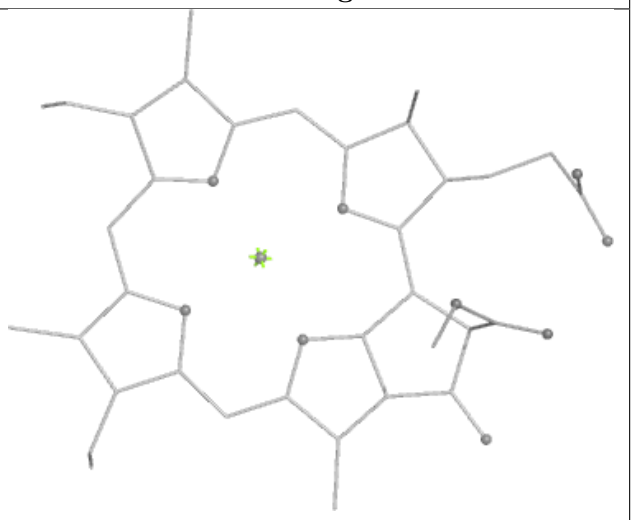
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Bond angles

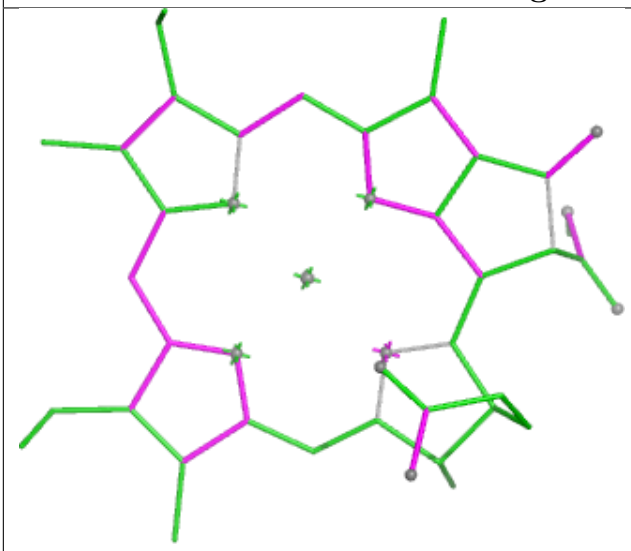


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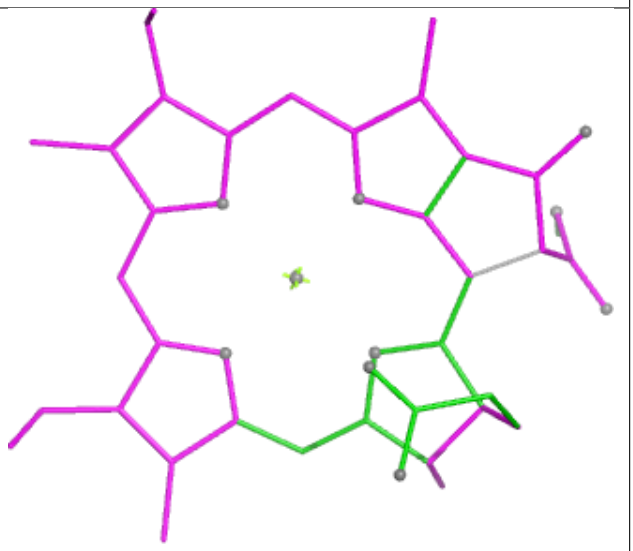


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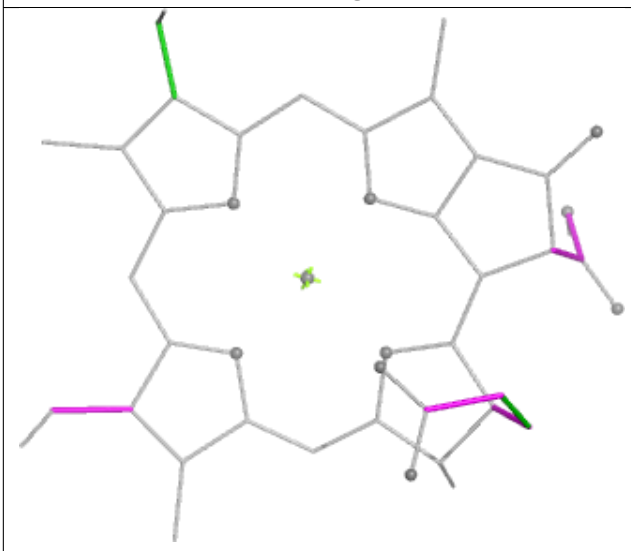
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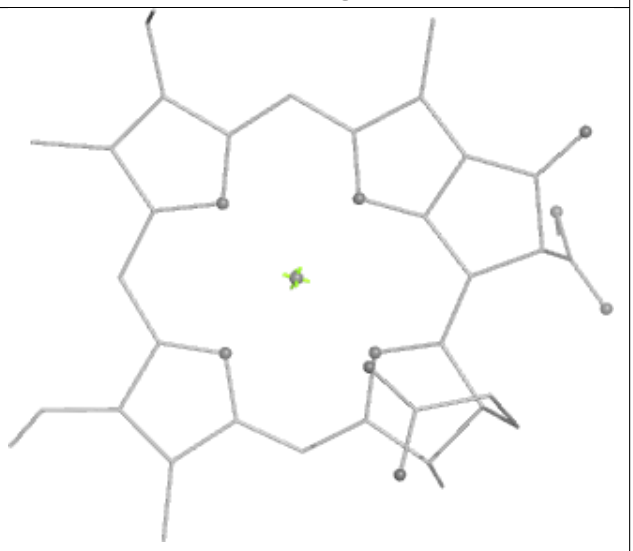
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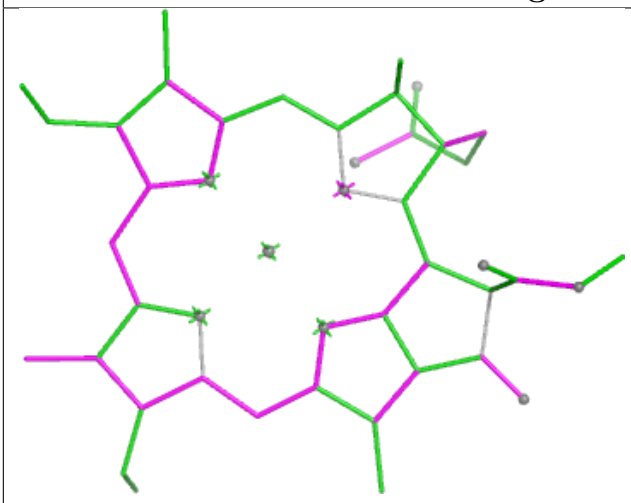


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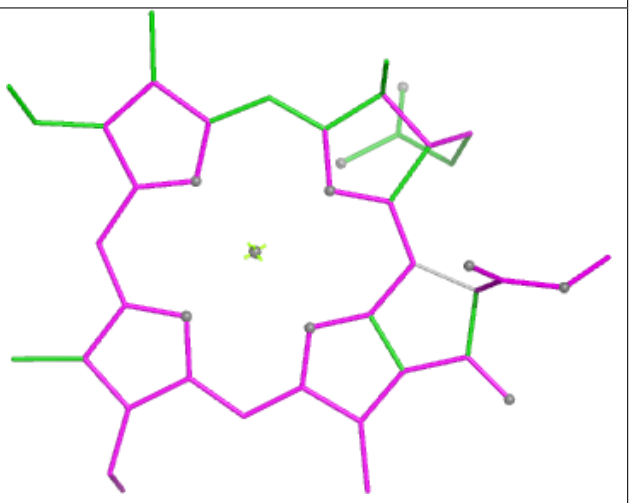


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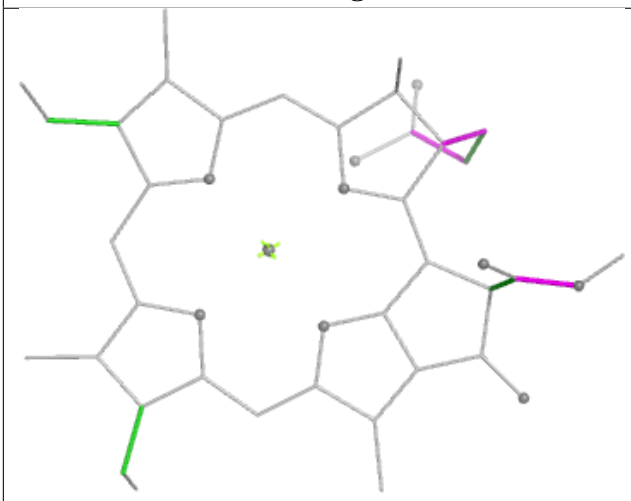
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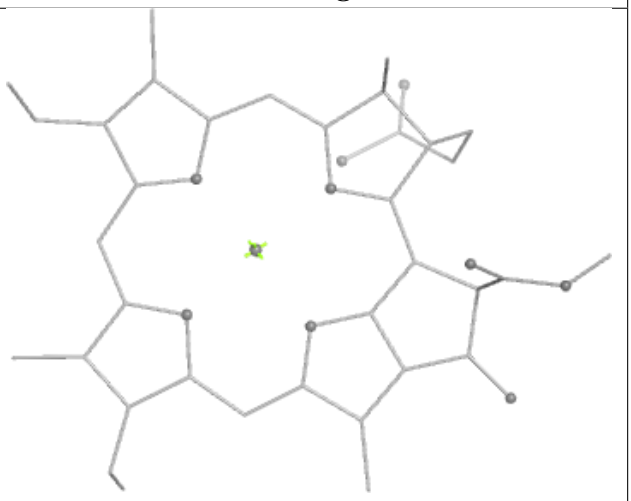
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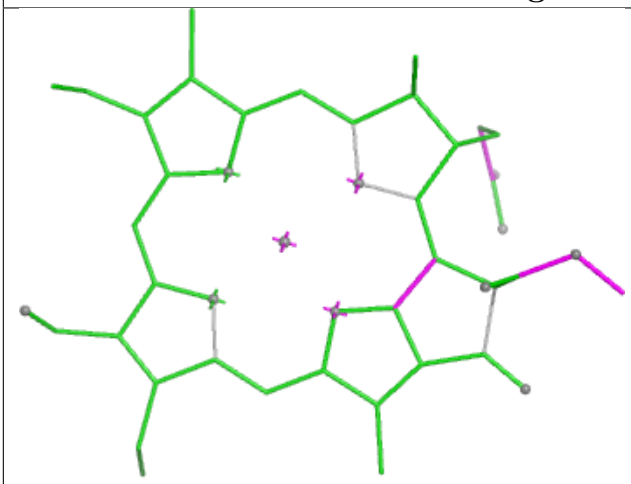


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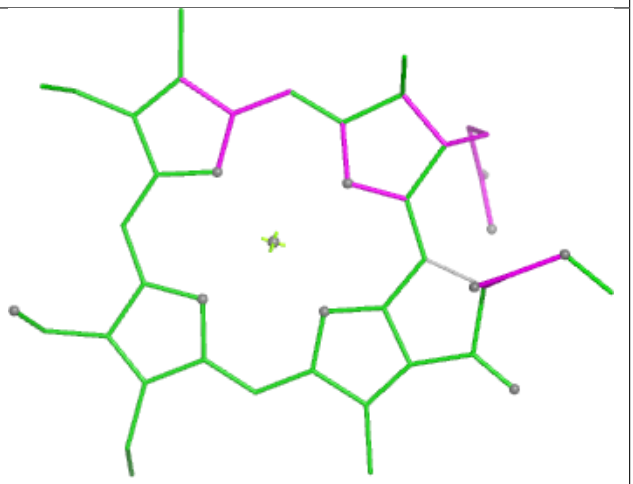


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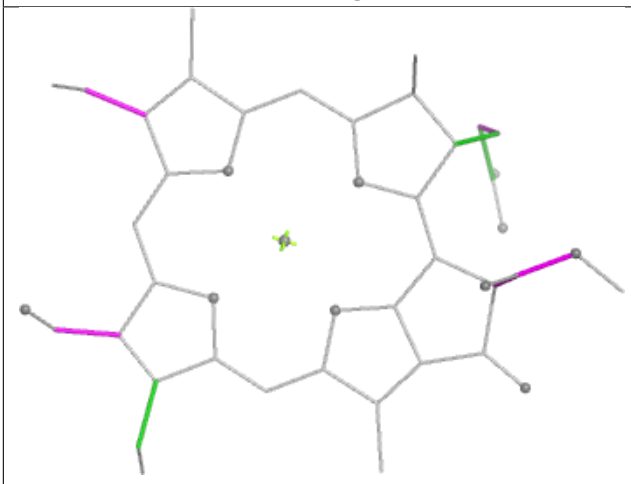
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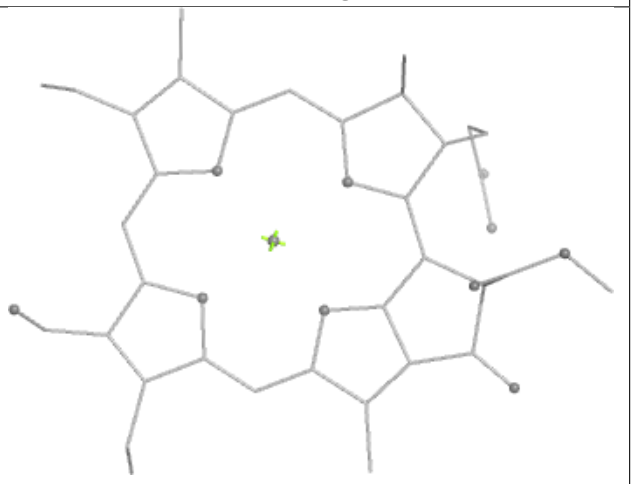
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Bond angles



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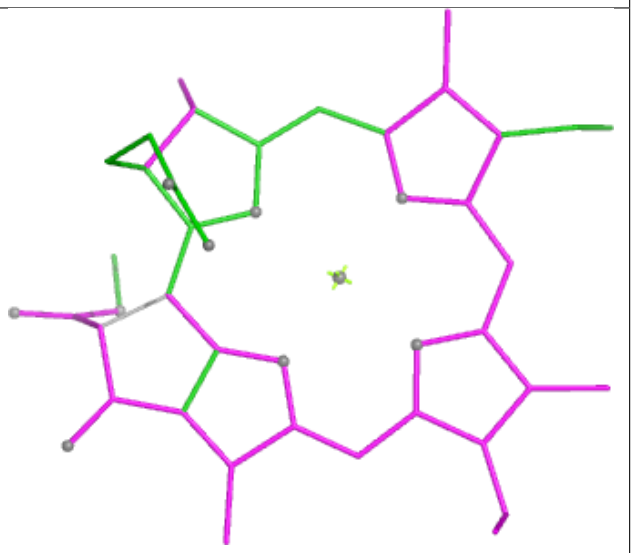


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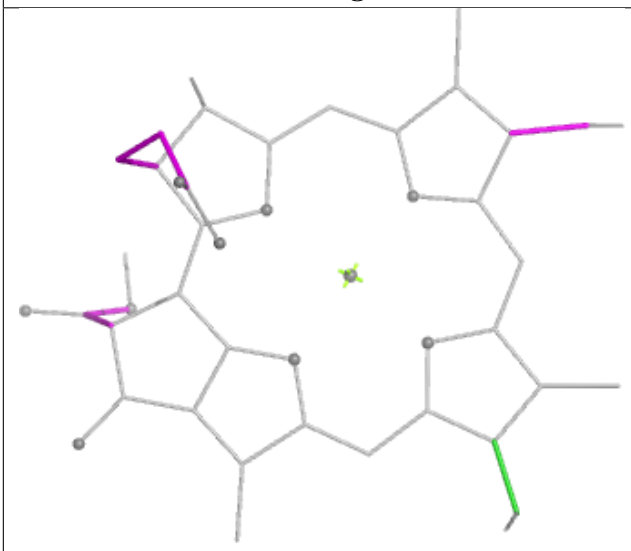
Ligand CLA 5 602



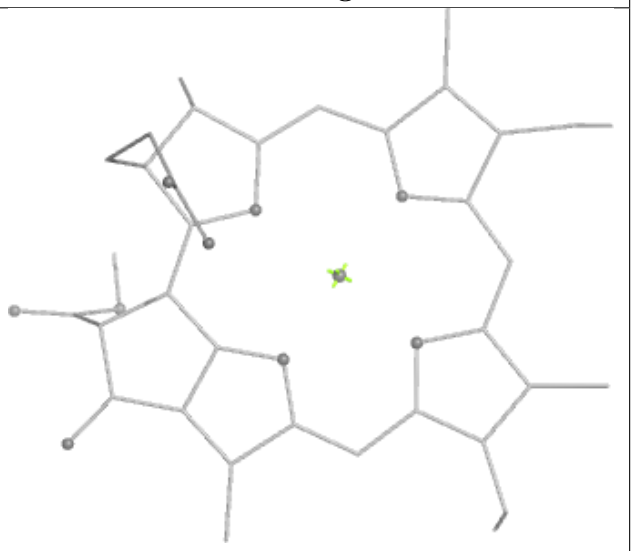
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Bond angles

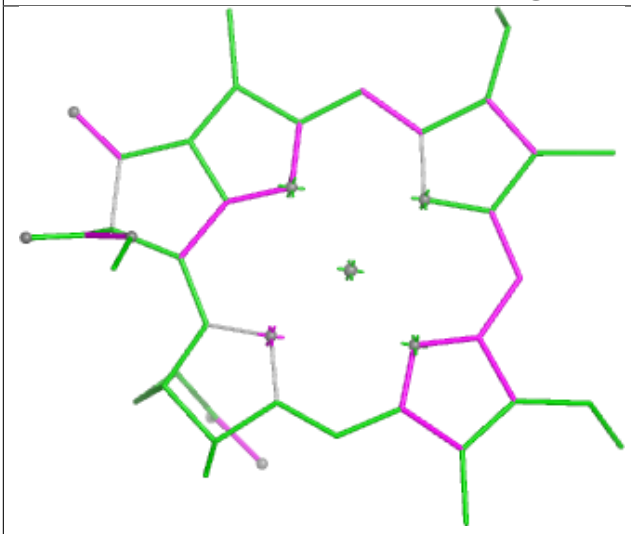


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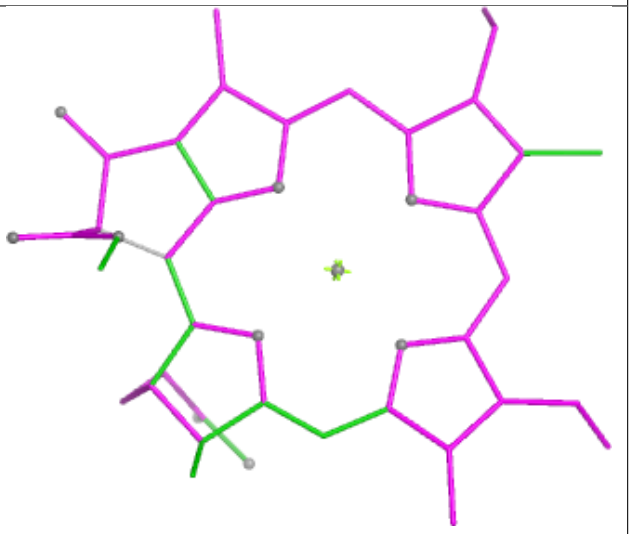


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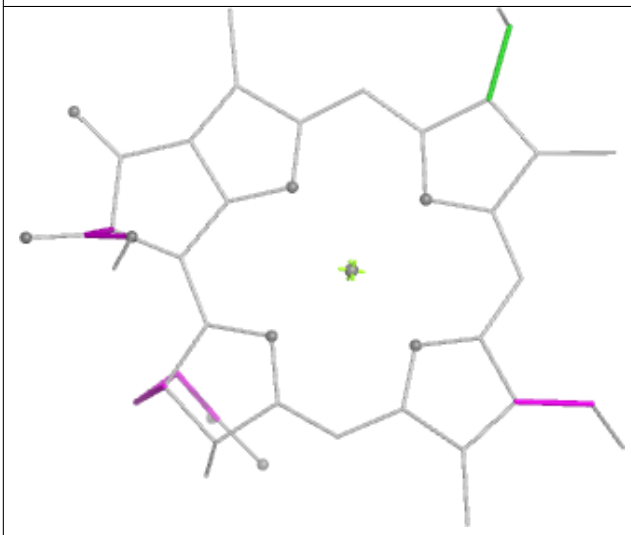
Ligand CLA n 604



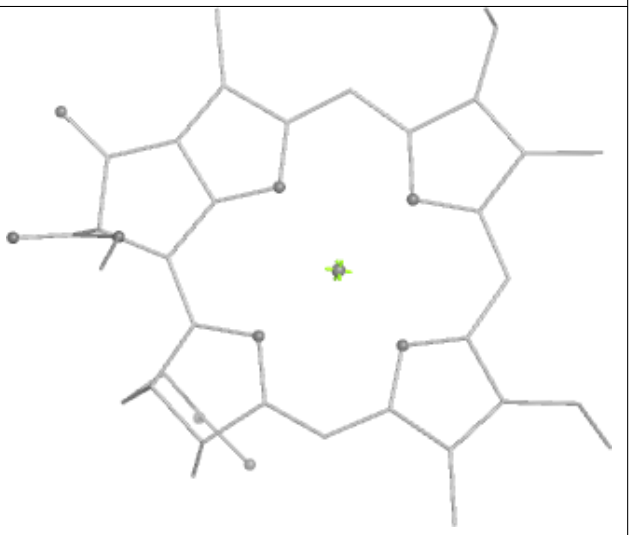
Bond lengths



Bond angles

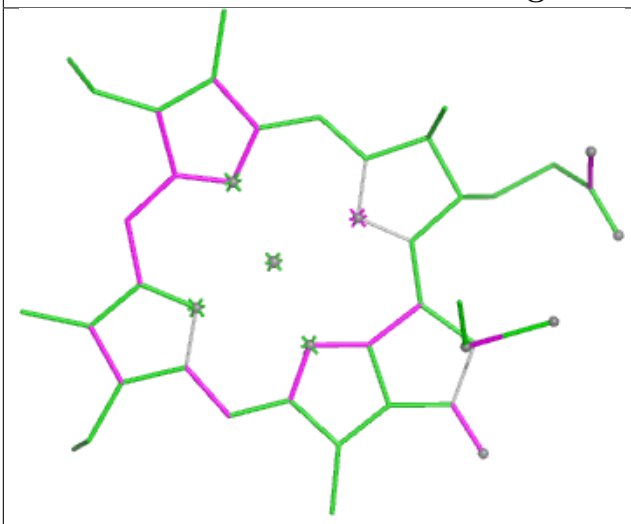


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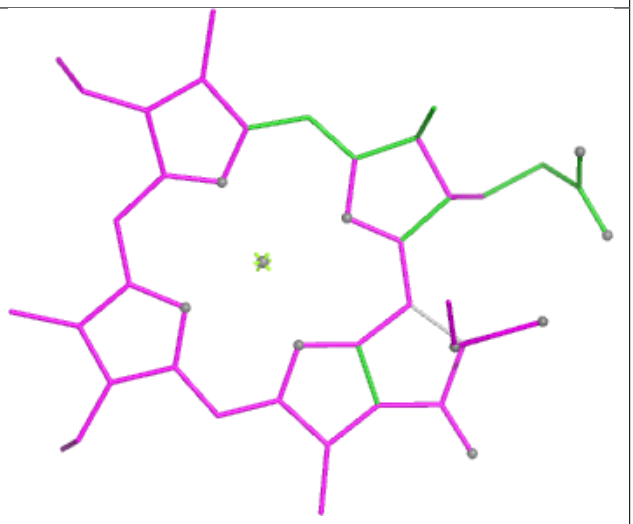


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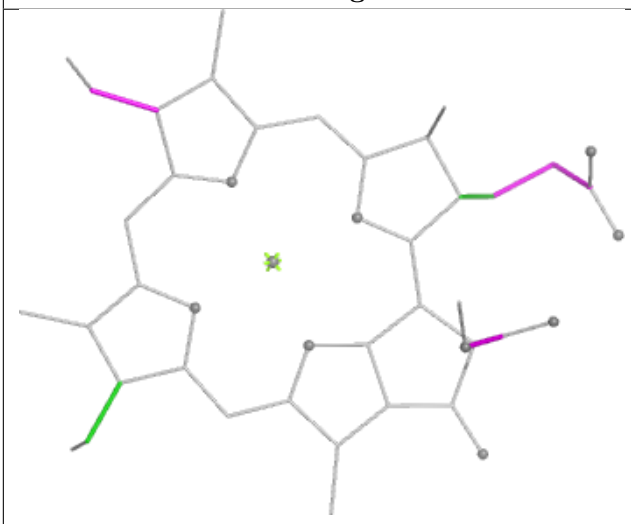
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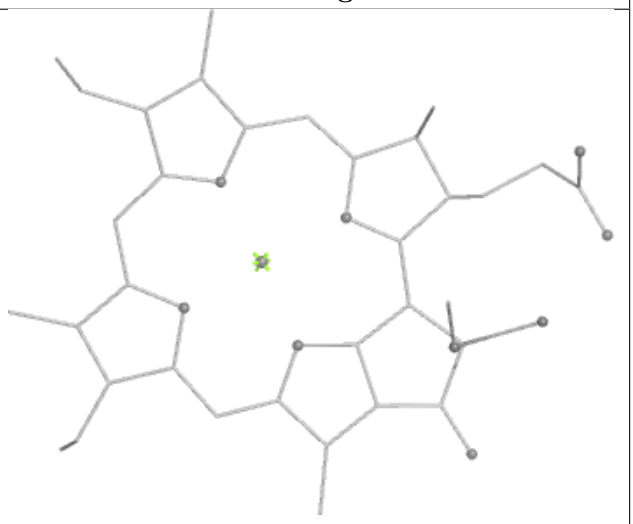
Bond lengths



Bond angles

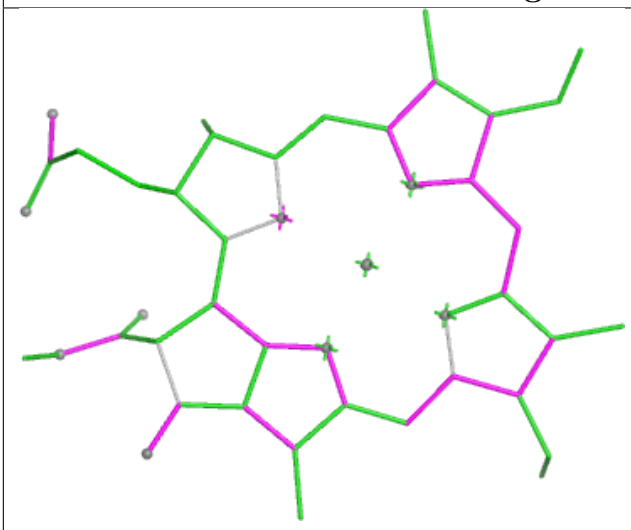


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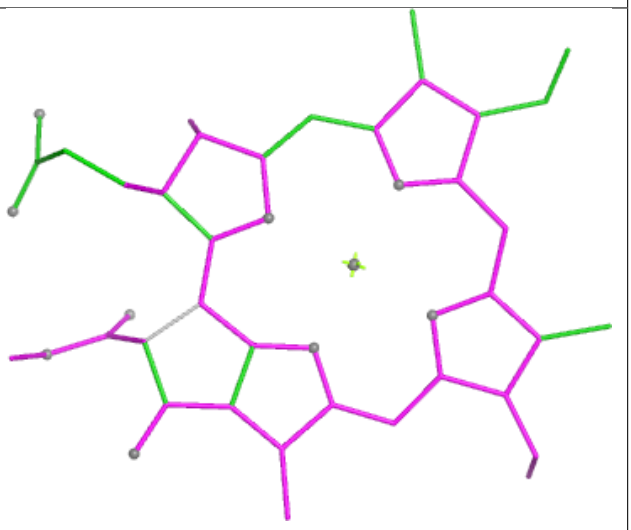


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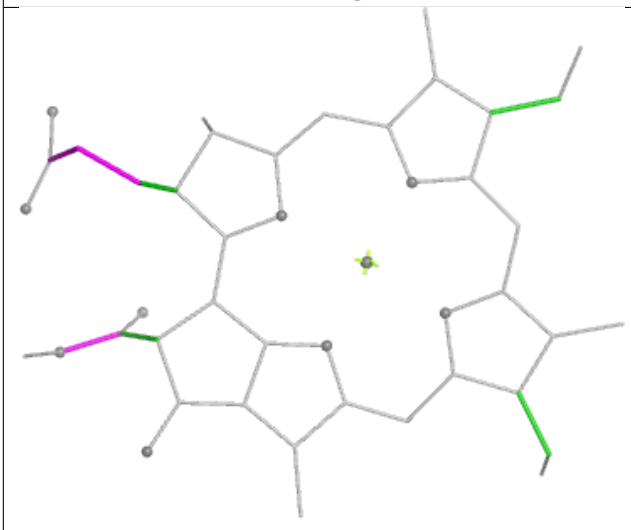
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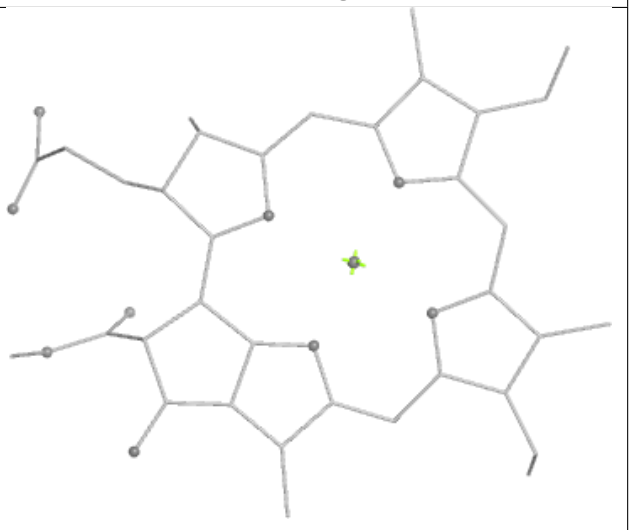
Bond lengths



Bond angles

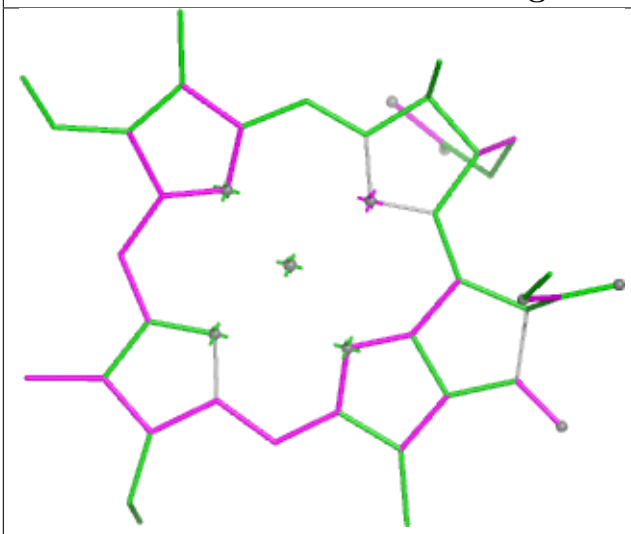


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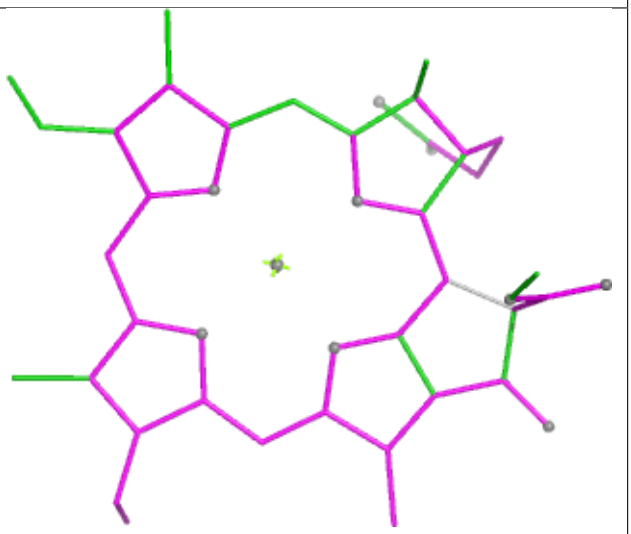


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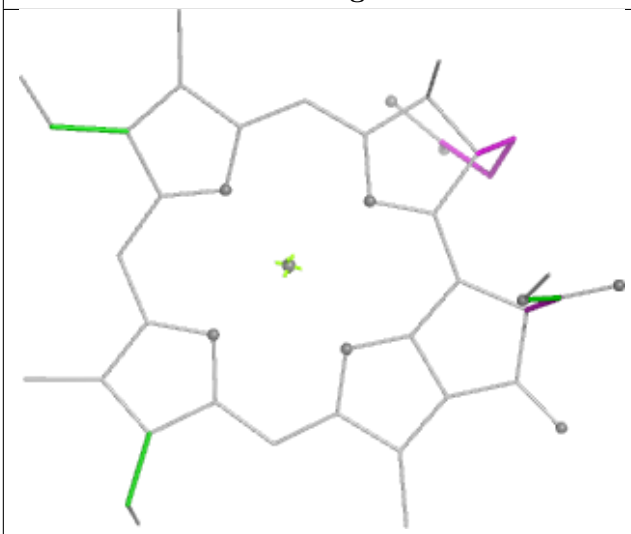
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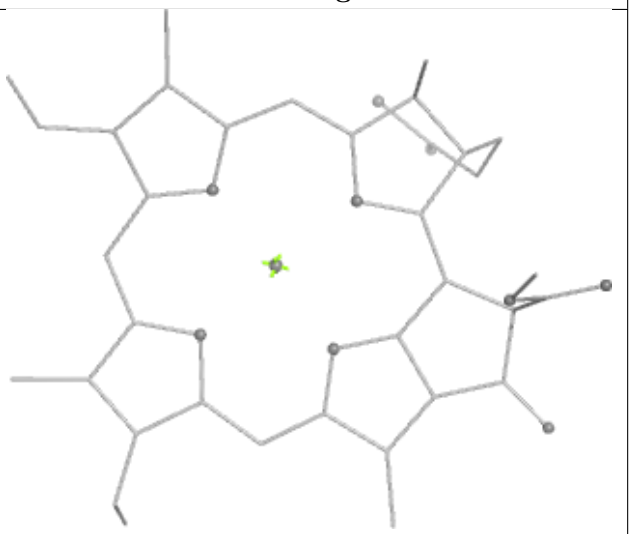
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Bond angles

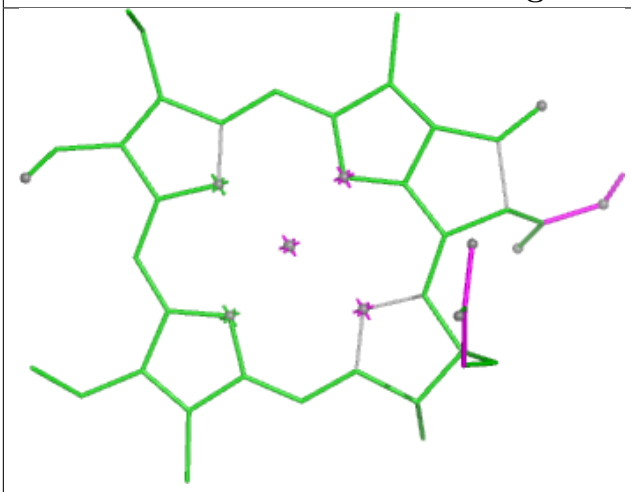


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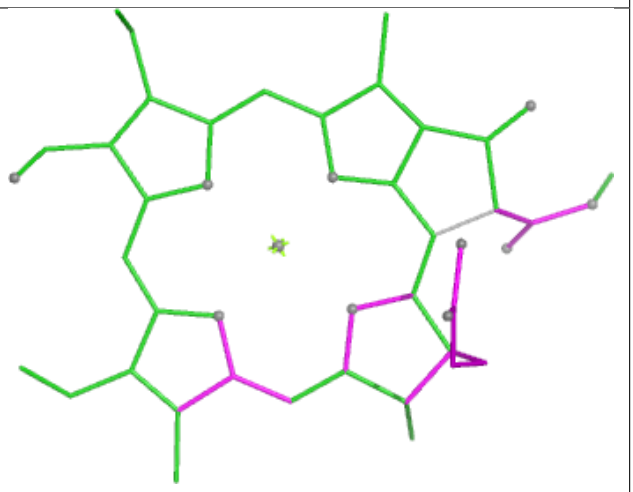


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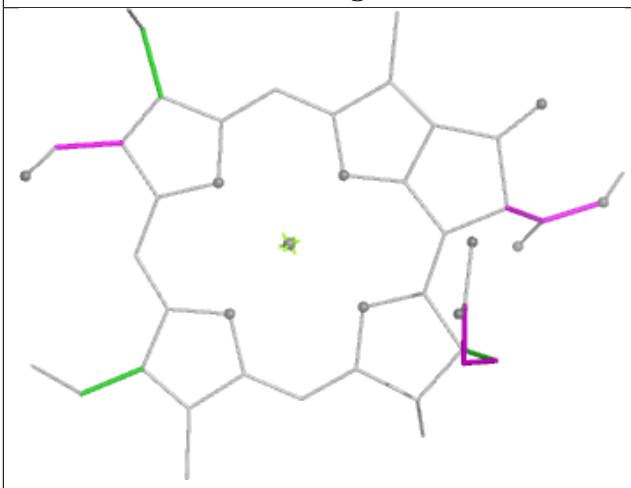
Ligand CHL n 608



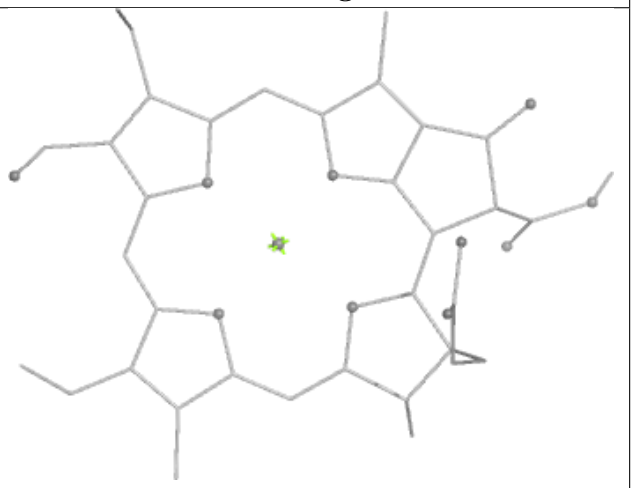
Bond lengths



Bond angles

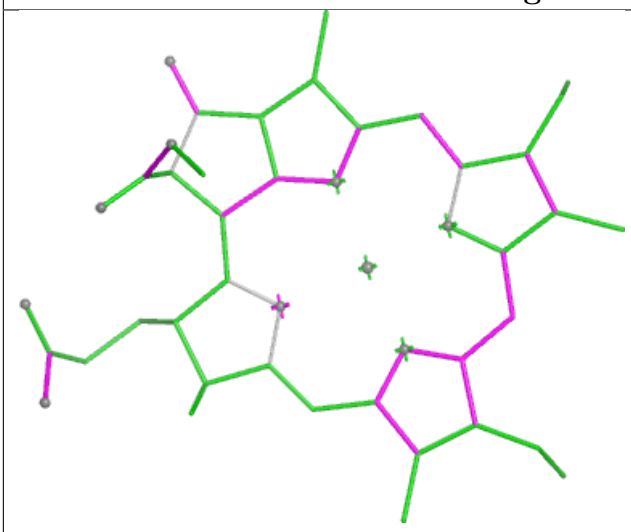


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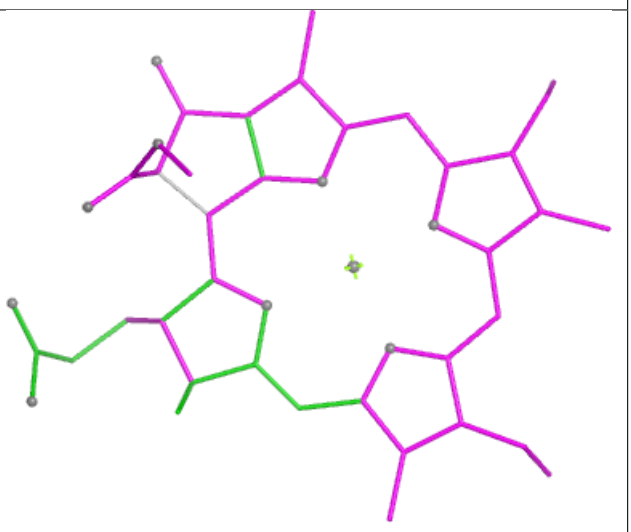


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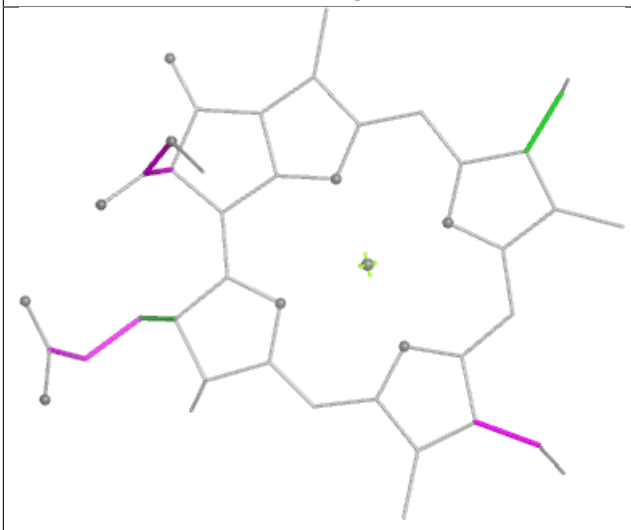
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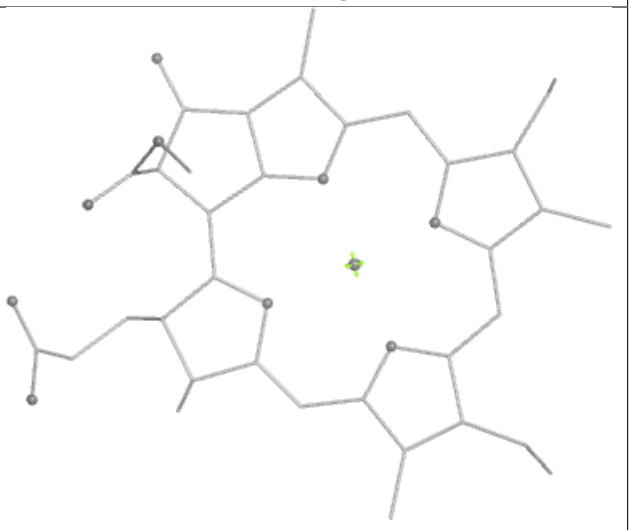
Bond lengths



Bond angles

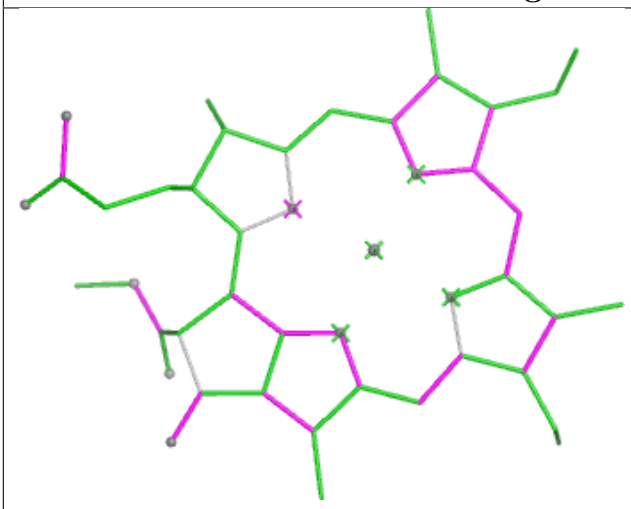


Torsions

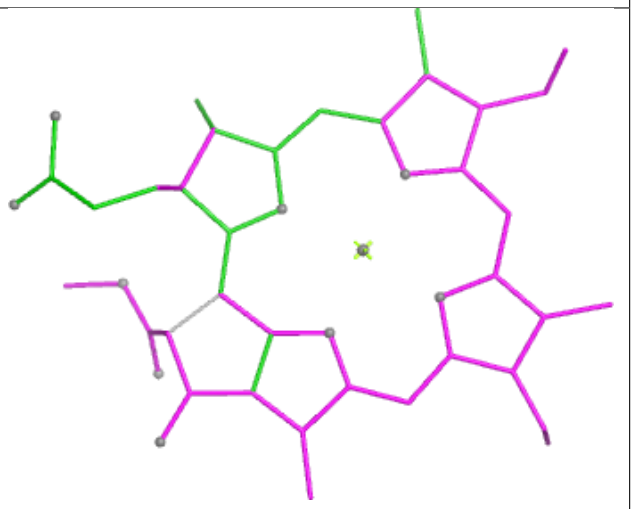


Rings

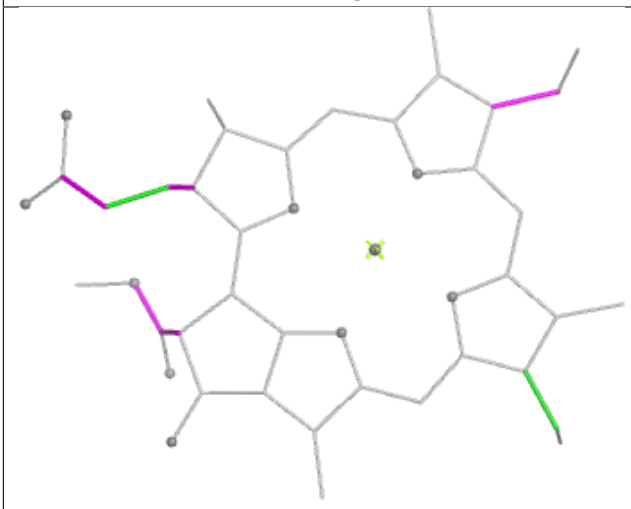
Ligand CLA B 615



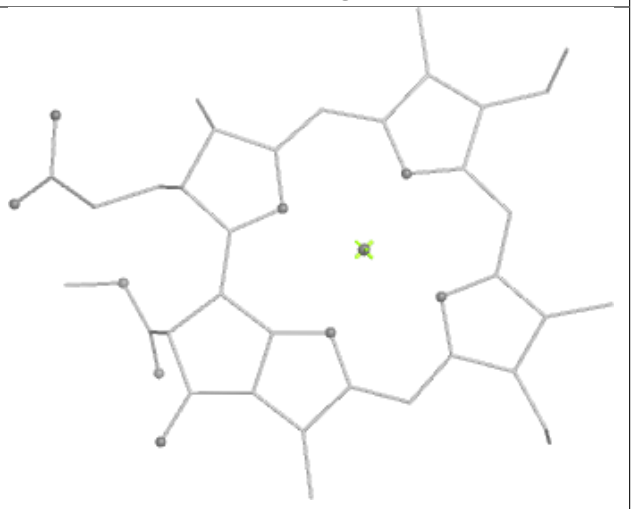
Bond lengths



Bond angles

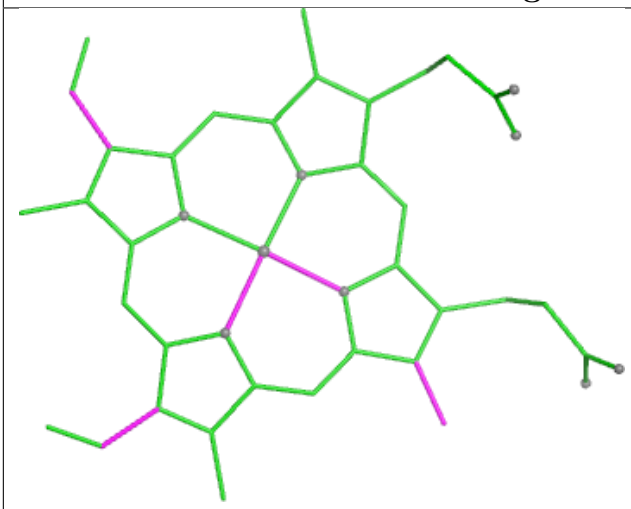


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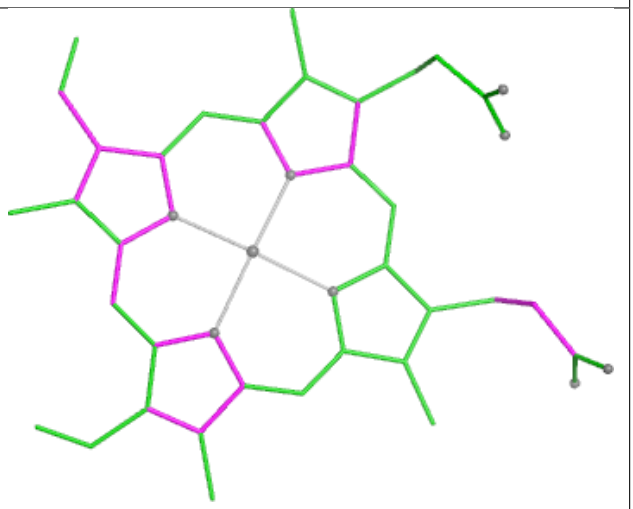


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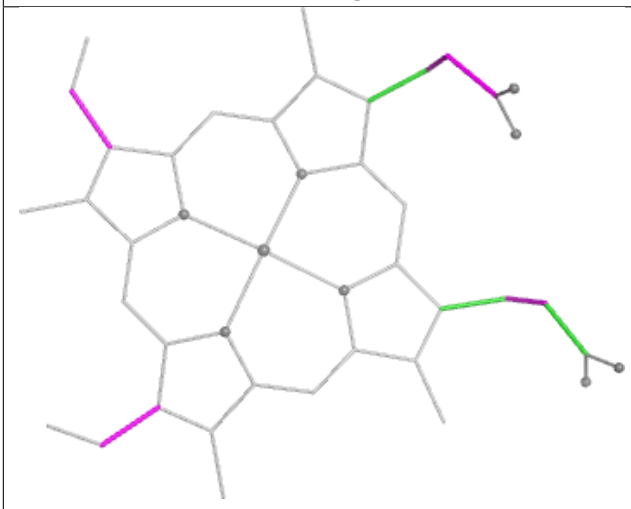
Ligand HEM e 101



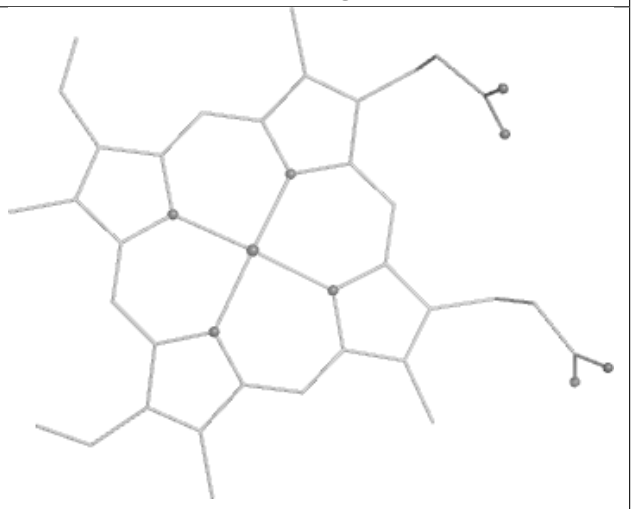
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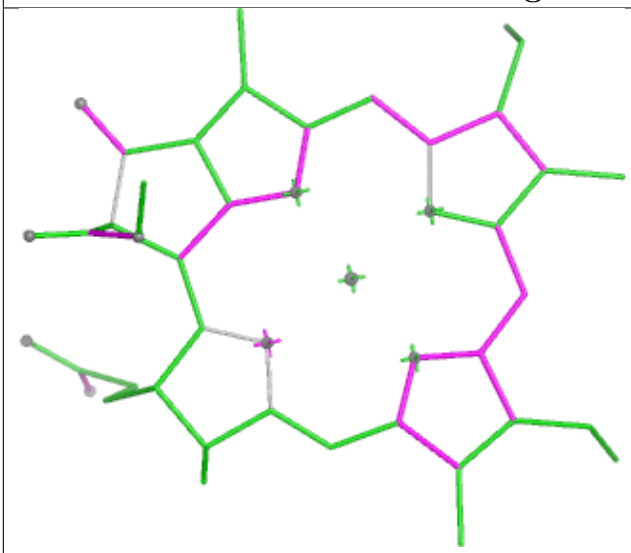


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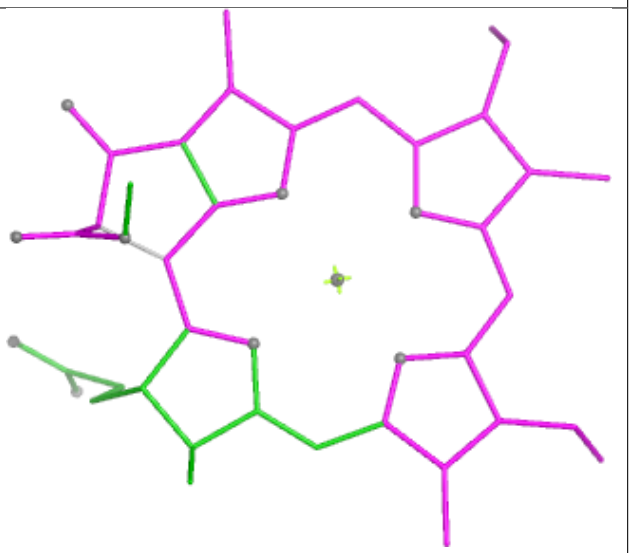


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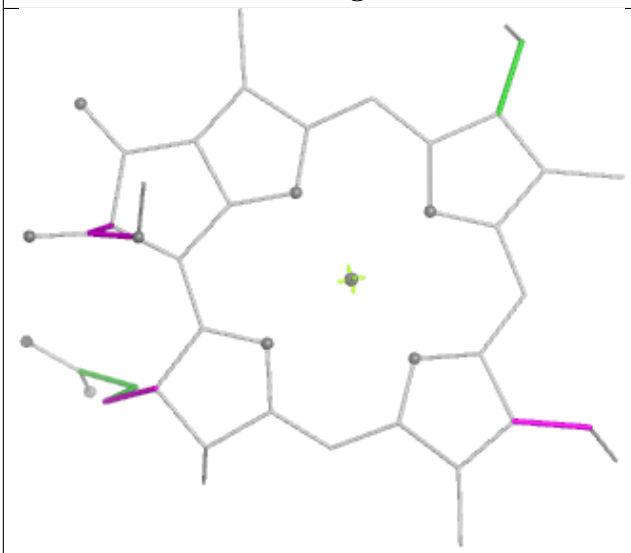
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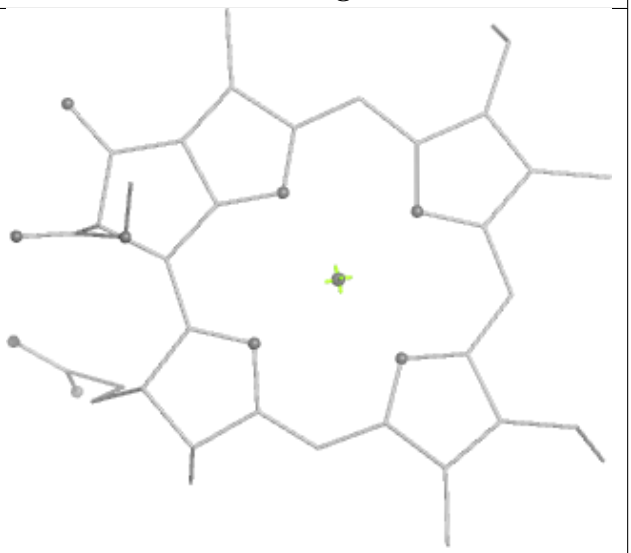
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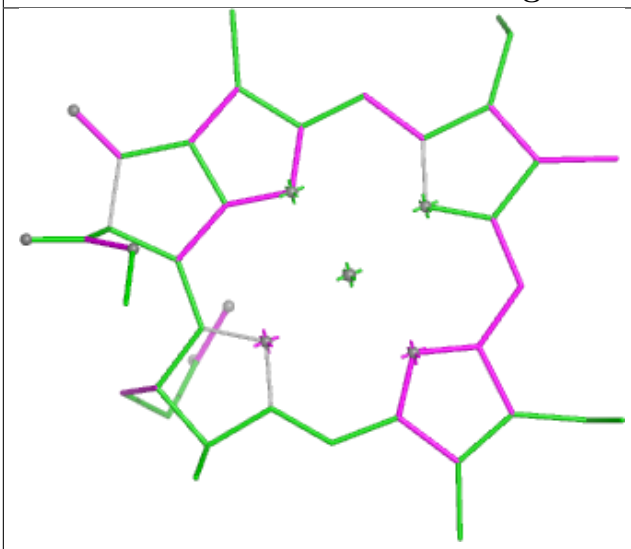


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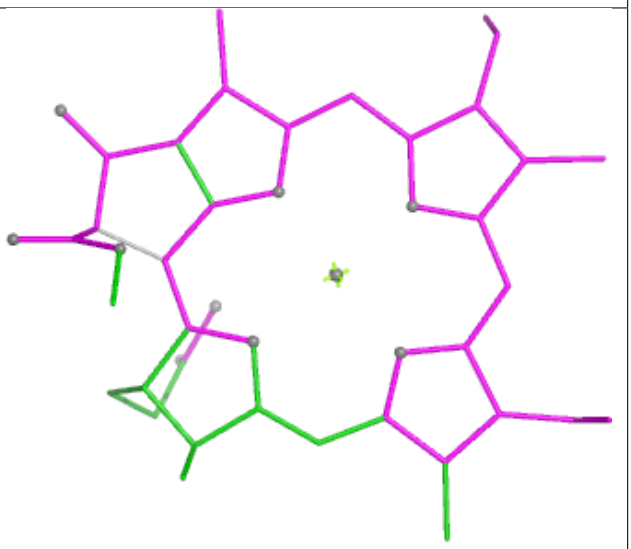


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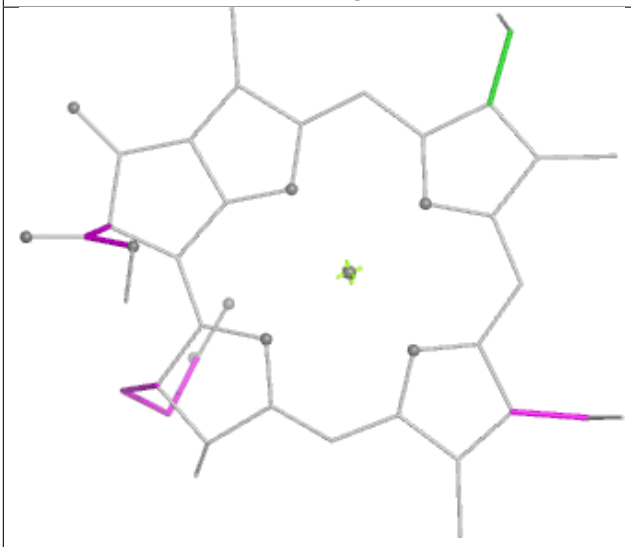
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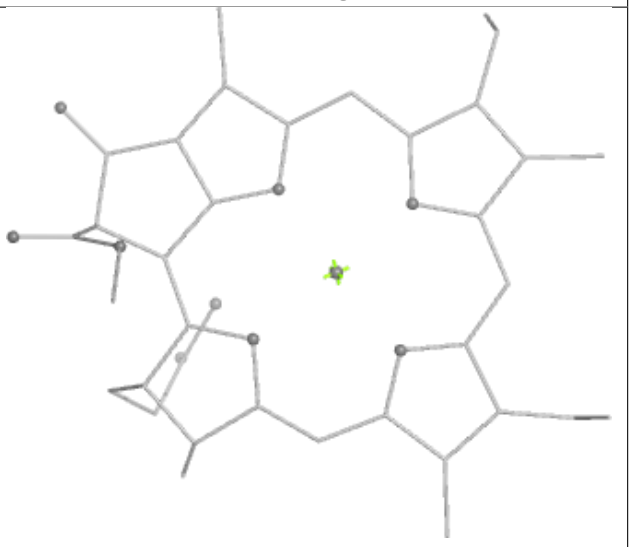
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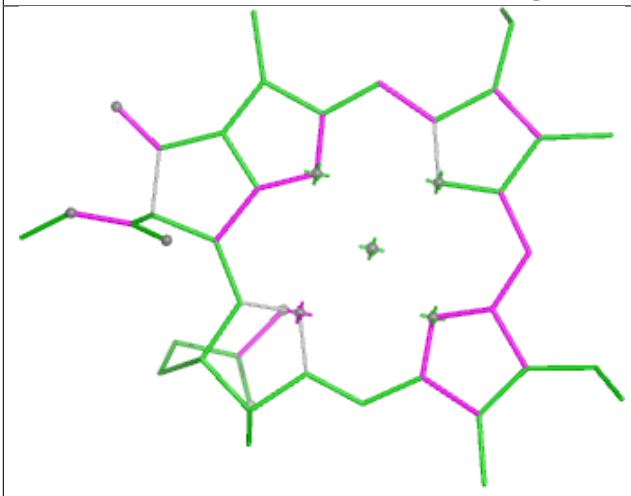


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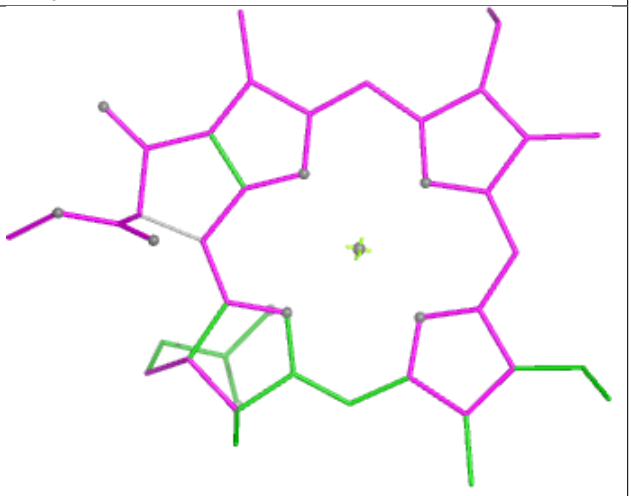


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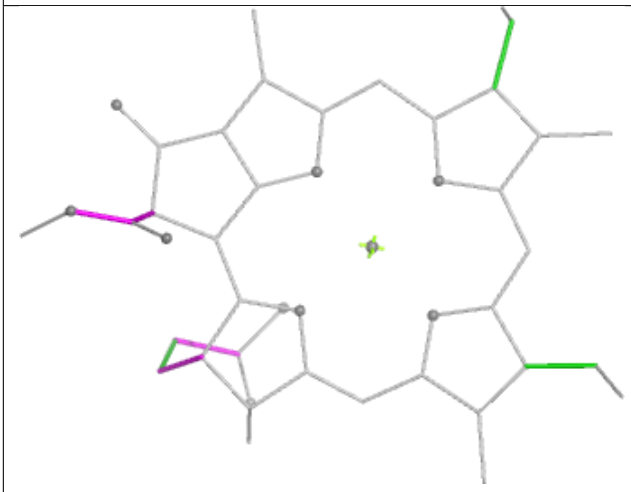
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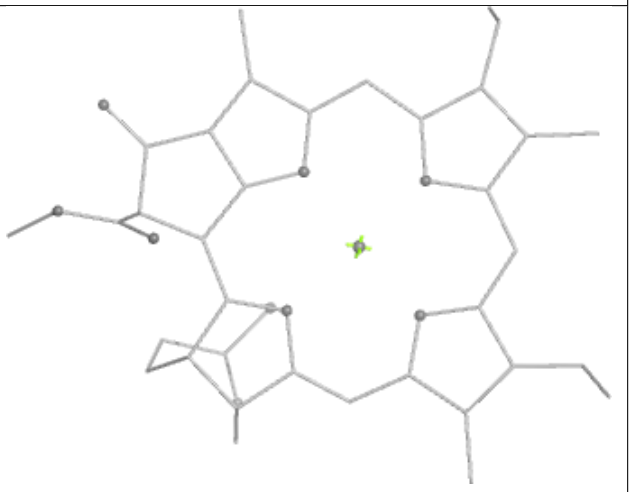
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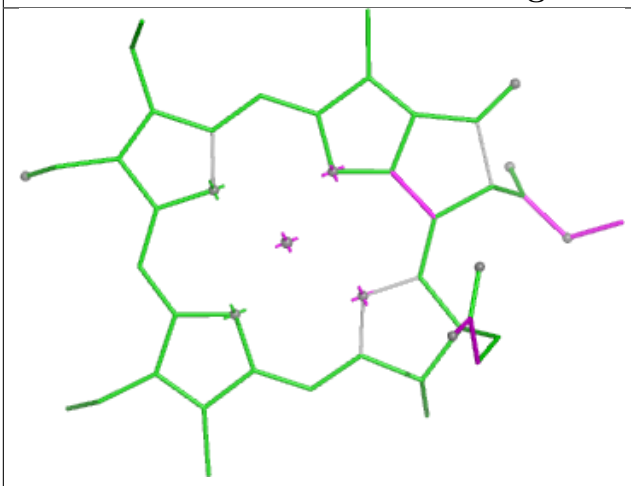


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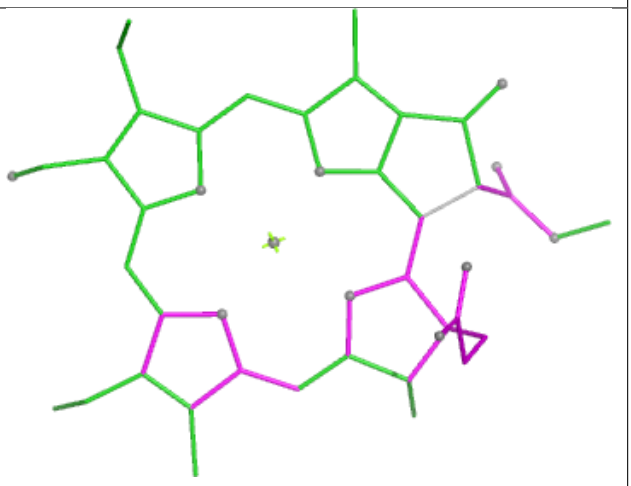


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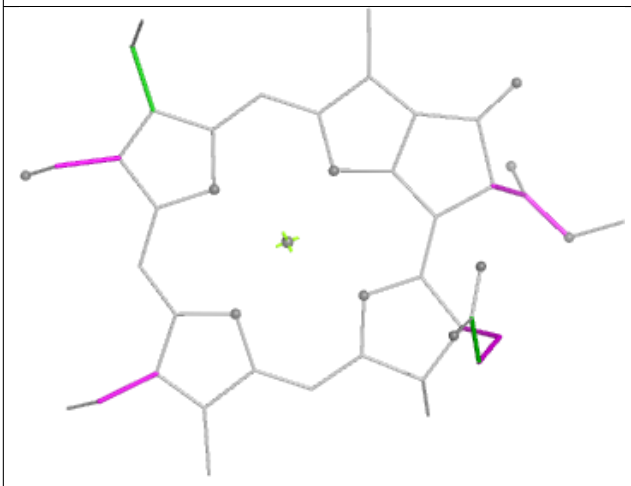
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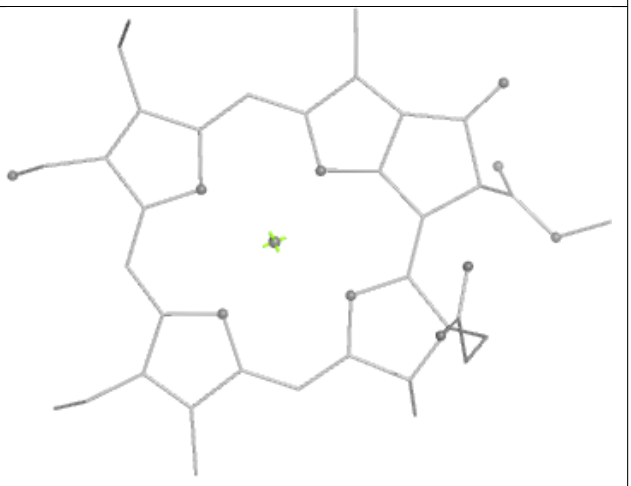
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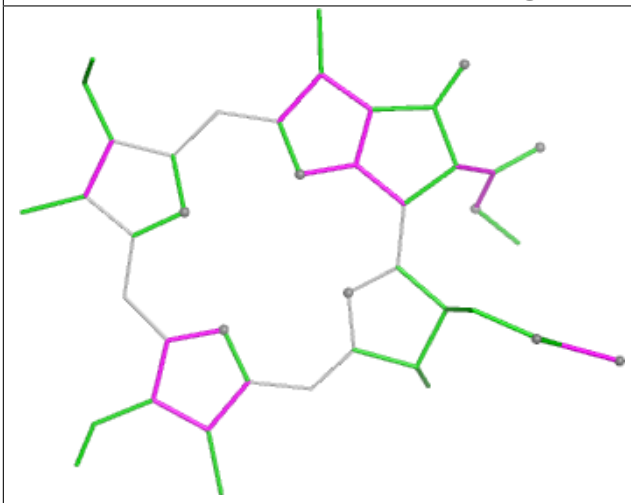


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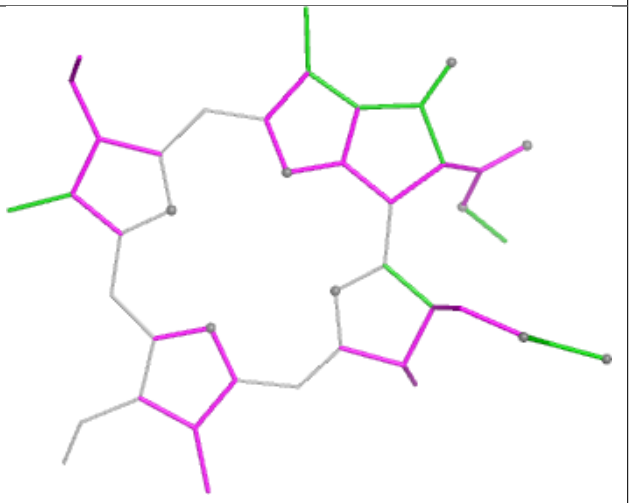


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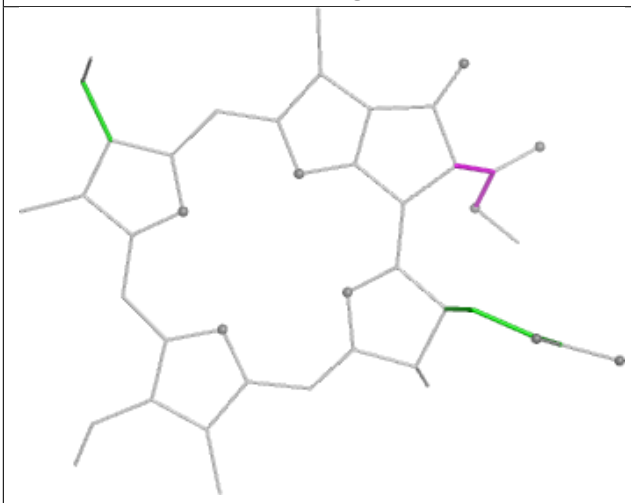
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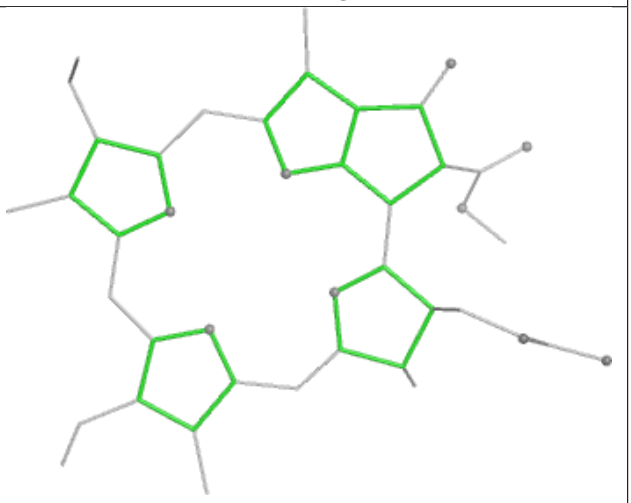
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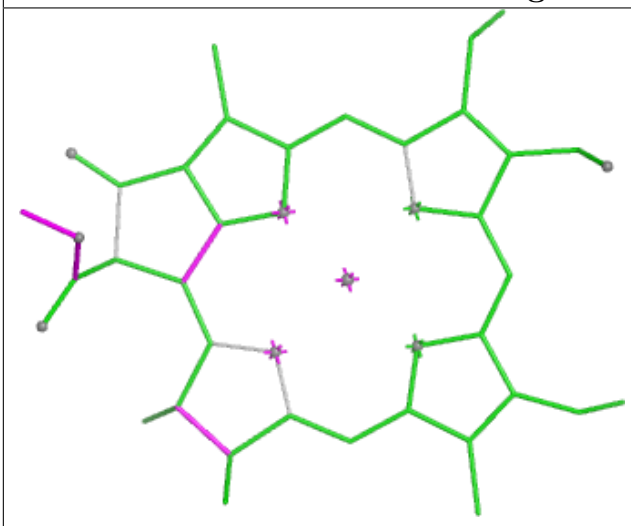


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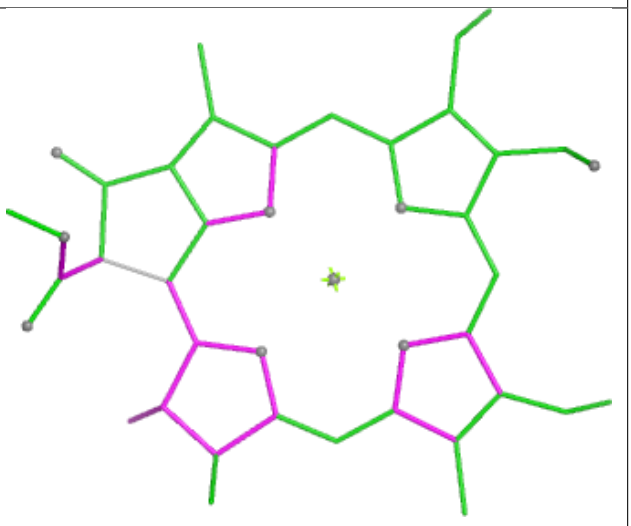


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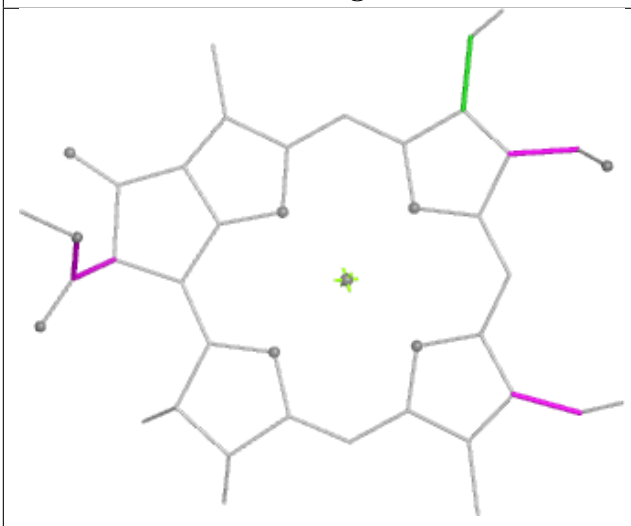
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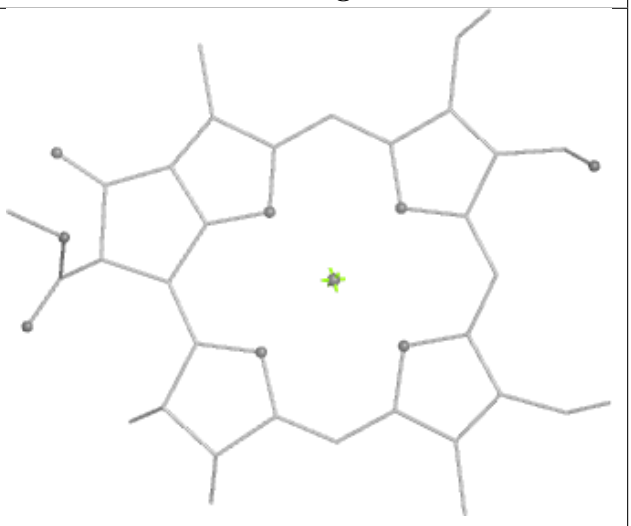
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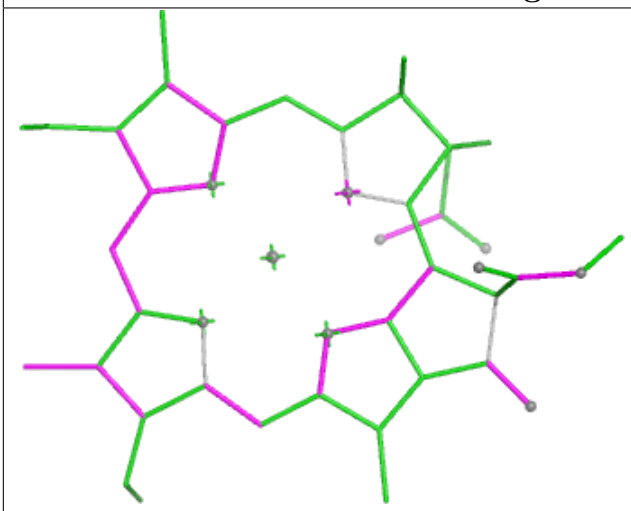


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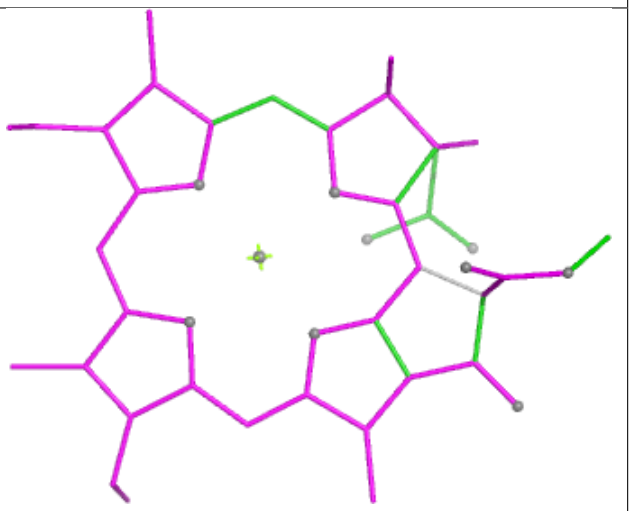


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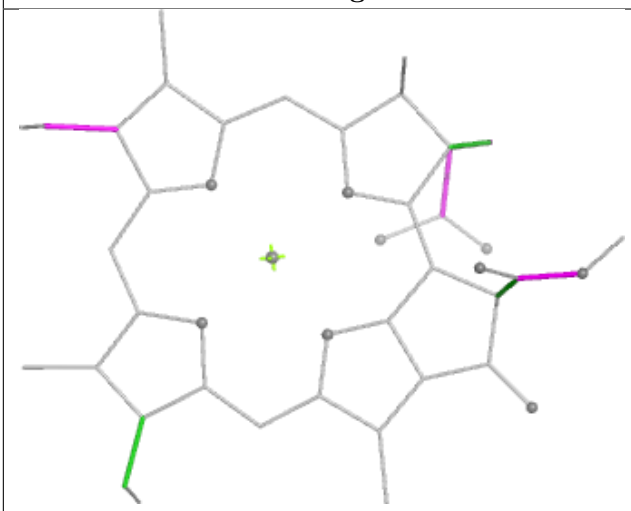
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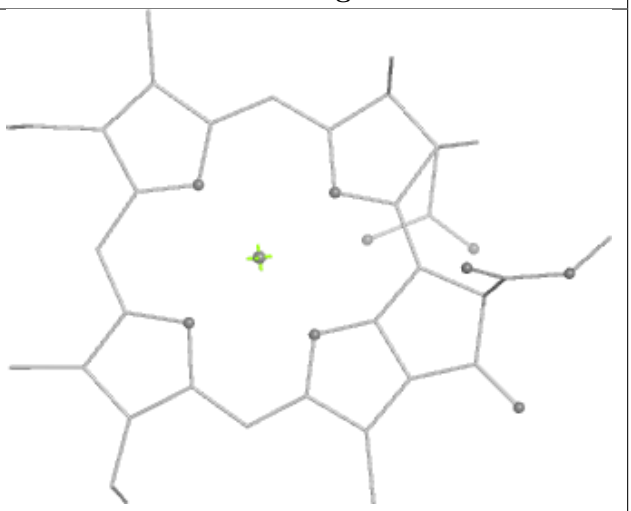
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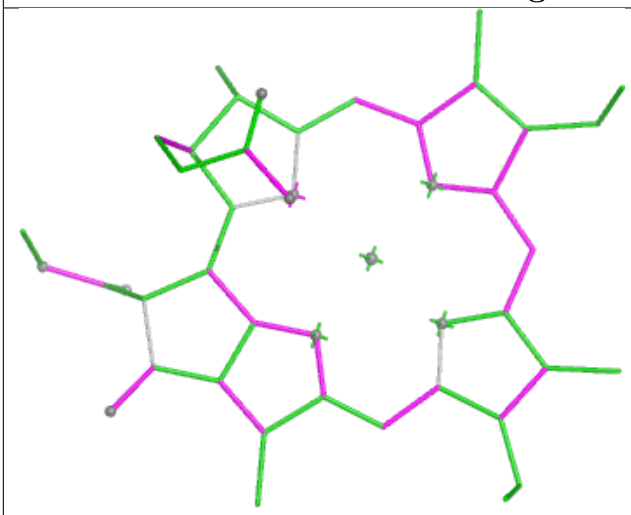


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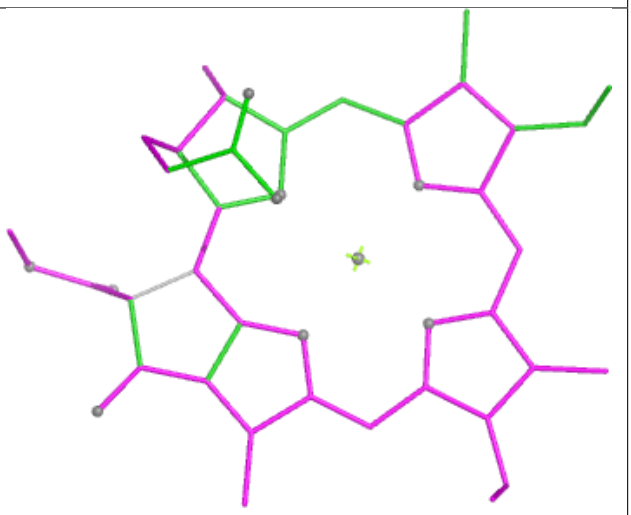


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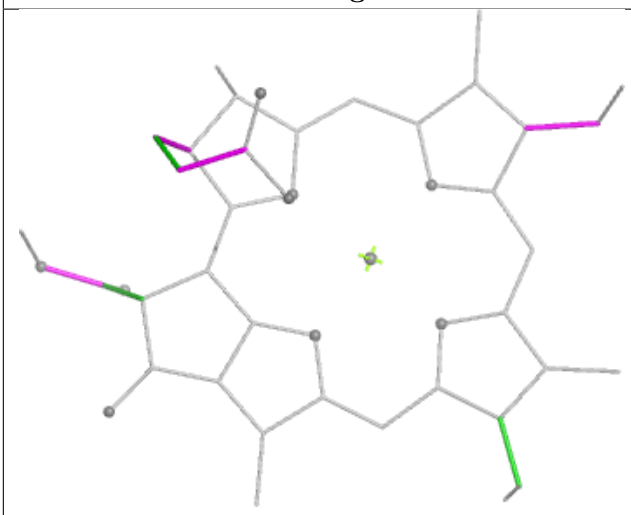
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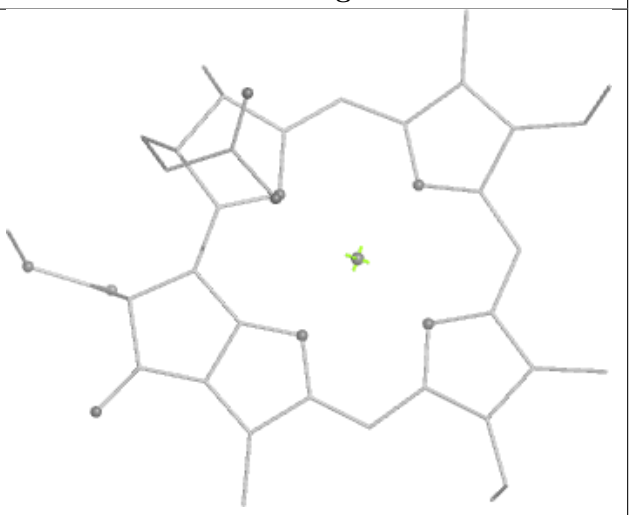
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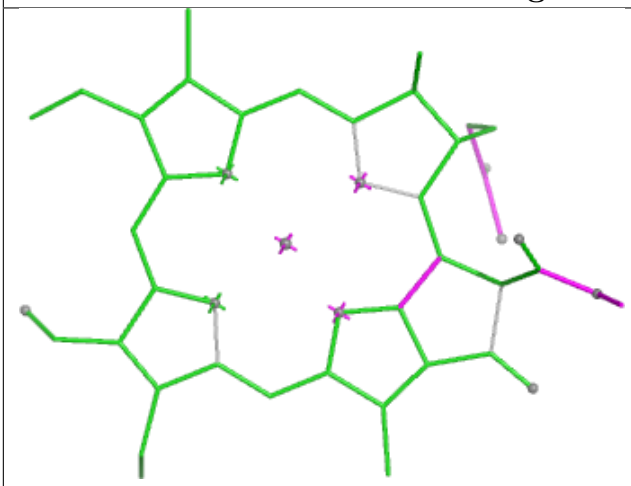


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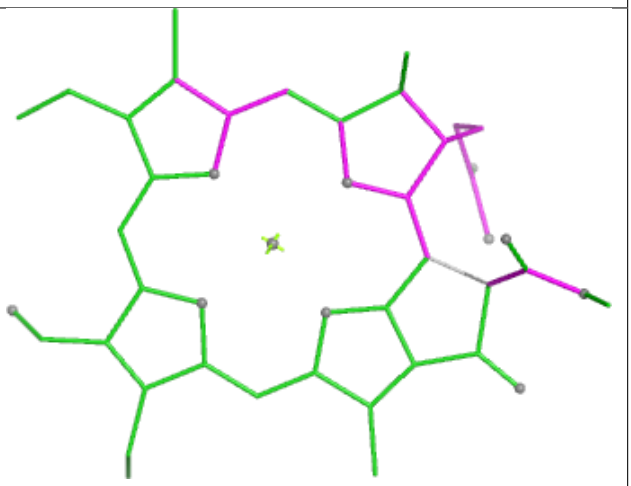


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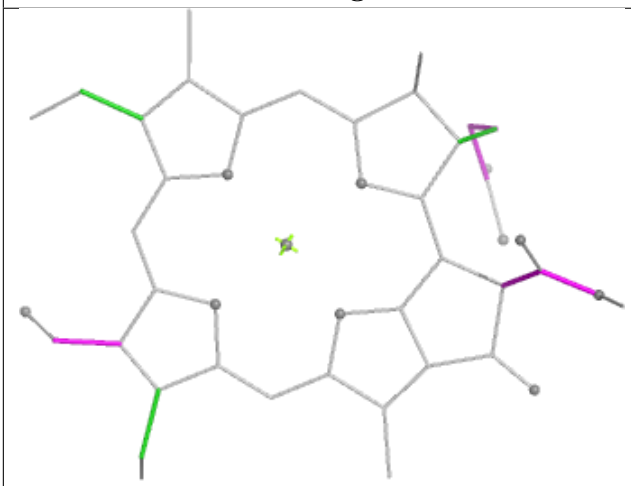
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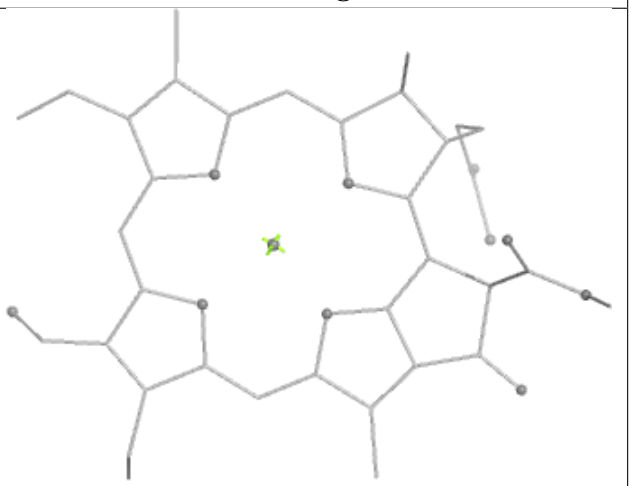
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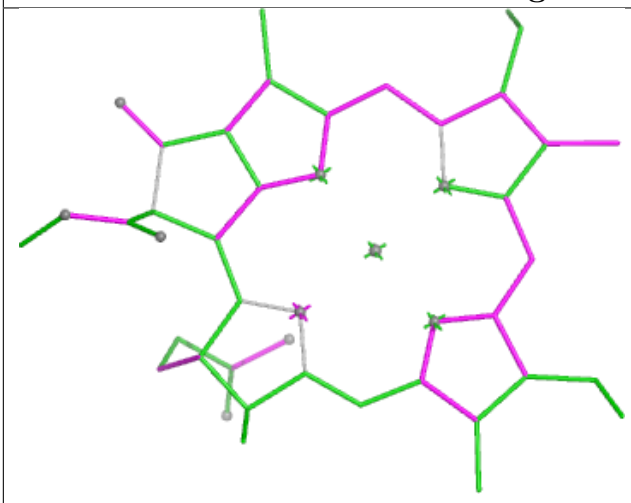


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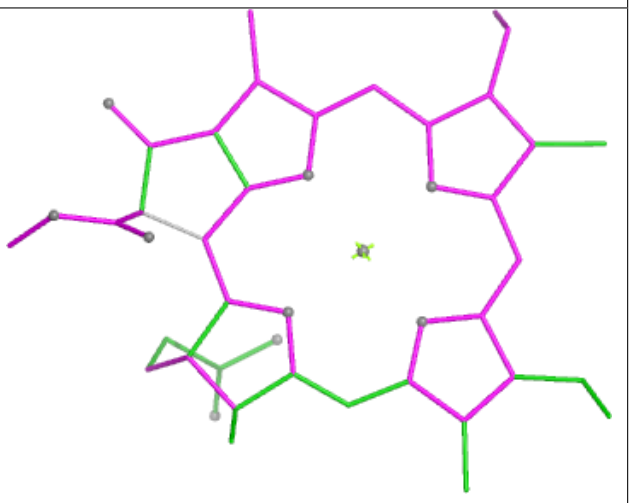


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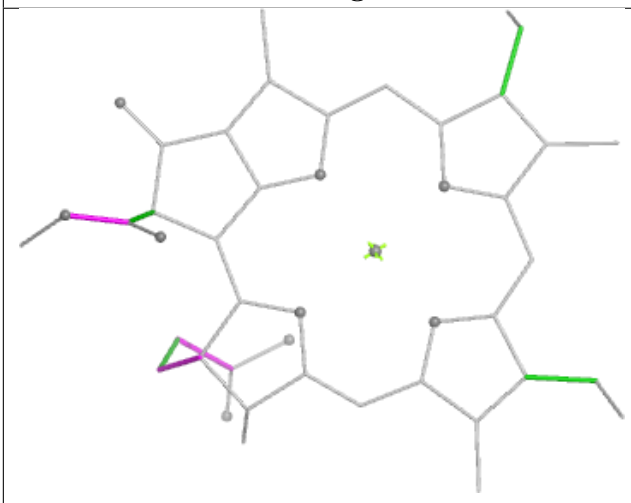
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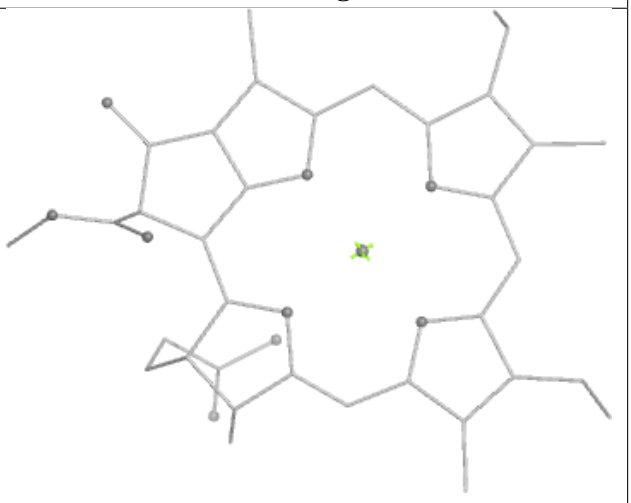
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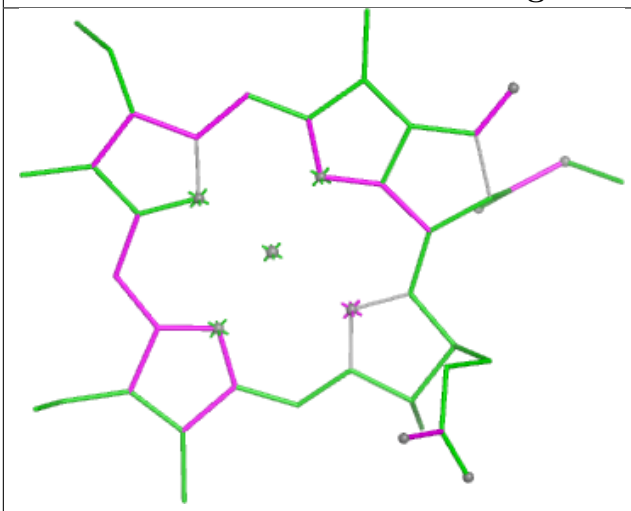


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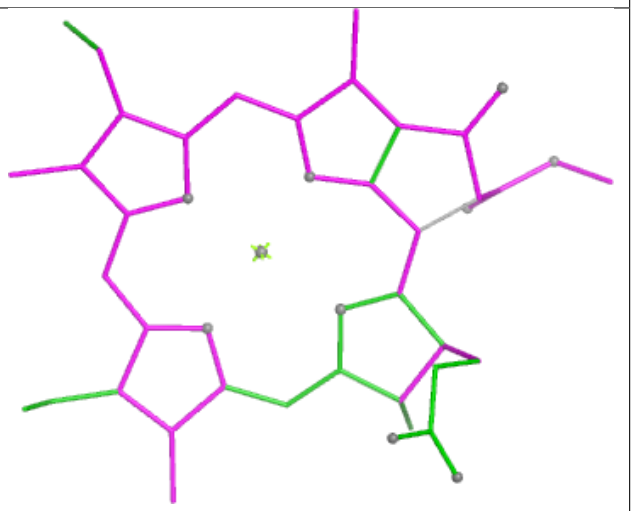


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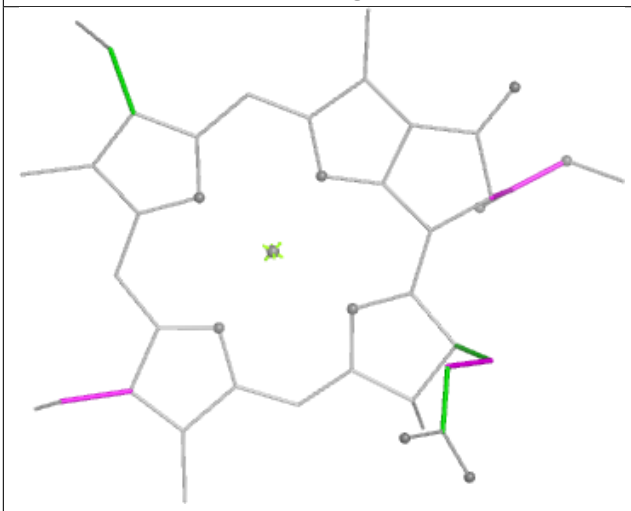
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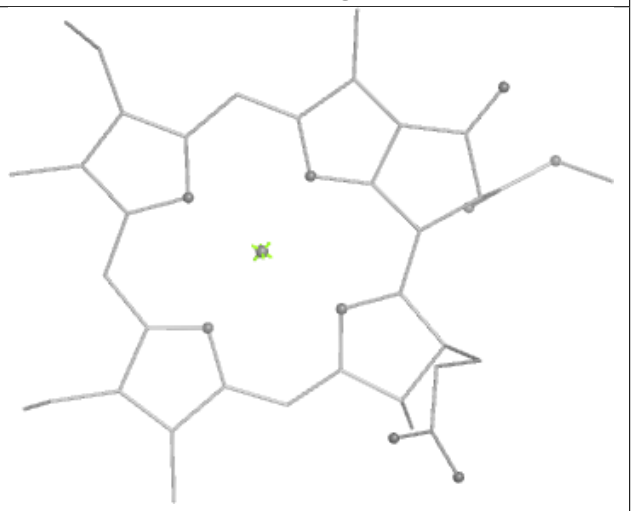
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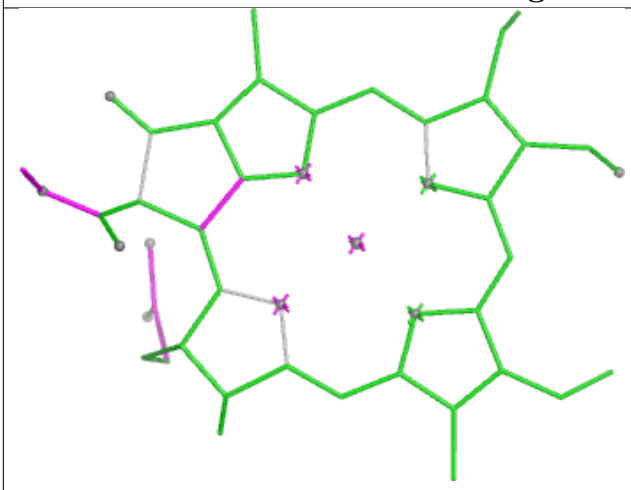


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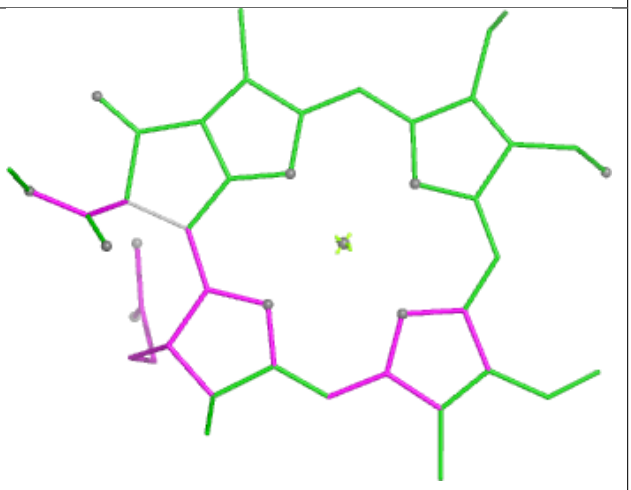


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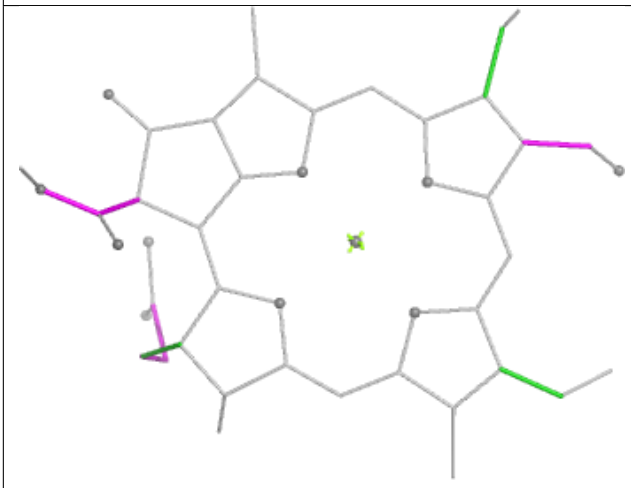
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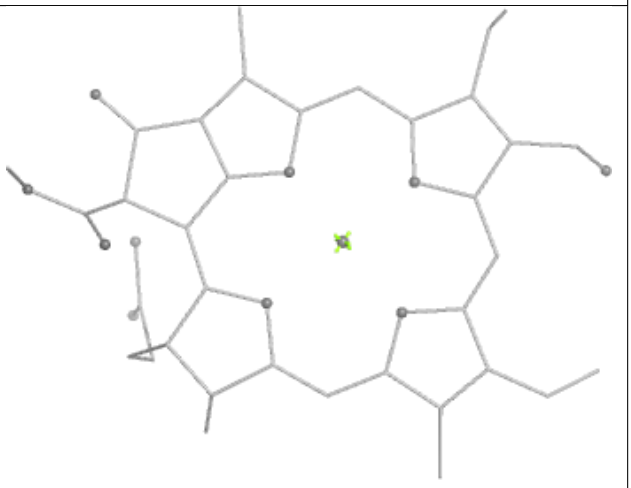
Bond lengths



Bond angles

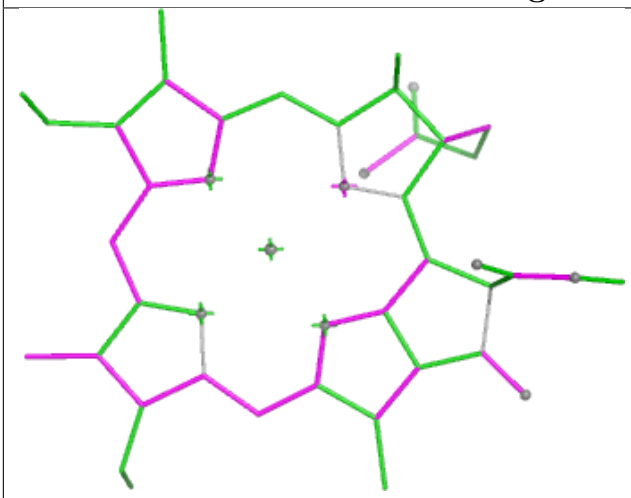


Torsions

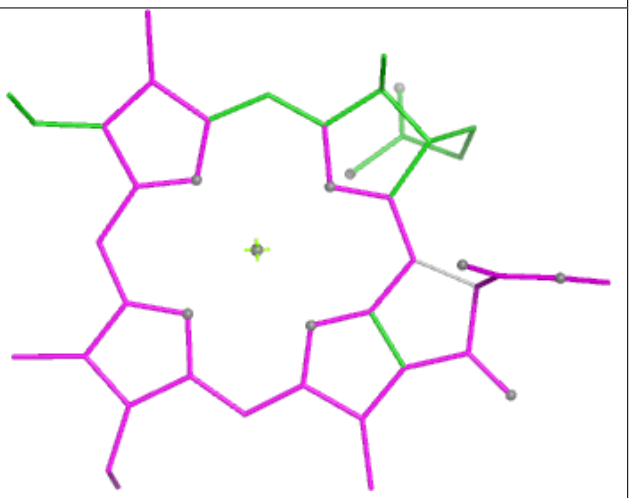


Rings

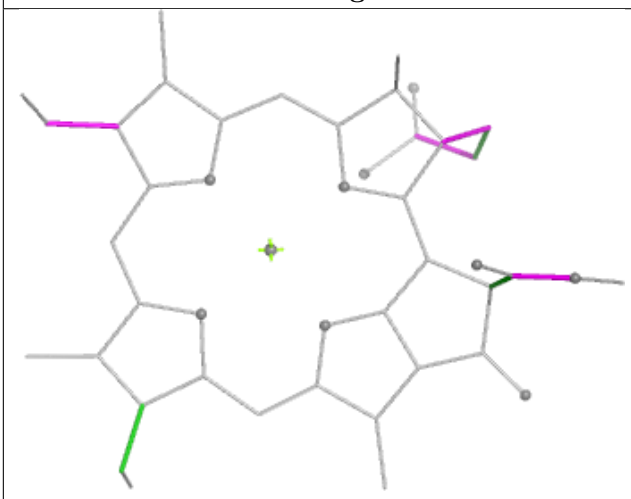
Ligand CLA 1 614



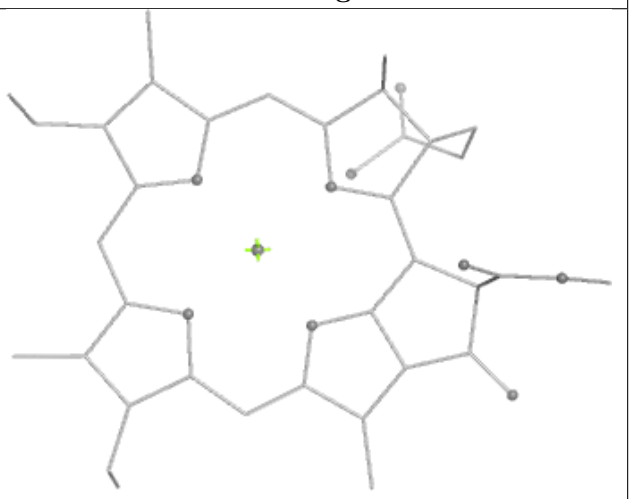
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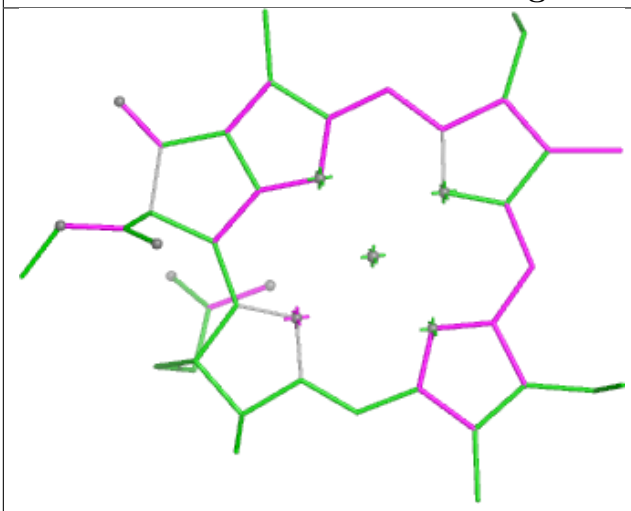
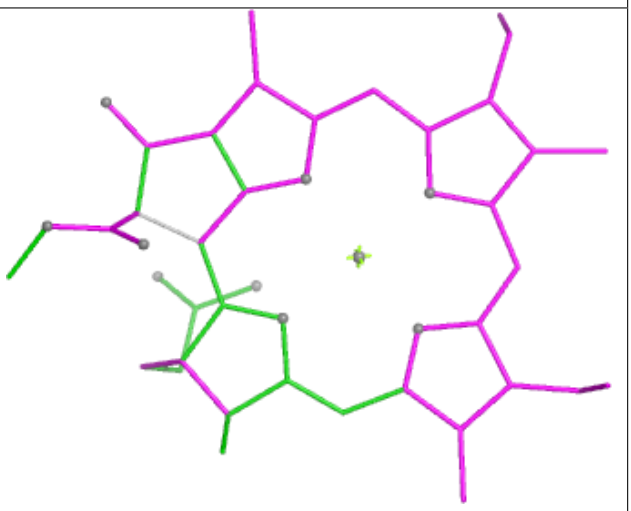
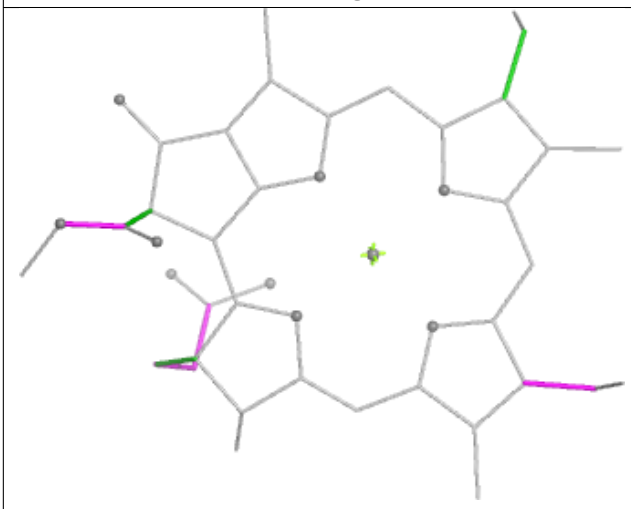
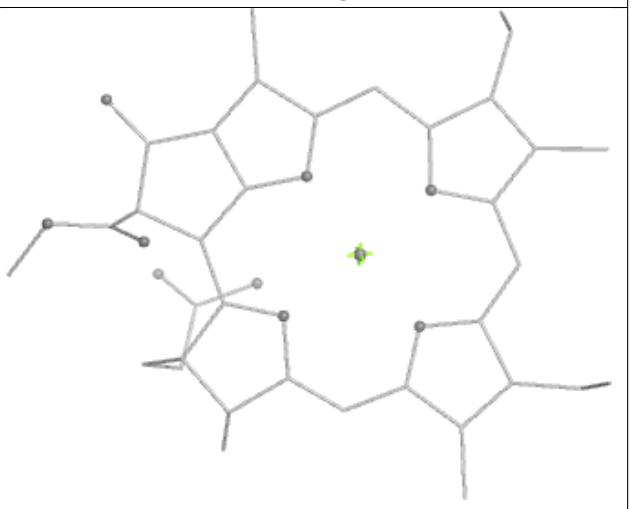
Bond angles



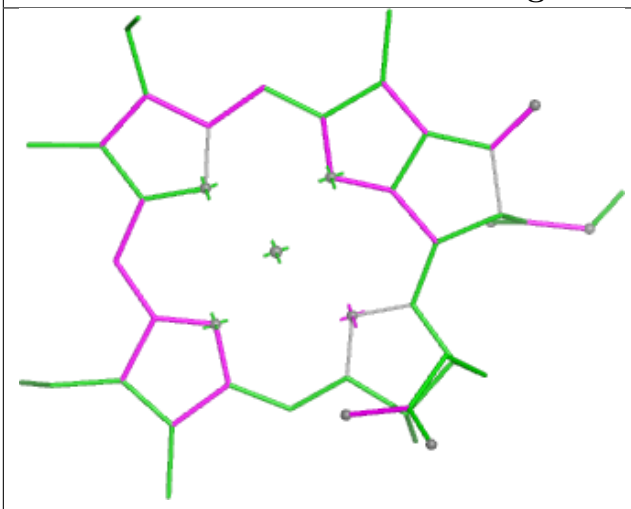
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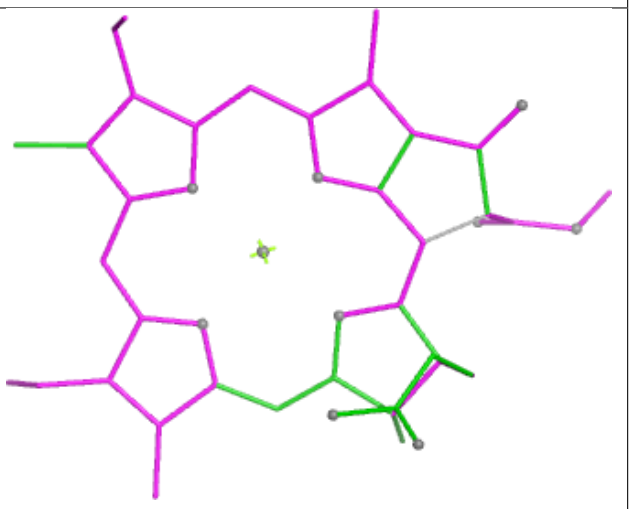
Rings

Ligand CLA 7 313	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

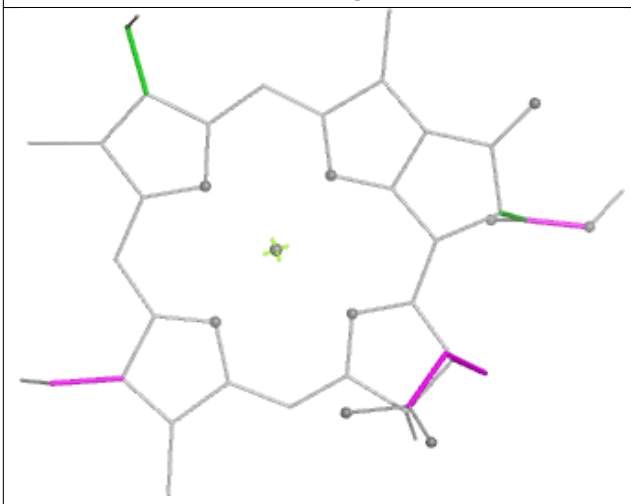
Ligand CLA d 404



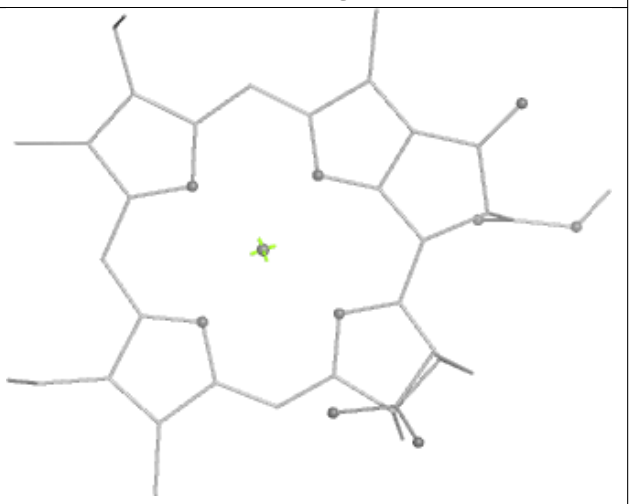
Bond lengths



Bond angles

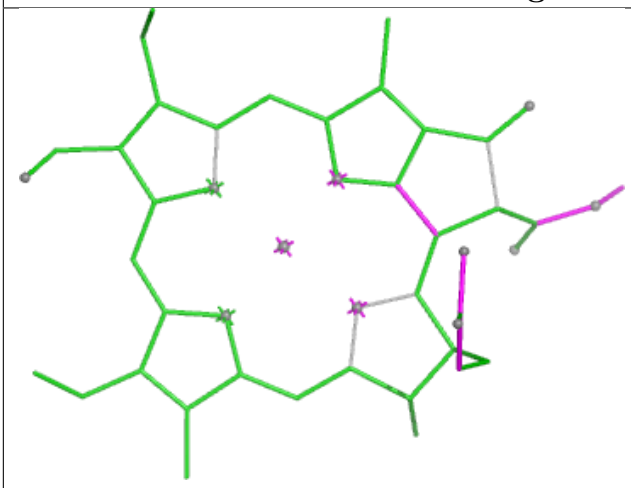


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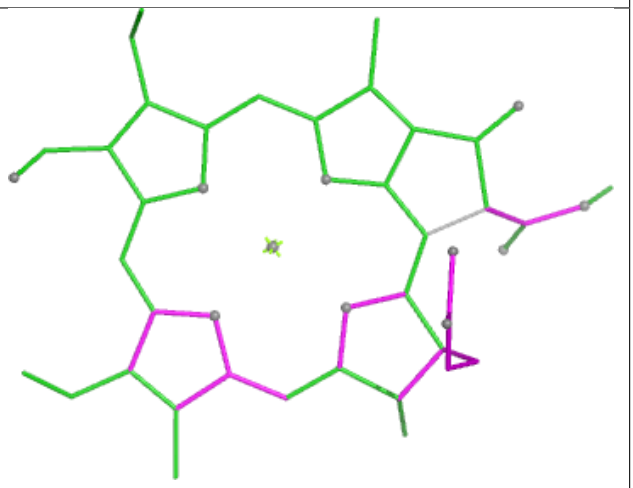


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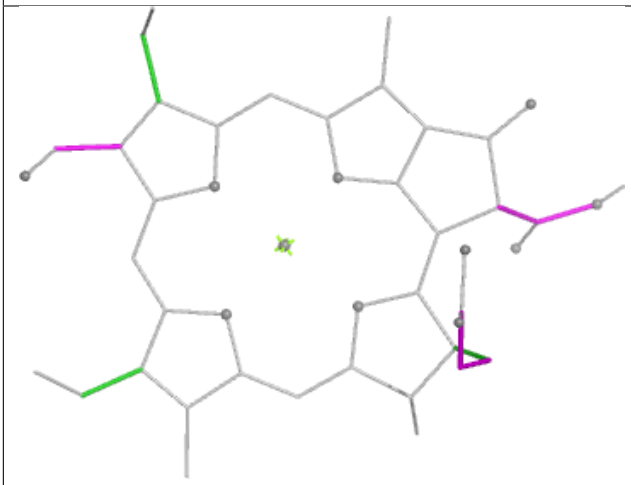
Ligand CHL 1 608



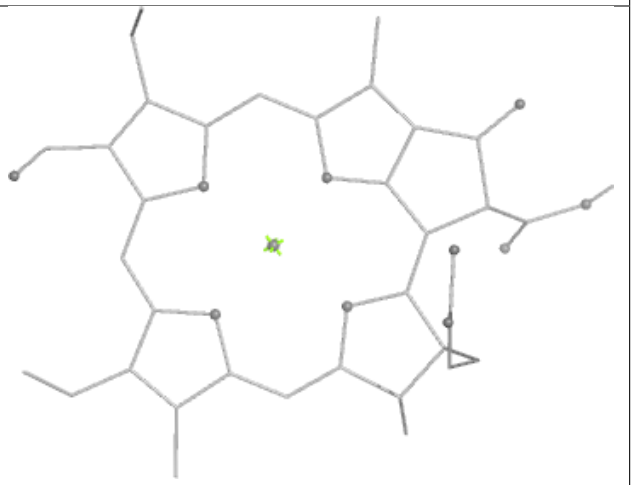
Bond lengths



Bond angles

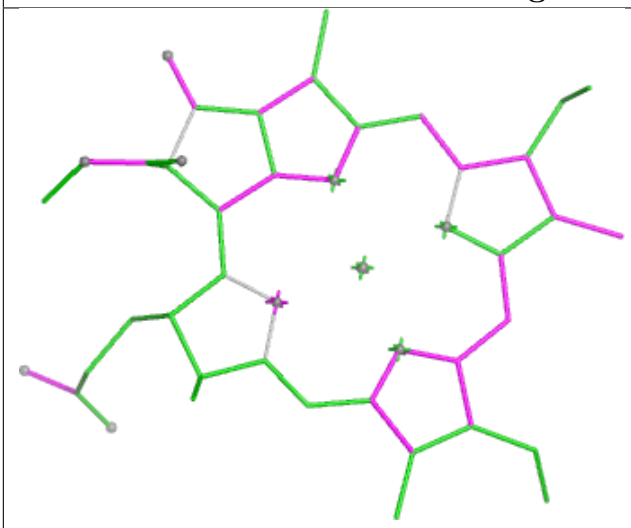


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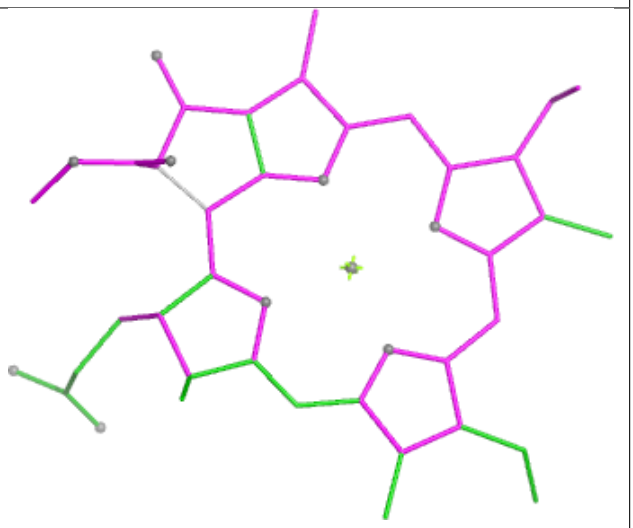


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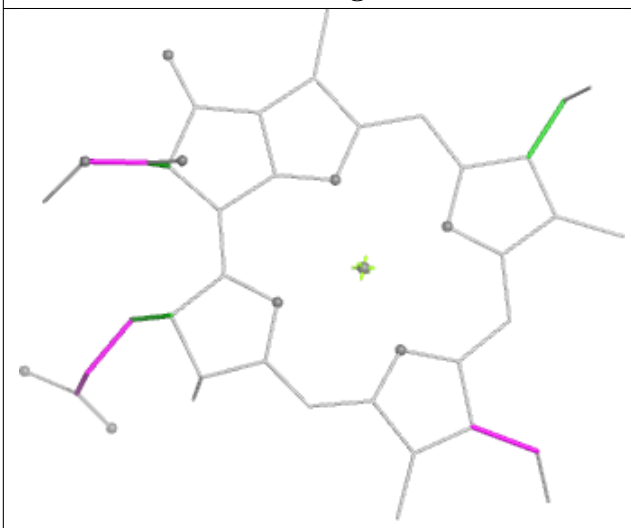
Ligand CLA 8 301



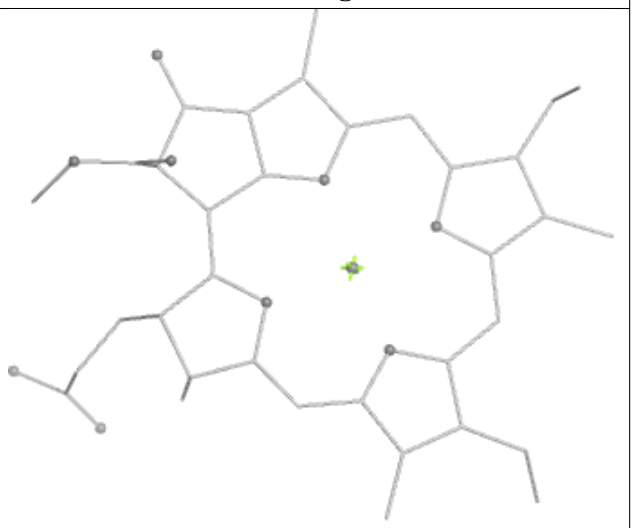
Bond lengths



Bond angles

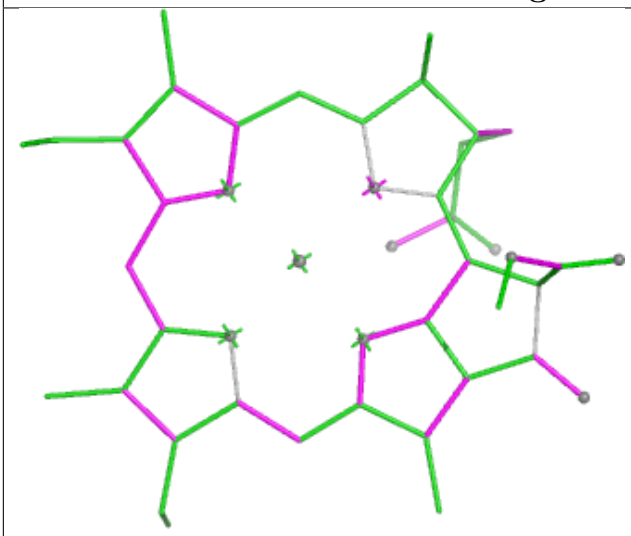


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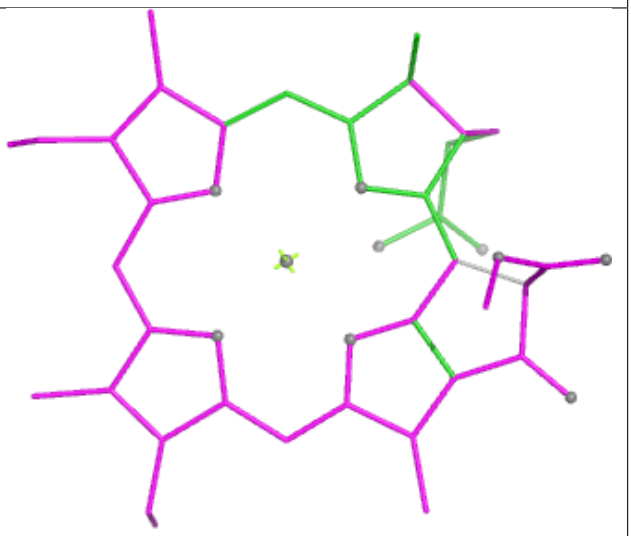


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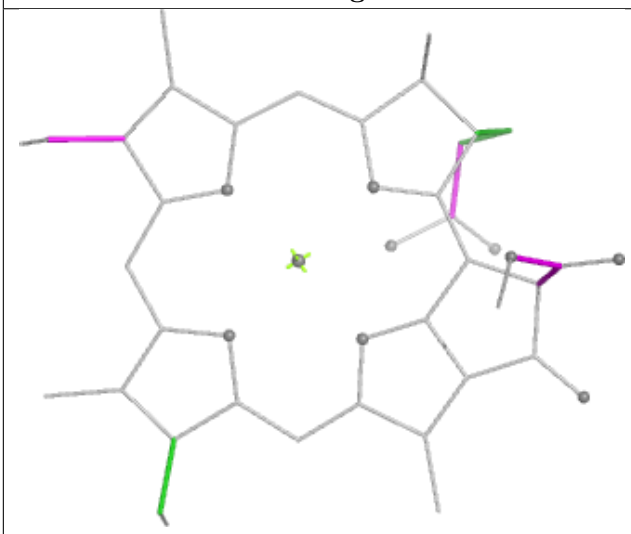
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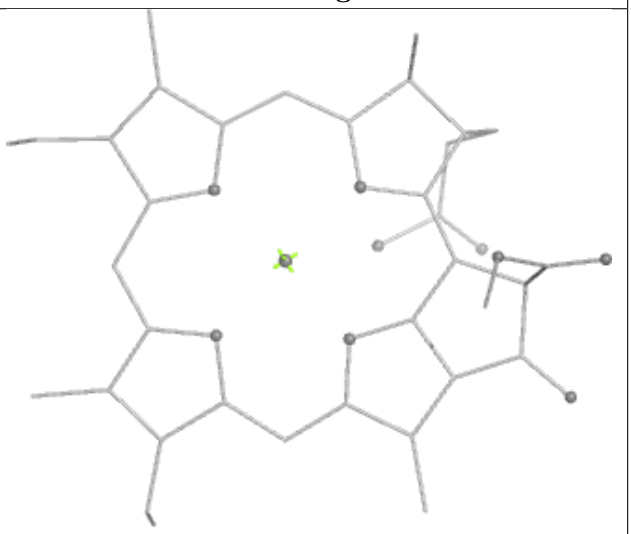
Bond lengths



Bond angles

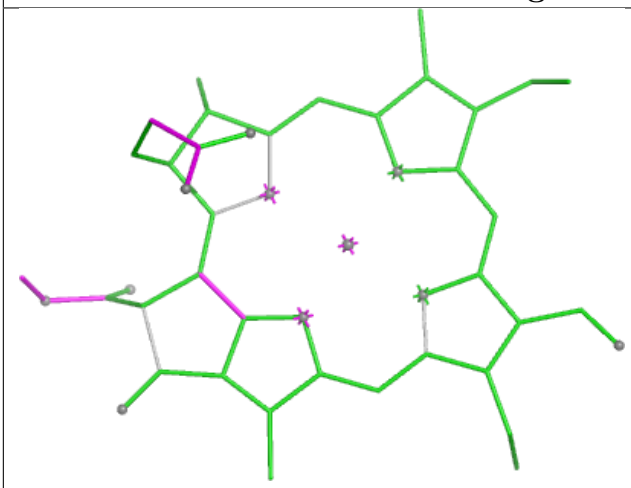


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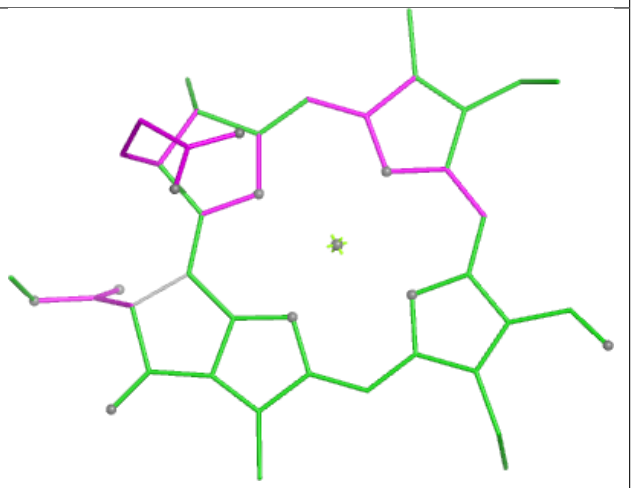


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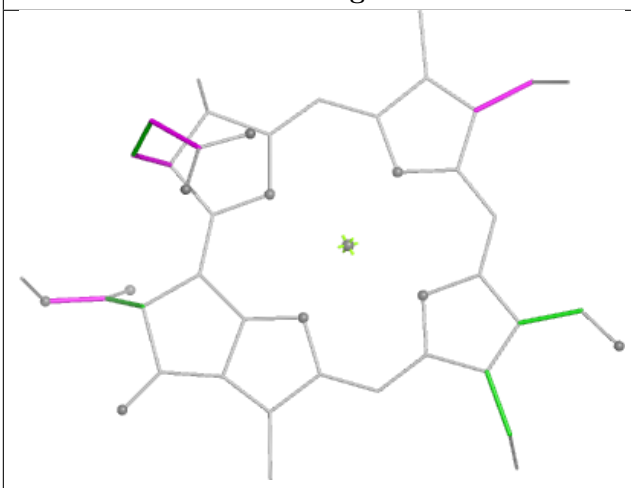
Ligand CHL 1 606



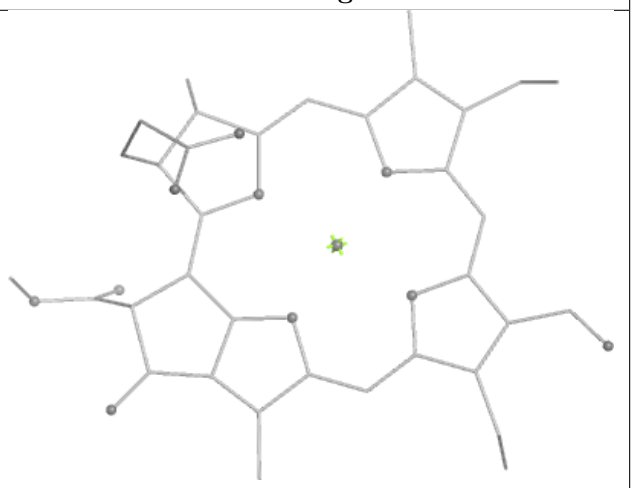
Bond lengths



Bond angles

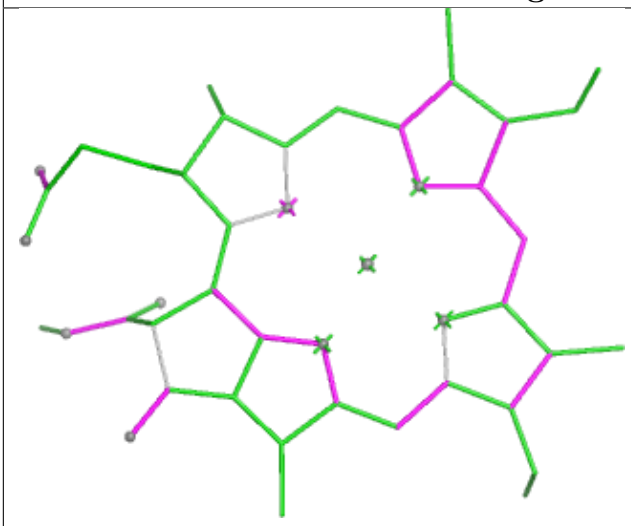


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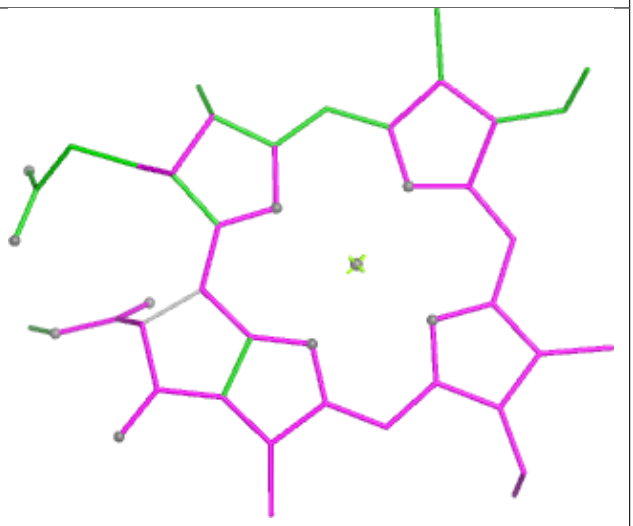


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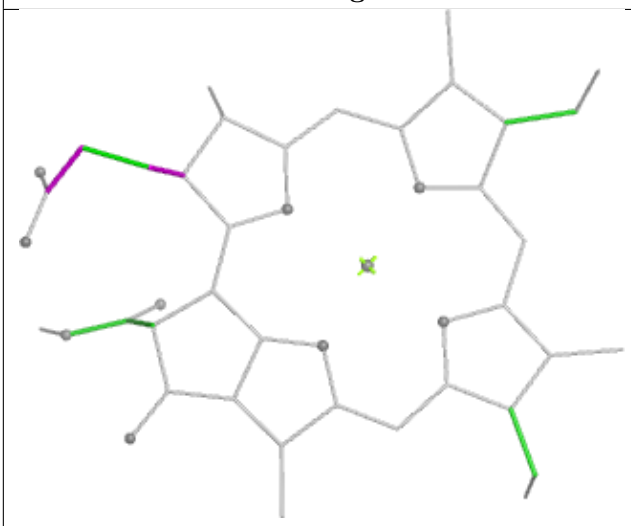
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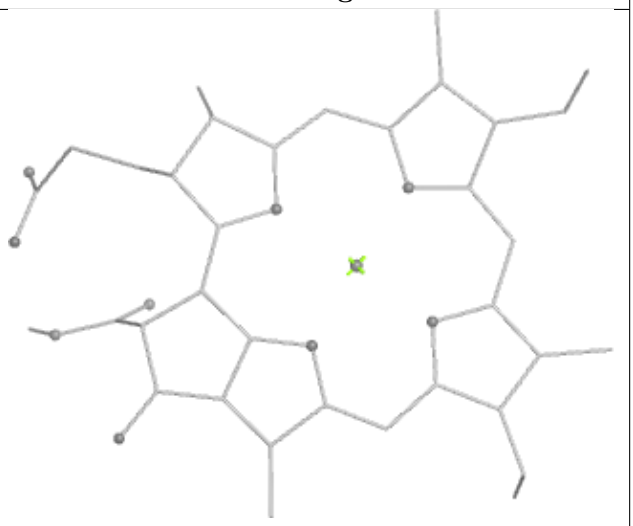
Bond lengths



Bond angles

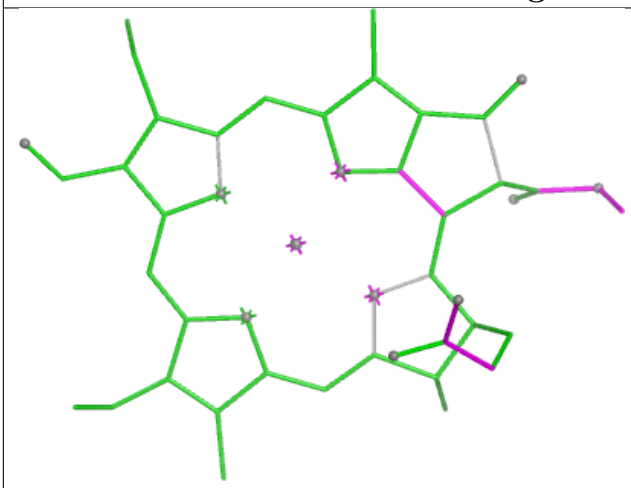


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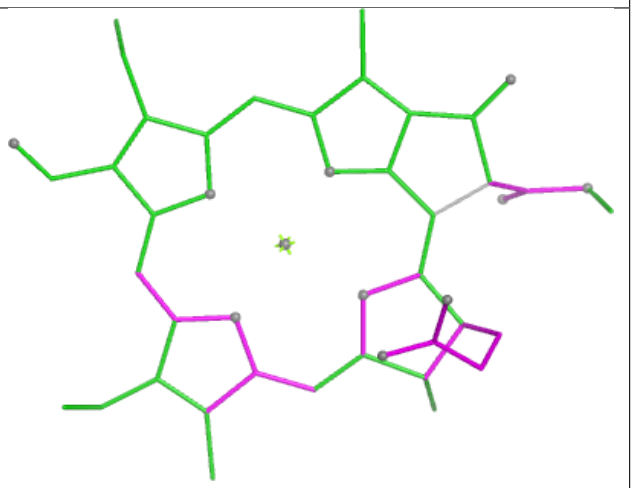


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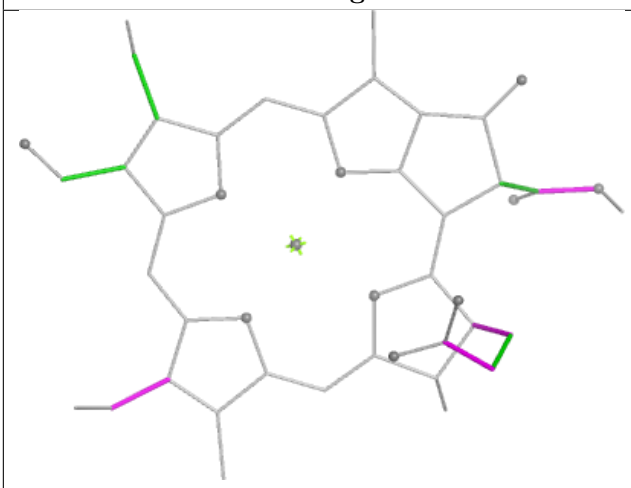
Ligand CHL 5 606



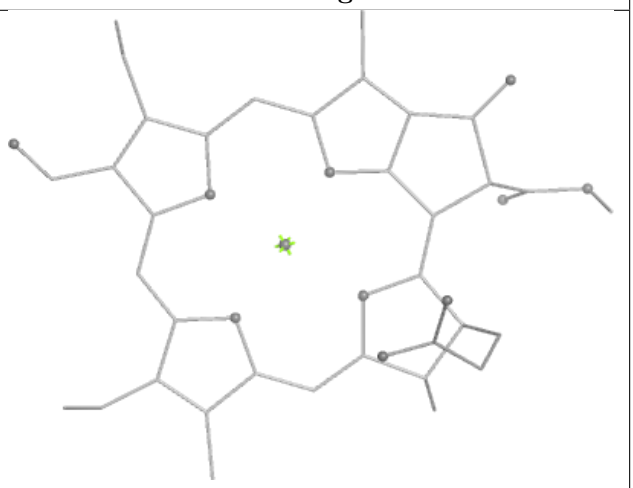
Bond lengths



Bond angles

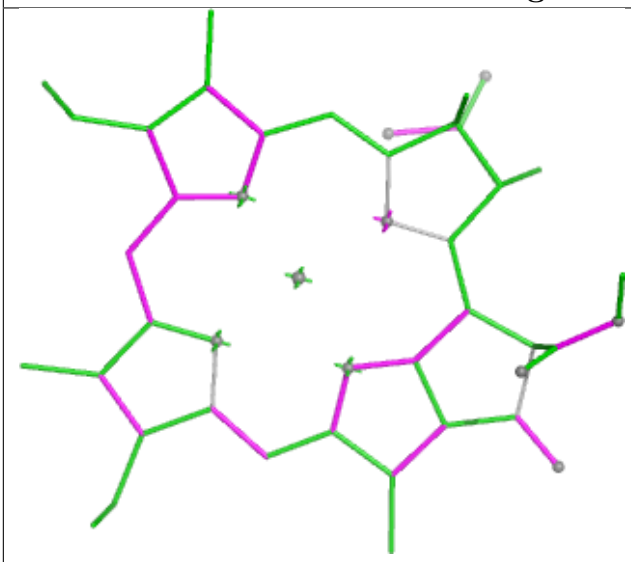


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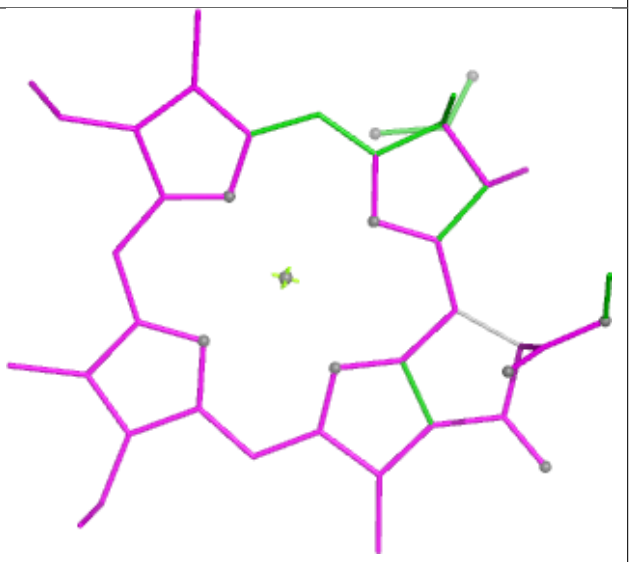


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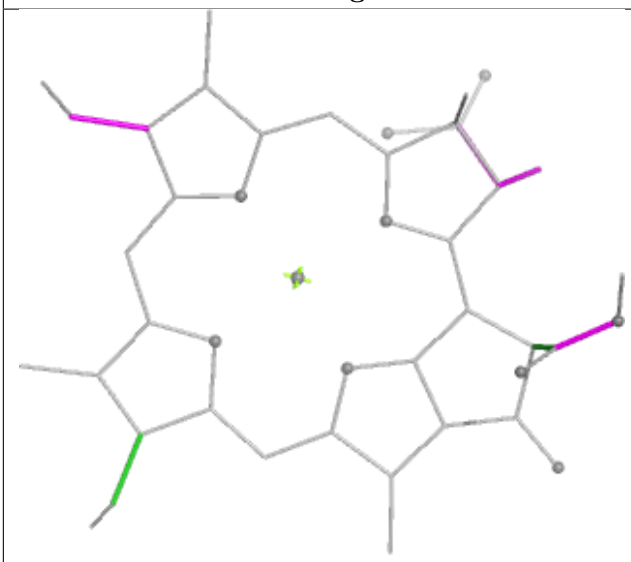
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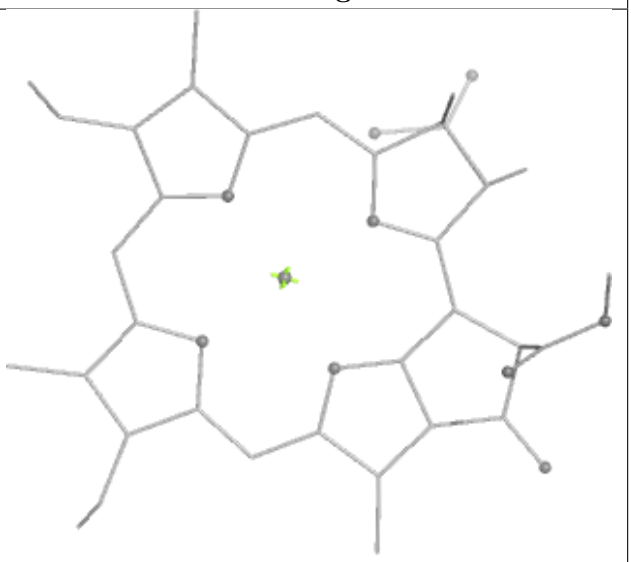
Bond lengths



Bond angles

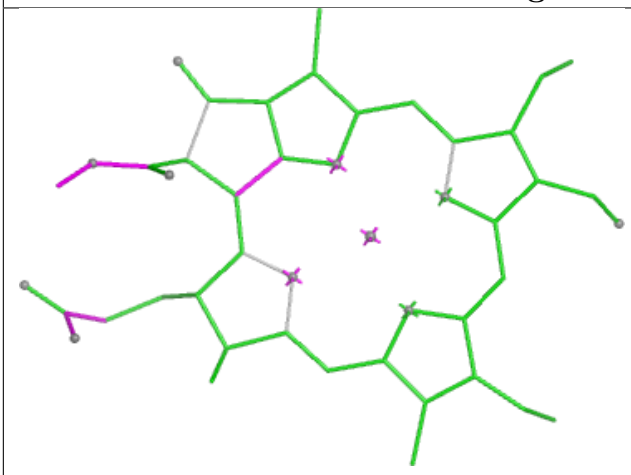


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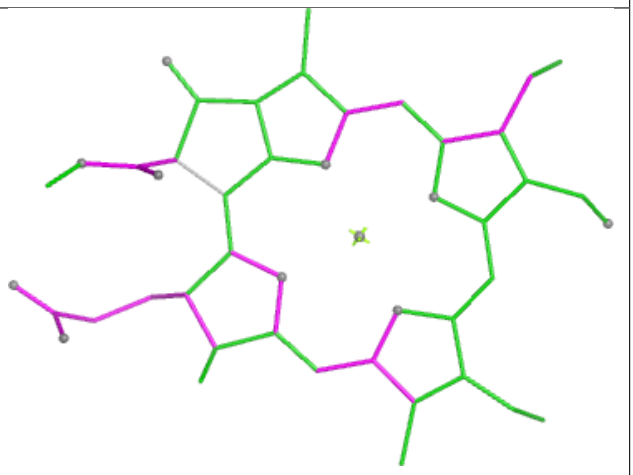


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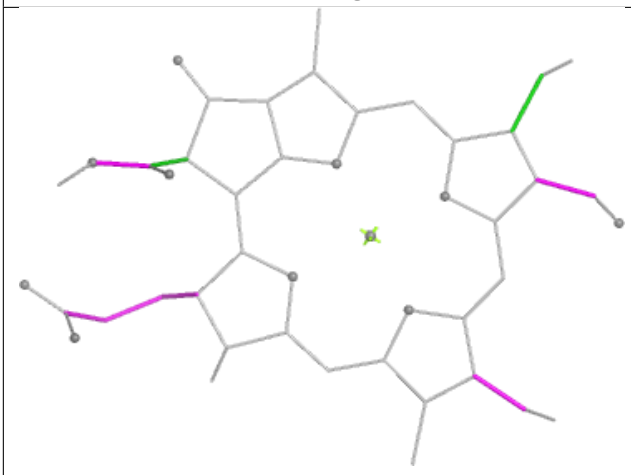
Ligand CHL 8 302



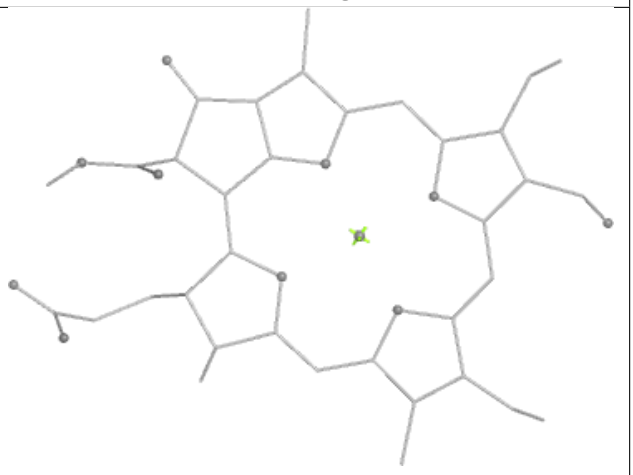
Bond lengths



Bond angles

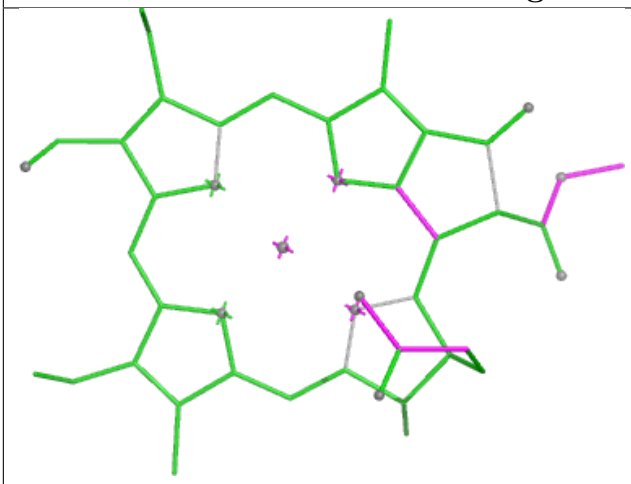


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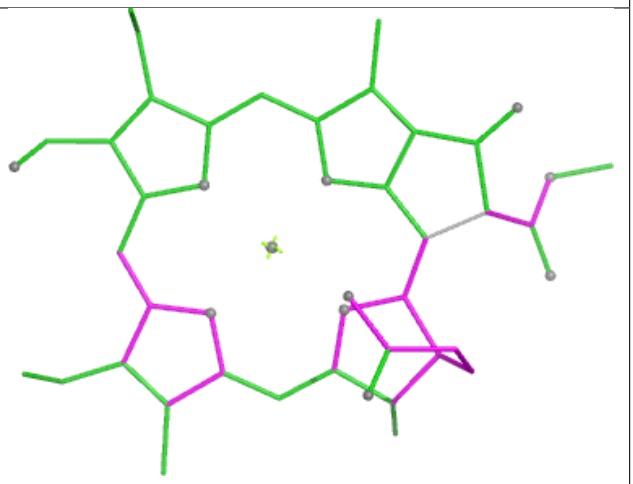


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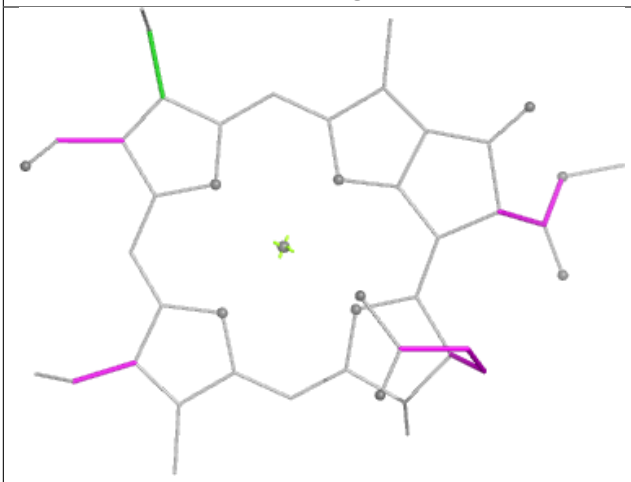
Ligand CHL n 609



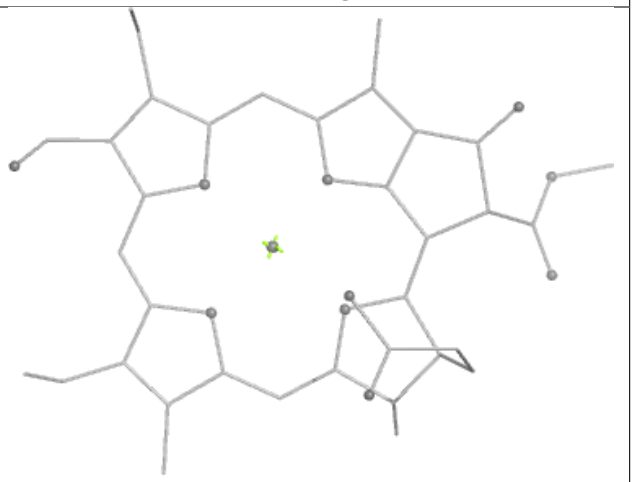
Bond lengths



Bond angles

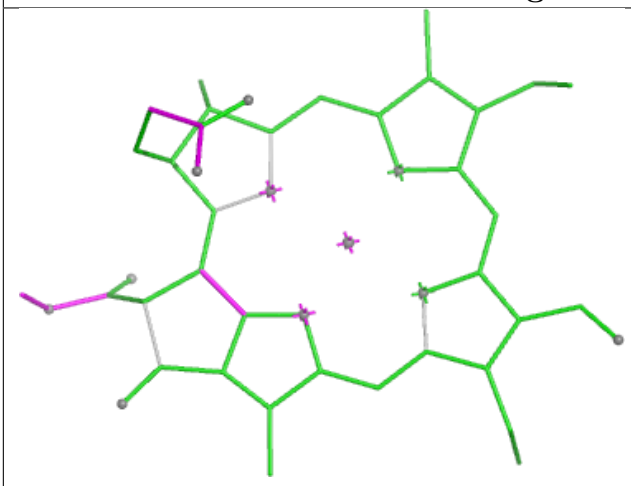


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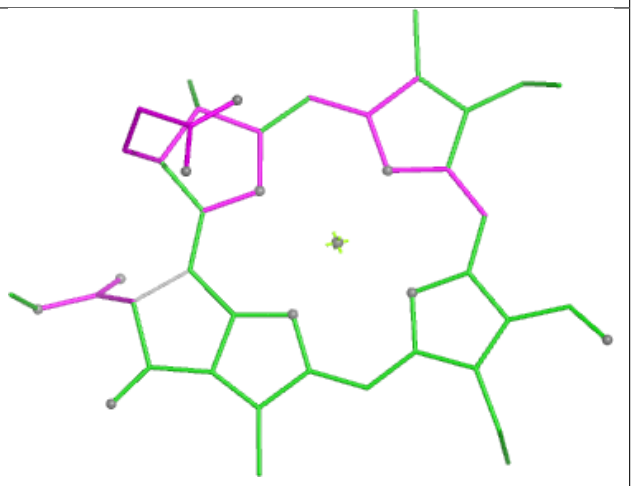


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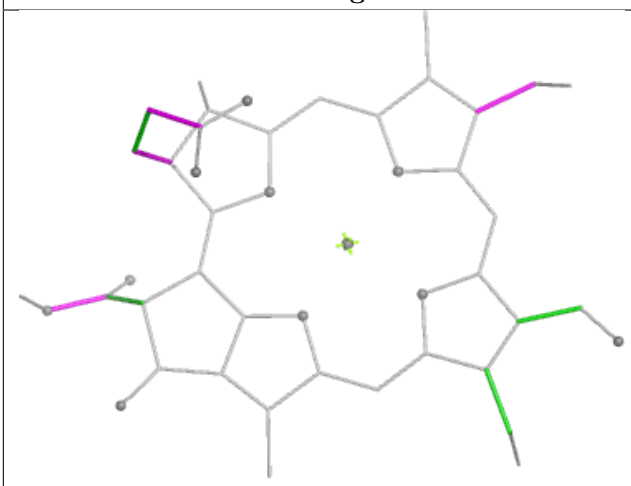
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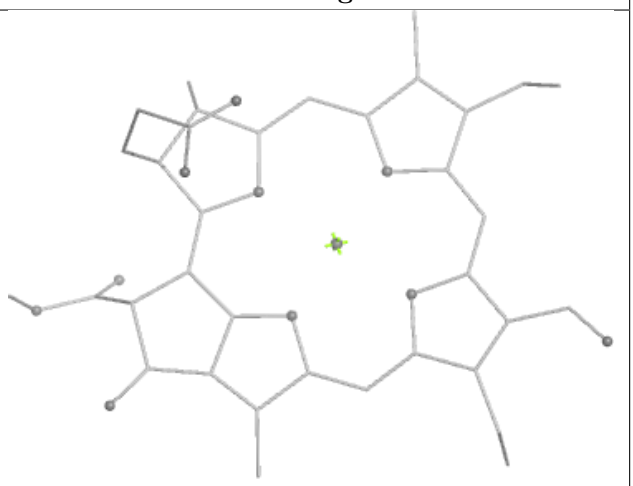
Bond lengths



Bond angles

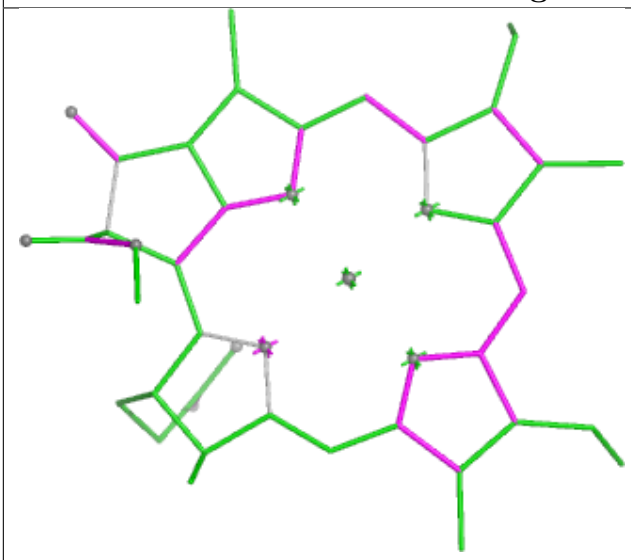


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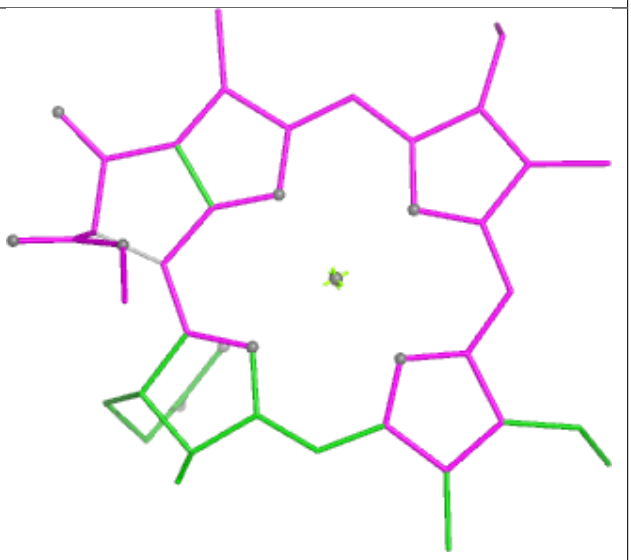


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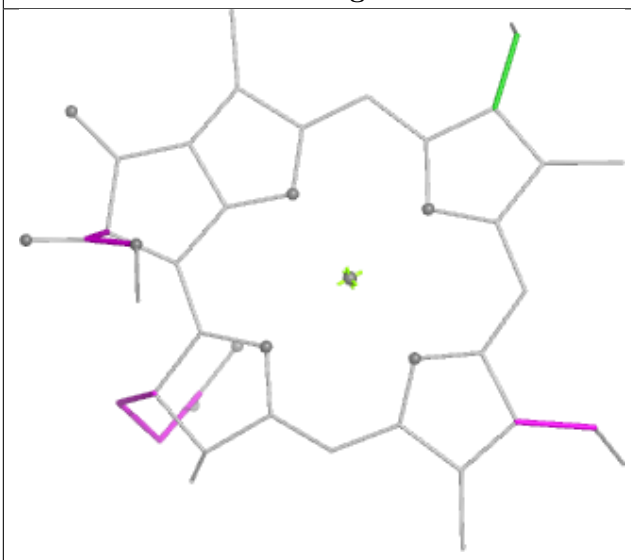
Ligand CLA s 303



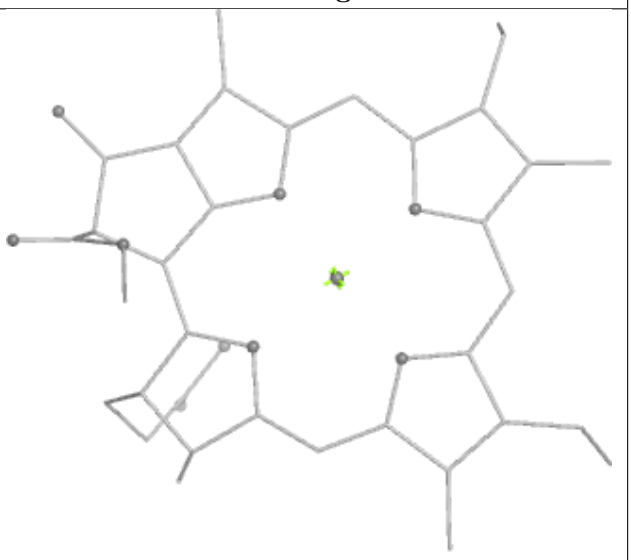
Bond lengths



Bond angles

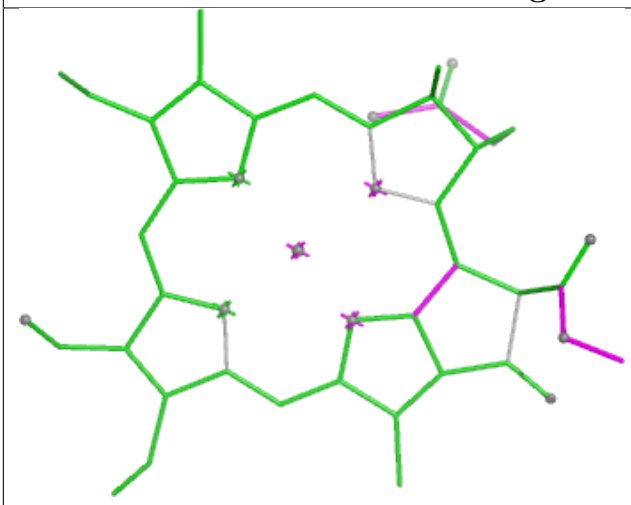


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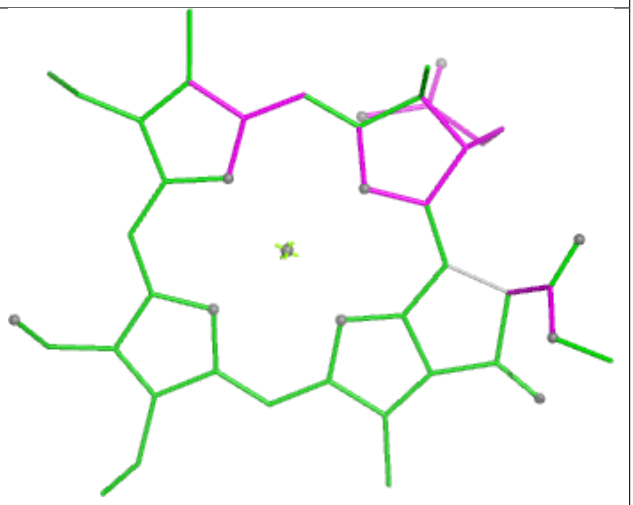


Rings

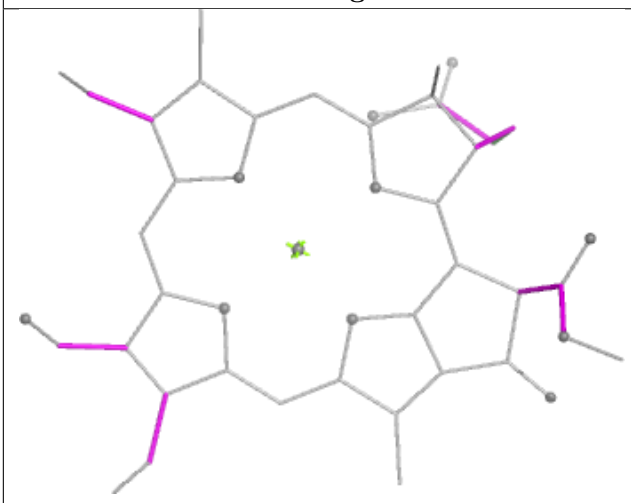
Ligand CHL r 306



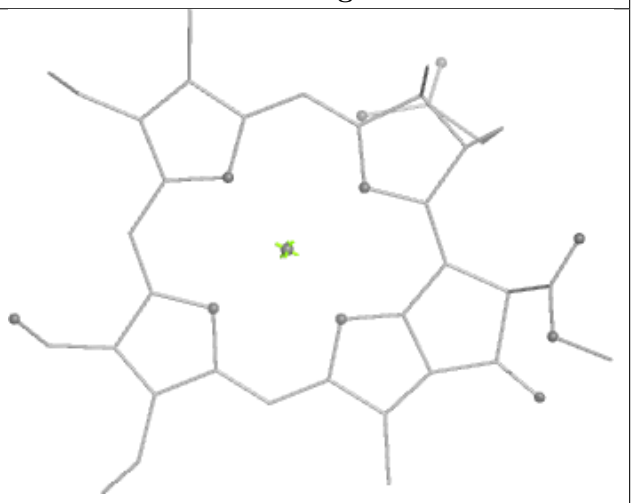
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Bond angles

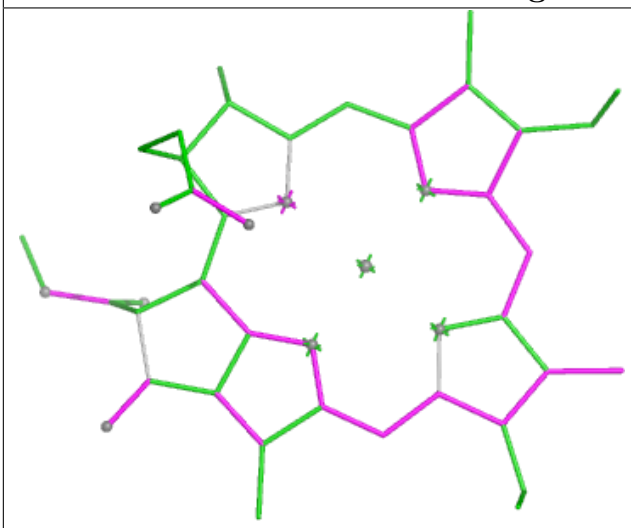


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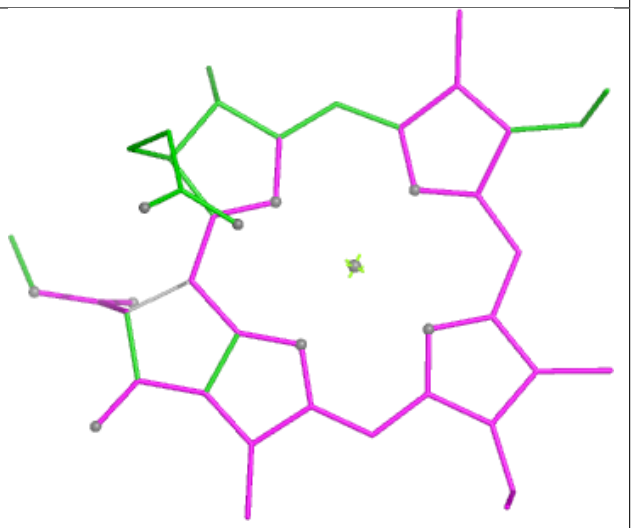


Rings

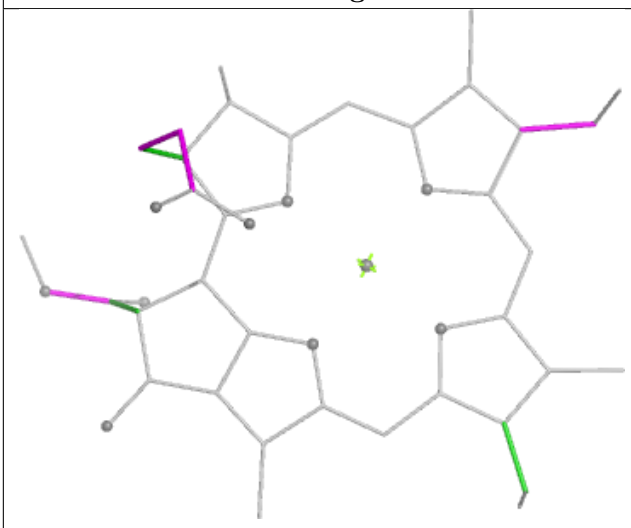
Ligand CLA 1 611



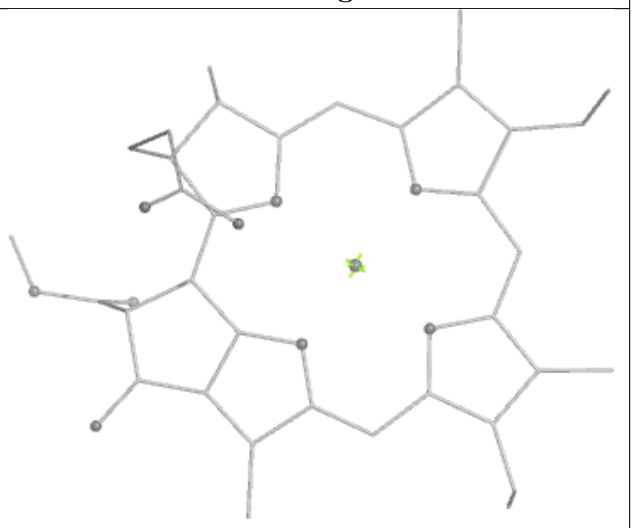
Bond lengths



Bond angles

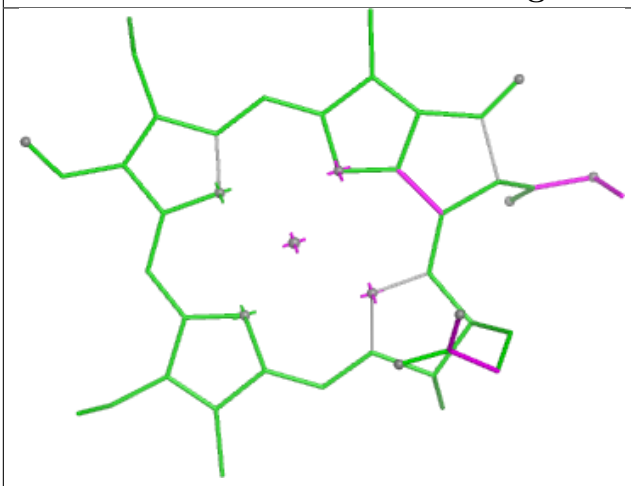


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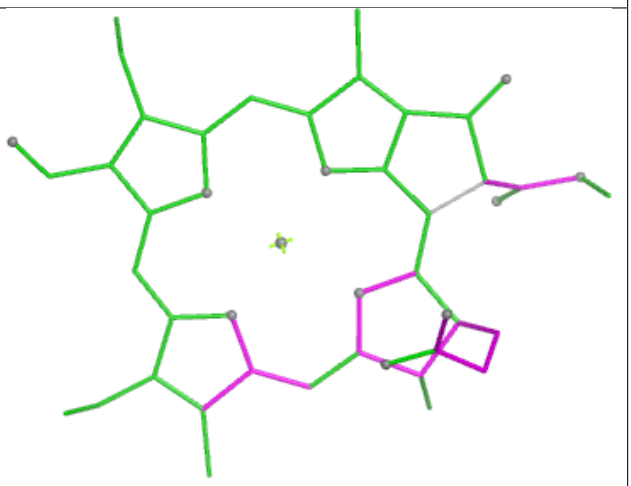


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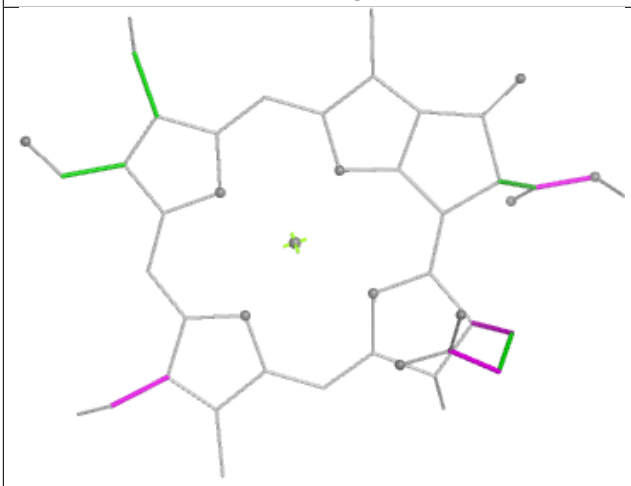
Ligand CHL 3 307



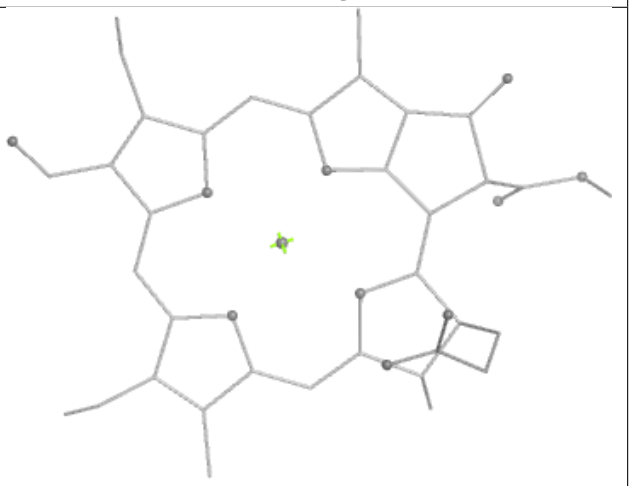
Bond lengths



Bond angles

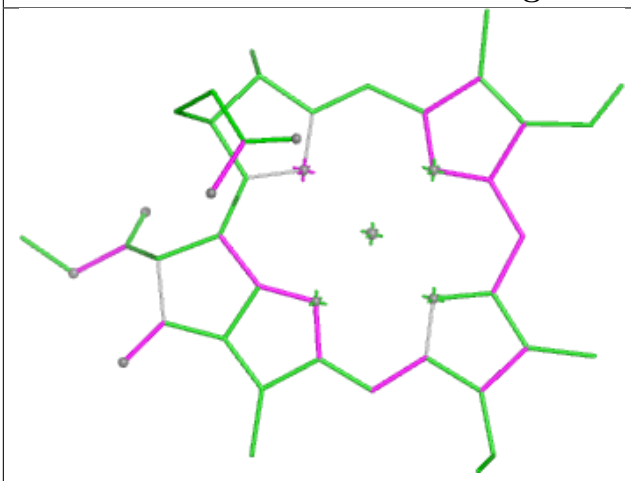


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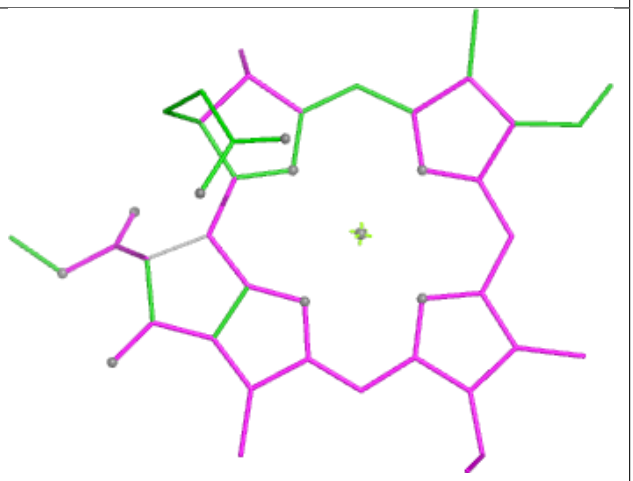


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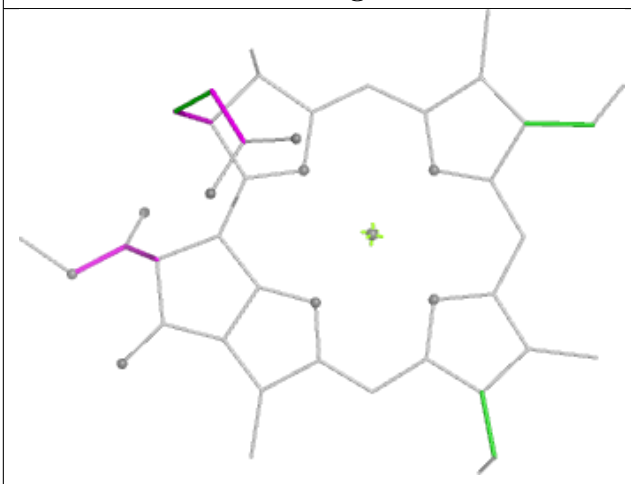
Ligand CLA G 610



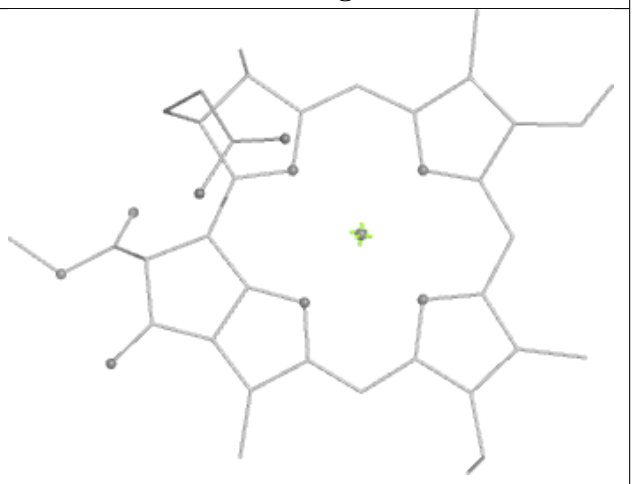
Bond lengths



Bond angles

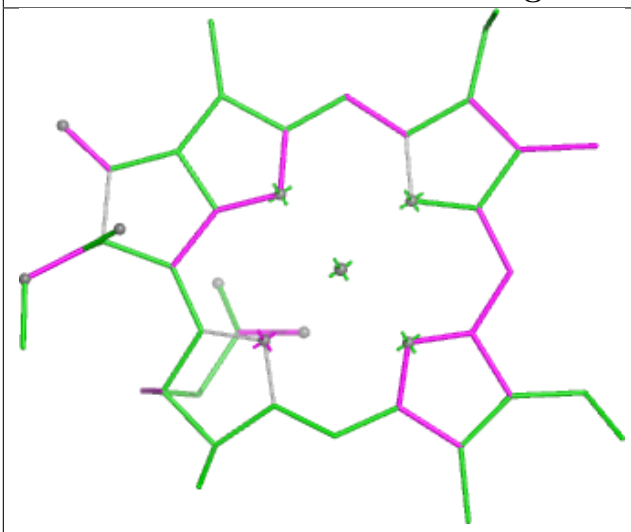


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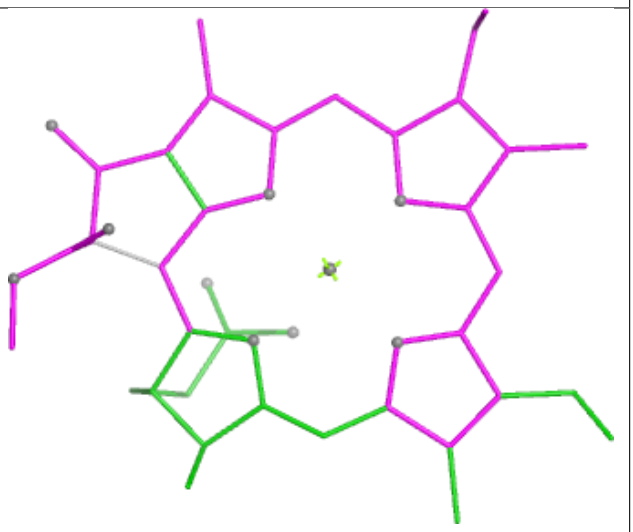


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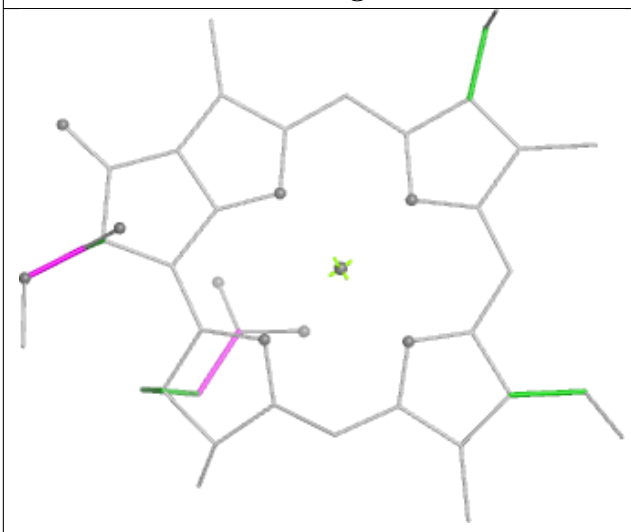
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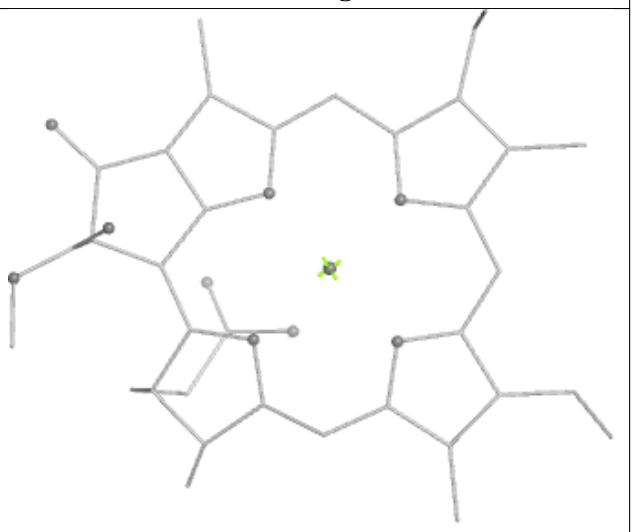
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Bond angles

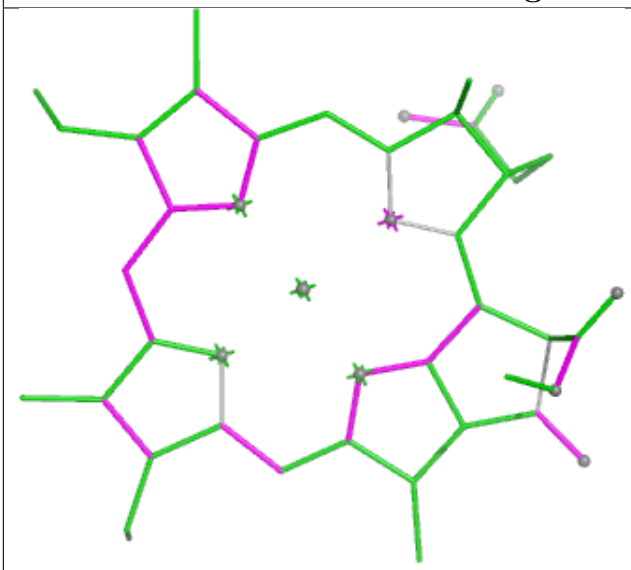


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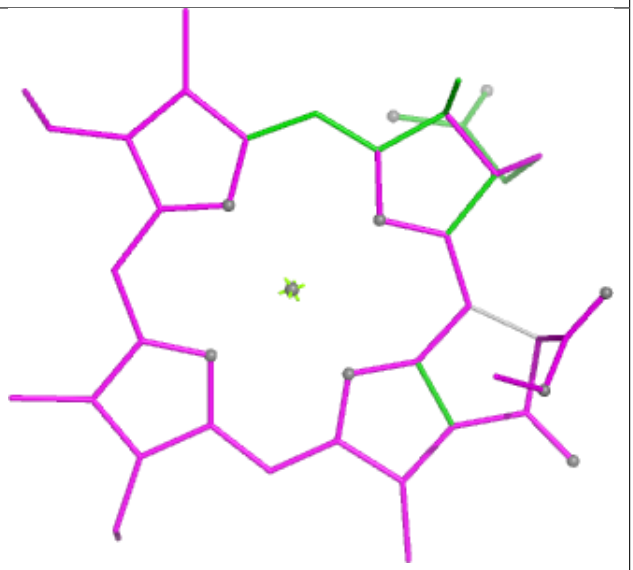


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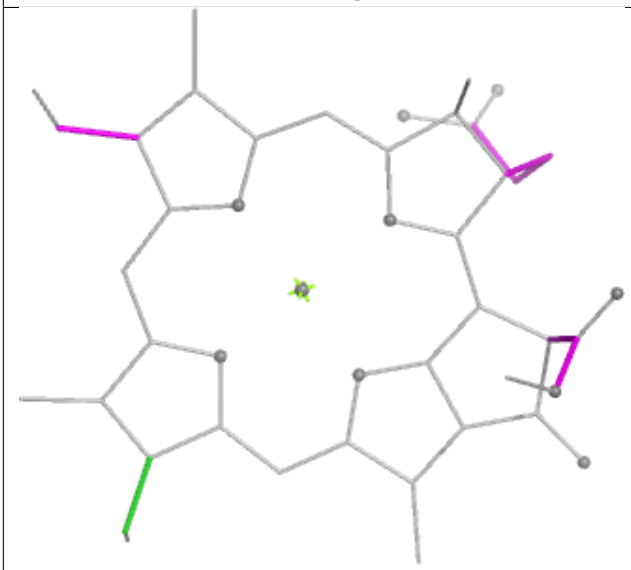
Ligand CLA C 503



Bond lengths



Bond angles

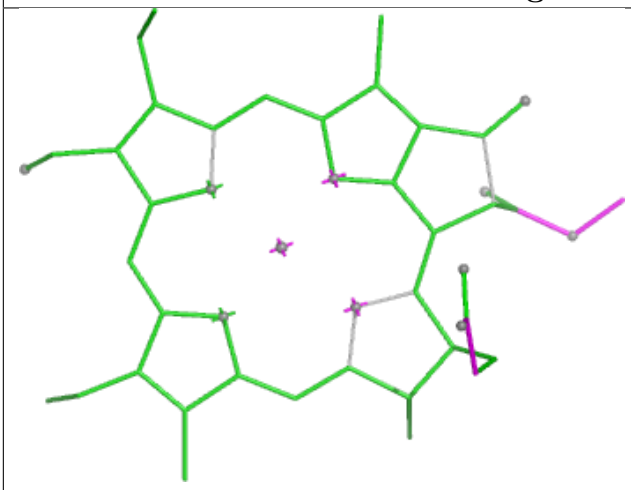


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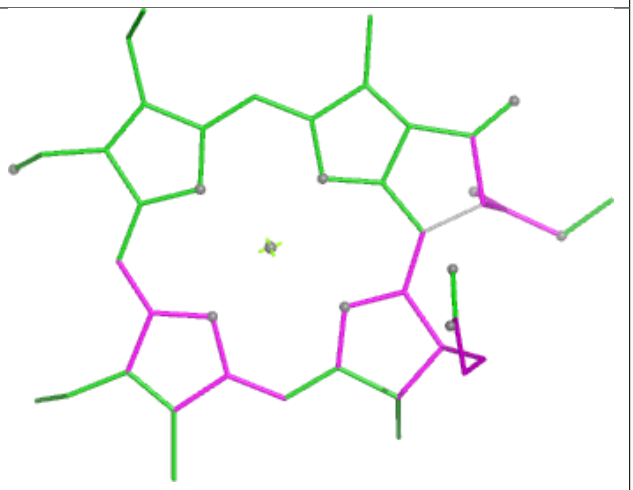


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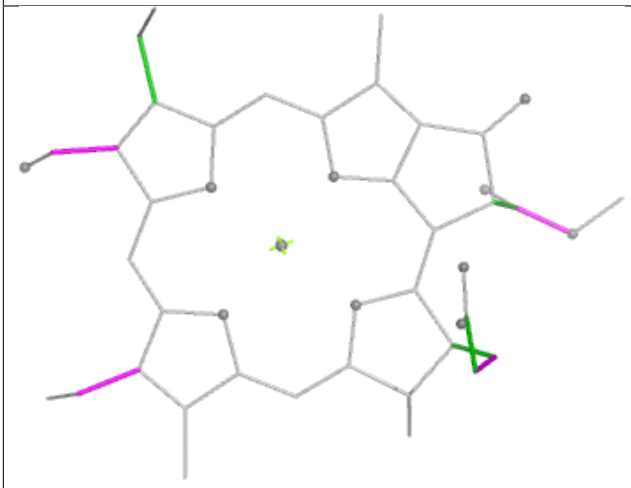
Ligand CHL n 607



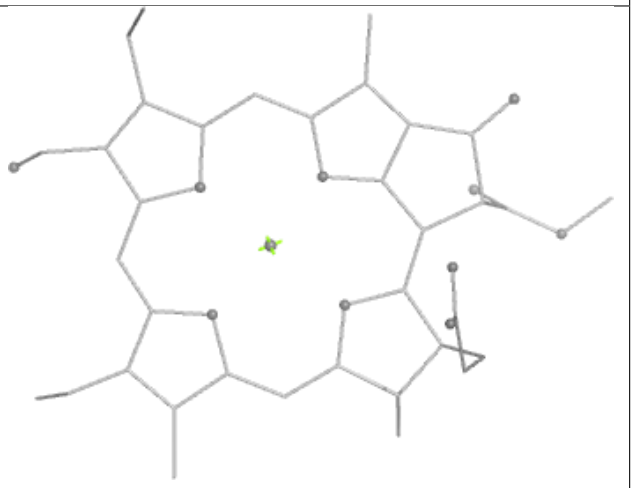
Bond lengths



Bond angles

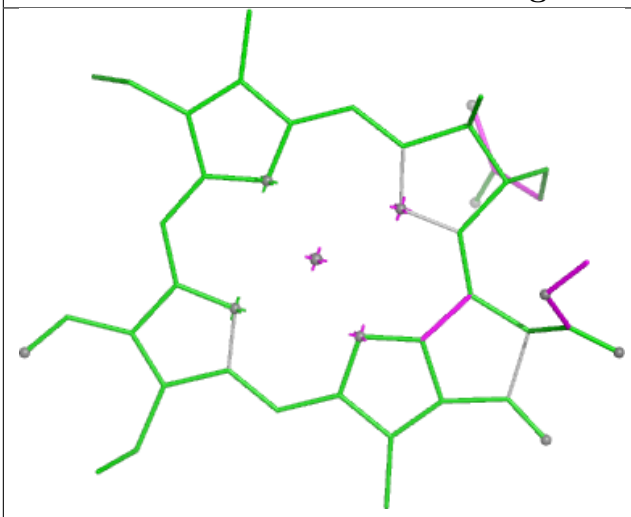


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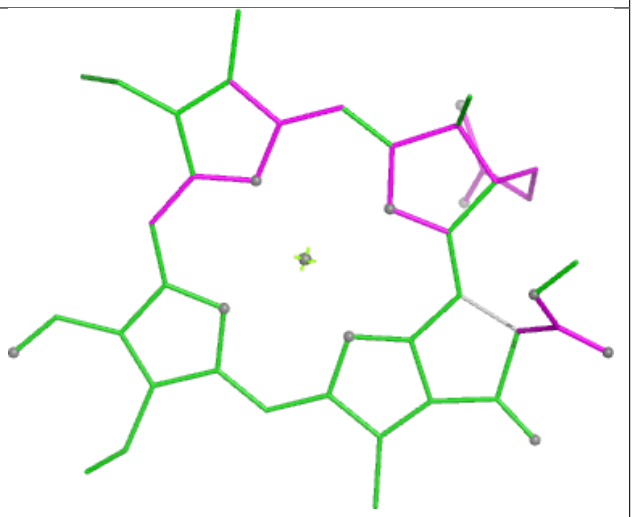


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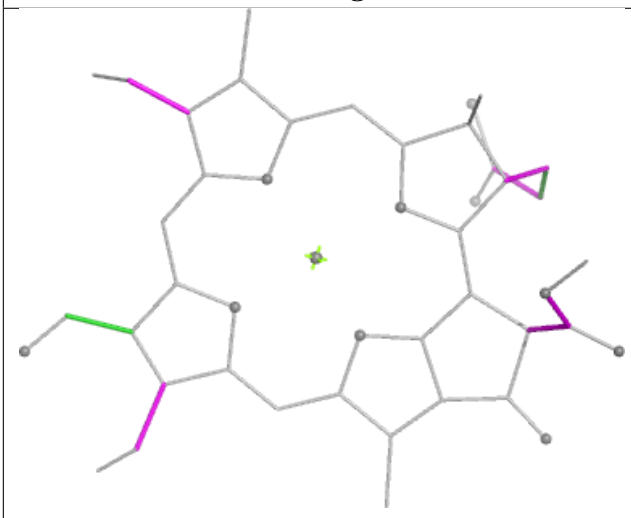
Ligand CHL r 304



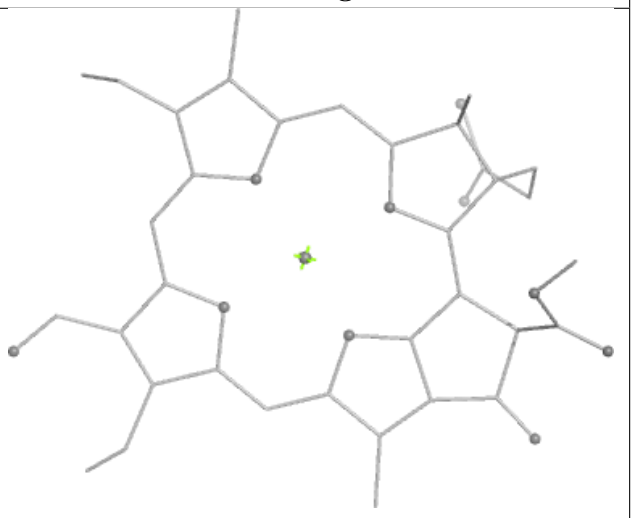
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Bond angles

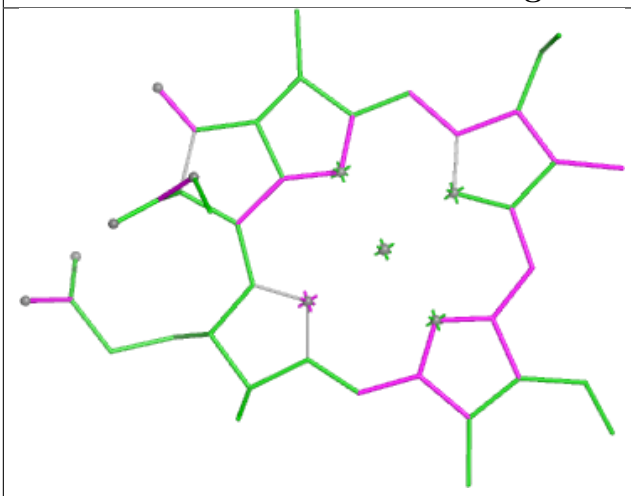


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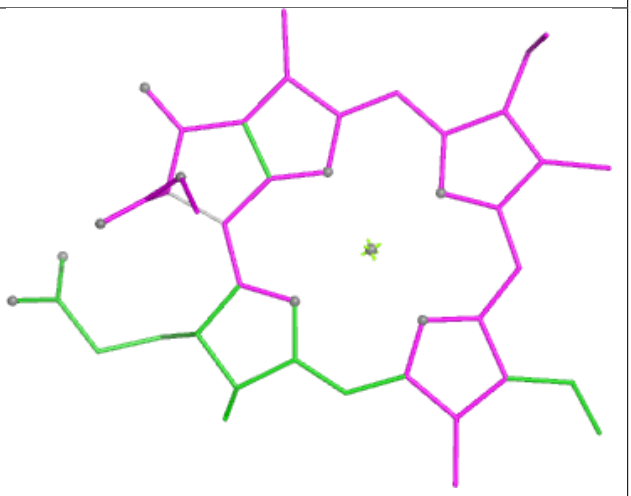


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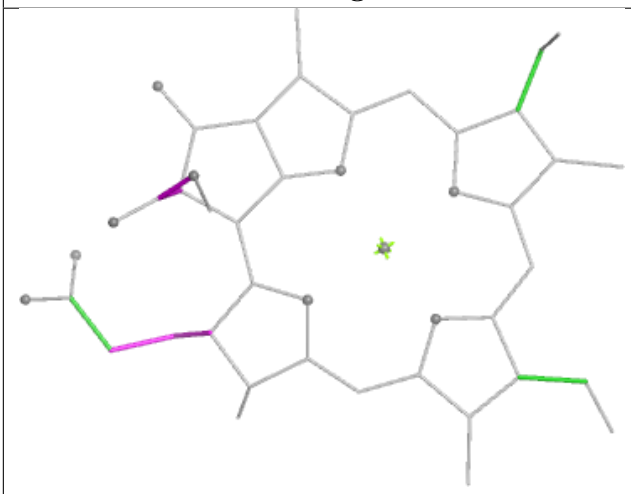
Ligand CLA B 616



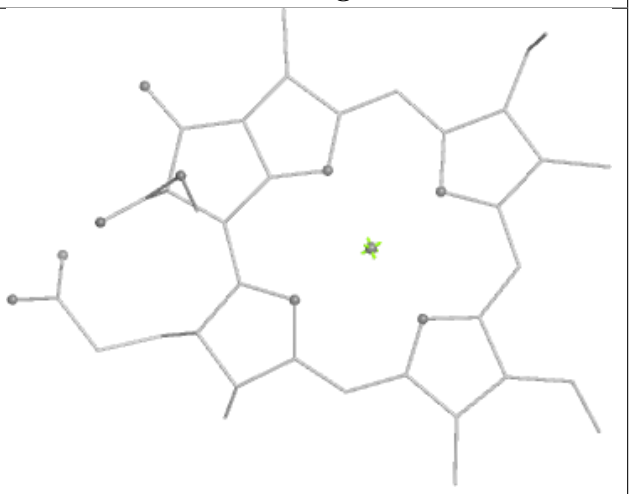
Bond lengths



Bond angles



Torsions

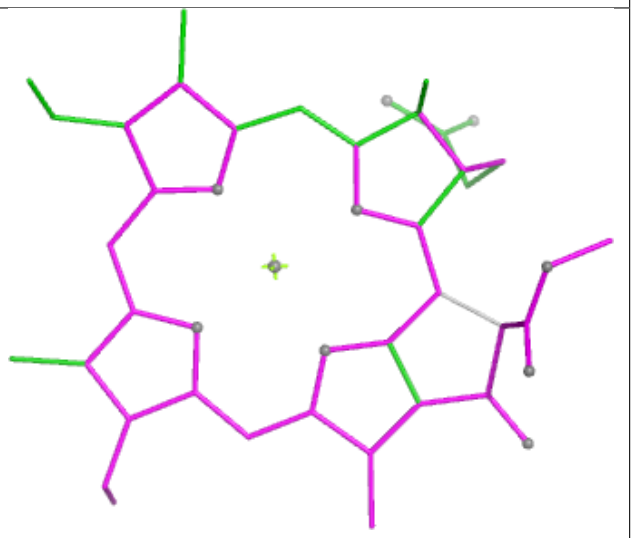


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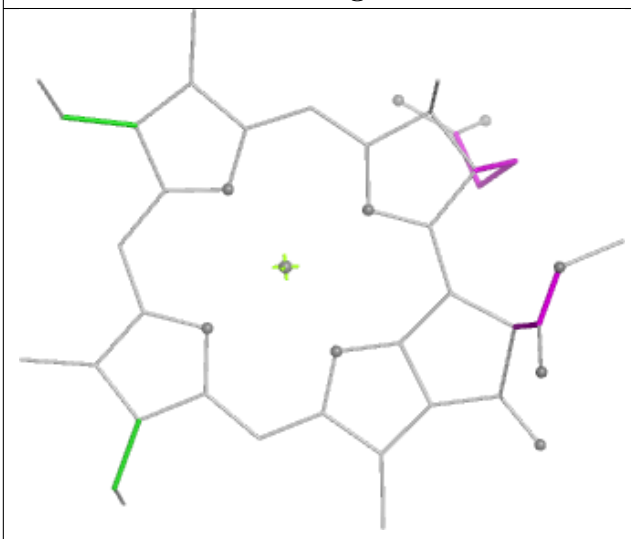
Ligand CLA s 305



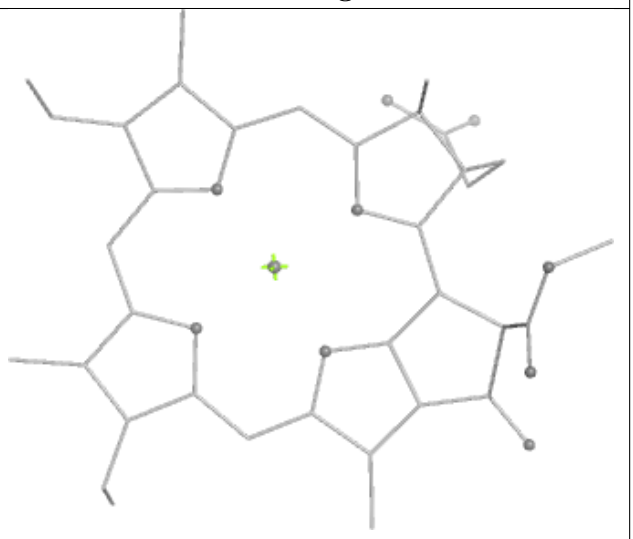
Bond lengths



Bond angles

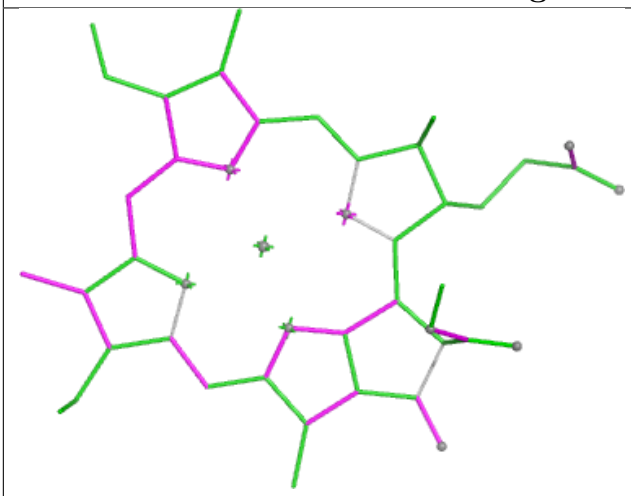


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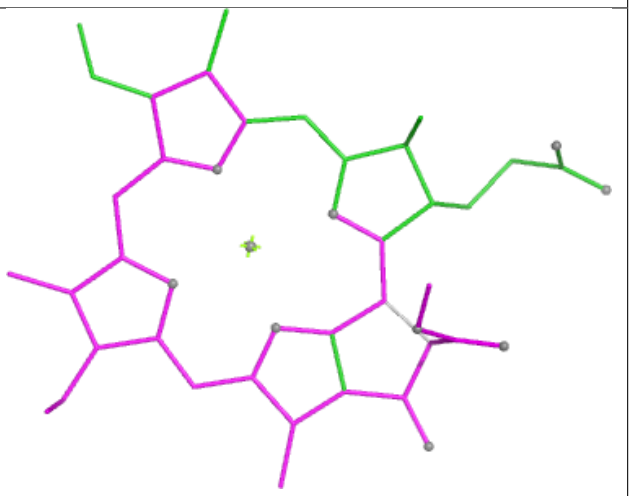


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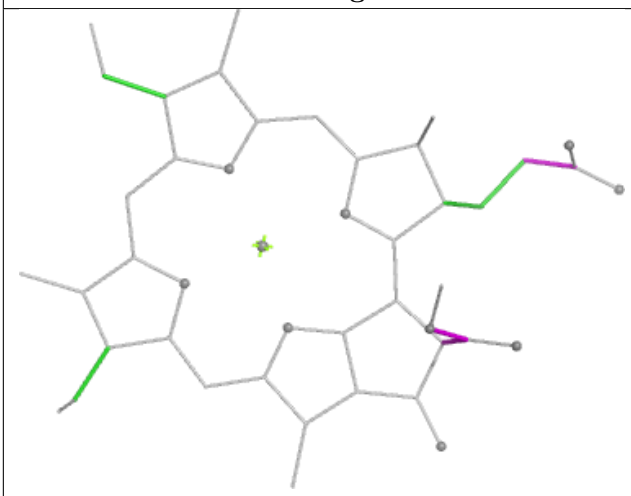
Ligand CLA c 510



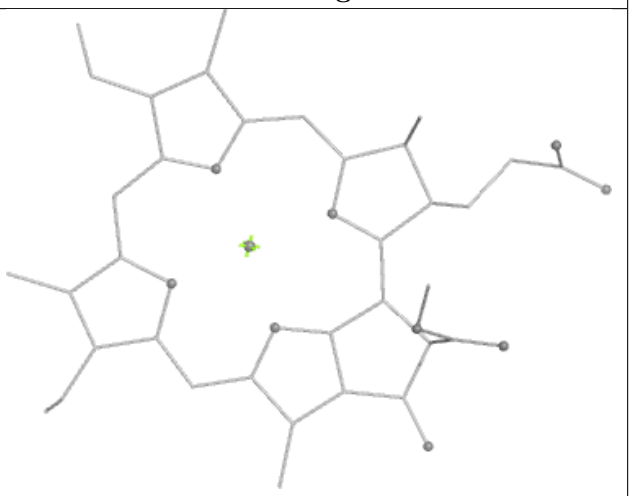
Bond lengths



Bond angles

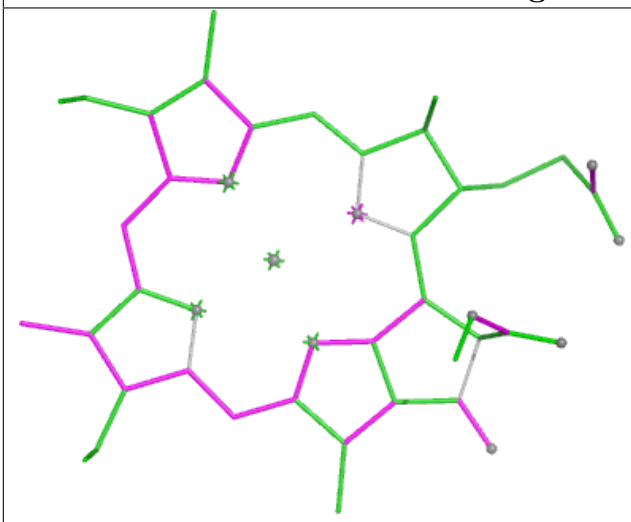


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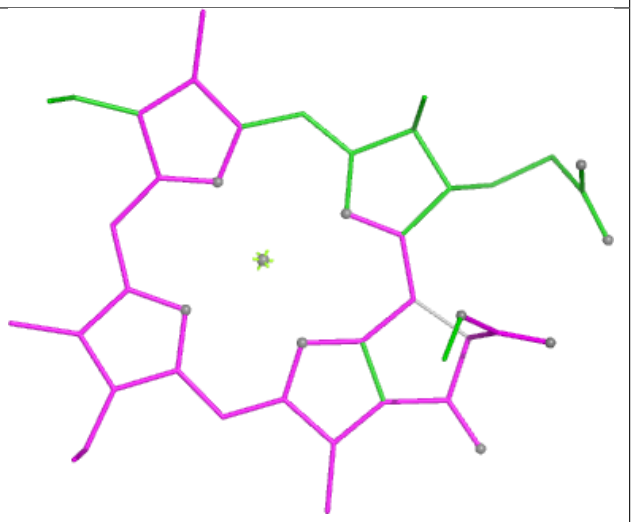


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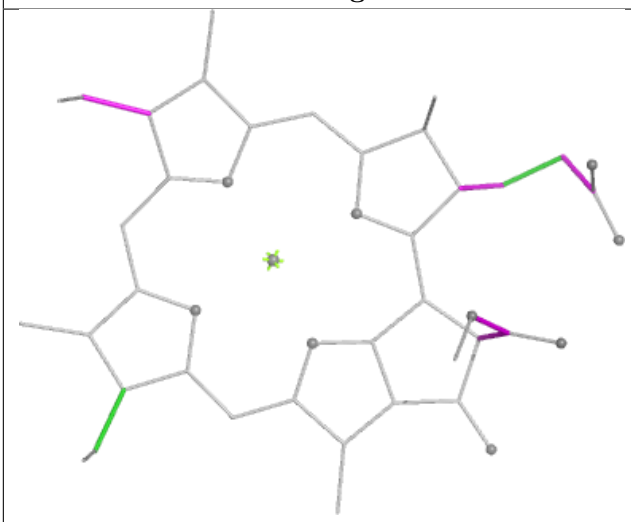
Ligand CLA 3 312



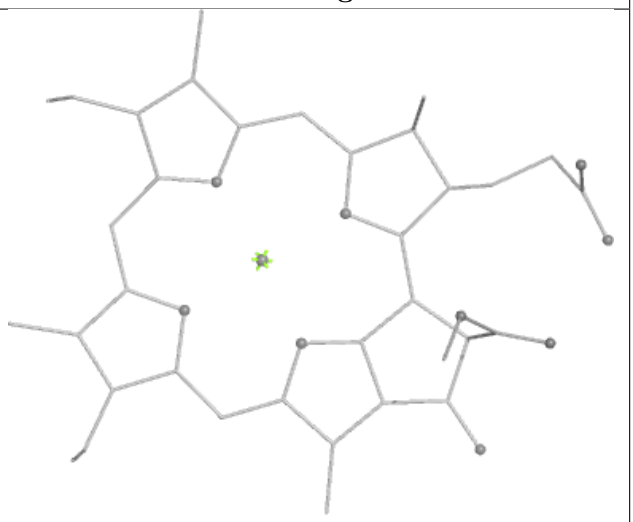
Bond lengths



Bond angles

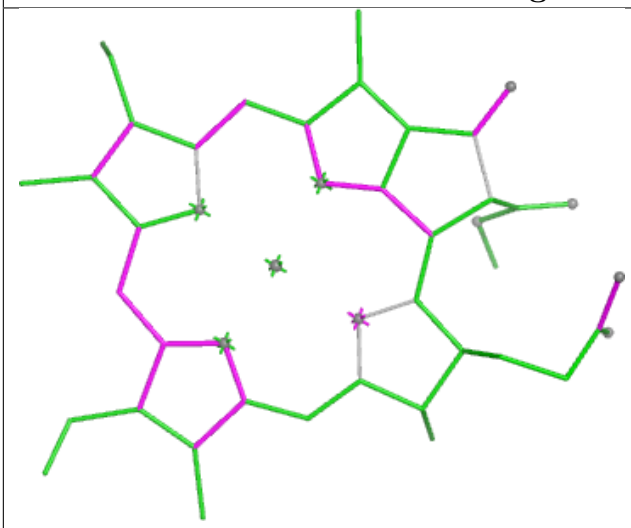


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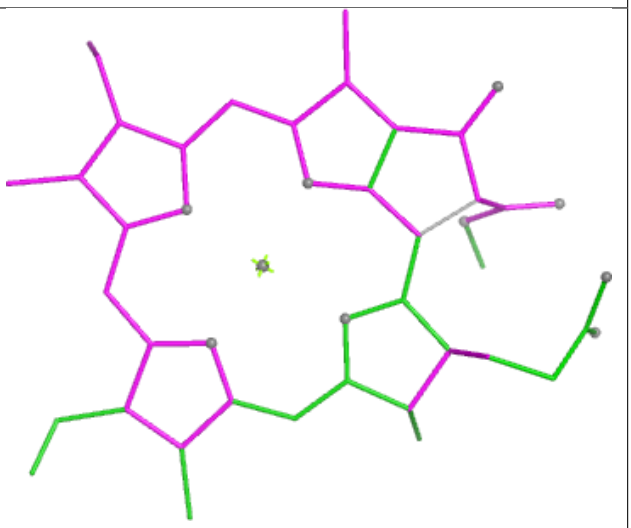


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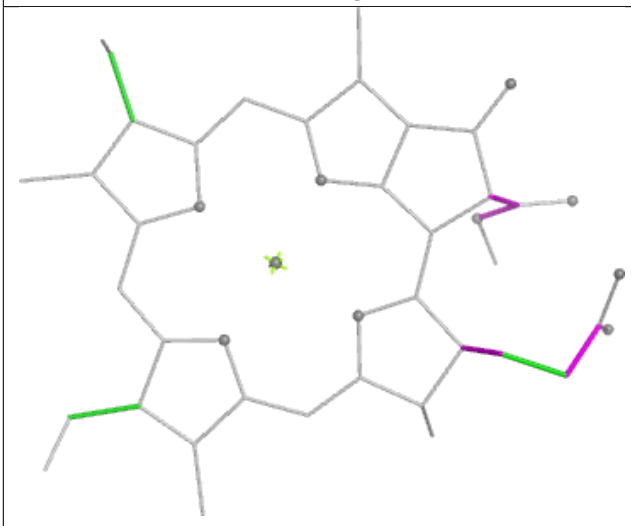
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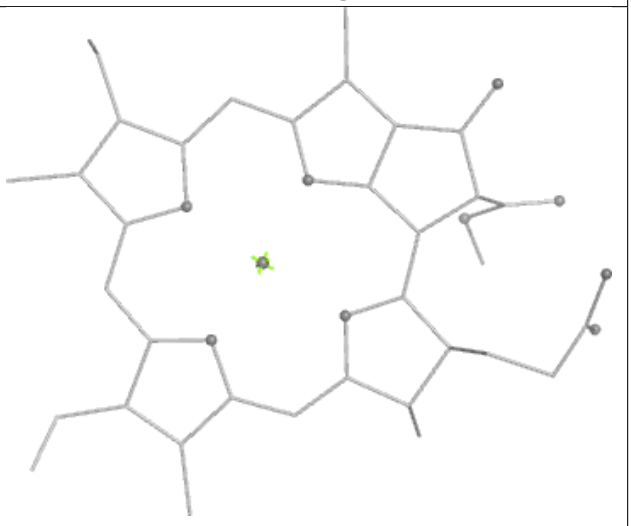
Bond lengths



Bond angles

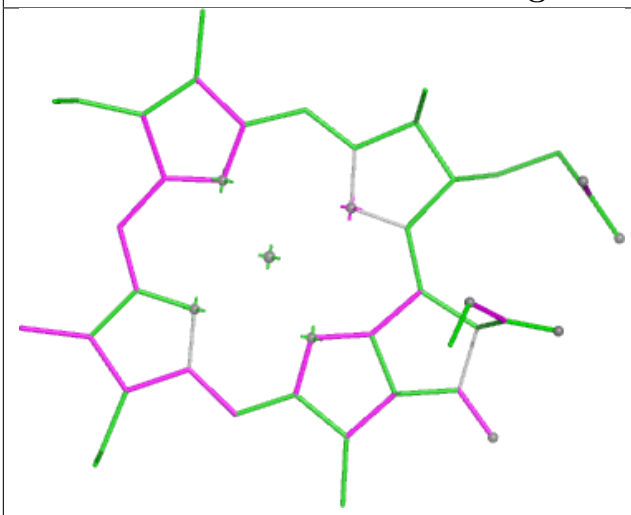


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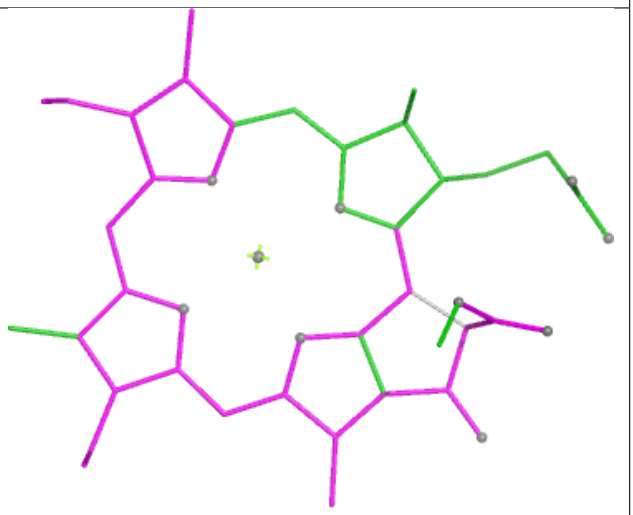


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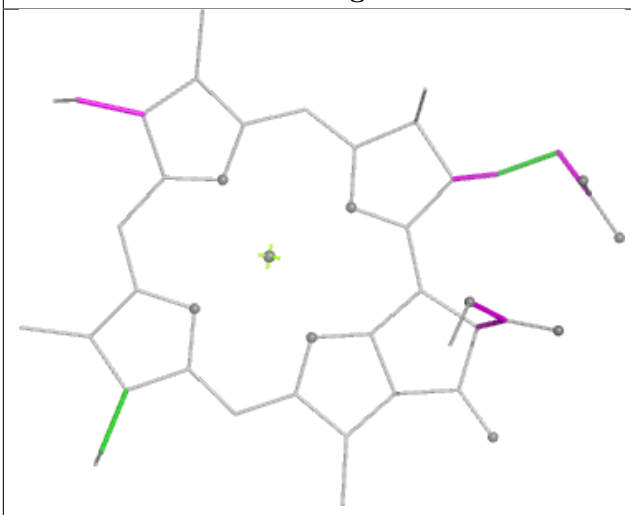
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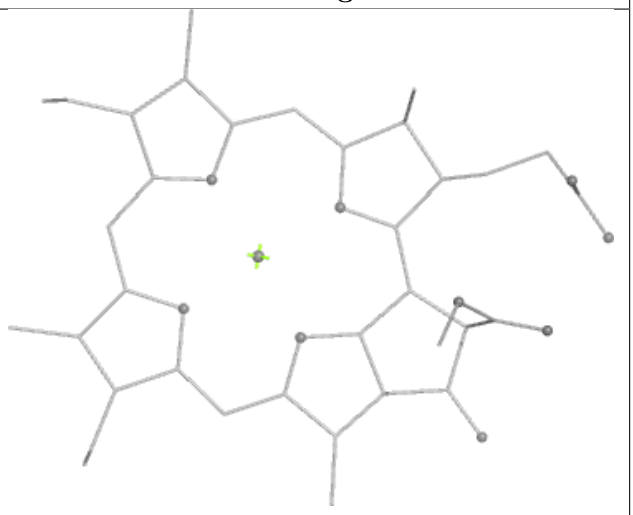
Bond lengths



Bond angles

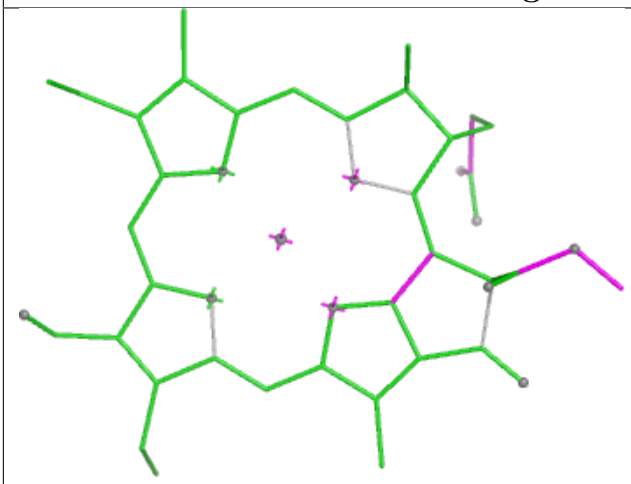


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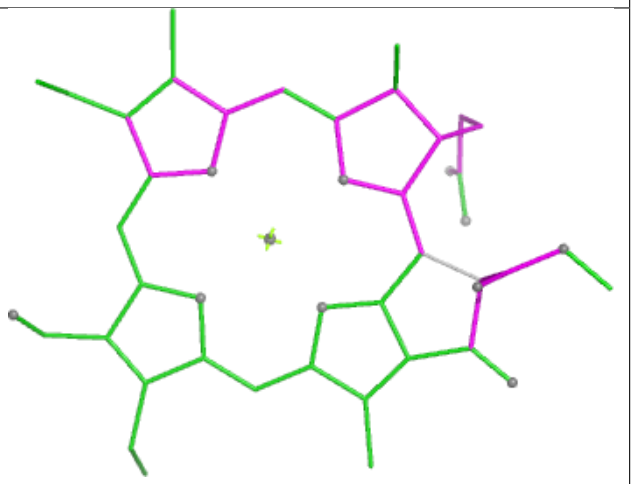


Rings

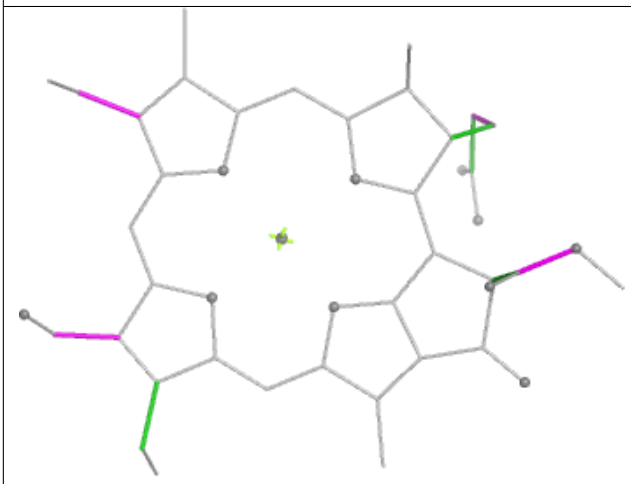
Ligand CHL G 607



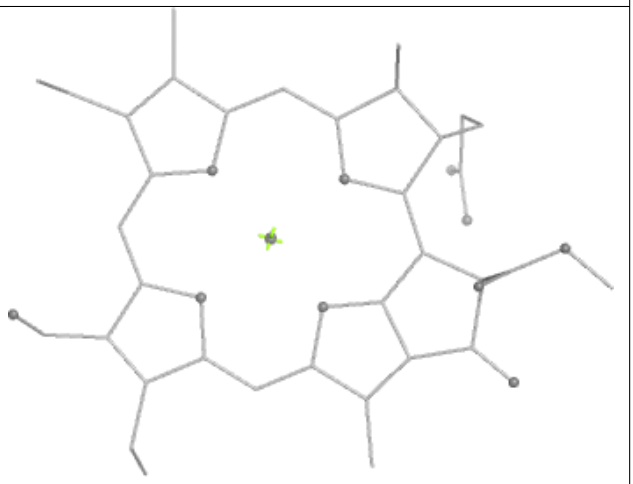
Bond lengths



Bond angles

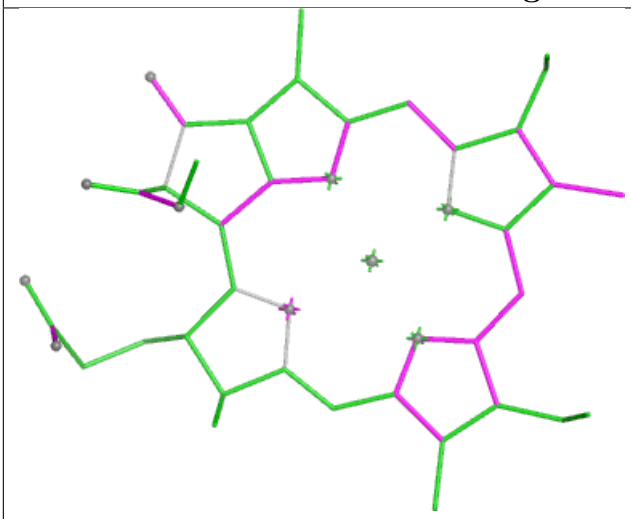


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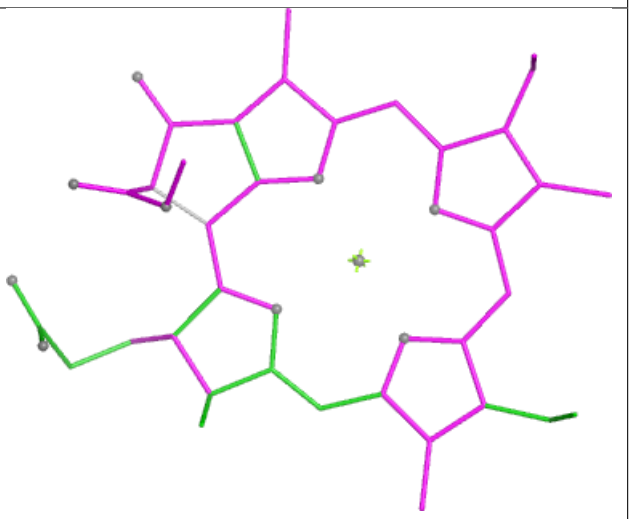


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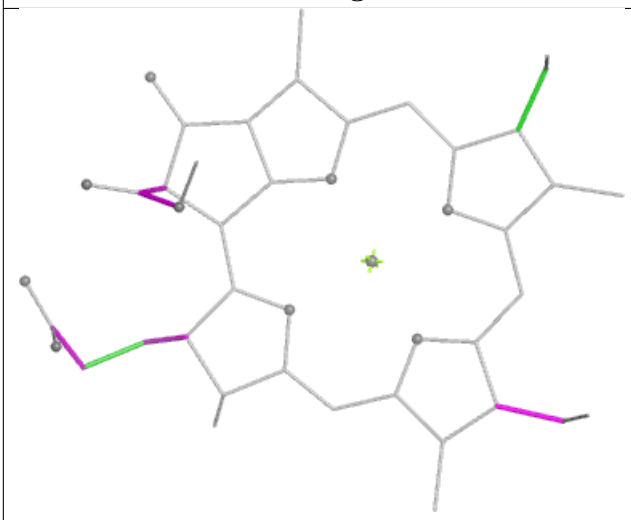
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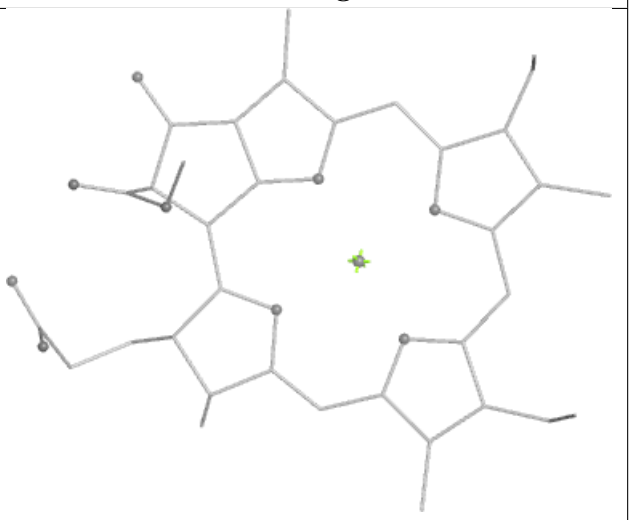
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Bond angles

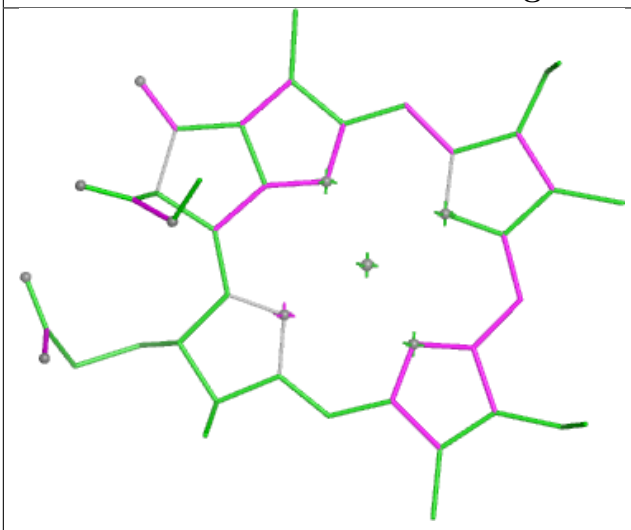


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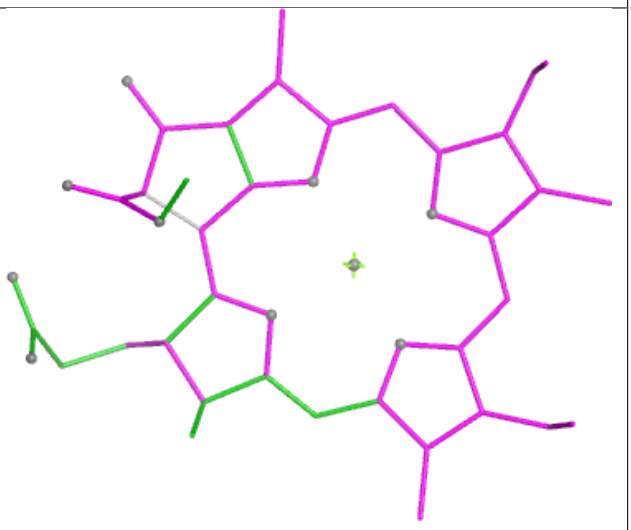


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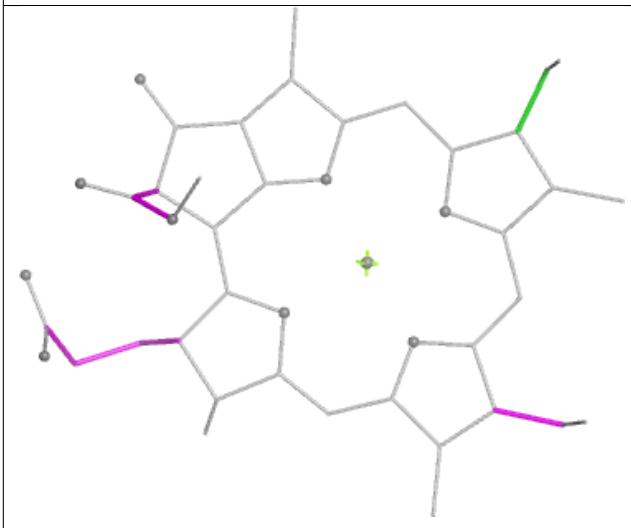
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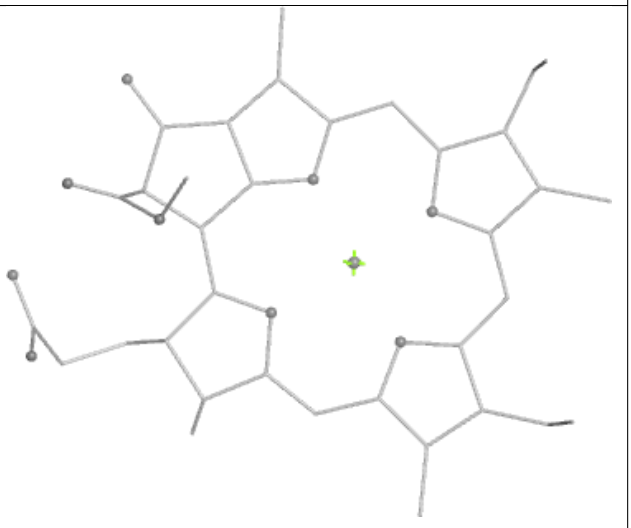
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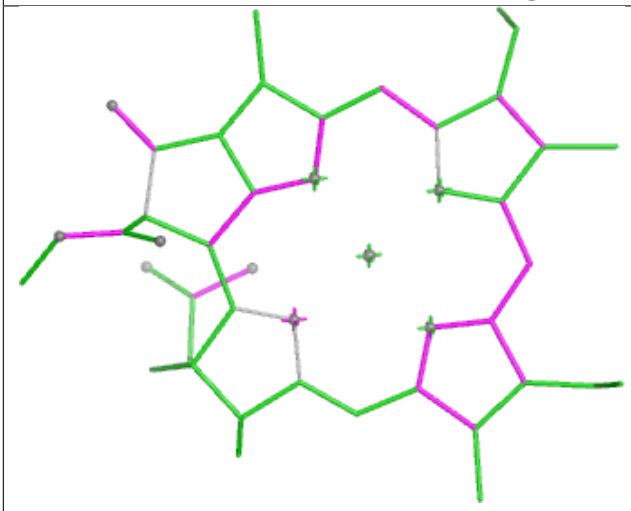


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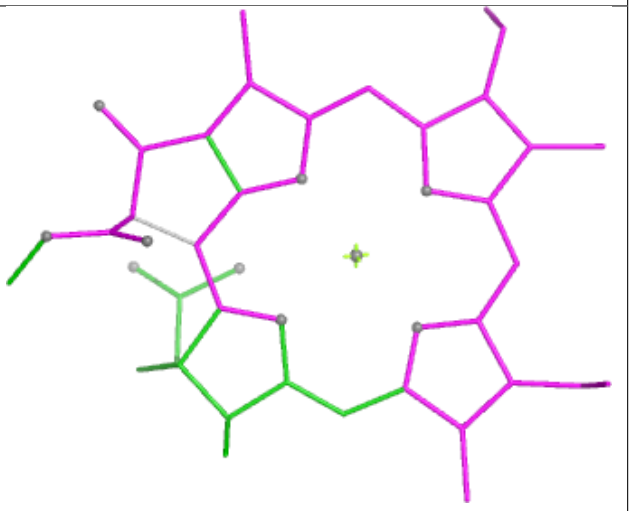


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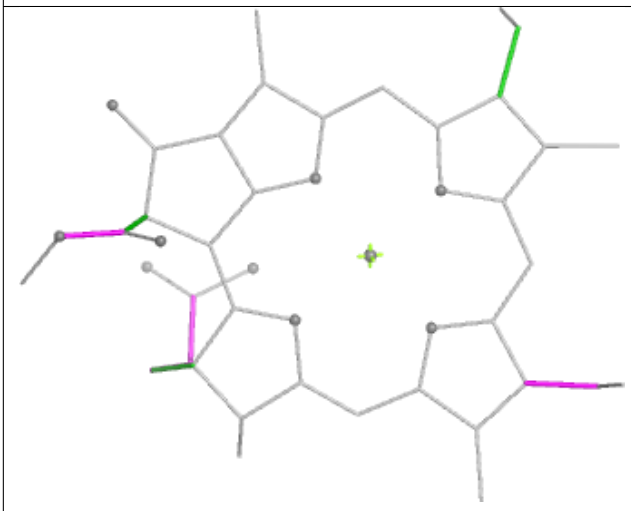
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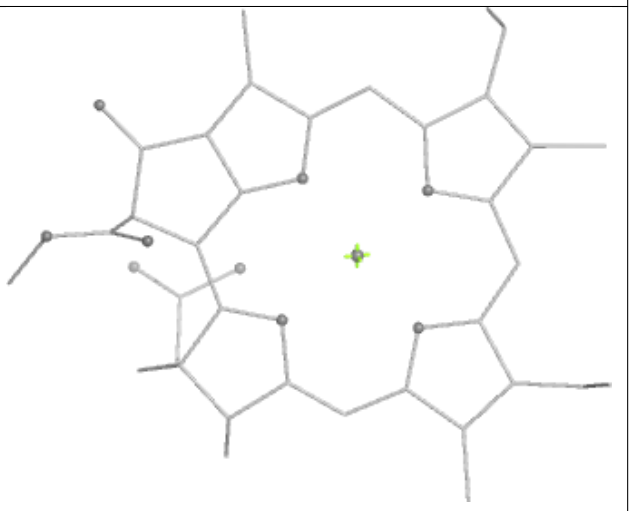
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Bond angles

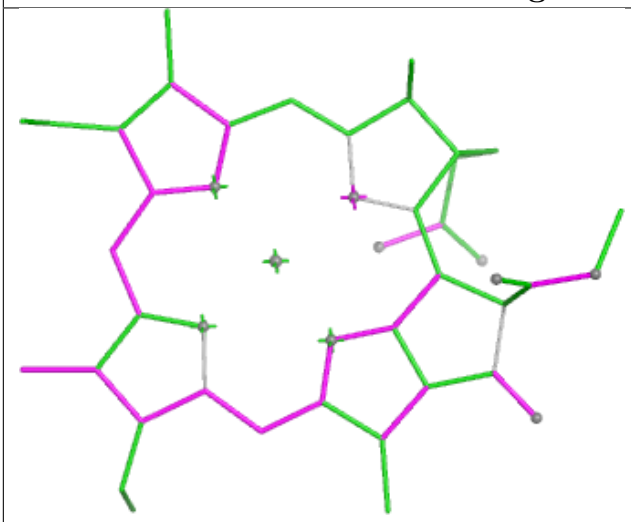


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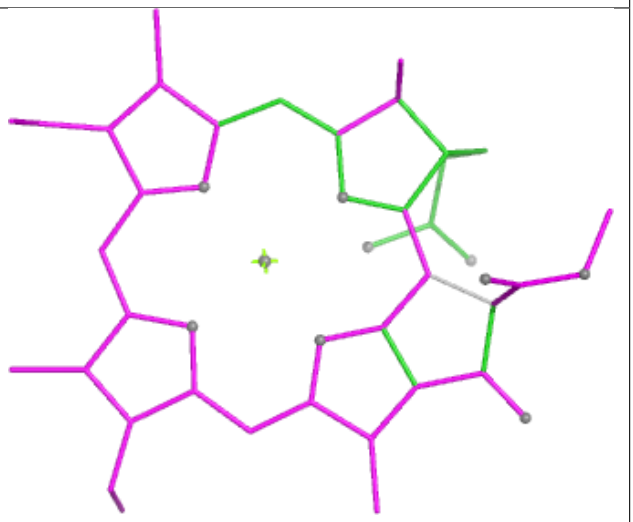


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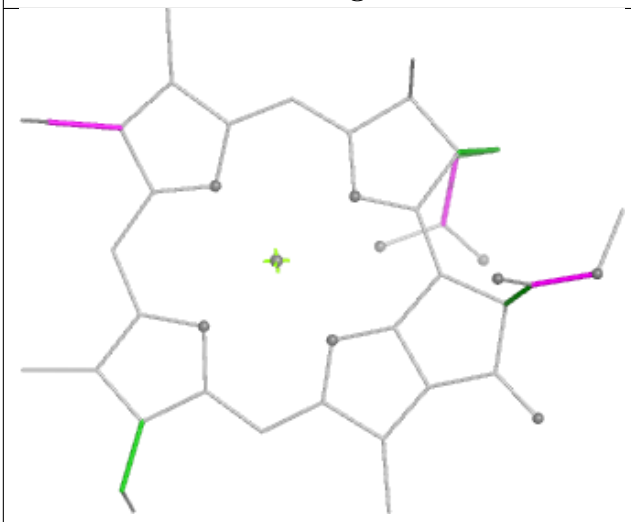
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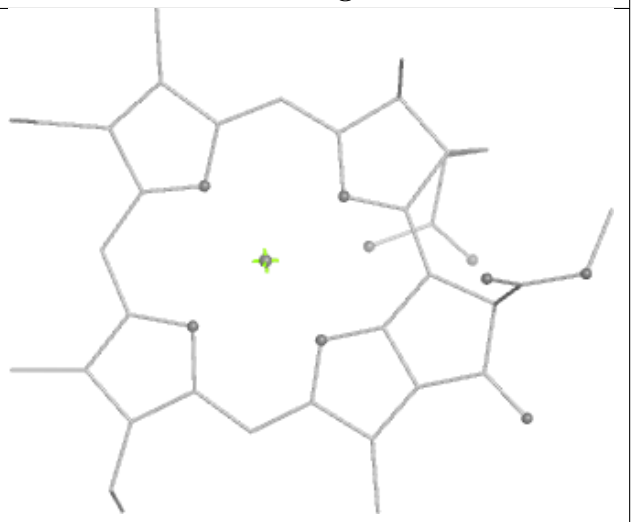
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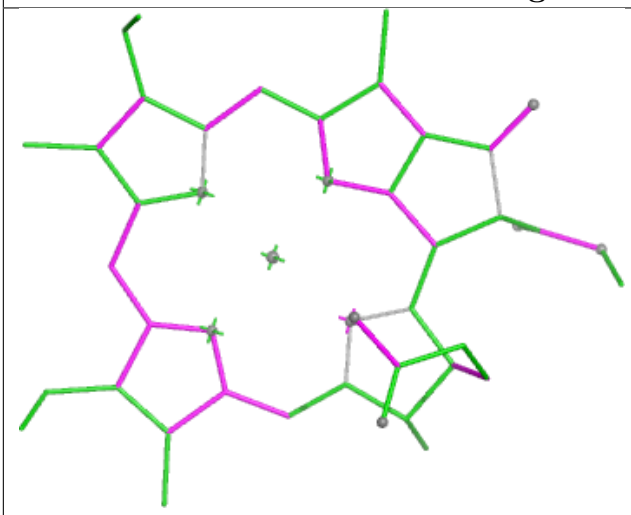


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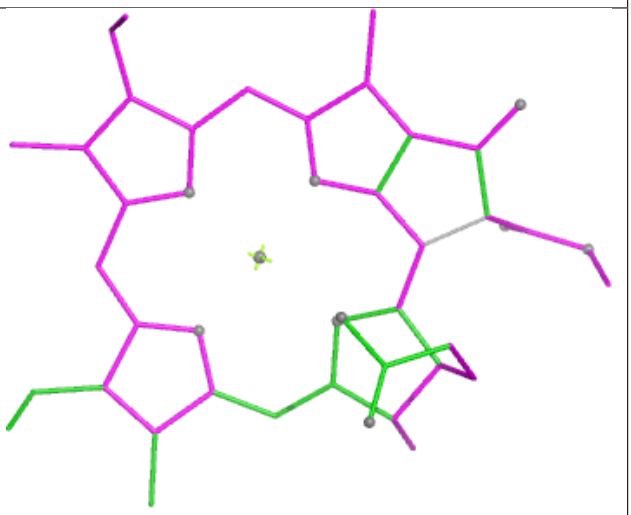


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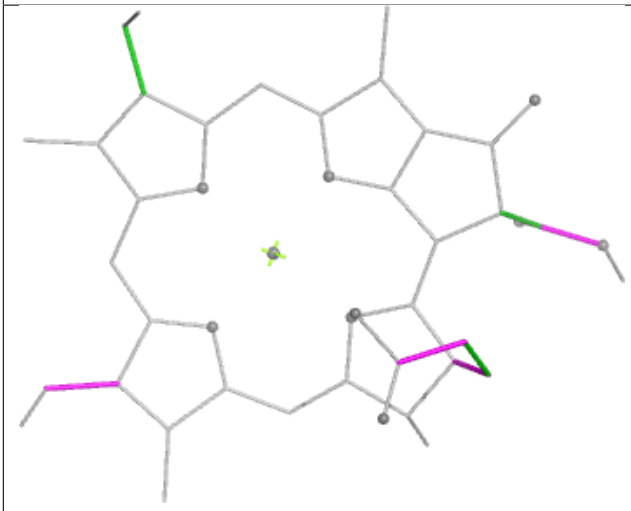
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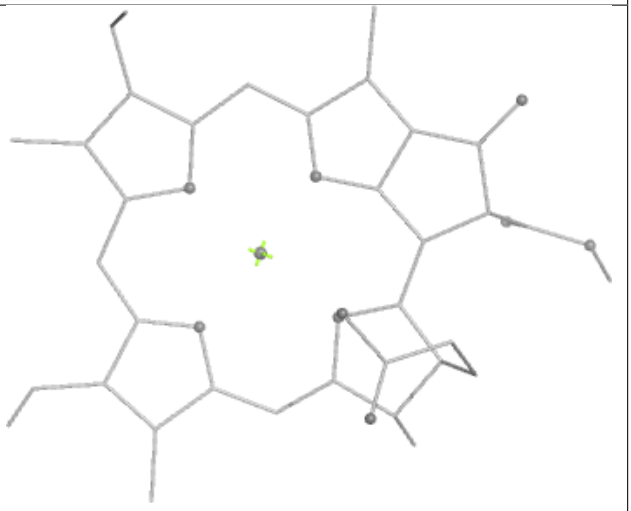
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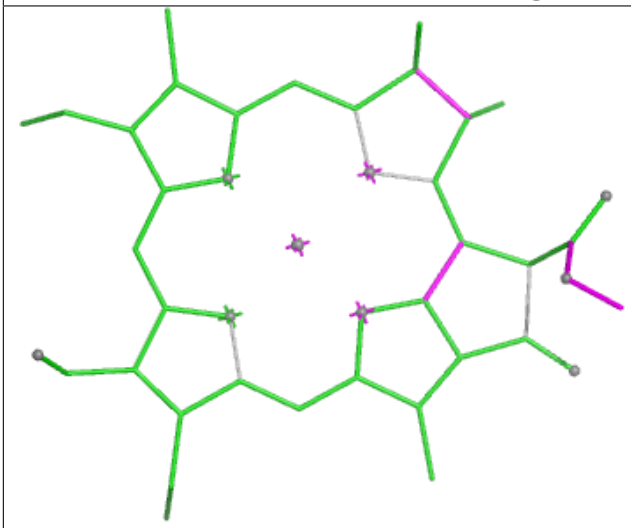


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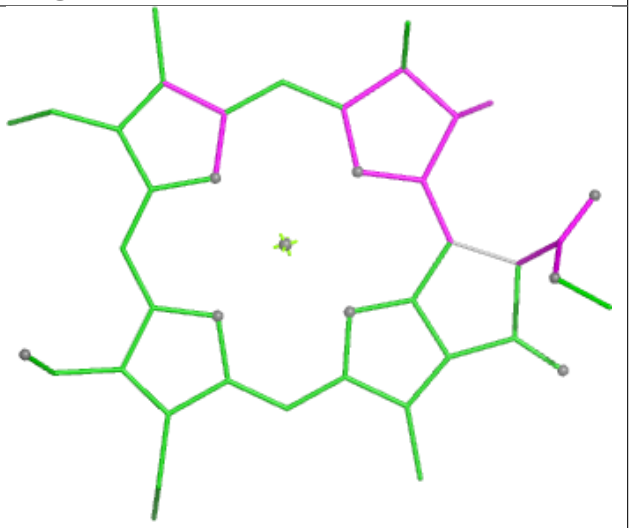


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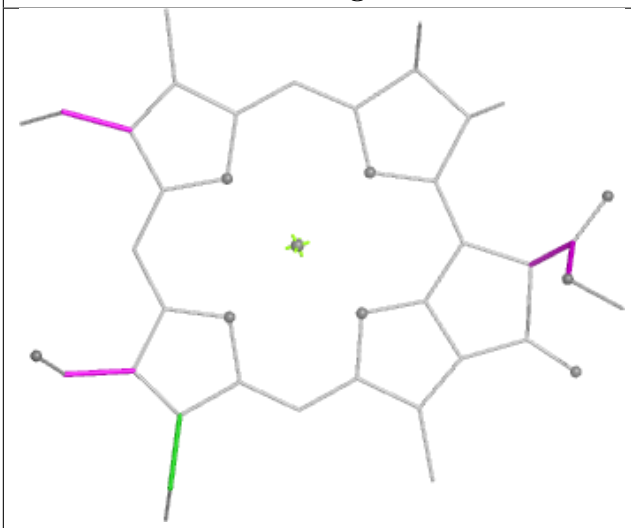
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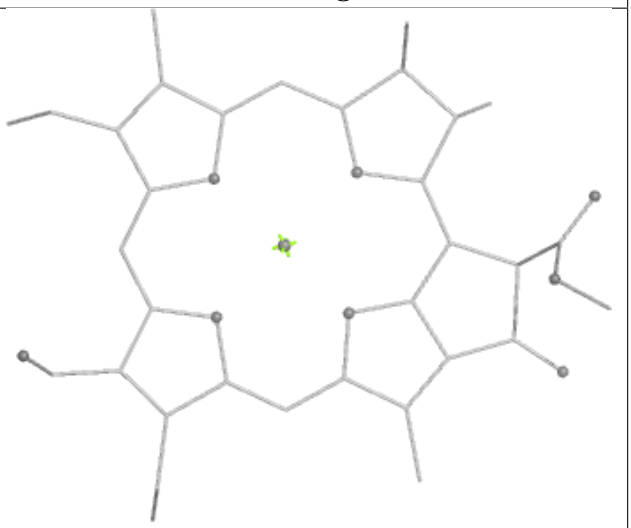
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Bond angles

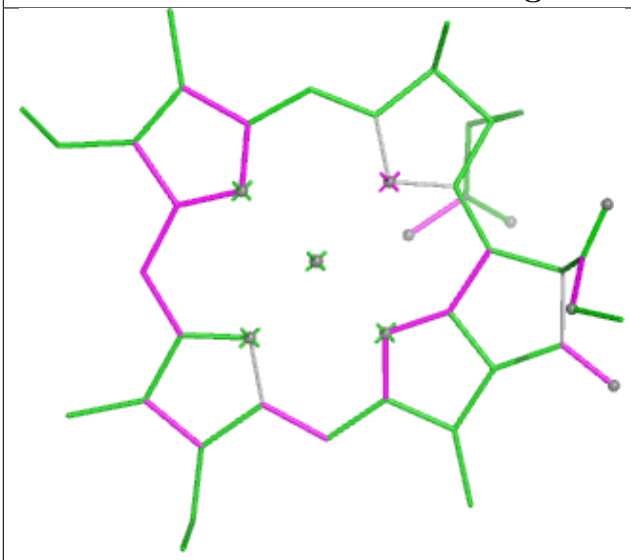


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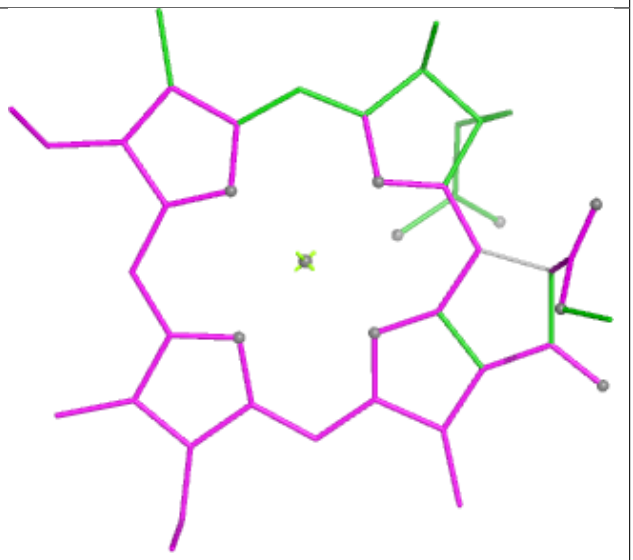


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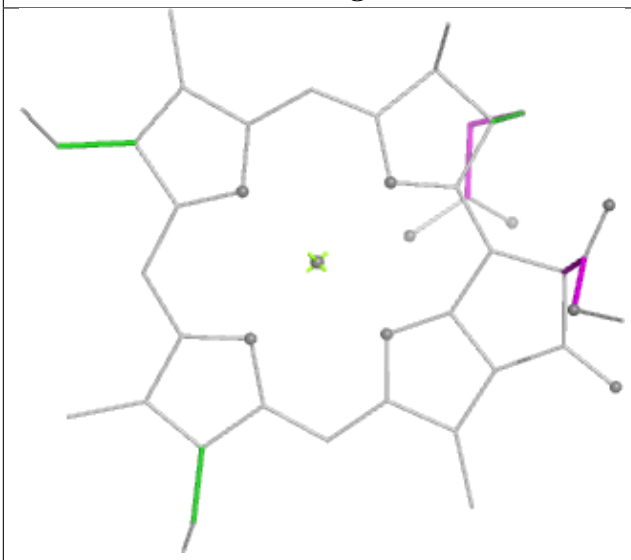
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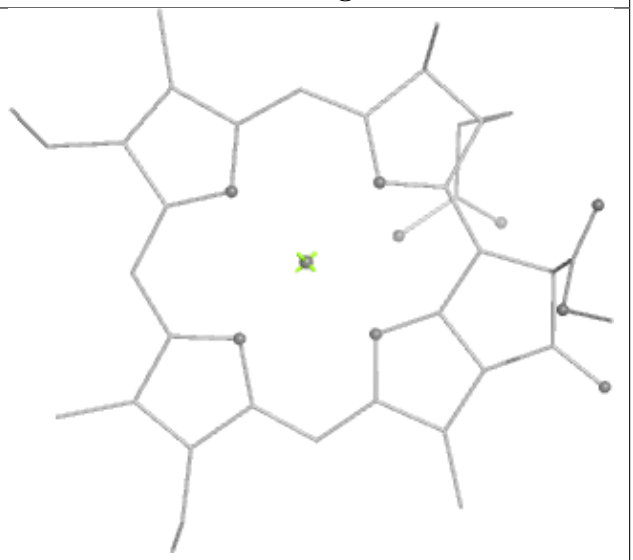
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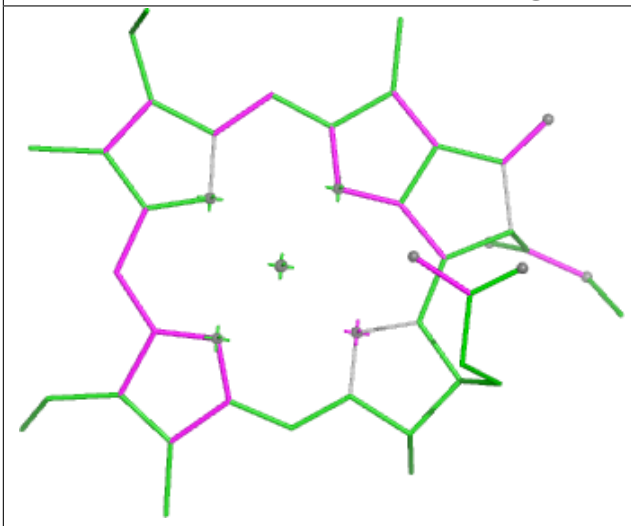


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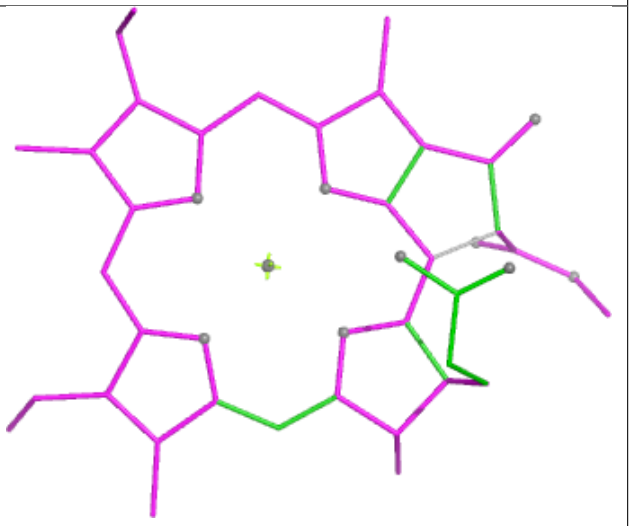


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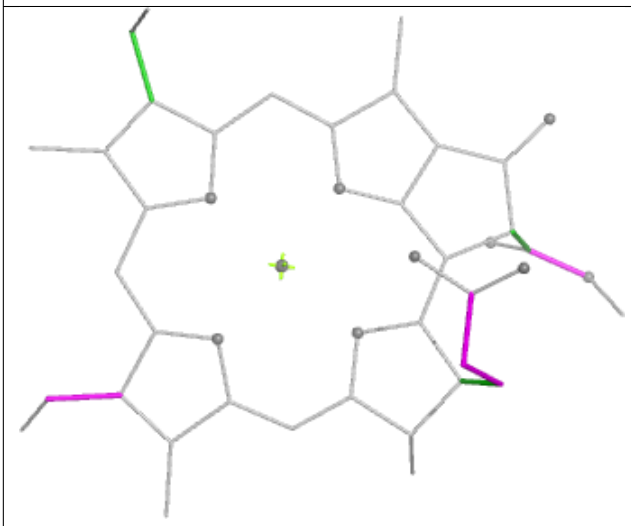
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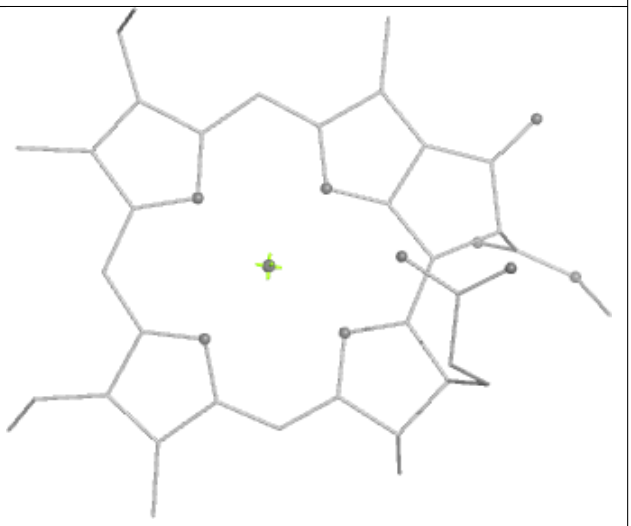
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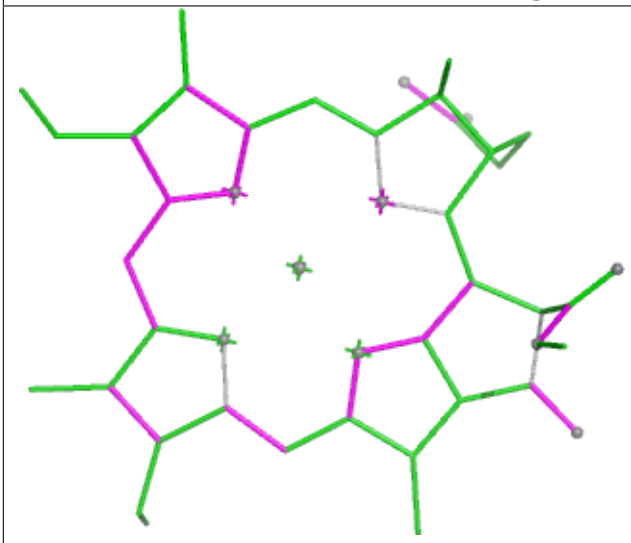


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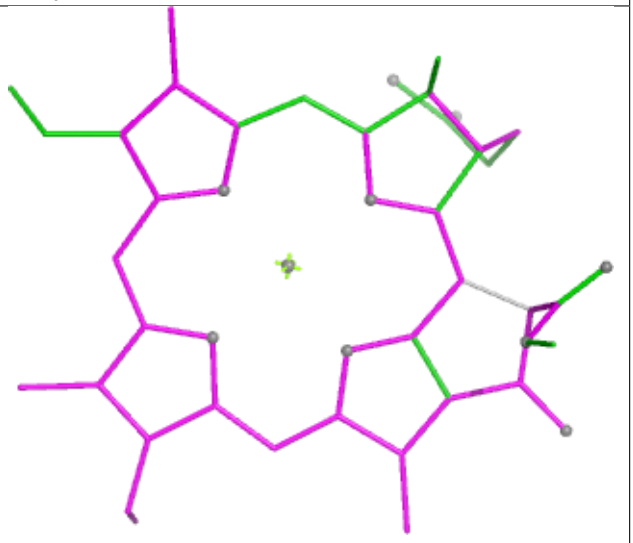


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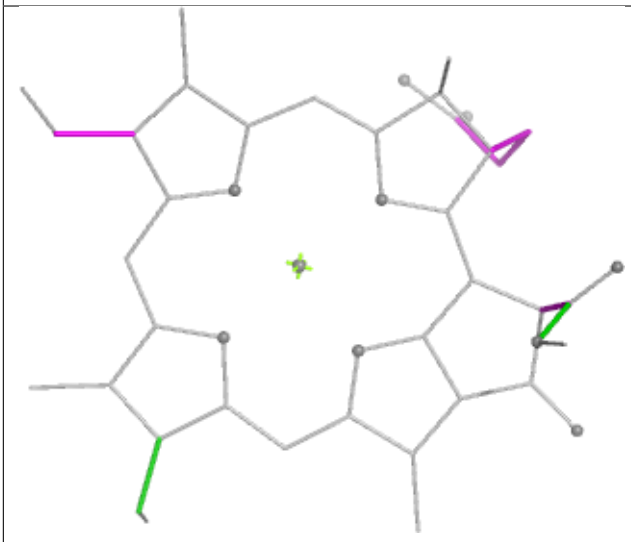
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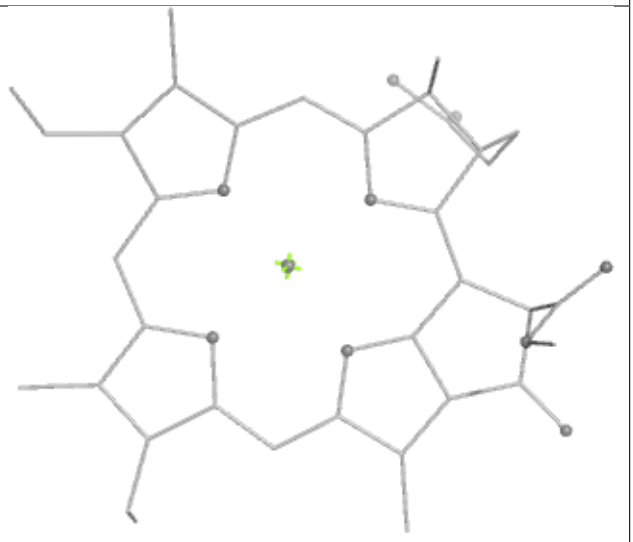
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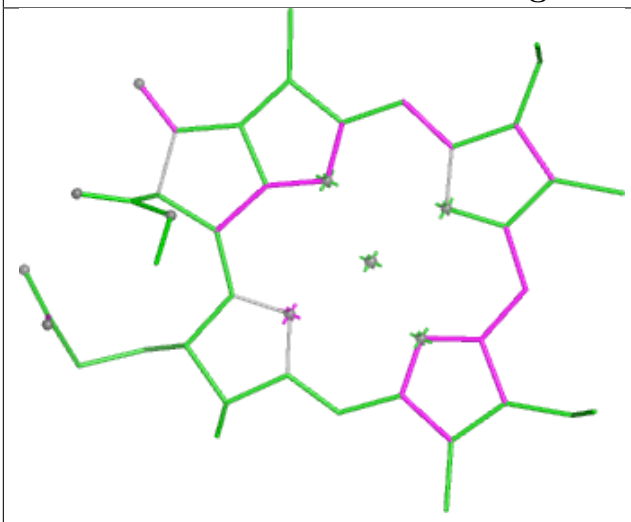


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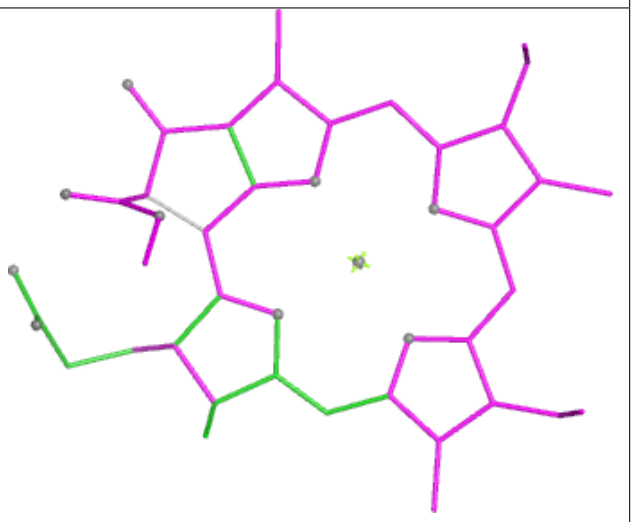


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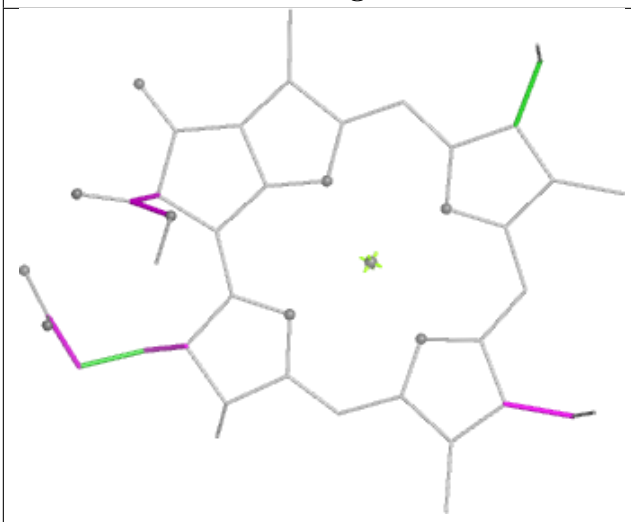
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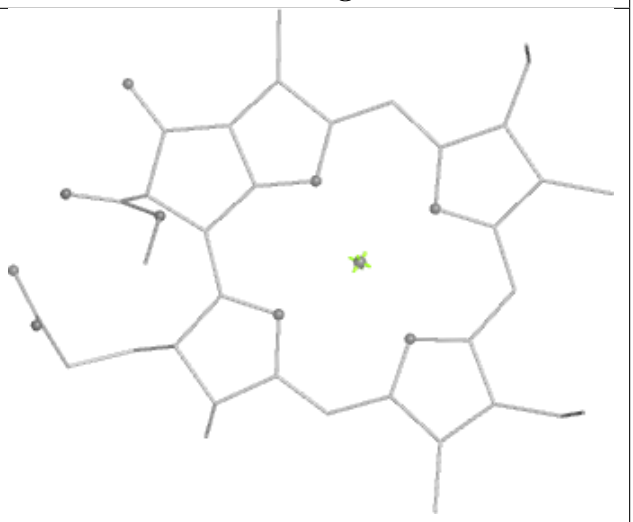
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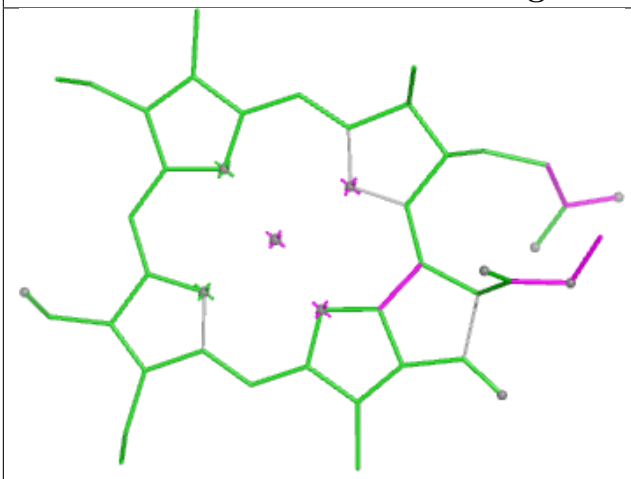


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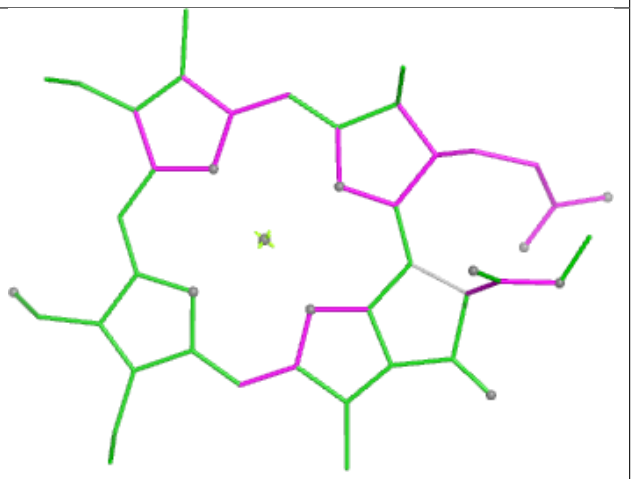


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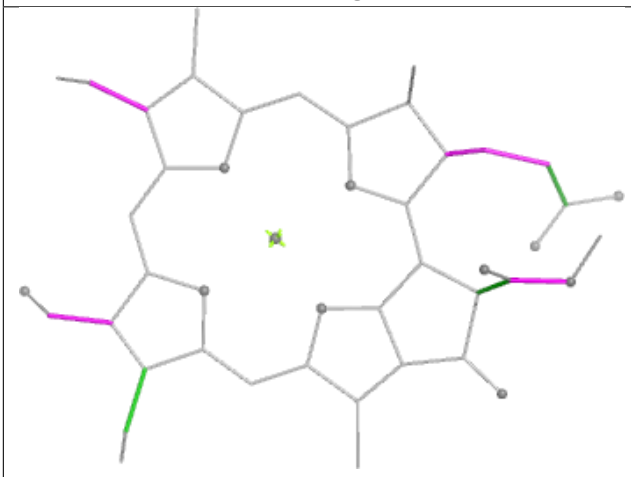
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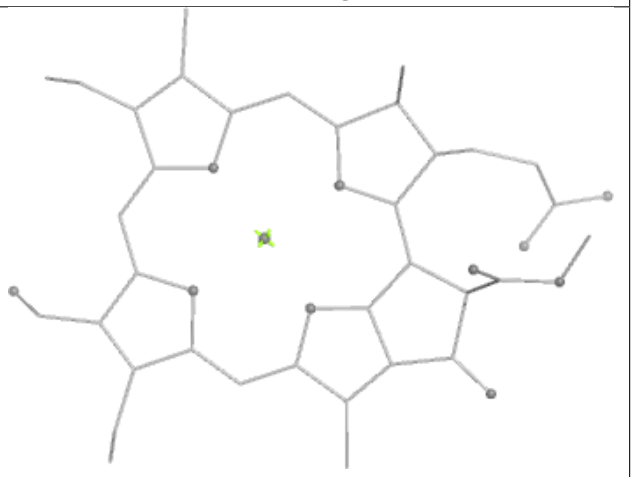
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Bond angles



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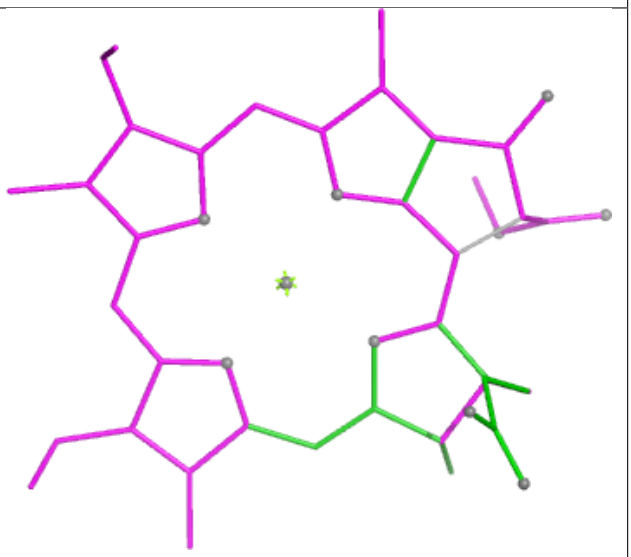


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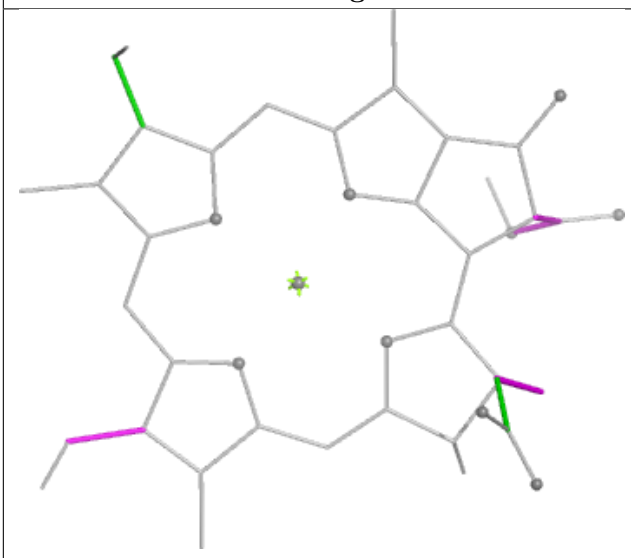
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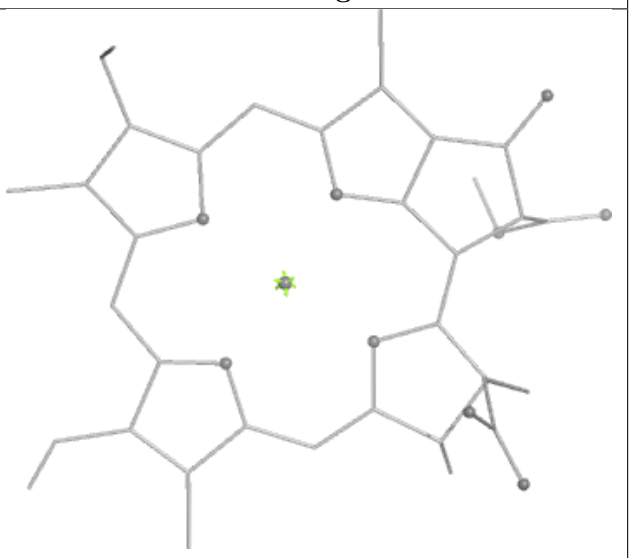
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Bond angles

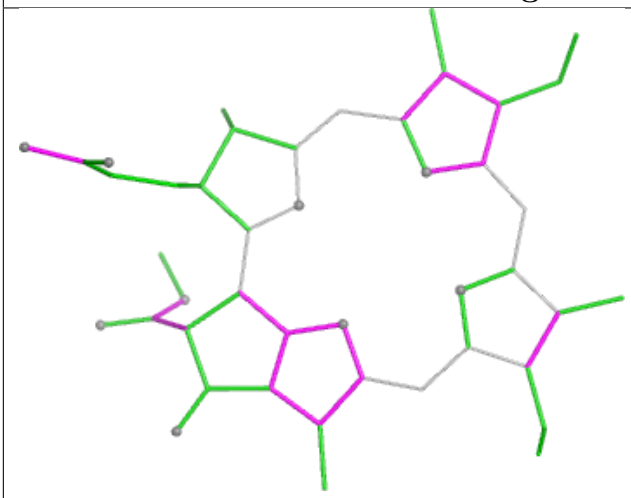


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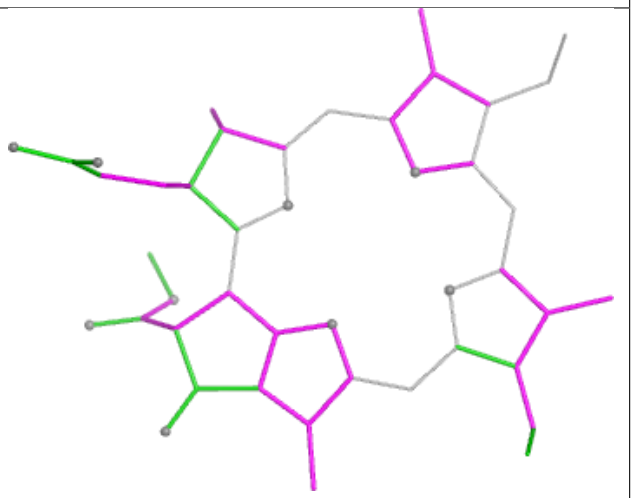


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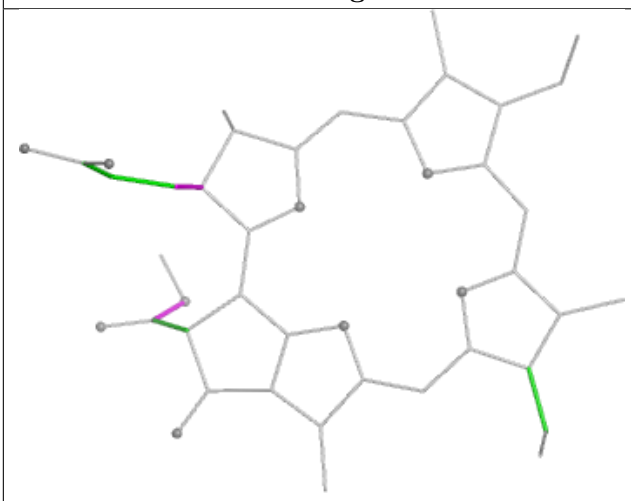
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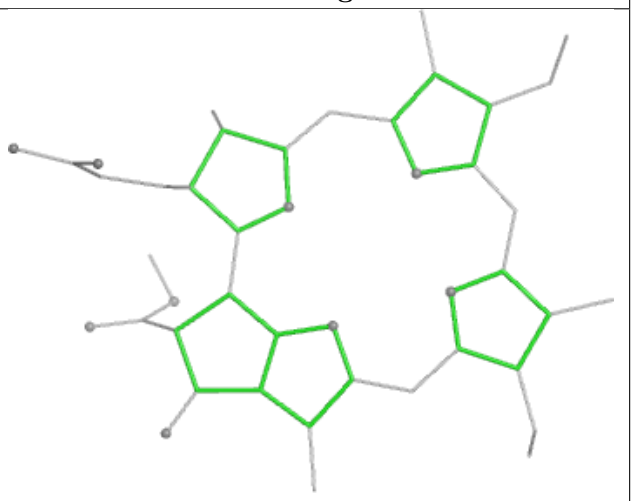
Bond lengths



Bond angles

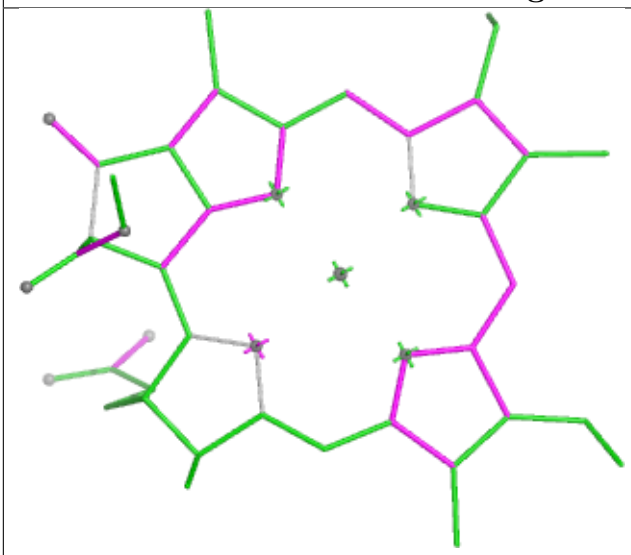


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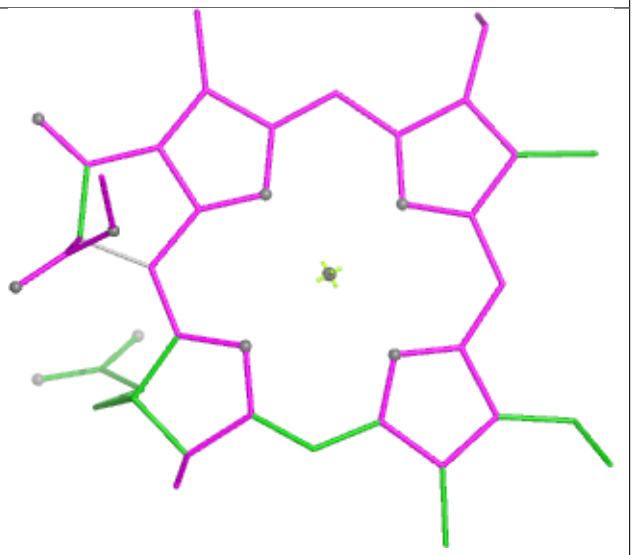


Rings

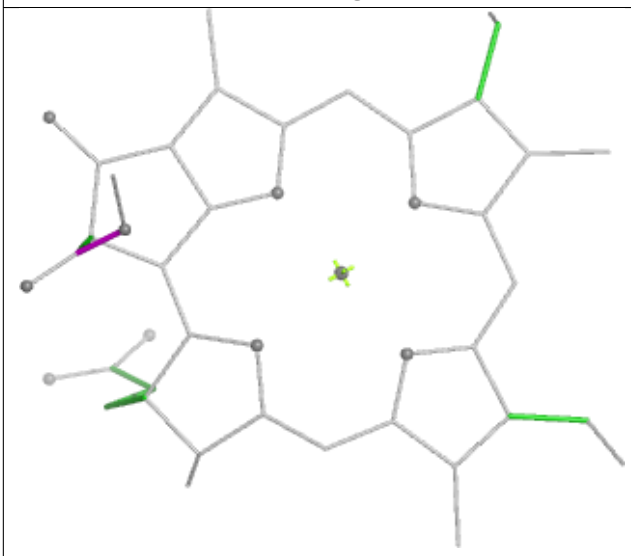
Ligand CLA b 605



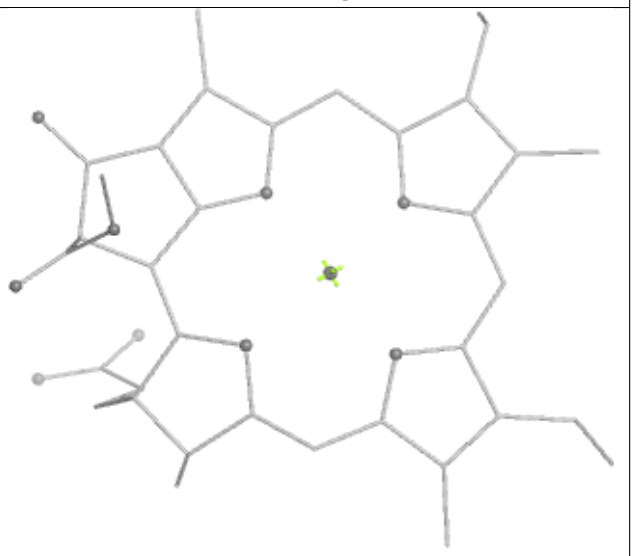
Bond lengths



Bond angles

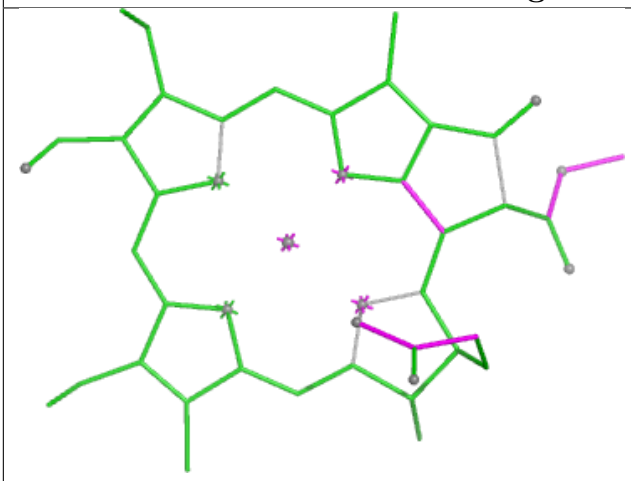


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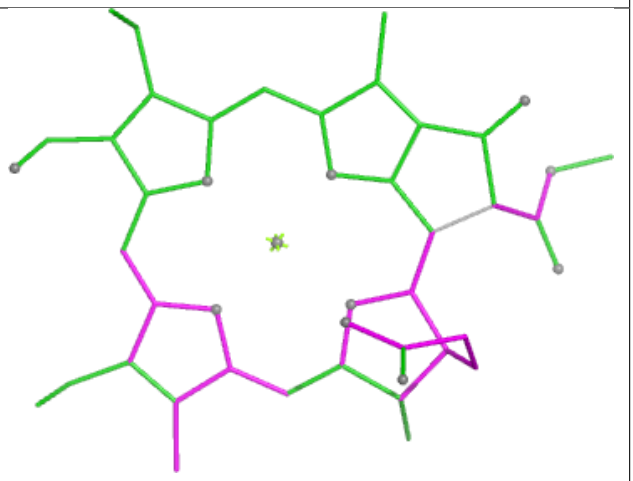


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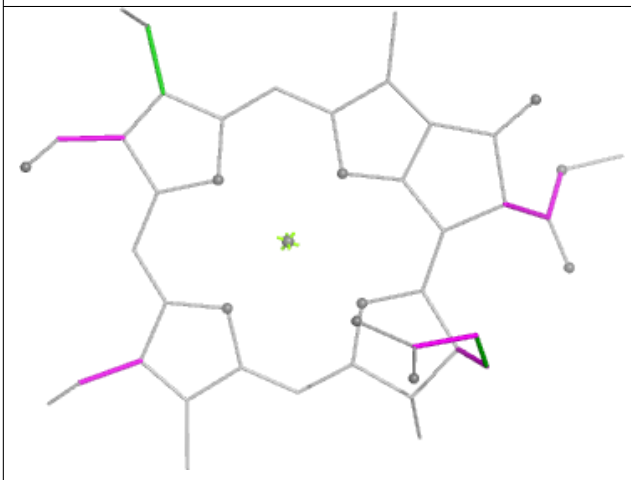
Ligand CHL 6 608



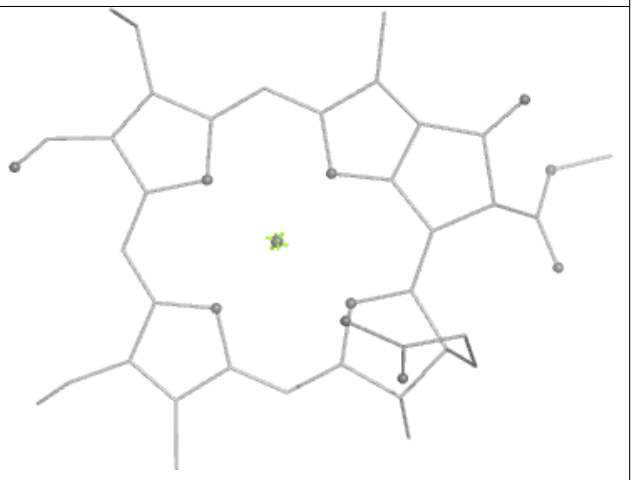
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Bond angles

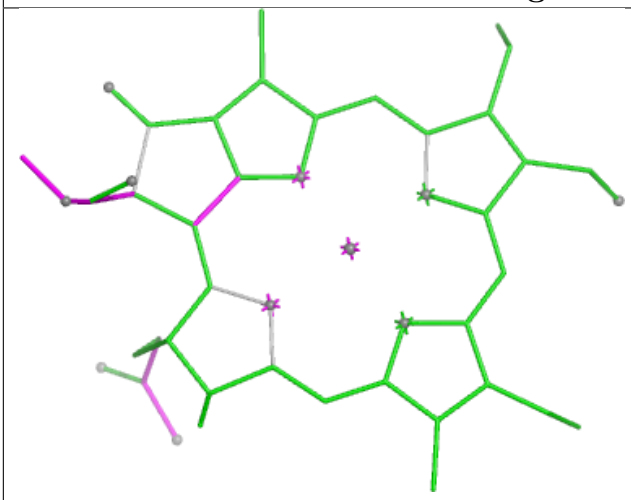


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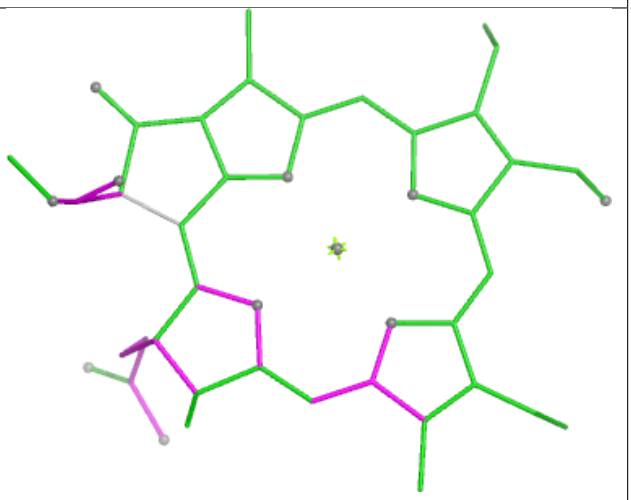


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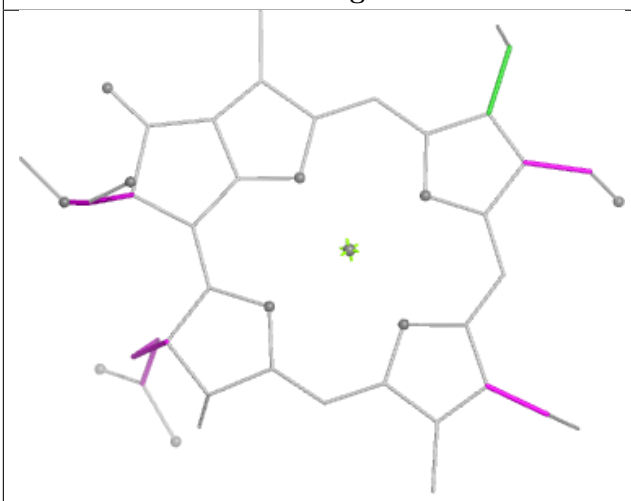
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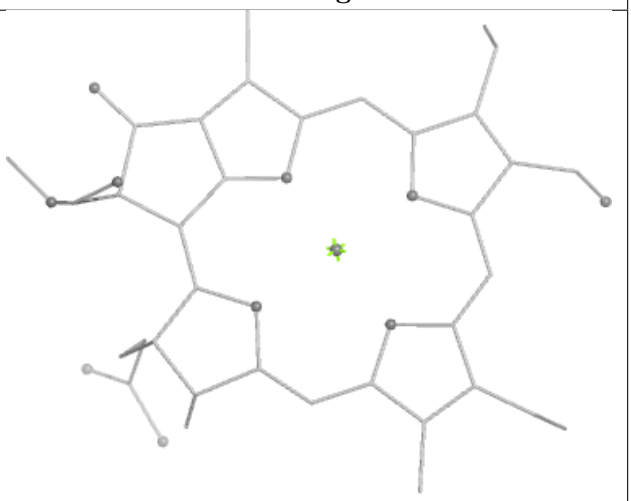
Bond lengths



Bond angles

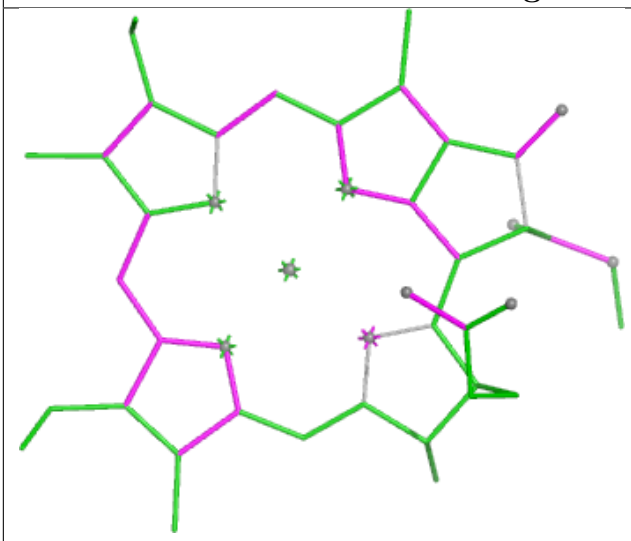


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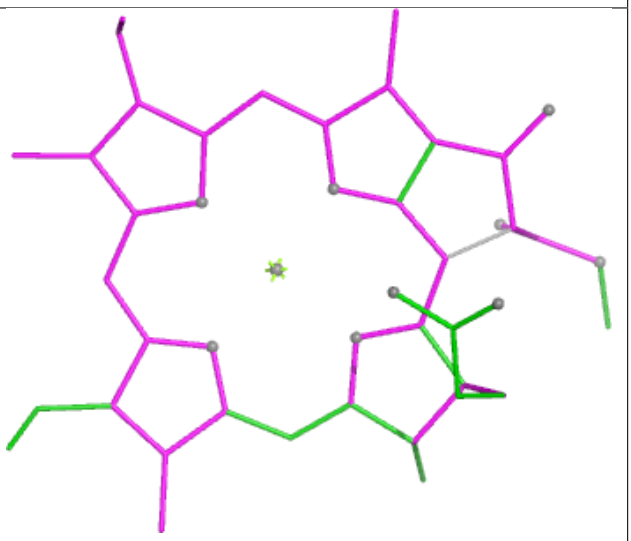


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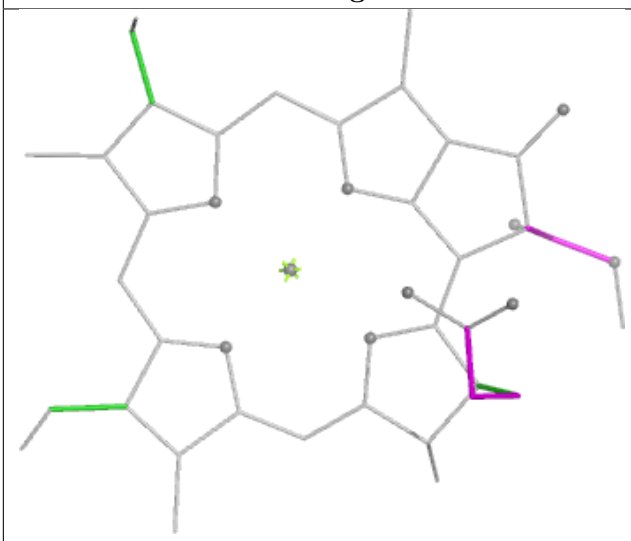
Ligand CLA N 611



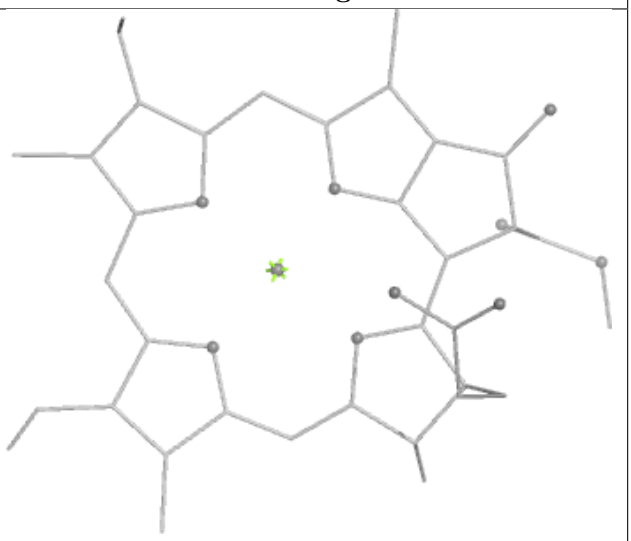
Bond lengths



Bond angles

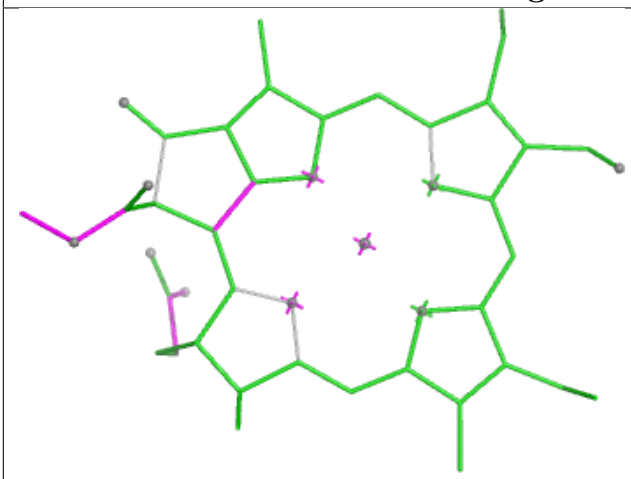


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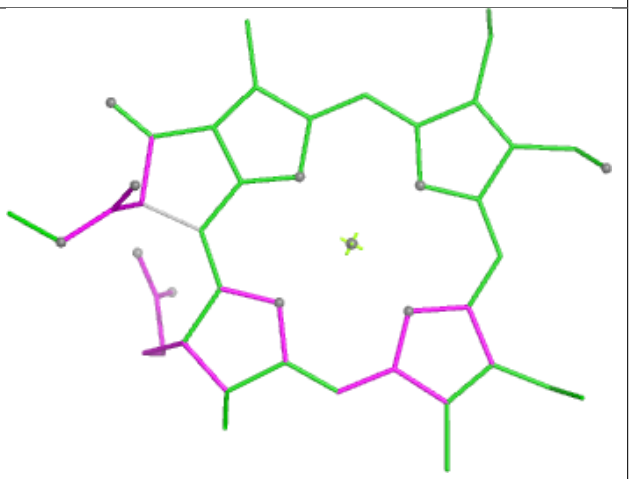


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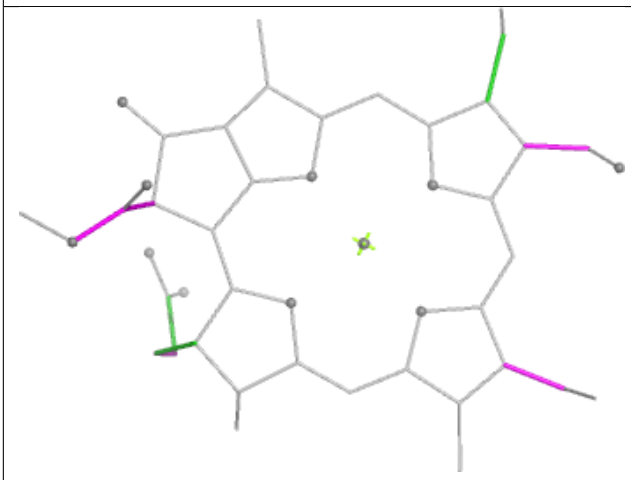
Ligand CHL 3 301



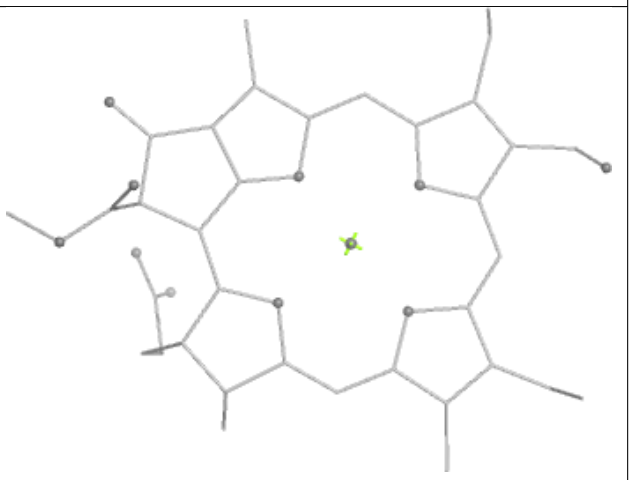
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Bond angles

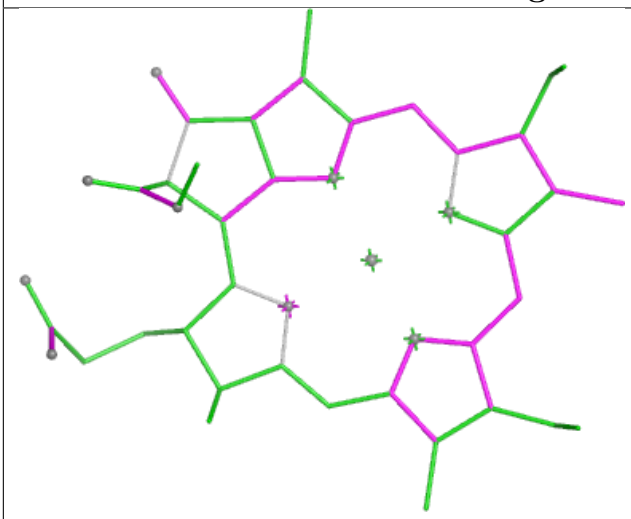


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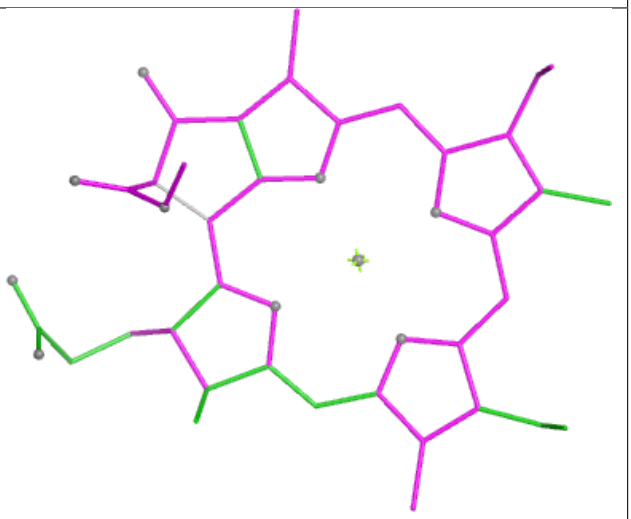


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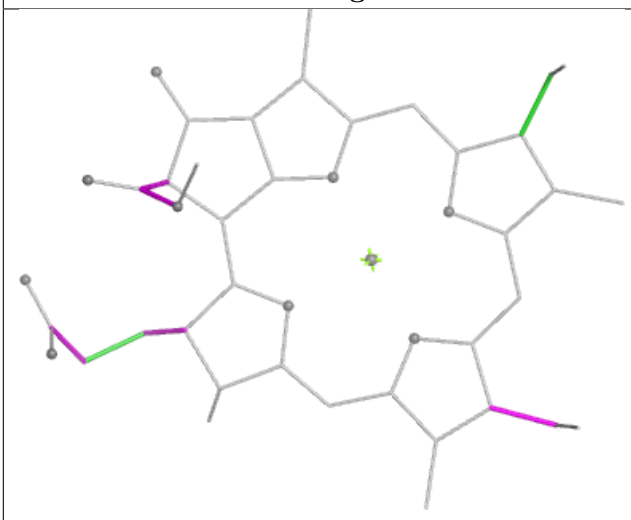
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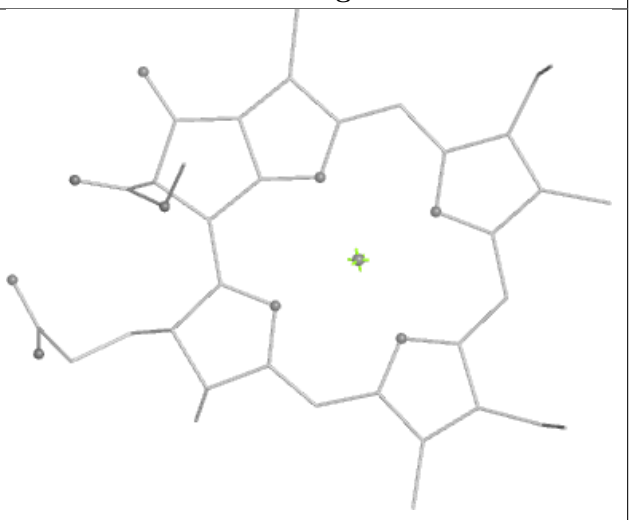
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Bond angles

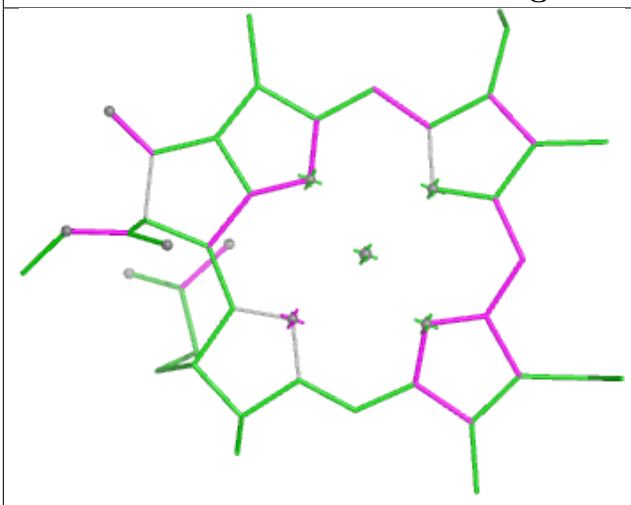


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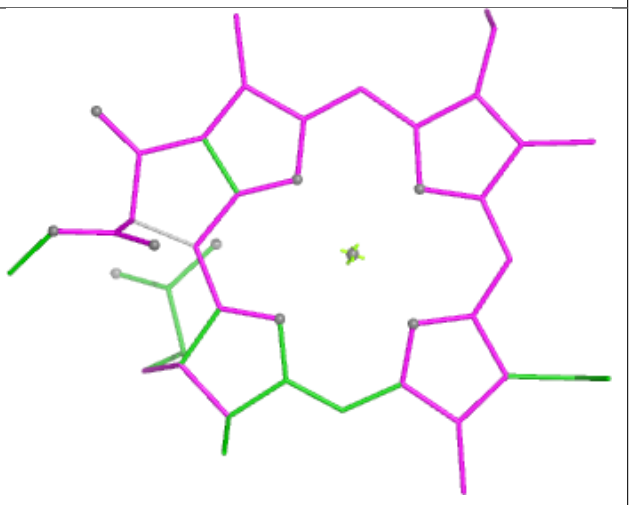


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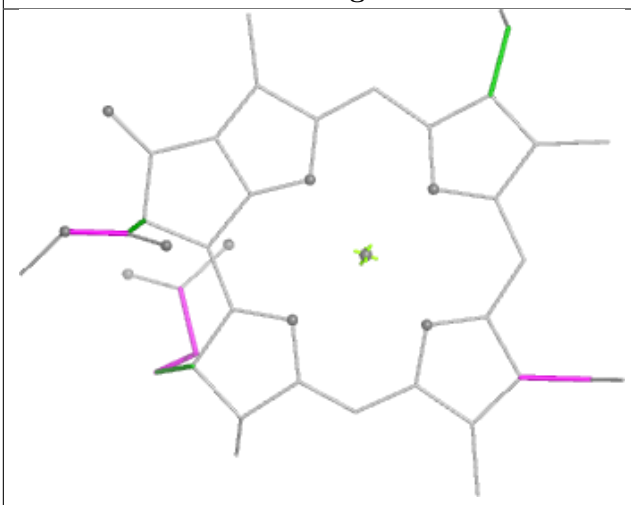
Ligand CLA s 314



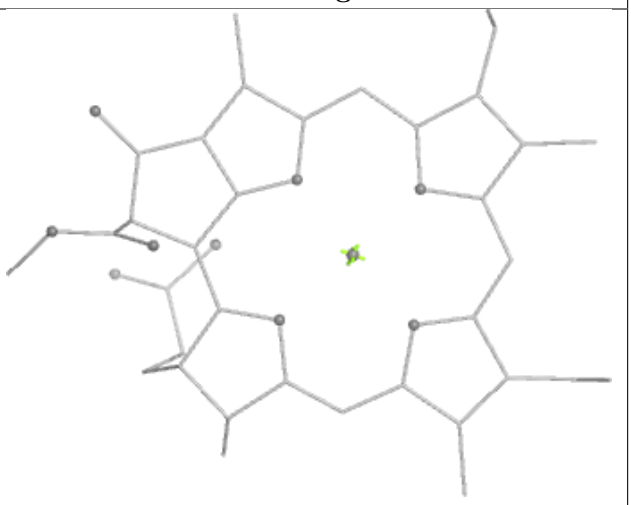
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Bond angles

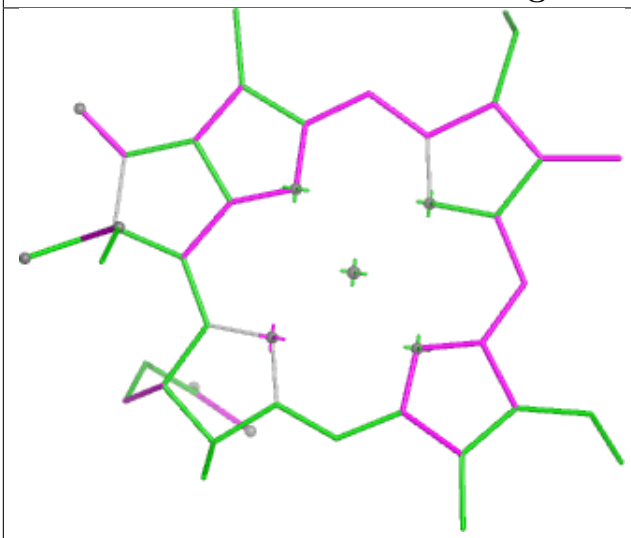


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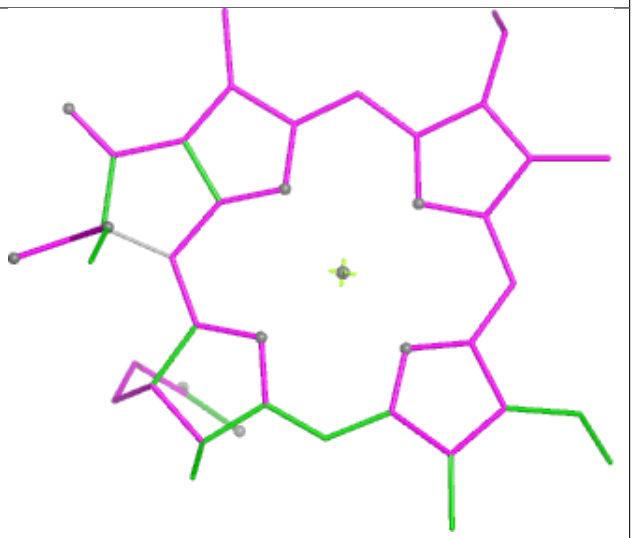


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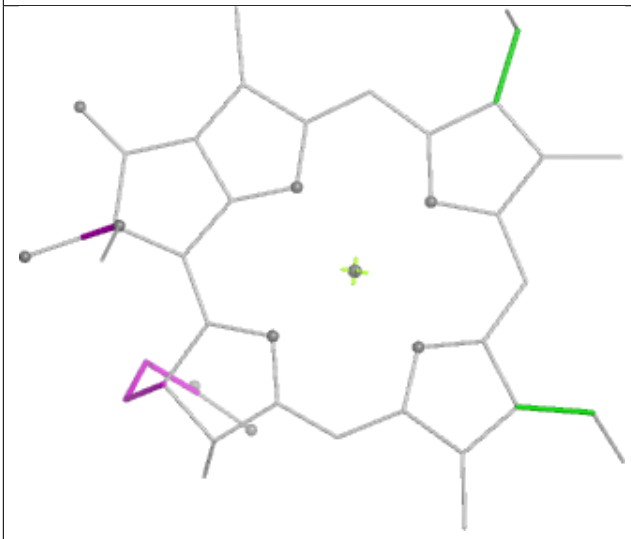
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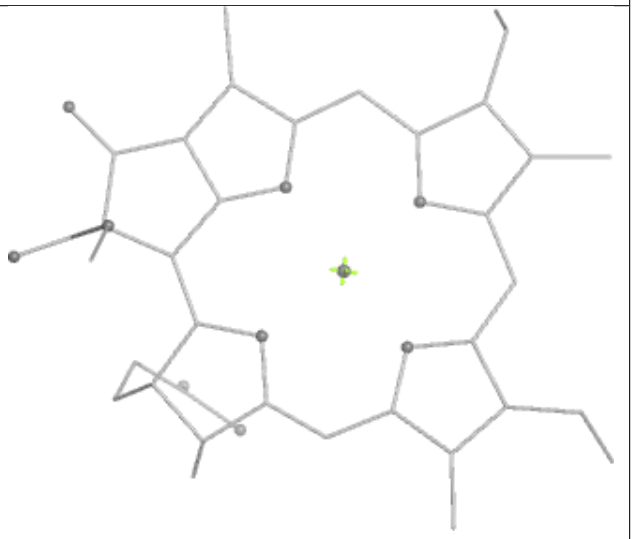
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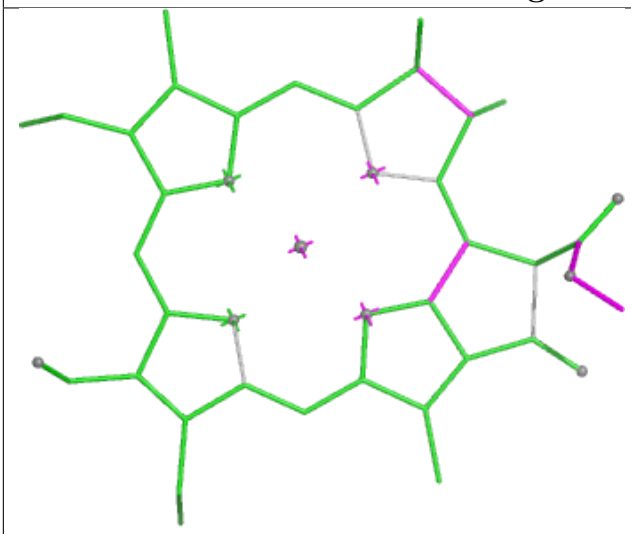


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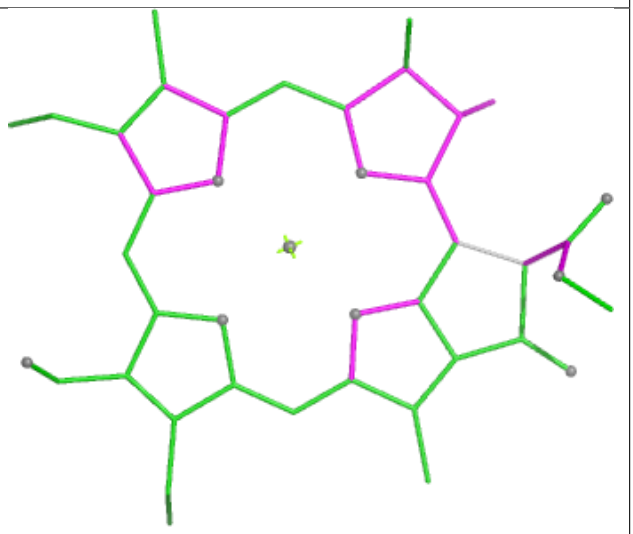


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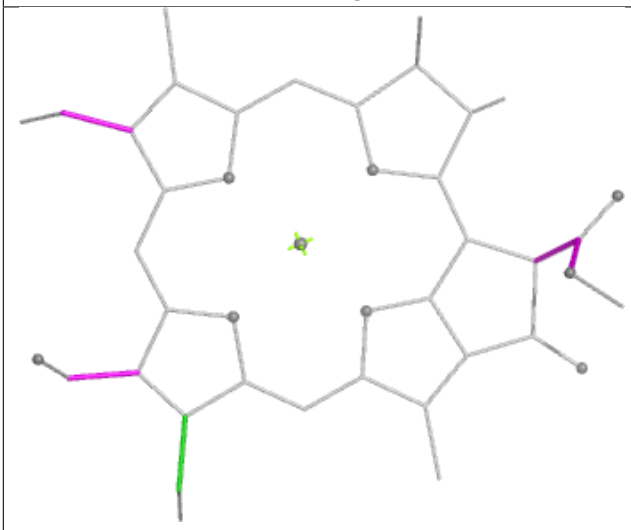
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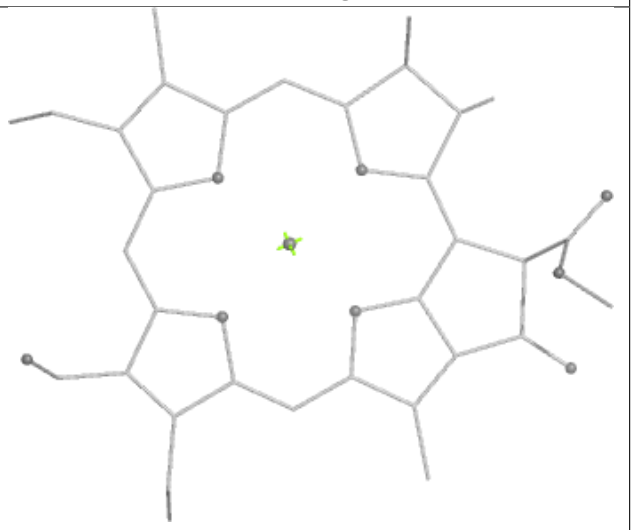
Bond lengths



Bond angles

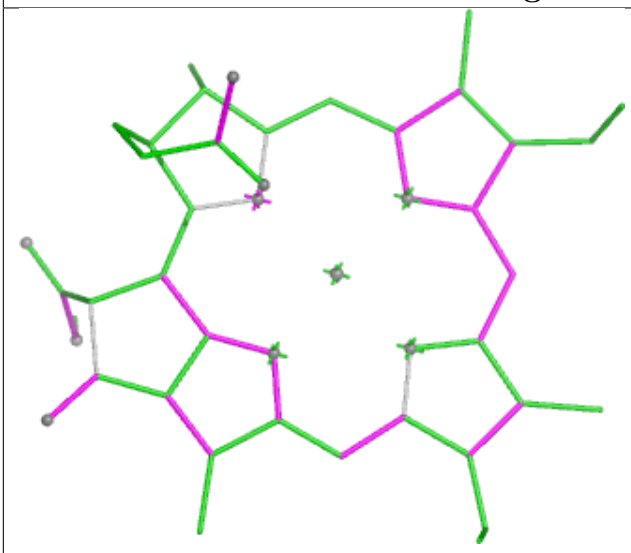


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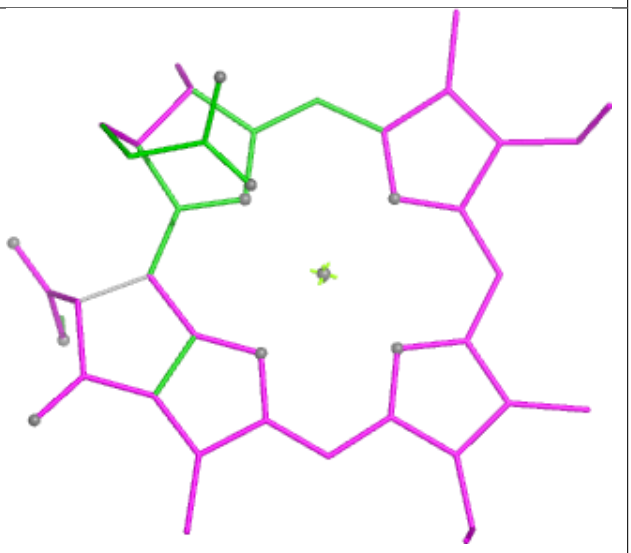


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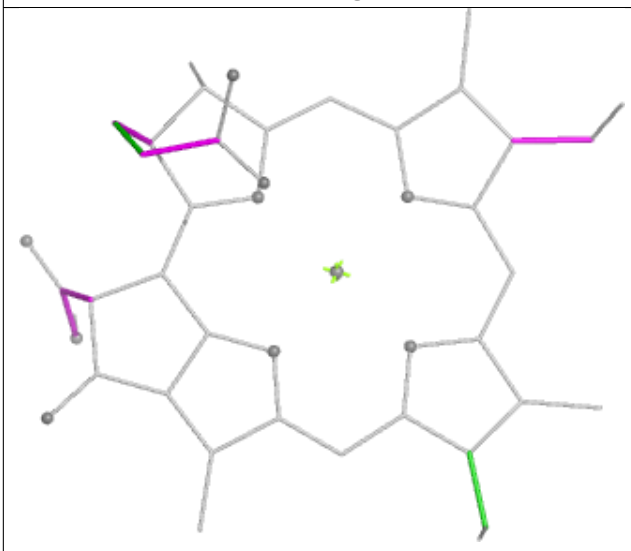
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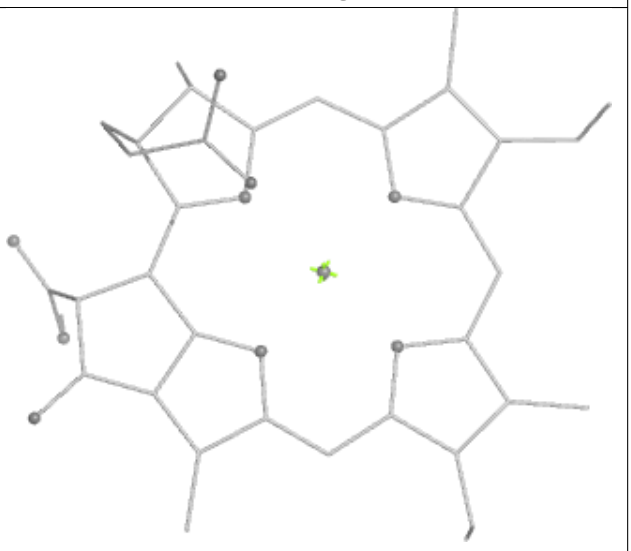
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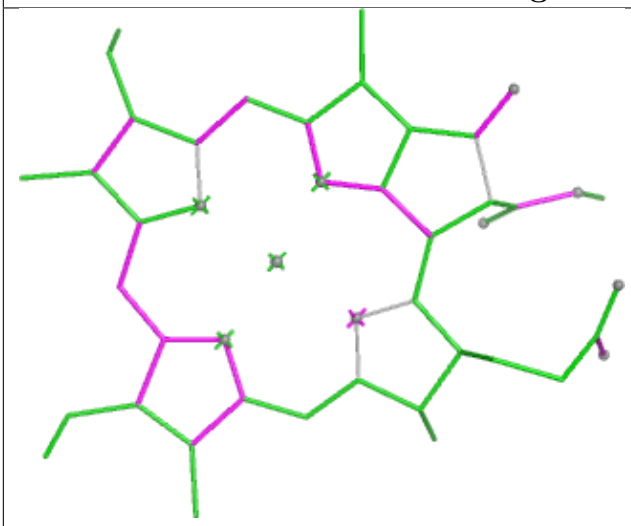


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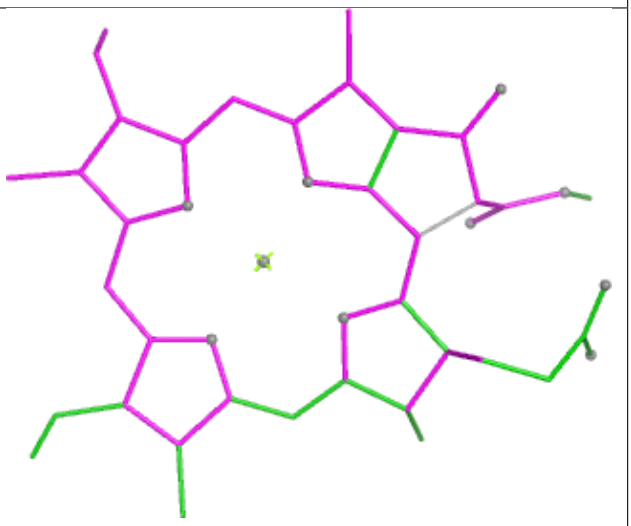


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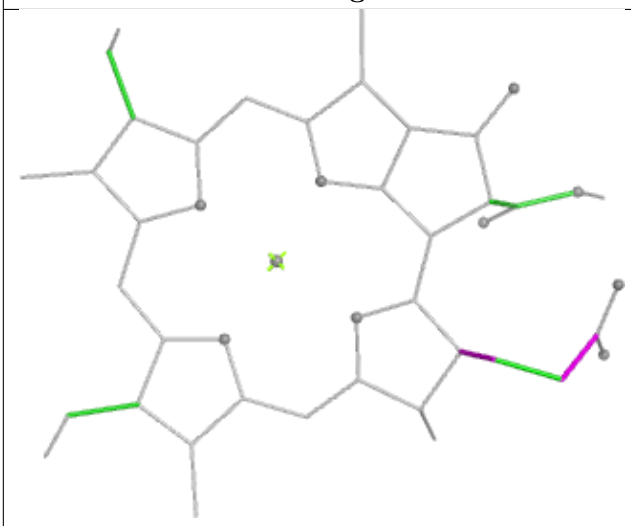
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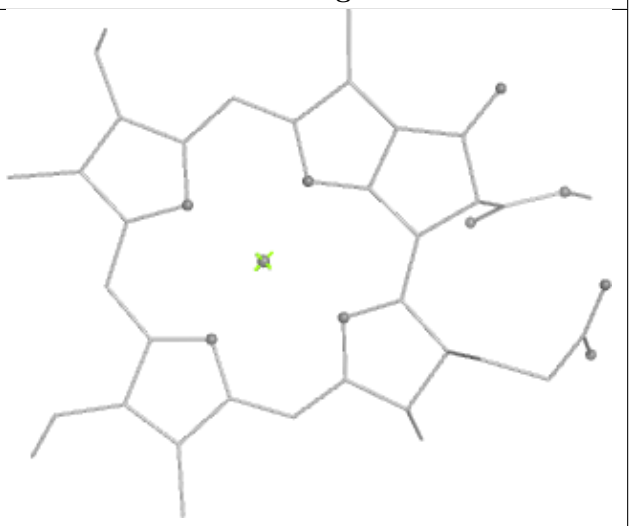
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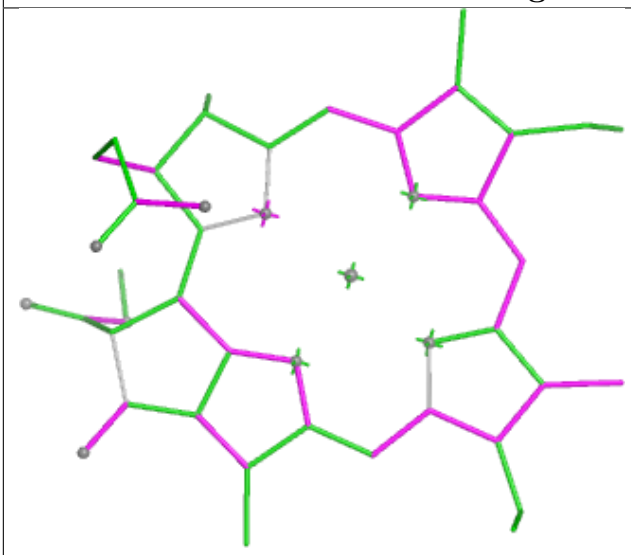


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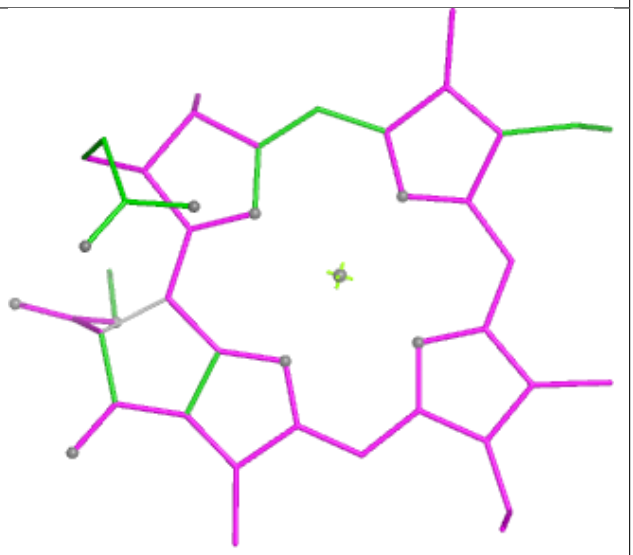


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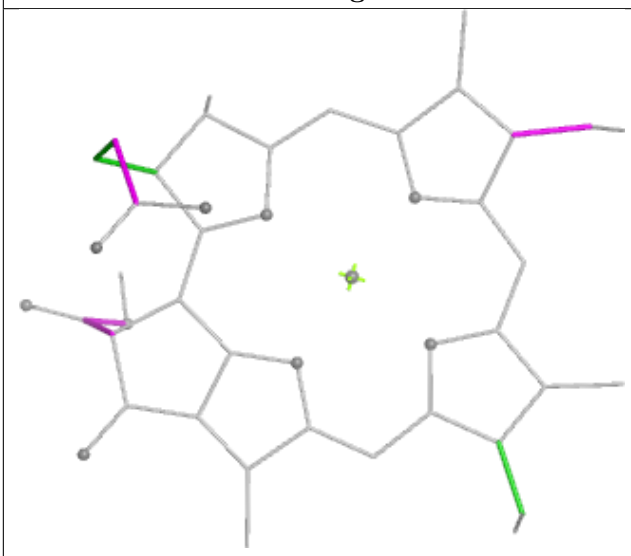
Ligand CLA 4 303



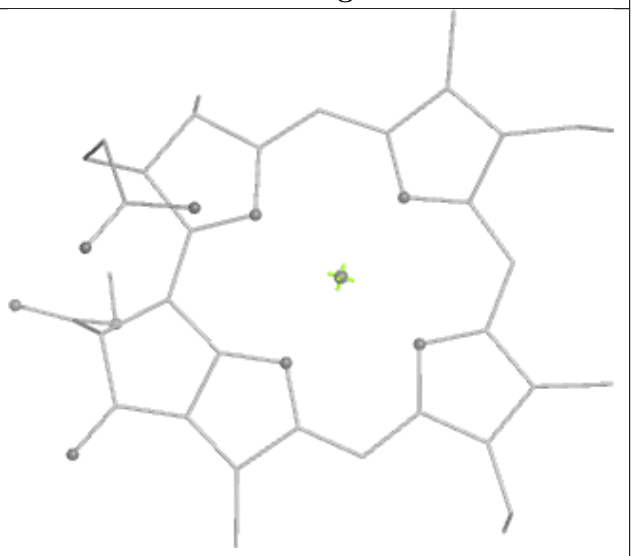
Bond lengths



Bond angles

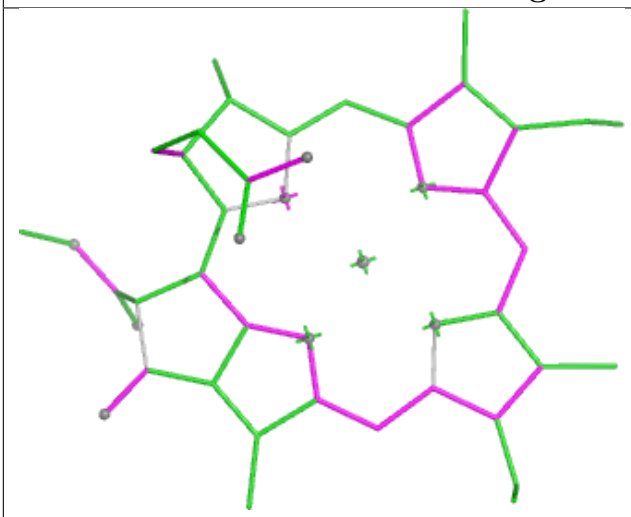


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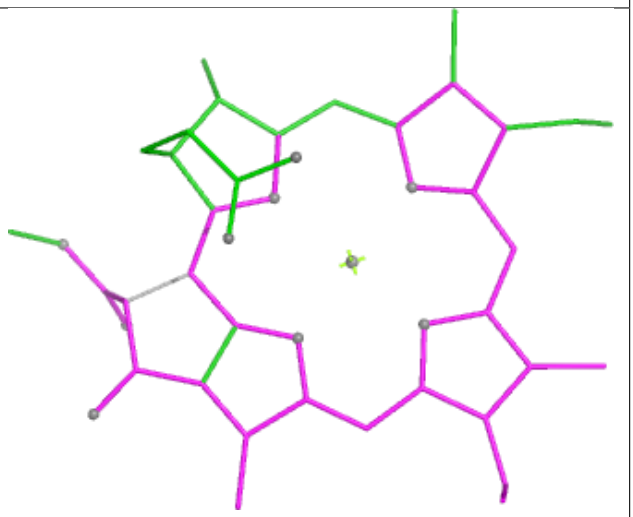


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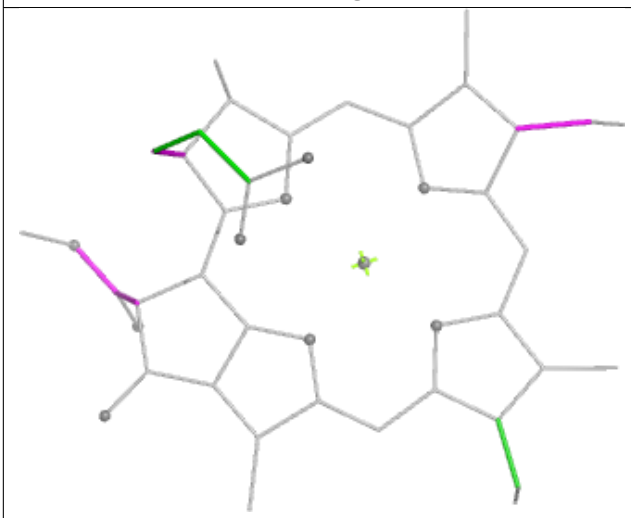
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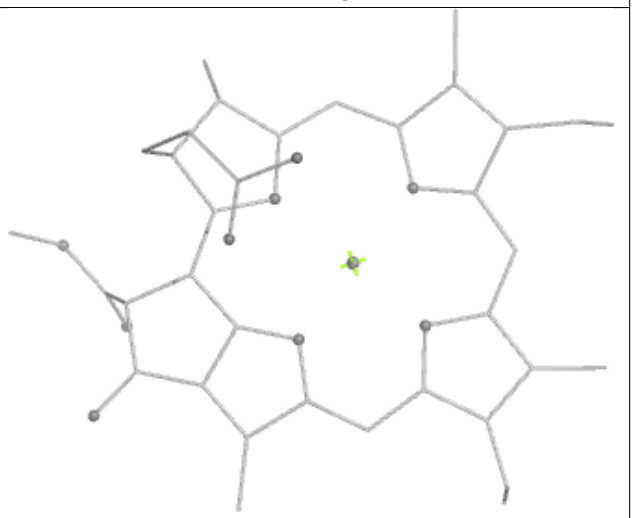
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Bond angles

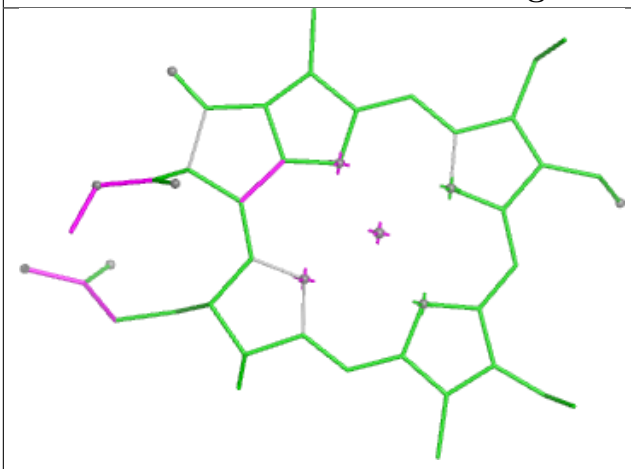


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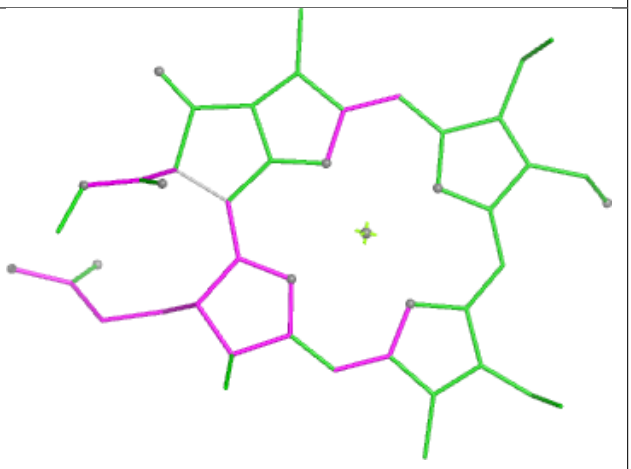


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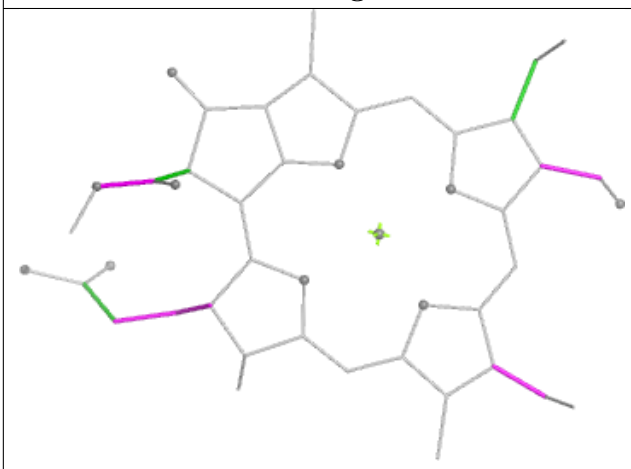
Ligand CHL 3 302



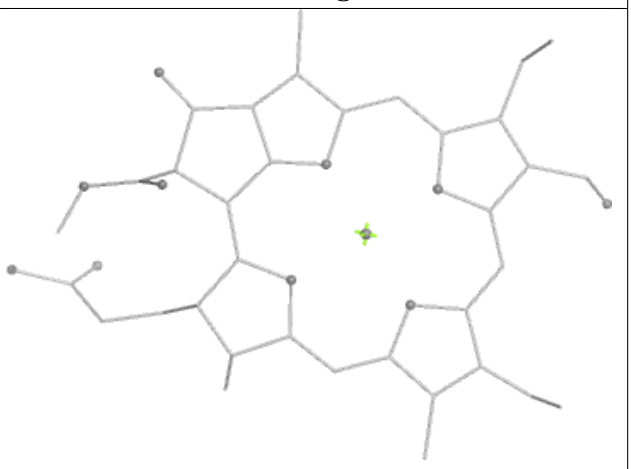
Bond lengths



Bond angles

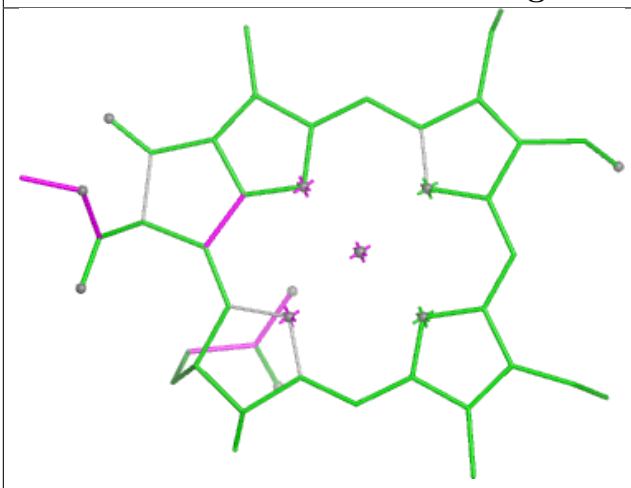


Torsions

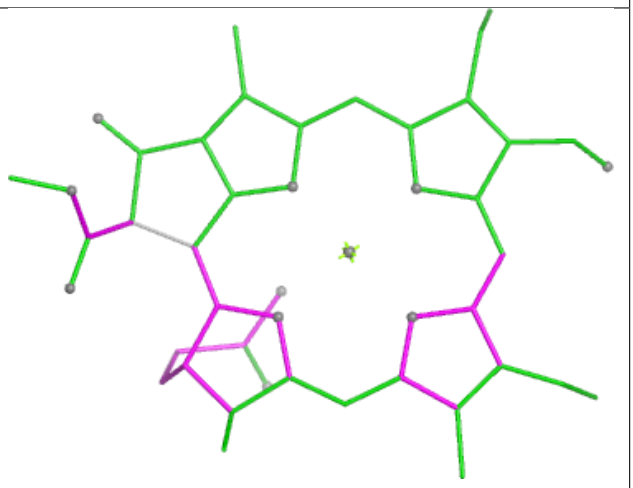


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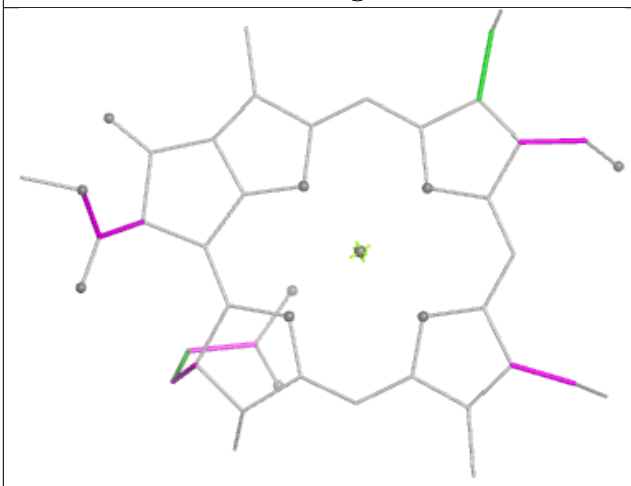
Ligand CHL 3 309



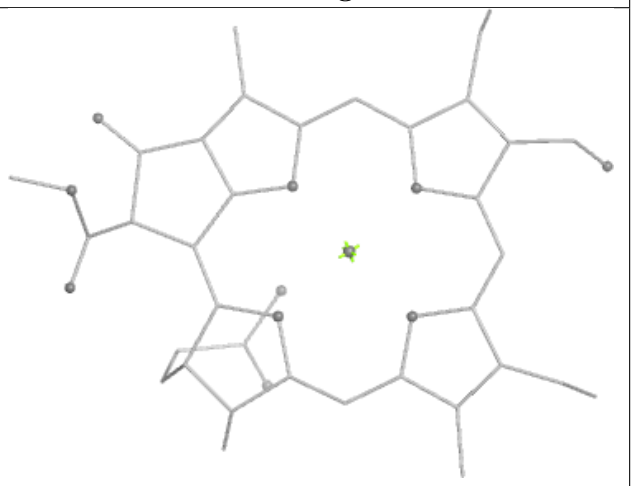
Bond lengths



Bond angles

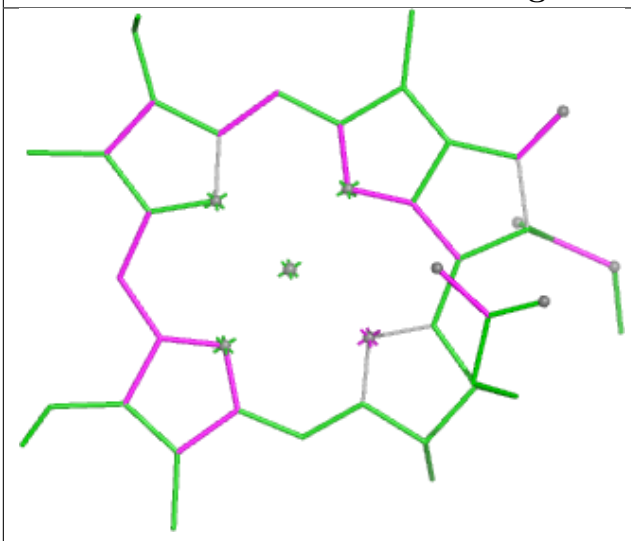


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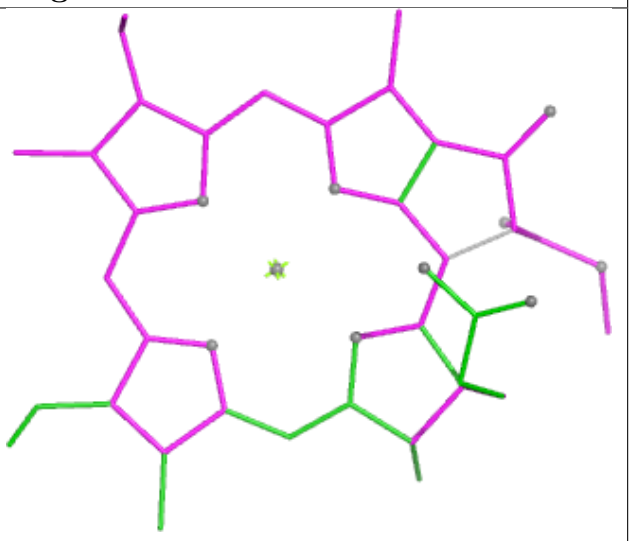


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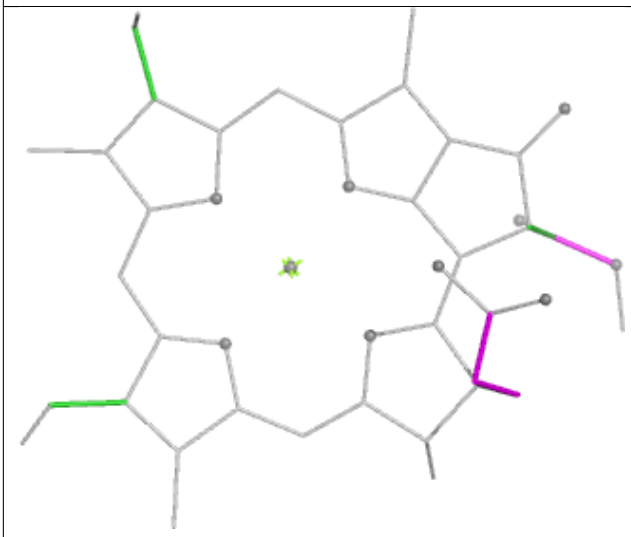
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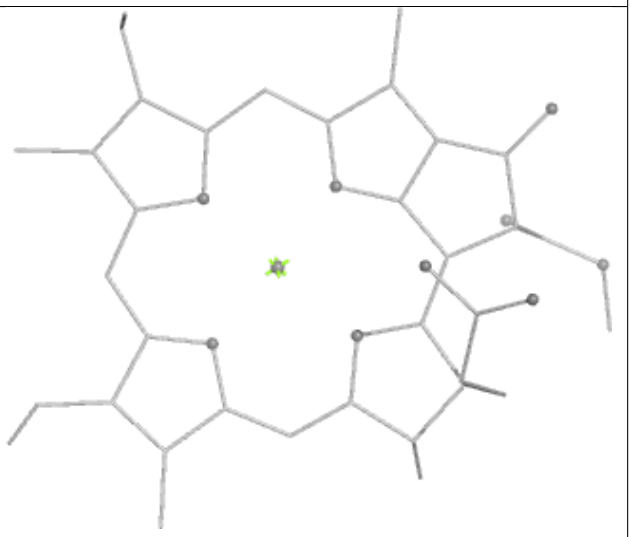
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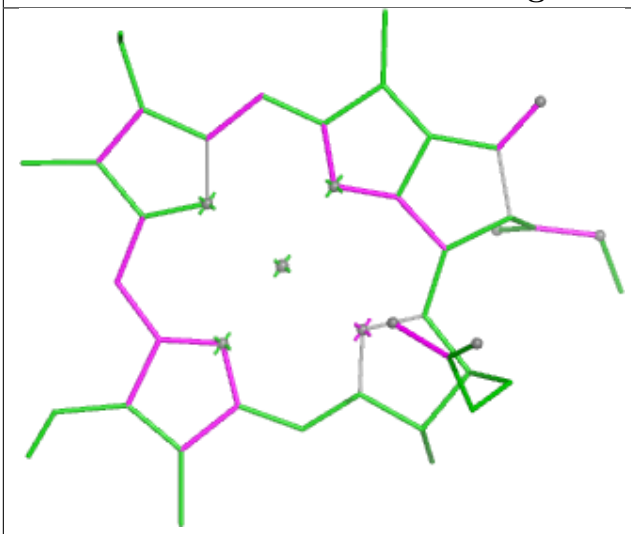


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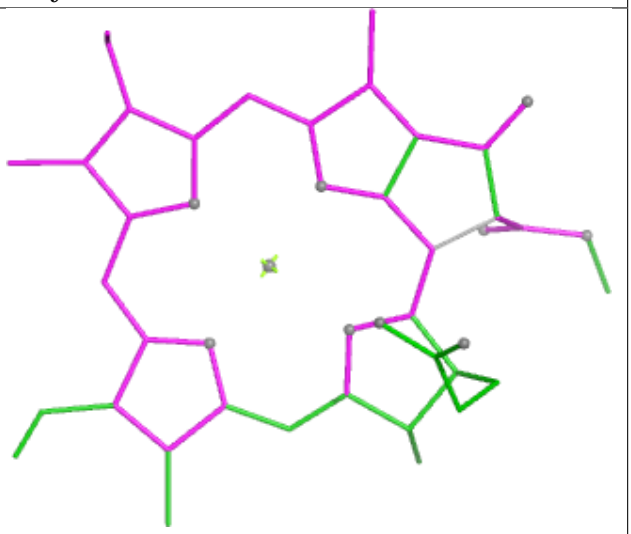


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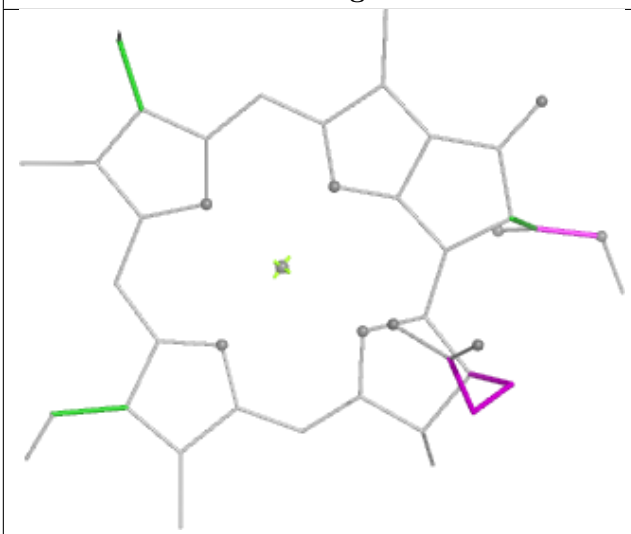
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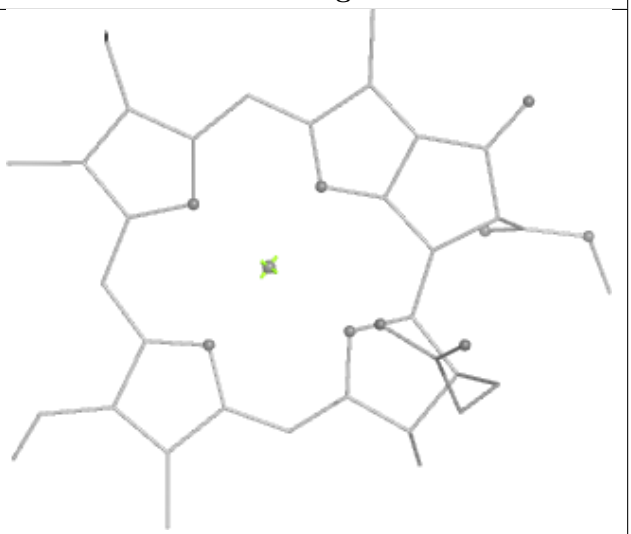
Bond lengths



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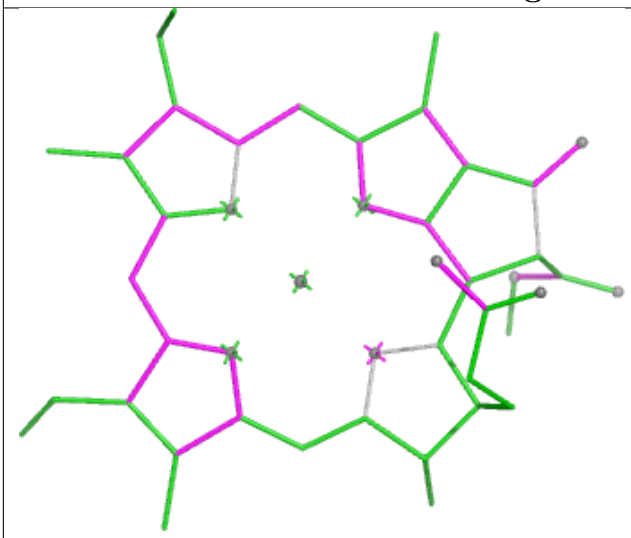


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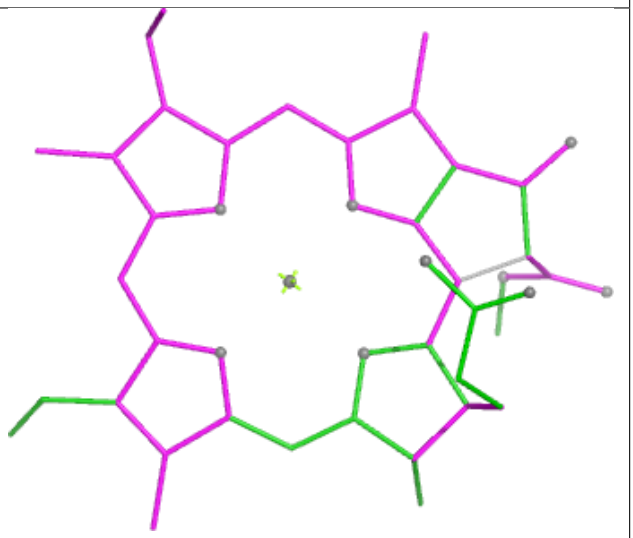


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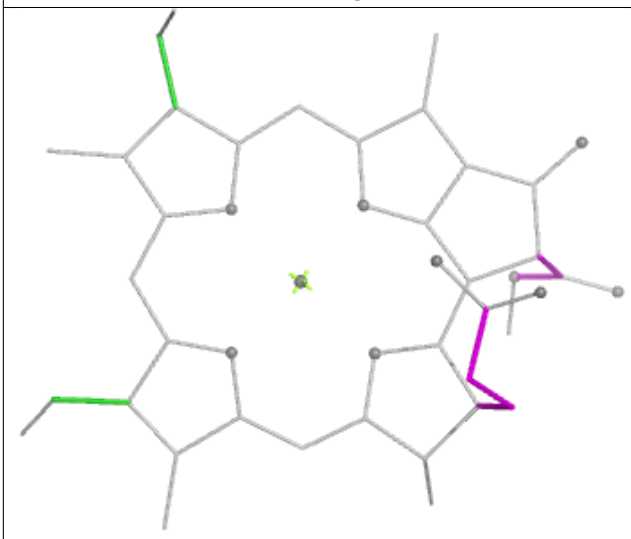
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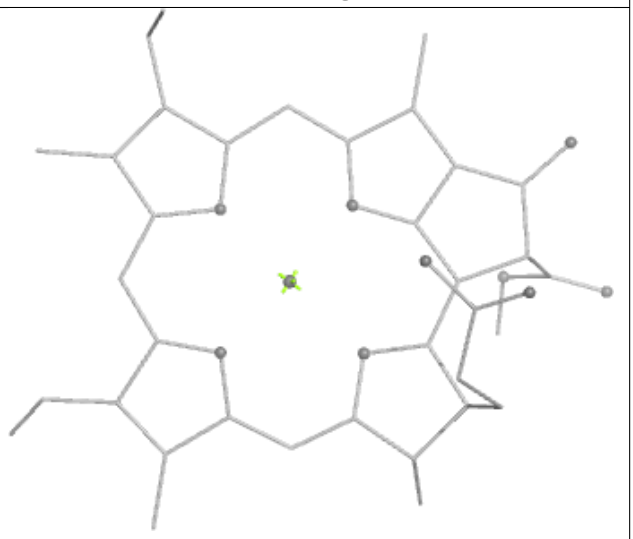
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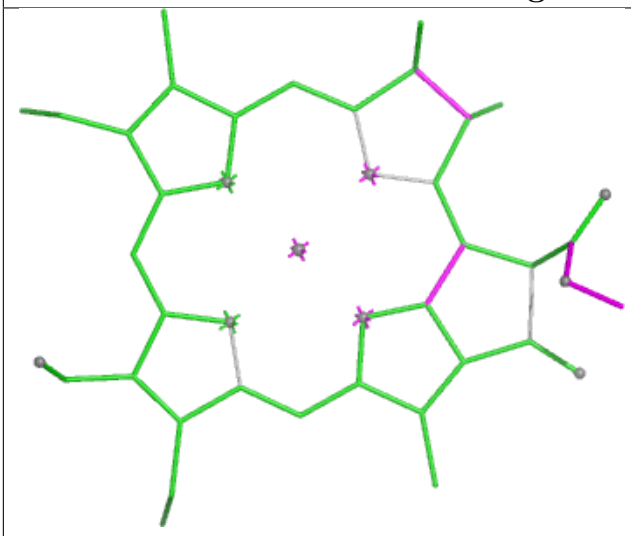


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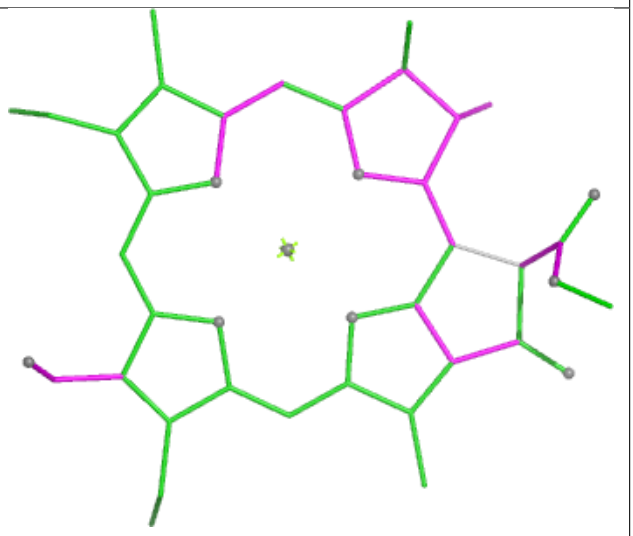


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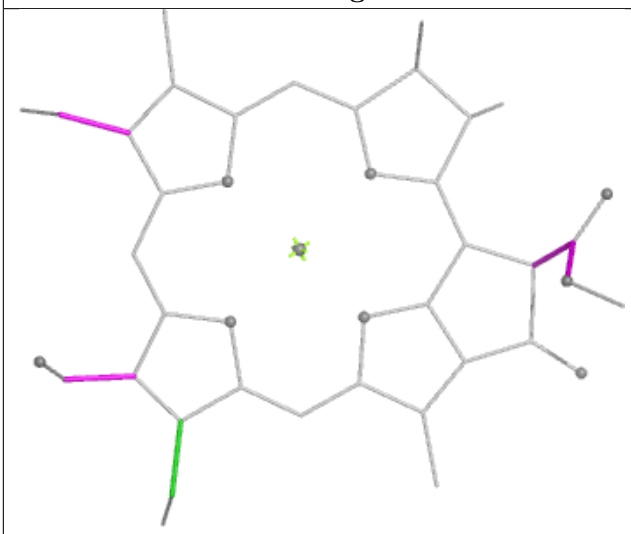
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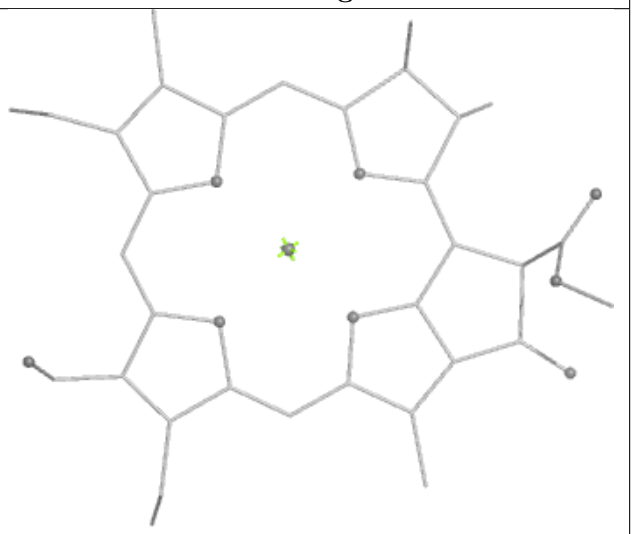
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Bond angles

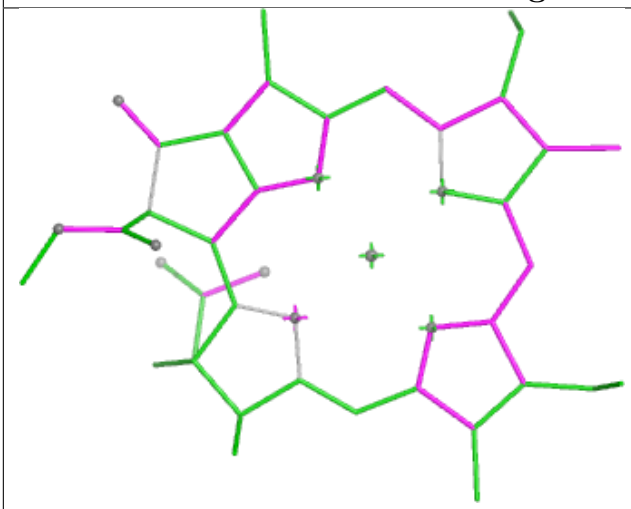


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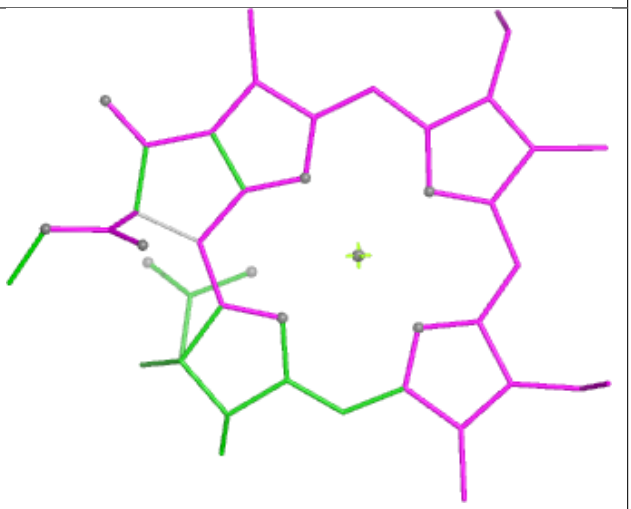


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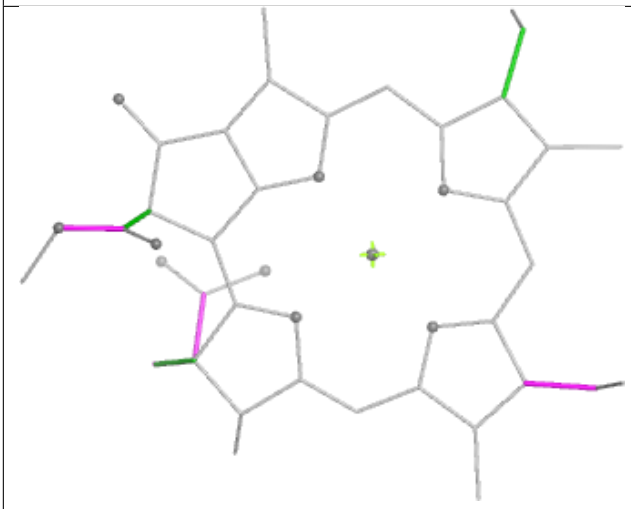
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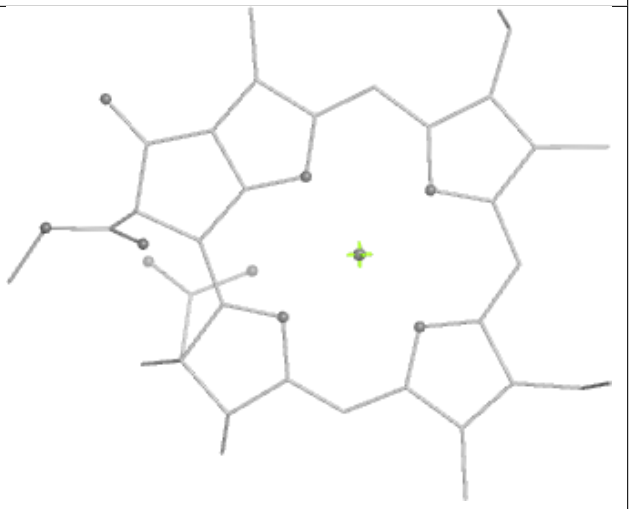
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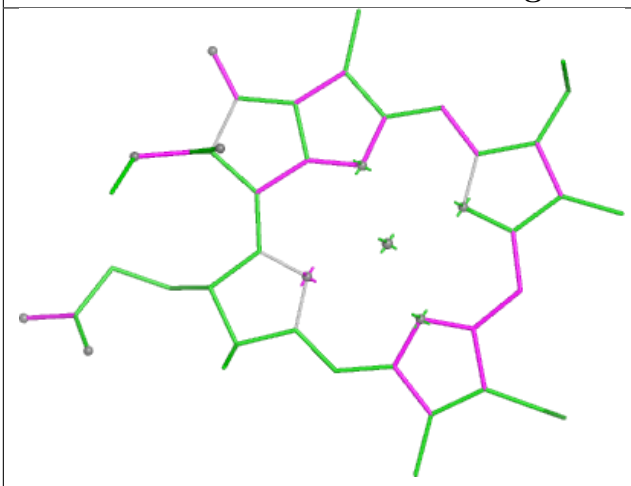


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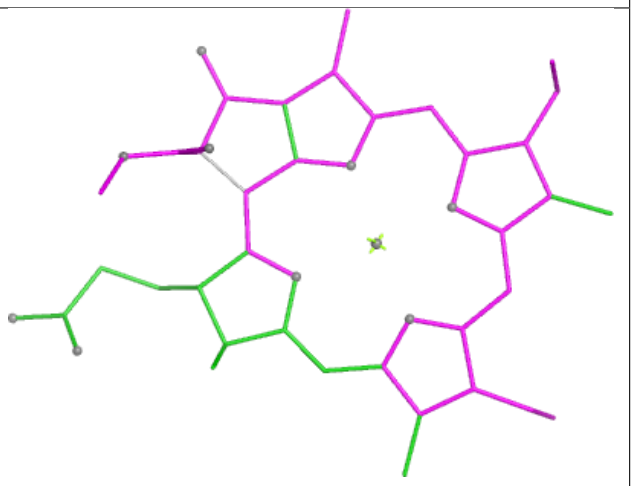


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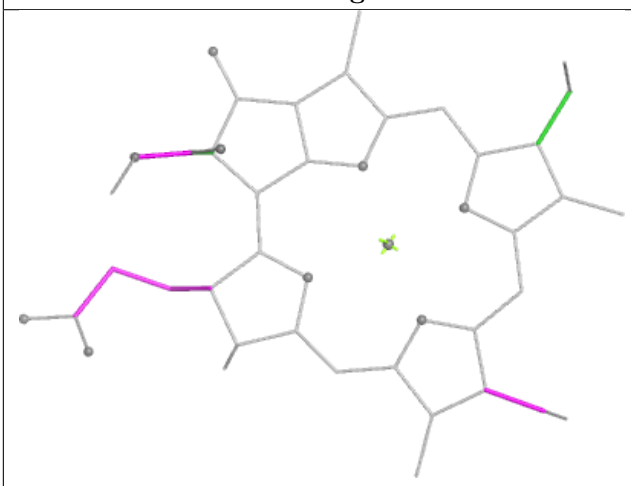
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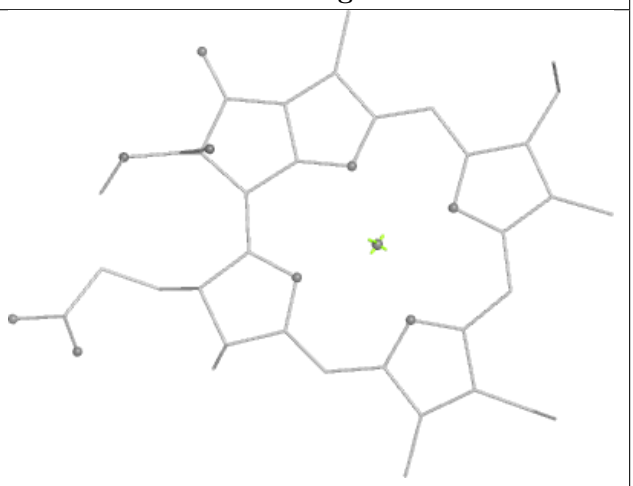
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Bond angles

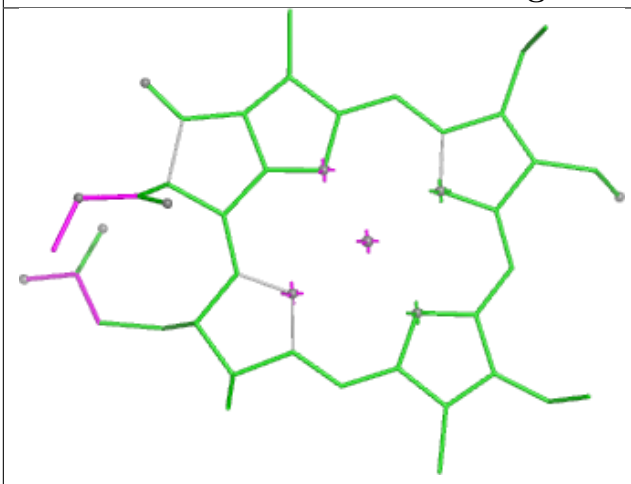


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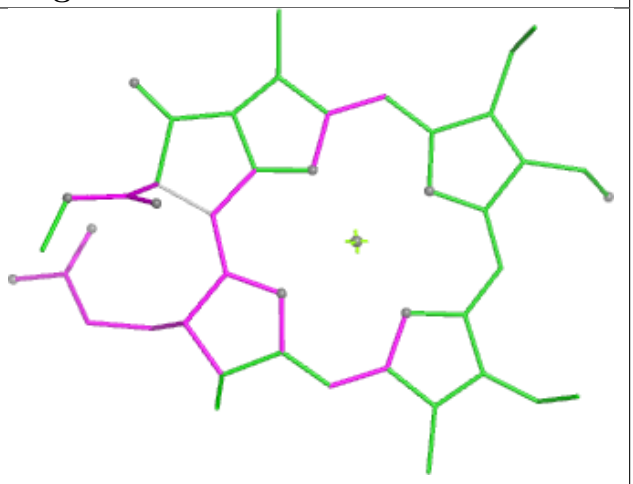


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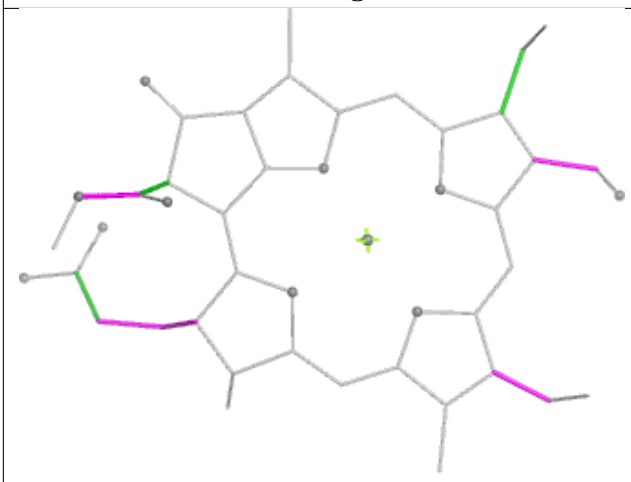
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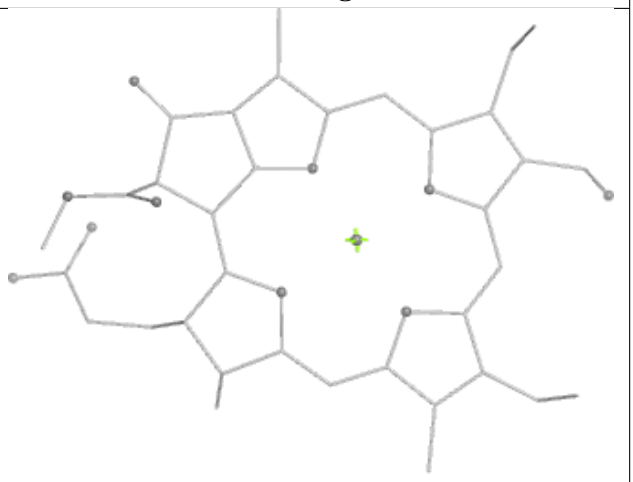
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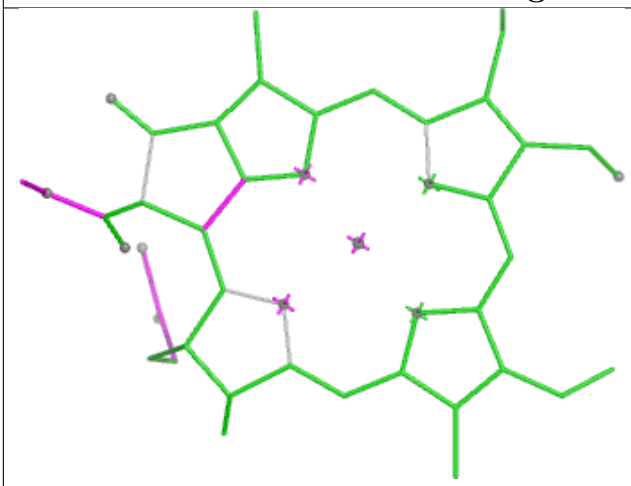


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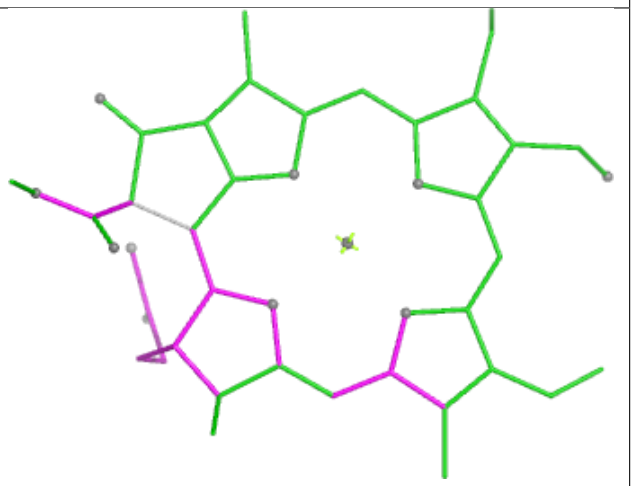


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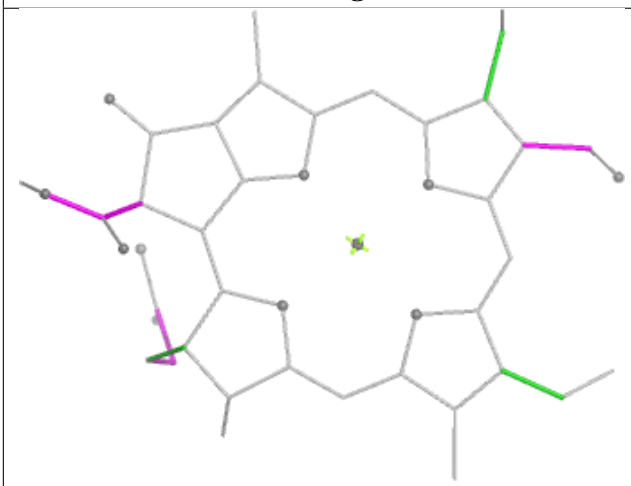
Ligand CHL 2 607



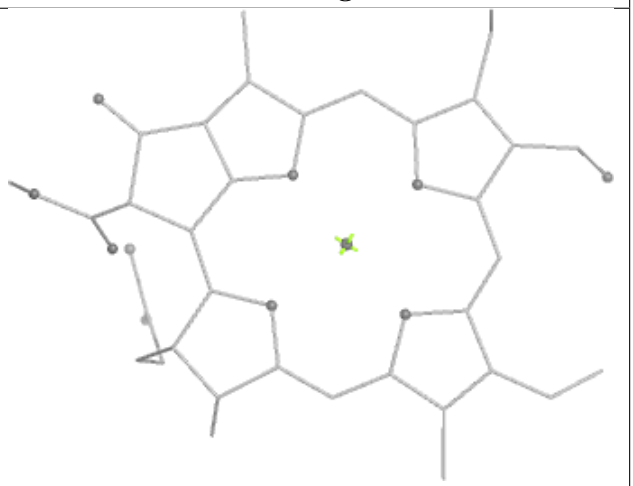
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Bond angles

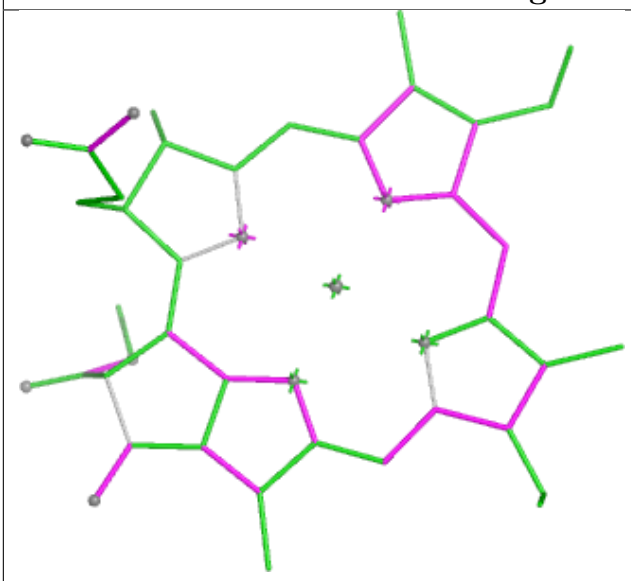


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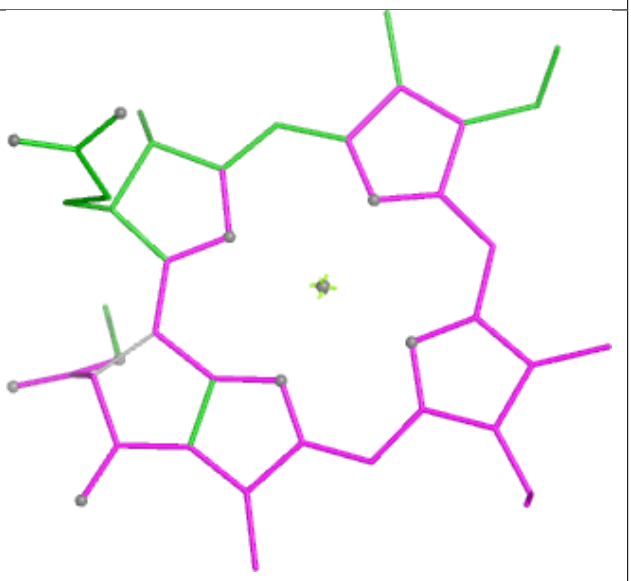


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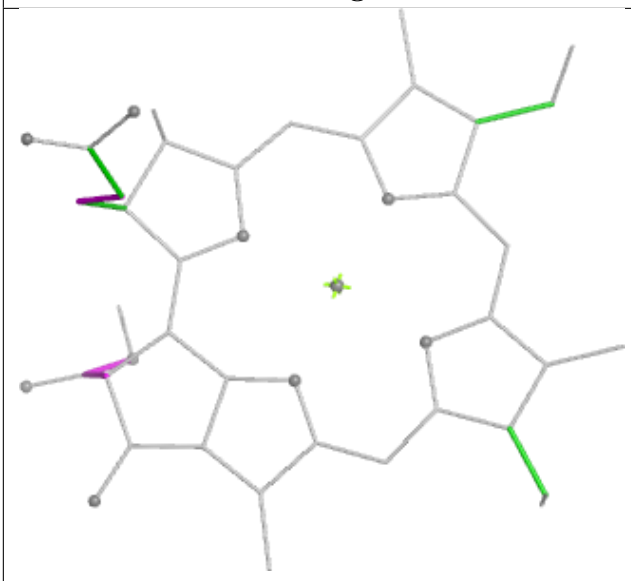
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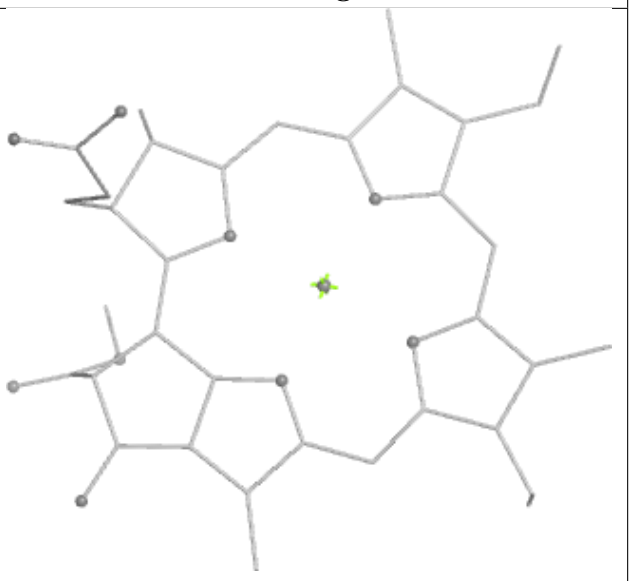
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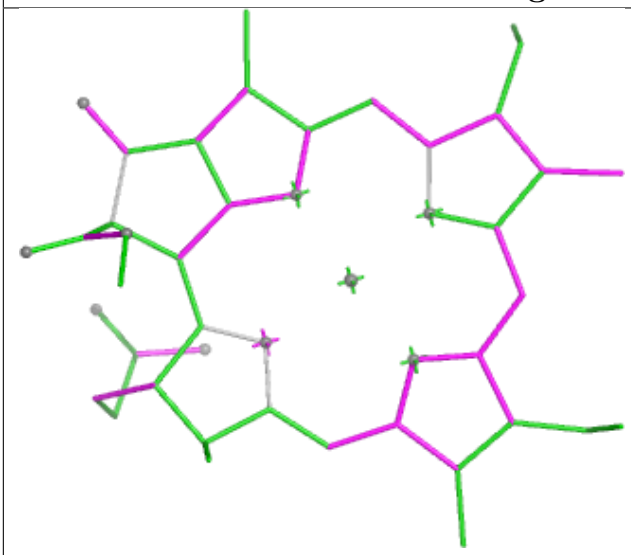


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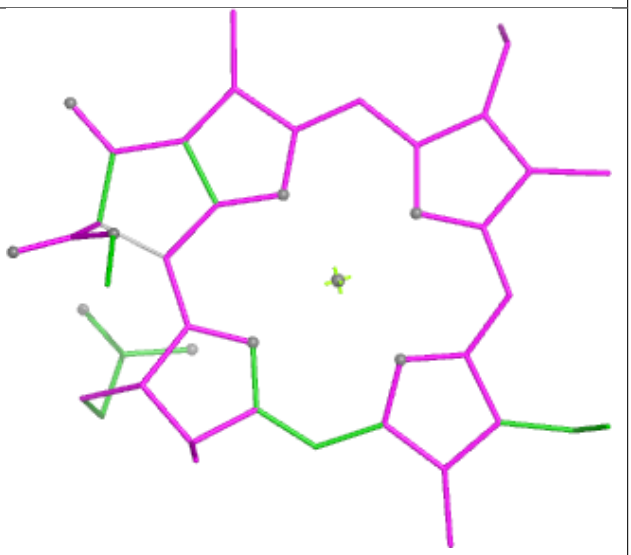


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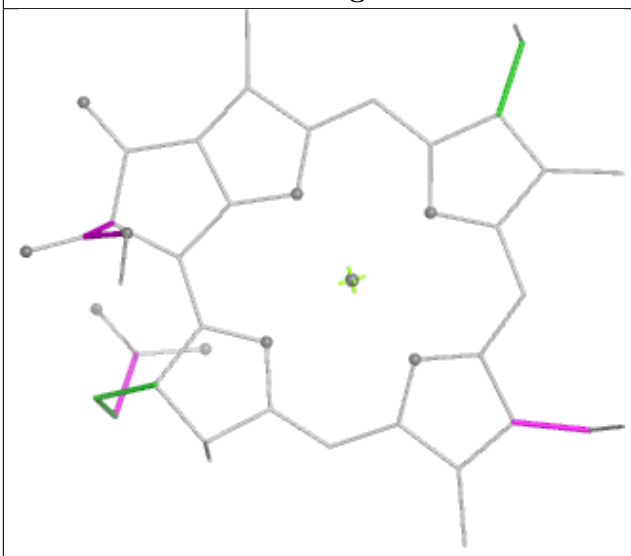
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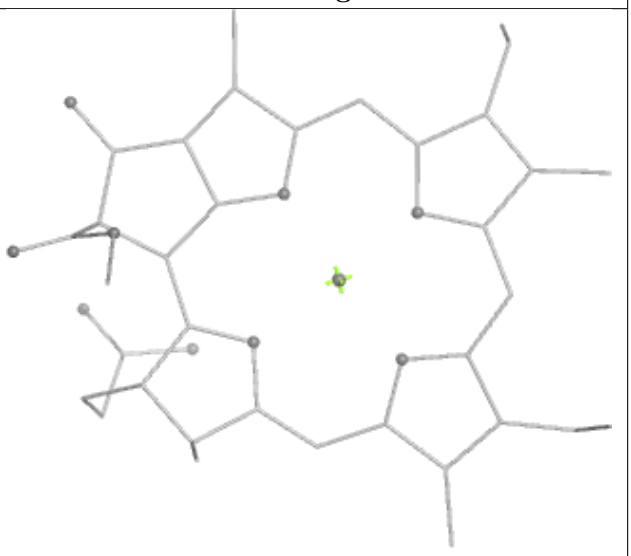
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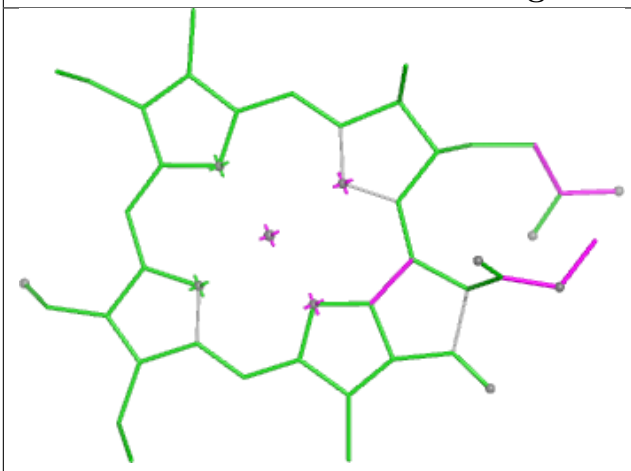


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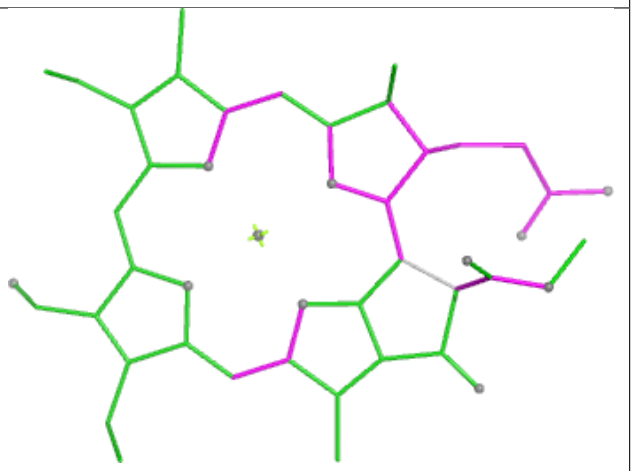


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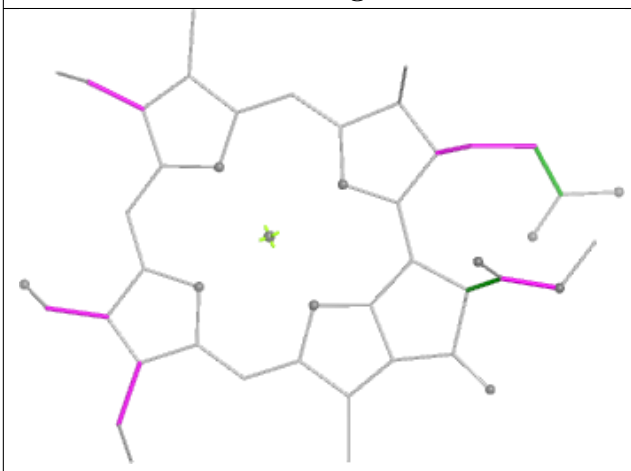
Ligand CHL 2 601



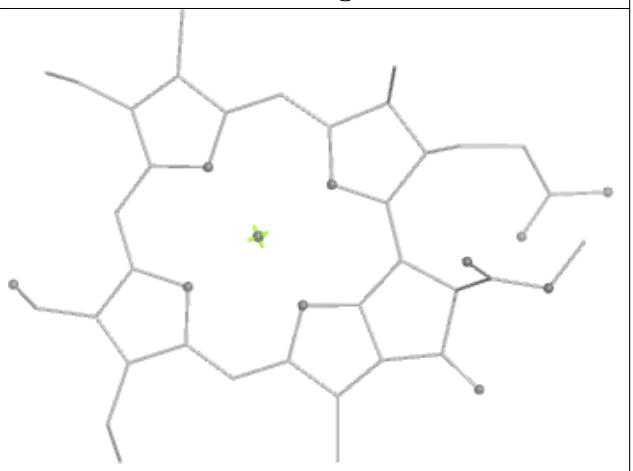
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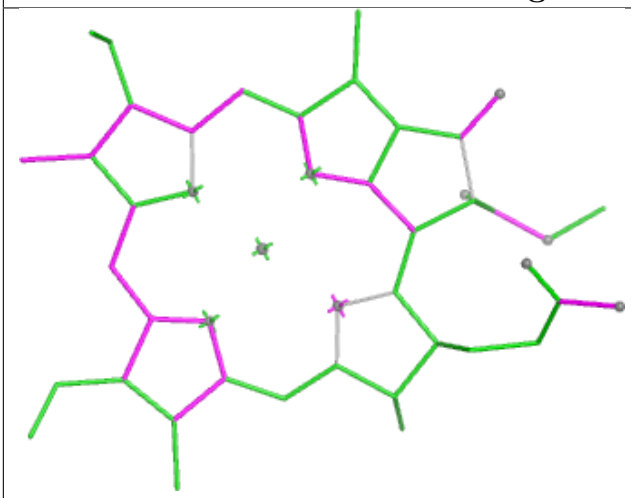


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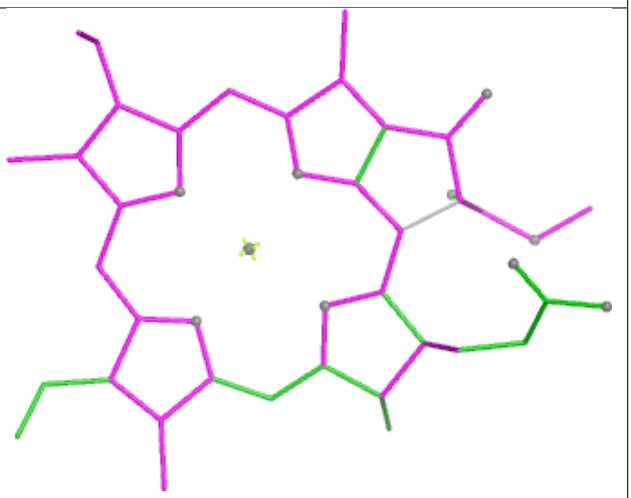


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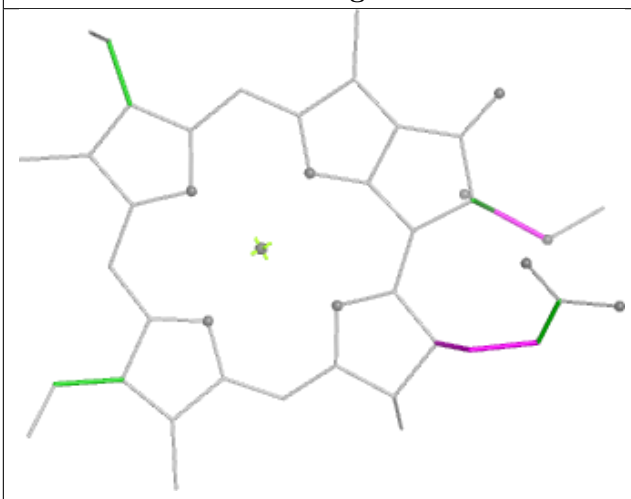
Ligand CLA a 402



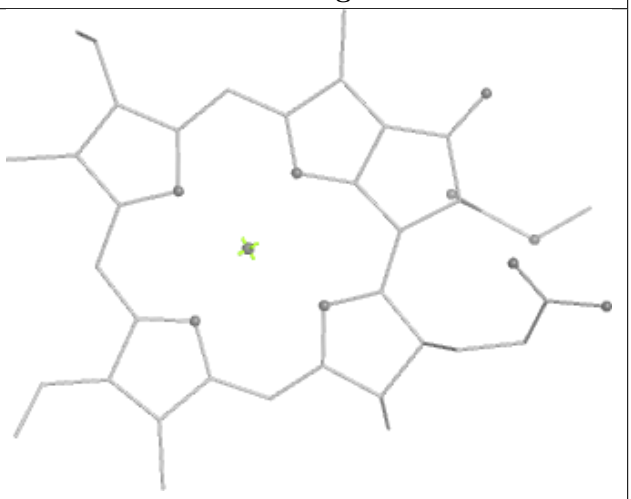
Bond lengths



Bond angles

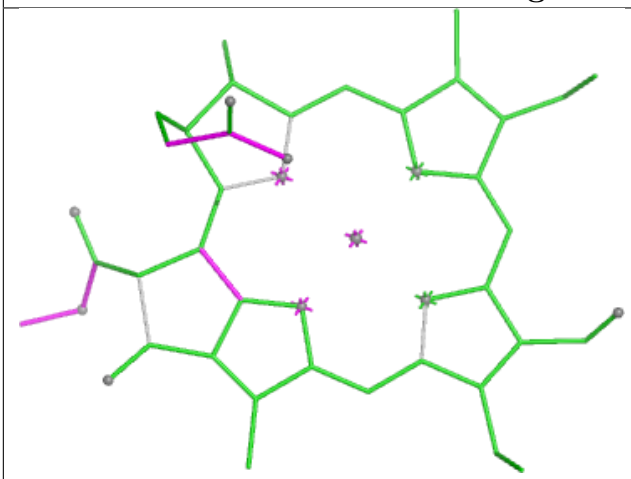


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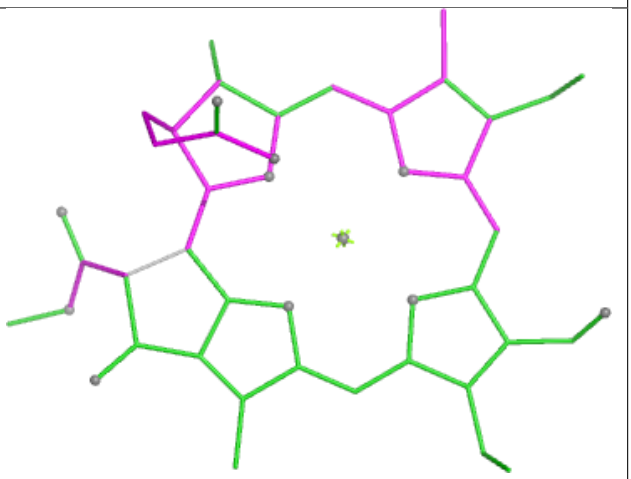


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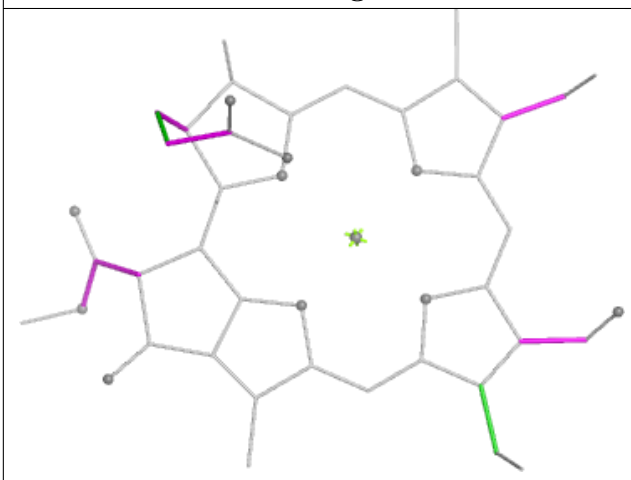
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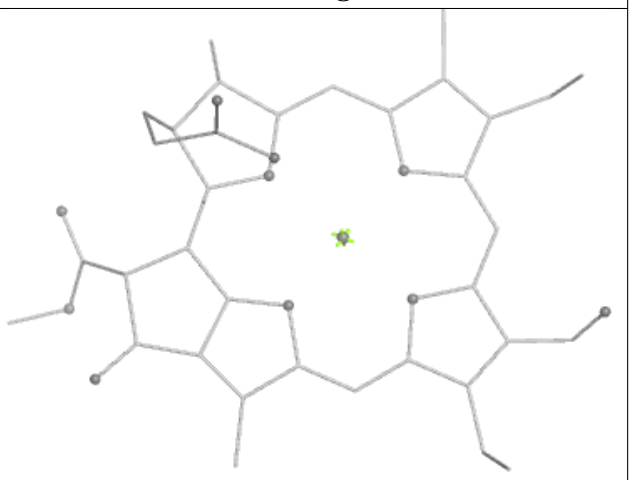
Bond lengths



Bond angles

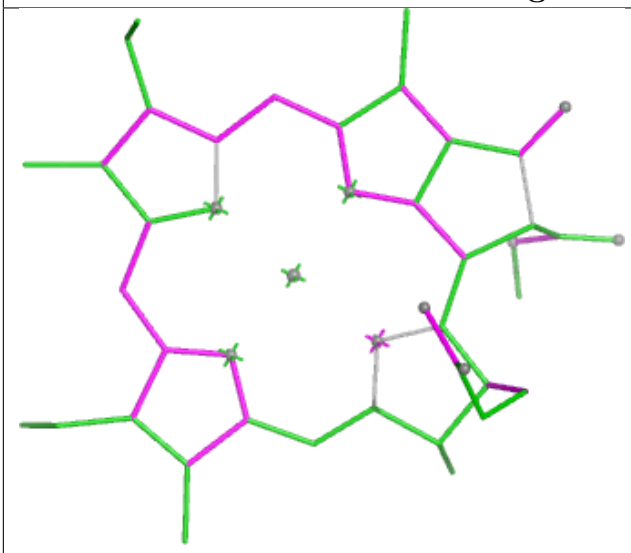


Torsions

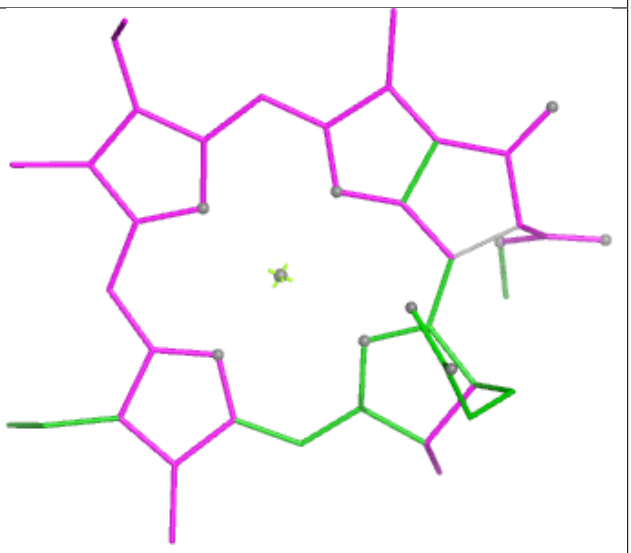


Rings

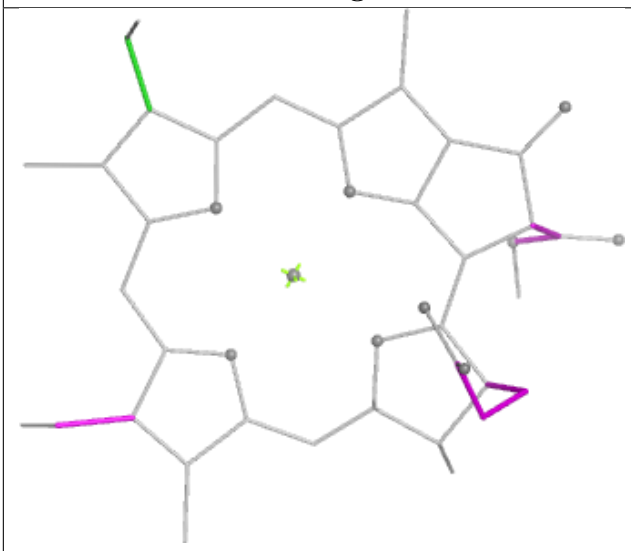
Ligand CLA 1 602



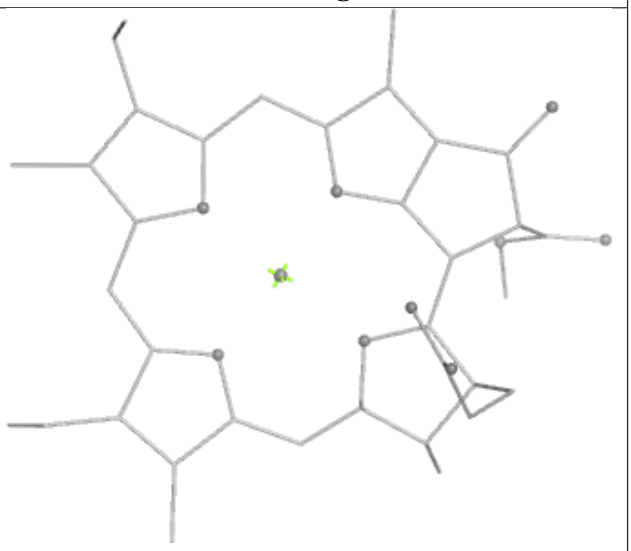
Bond lengths



Bond angles

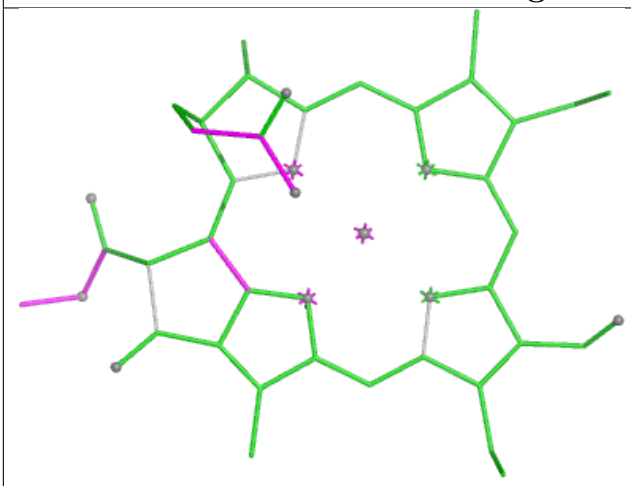


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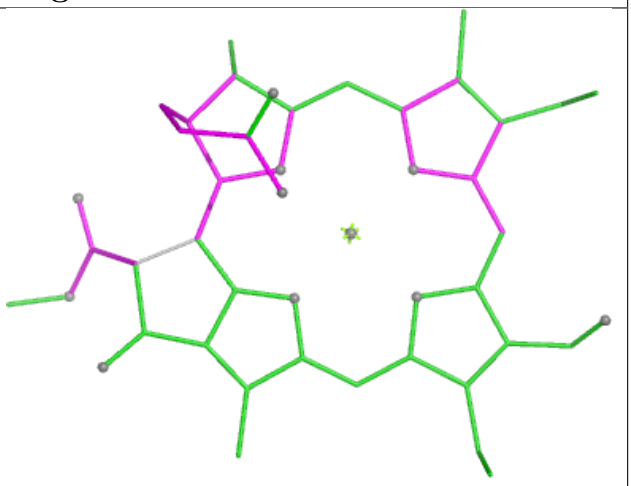


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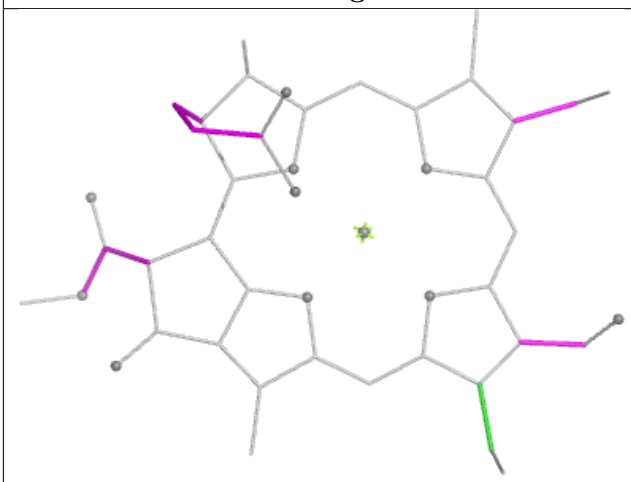
Ligand CHL g 609



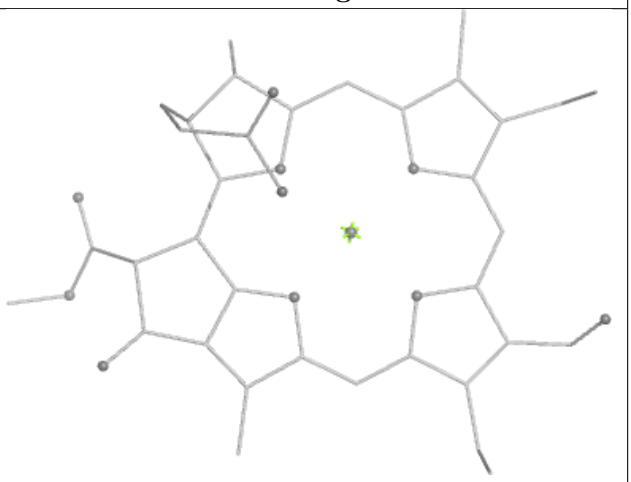
Bond lengths



Bond angles

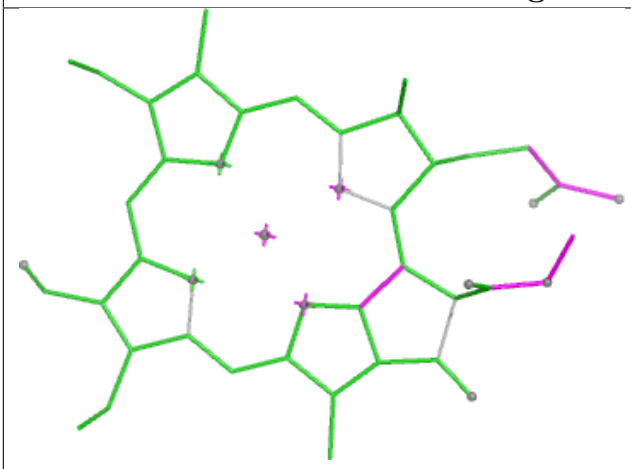


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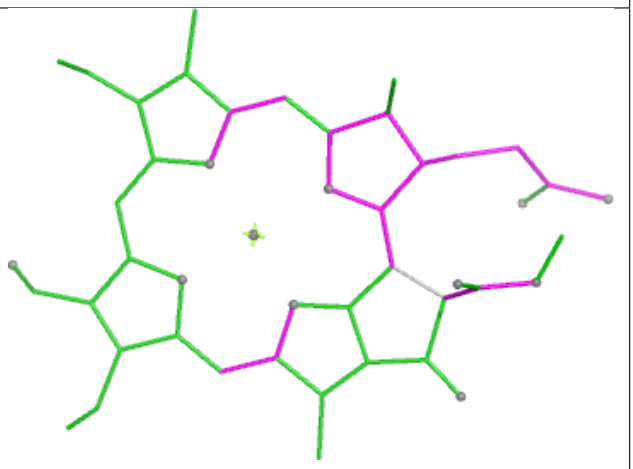


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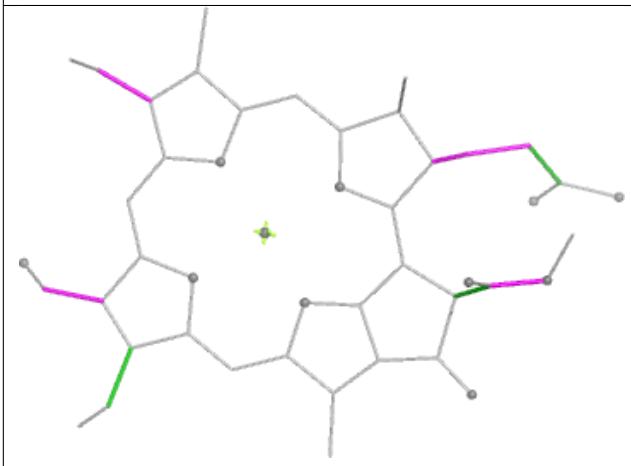
Ligand CHL 7 302



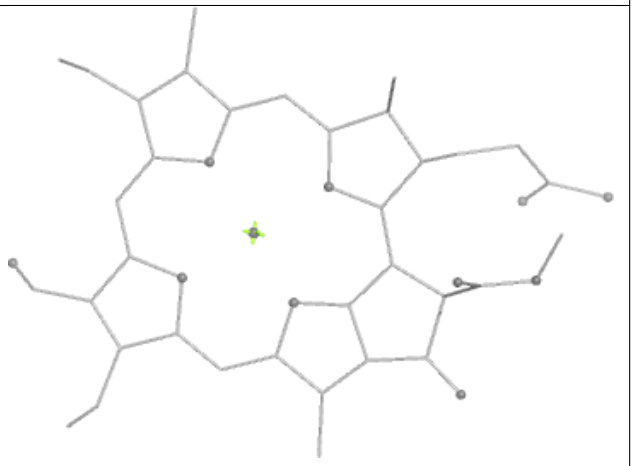
Bond lengths



Bond angles

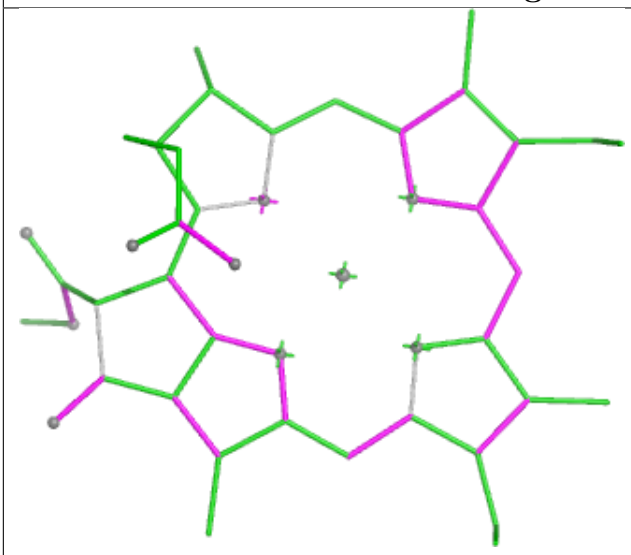


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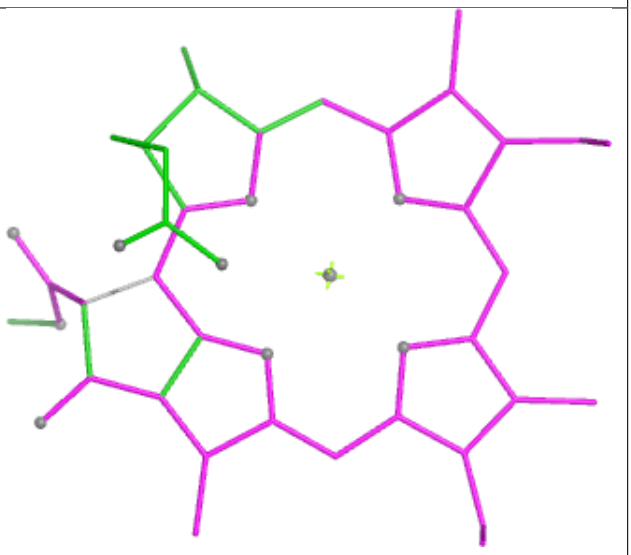


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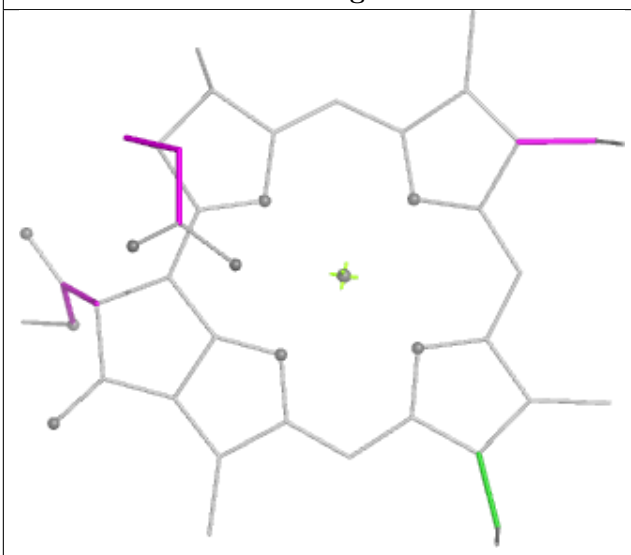
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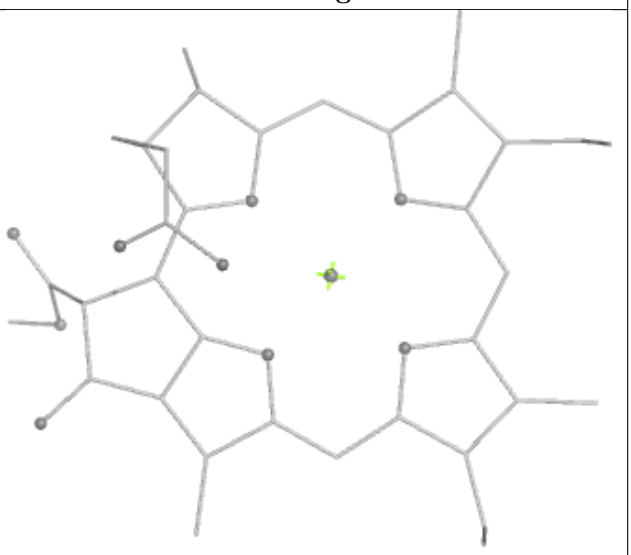
Bond lengths



Bond angles

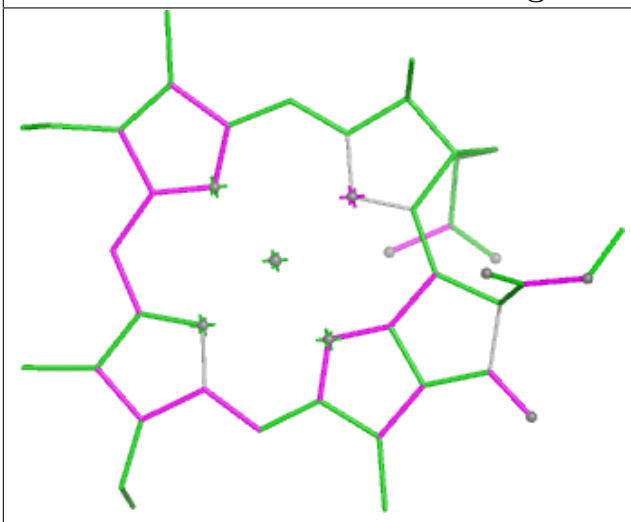


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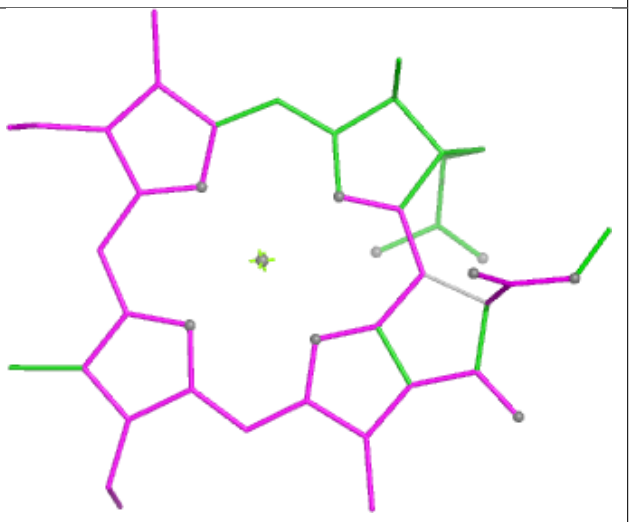


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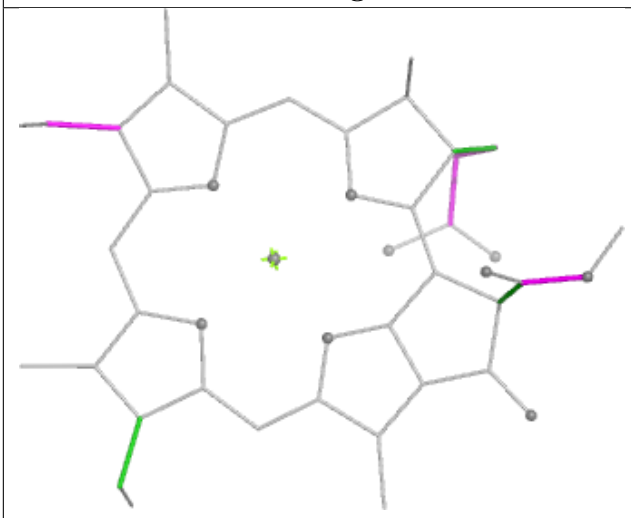
Ligand CLA n 613



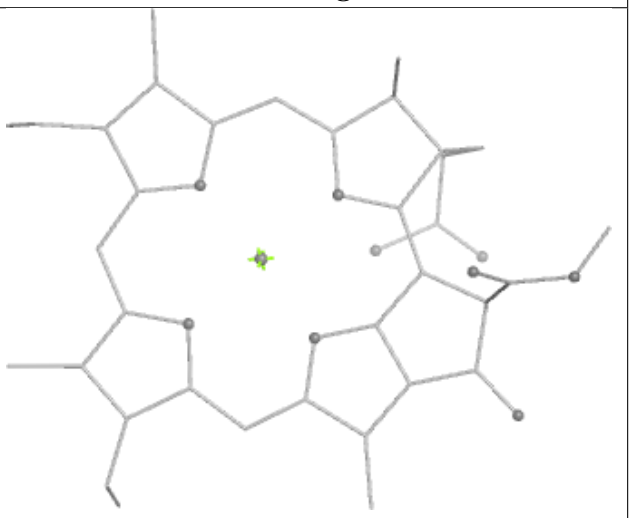
Bond lengths



Bond angles

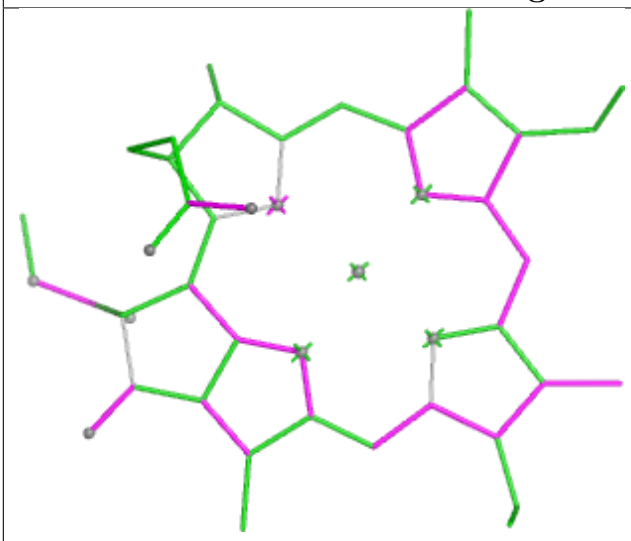


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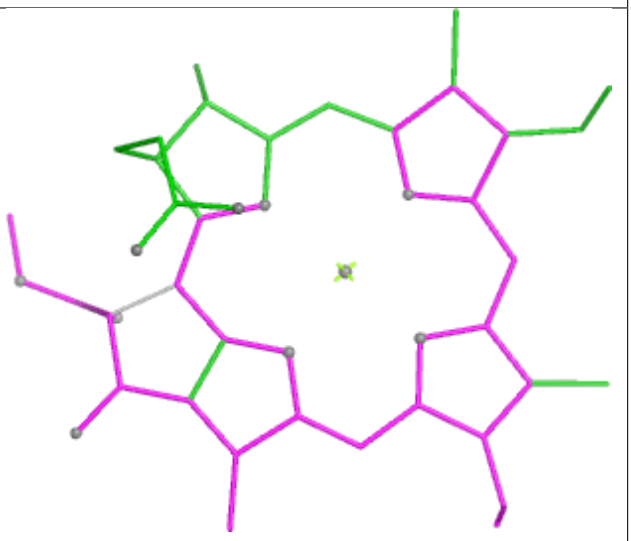


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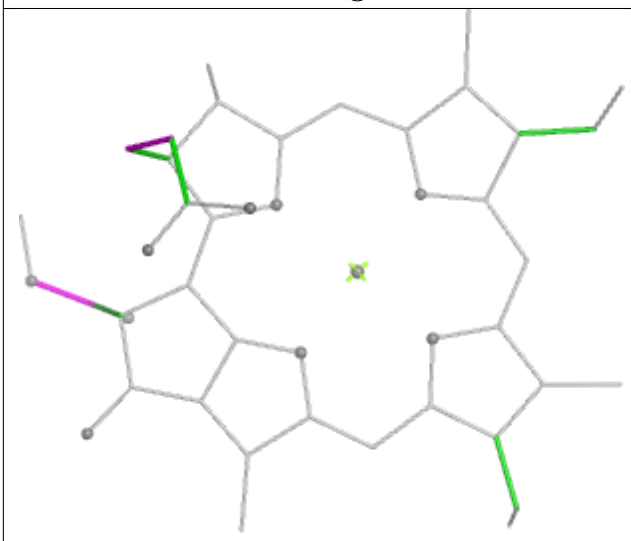
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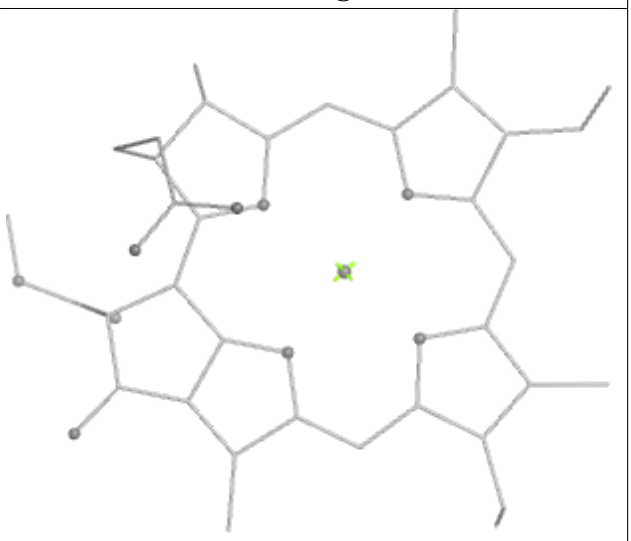
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Bond angles

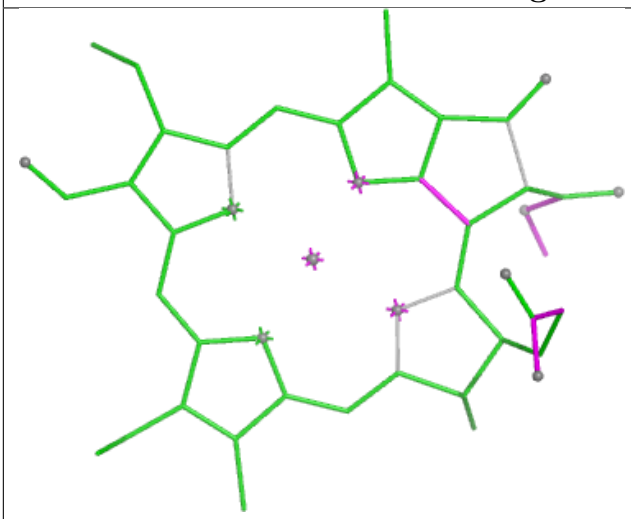


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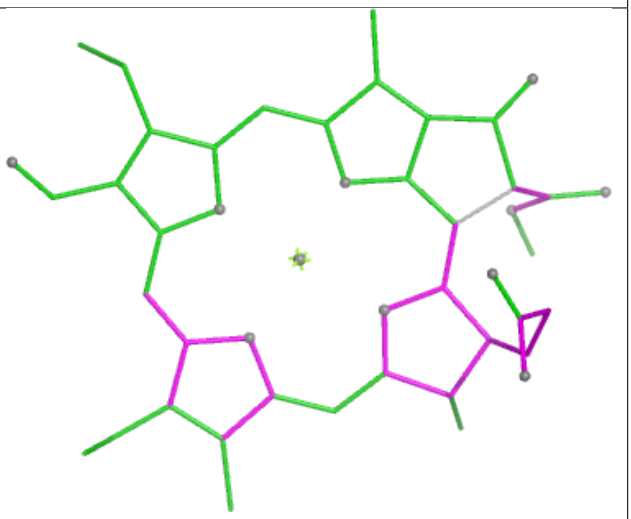


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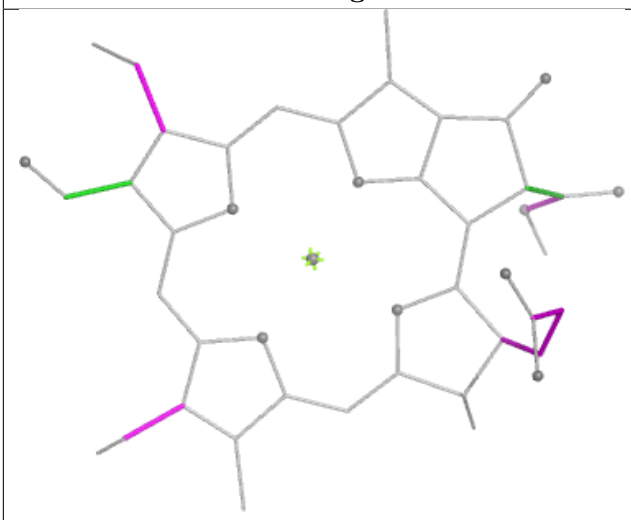
Ligand CHL s 306



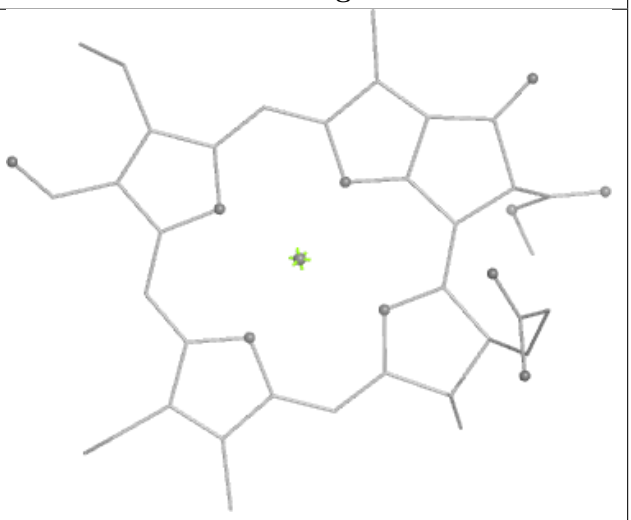
Bond lengths



Bond angles

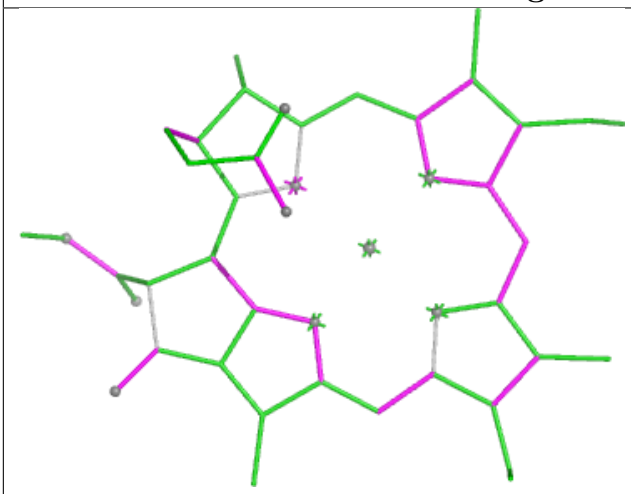


Torsions



Rings

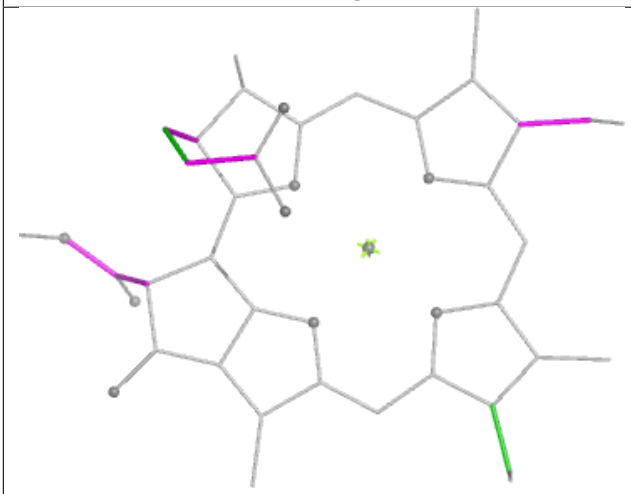
Ligand CLA S 310



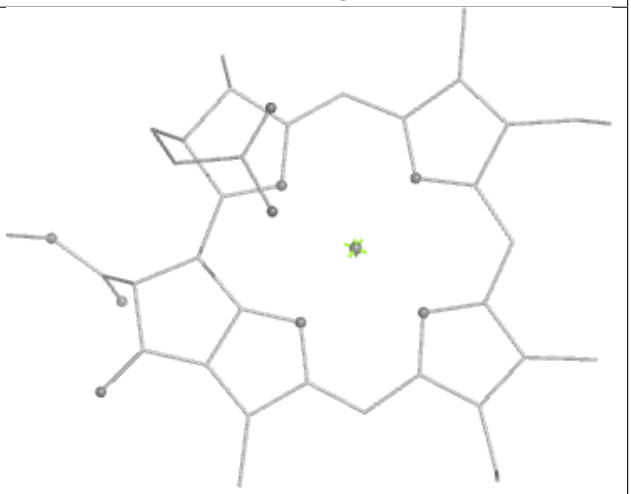
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Bond angles

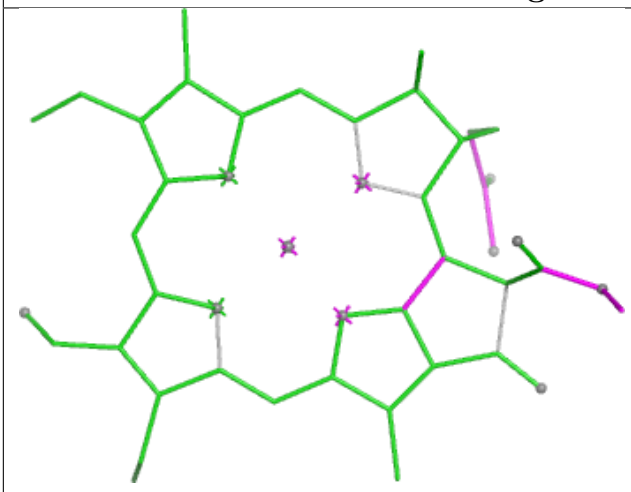


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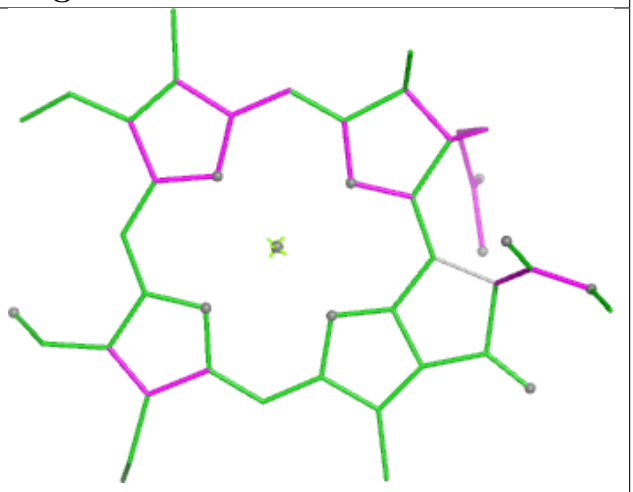


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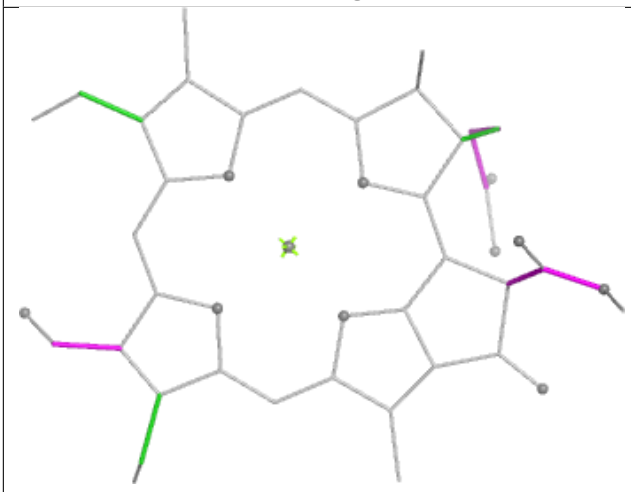
Ligand CHL g 608



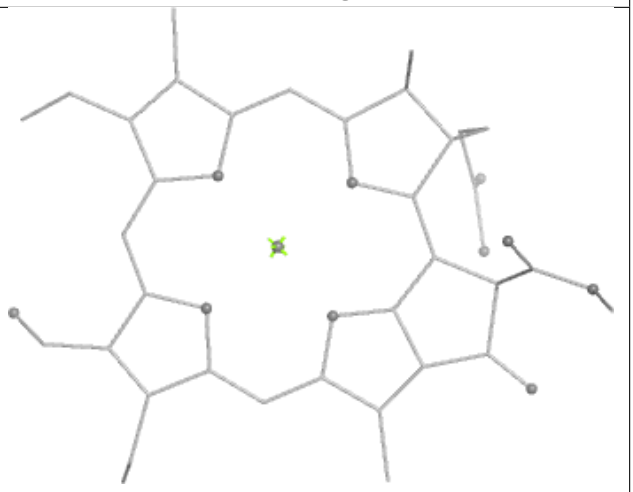
Bond lengths



Bond angles

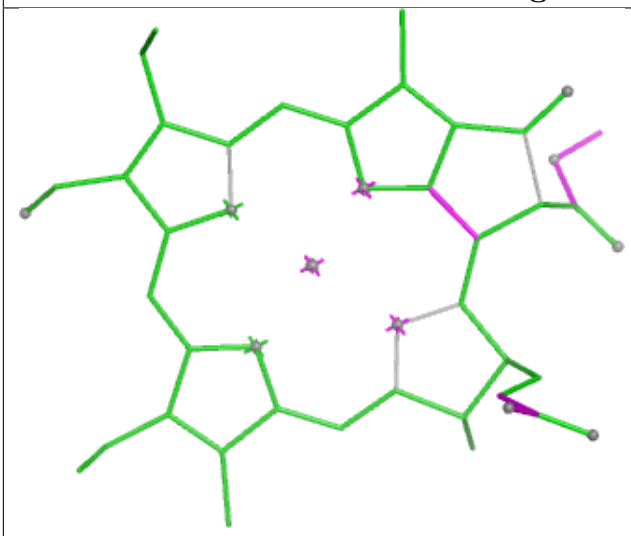


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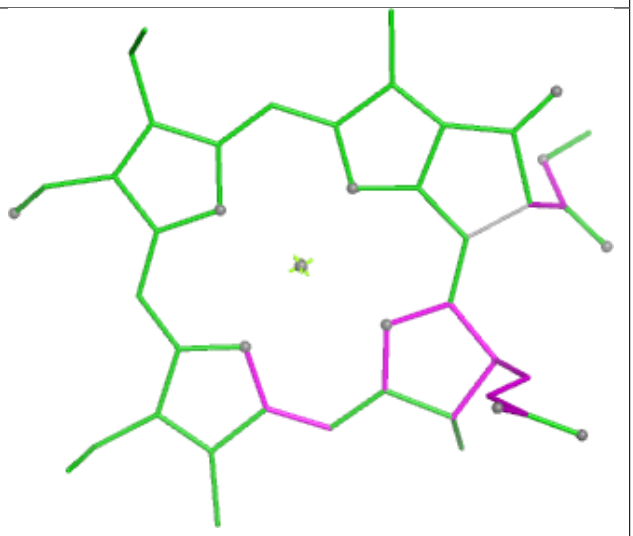


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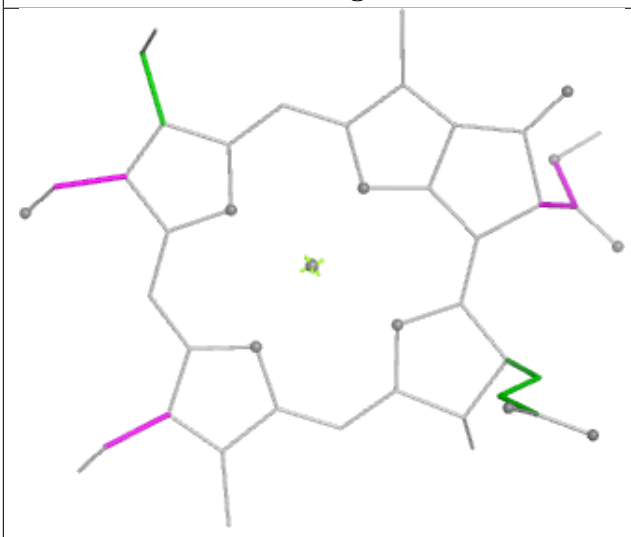
Ligand CHL s 308



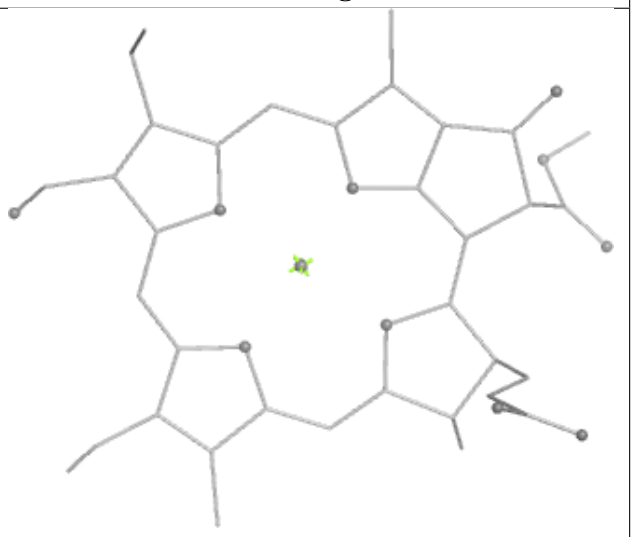
Bond lengths



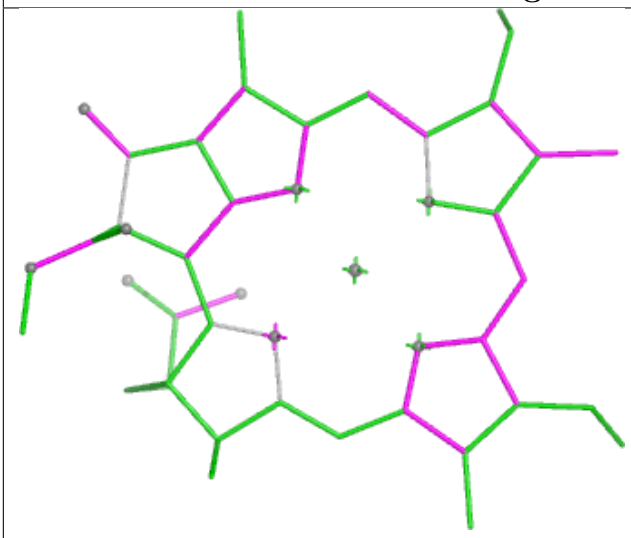
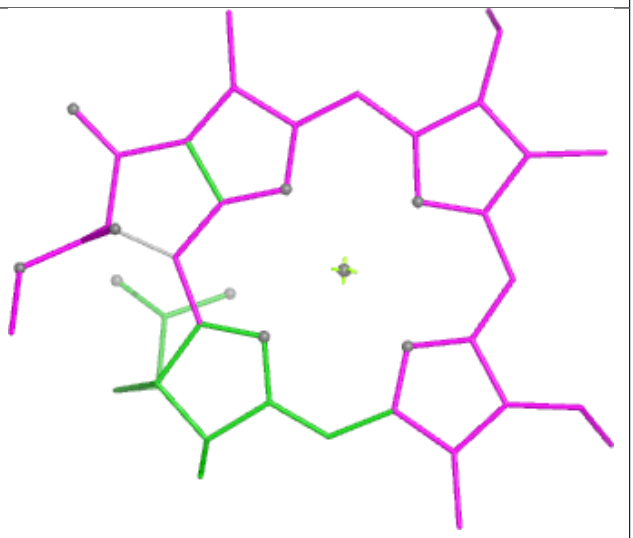
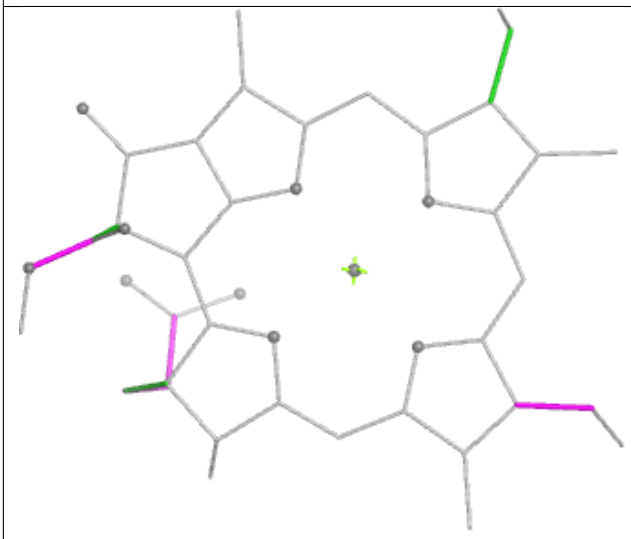
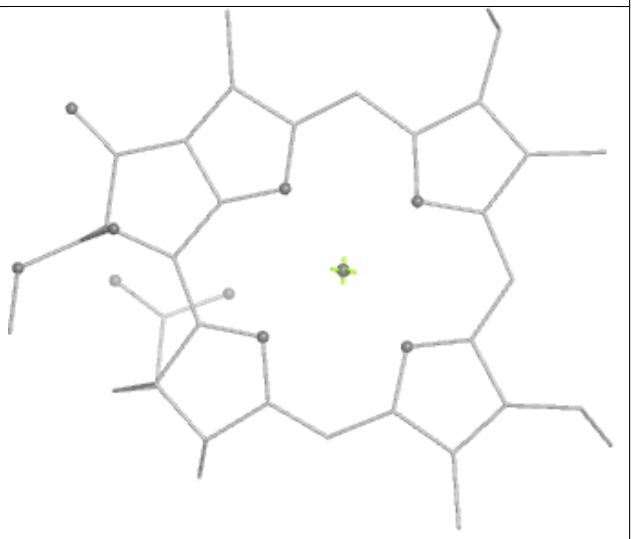
Bond angles



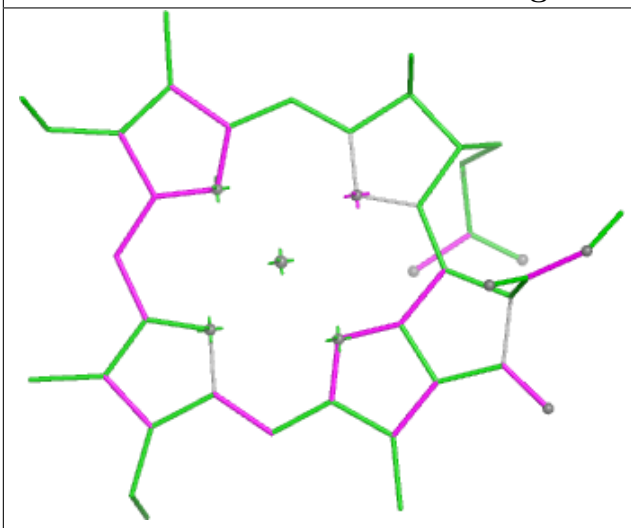
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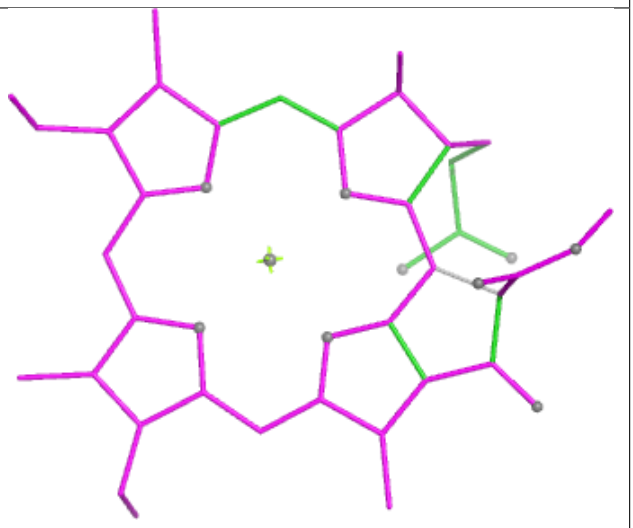
Rings

Ligand CLA R 311	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

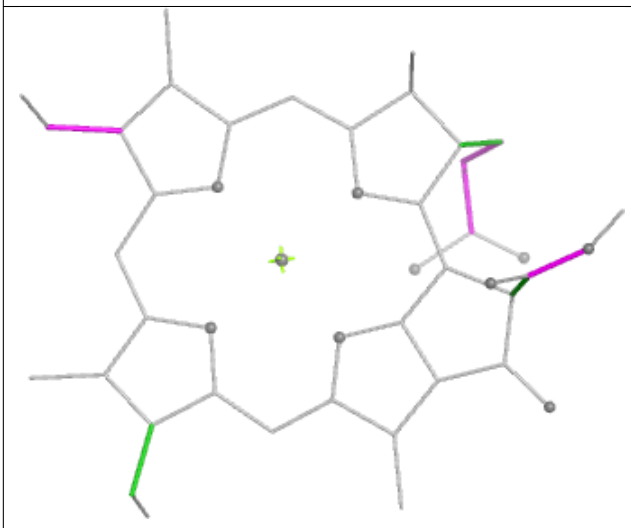
Ligand CLA s 313



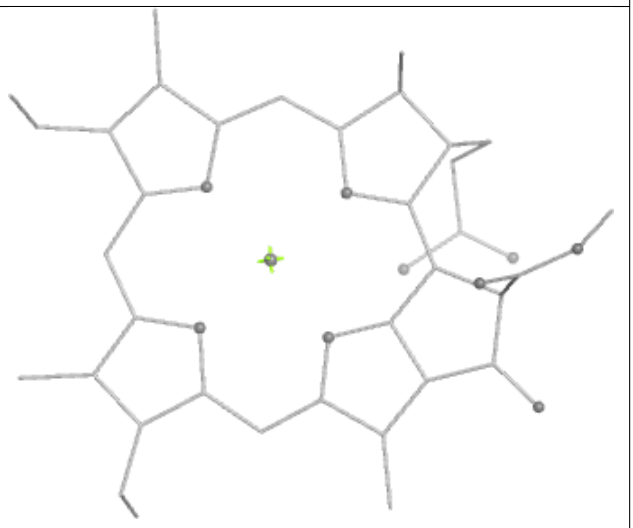
Bond lengths



Bond angles

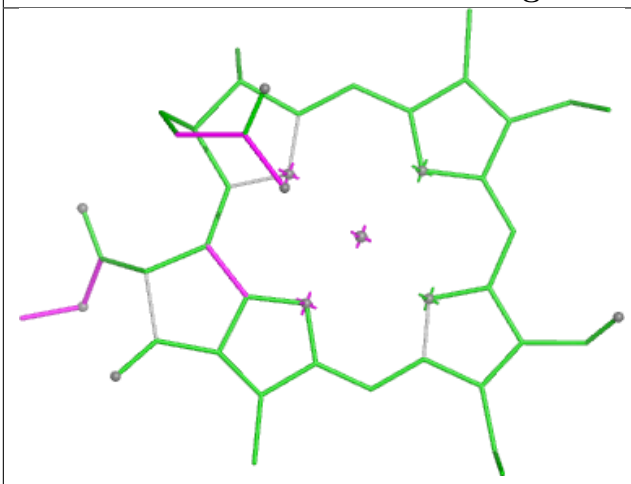


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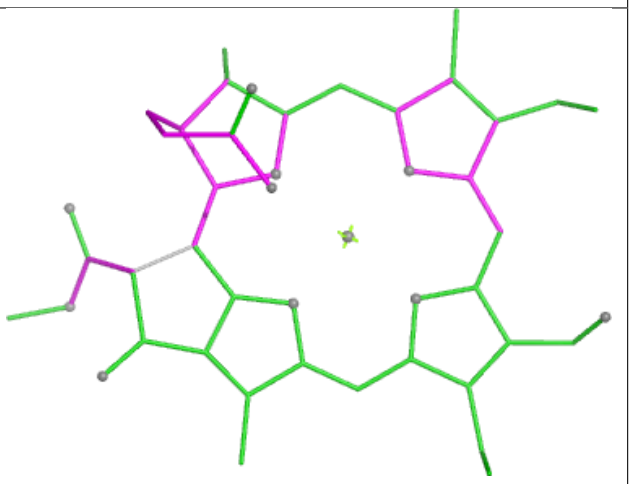


Rings

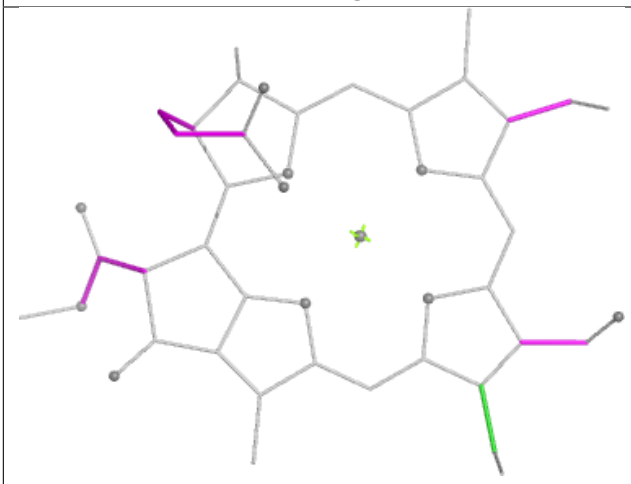
Ligand CHL N 609



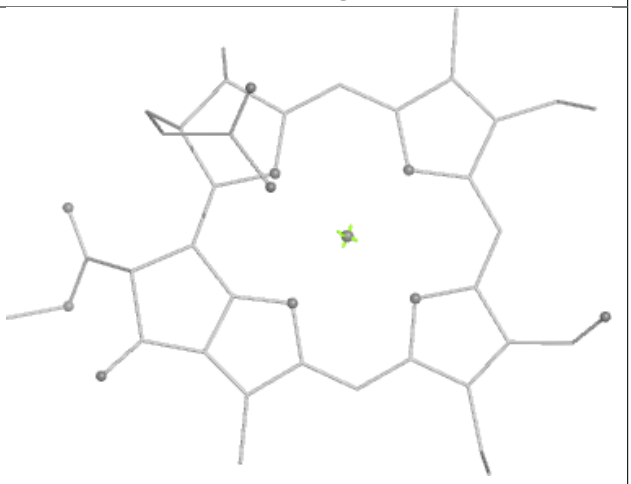
Bond lengths



Bond angles

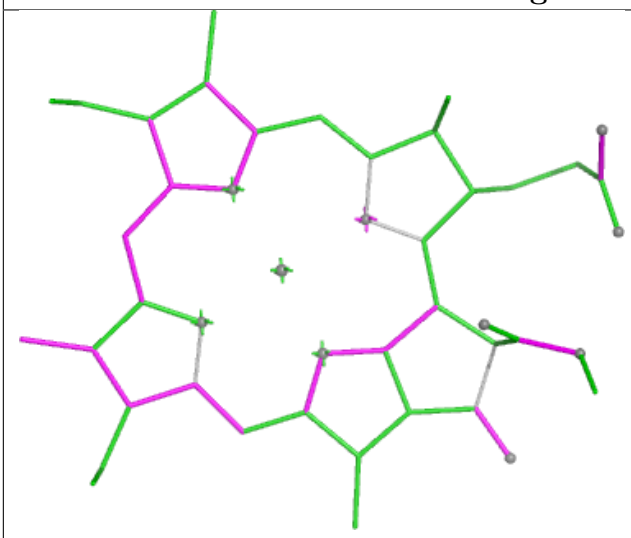


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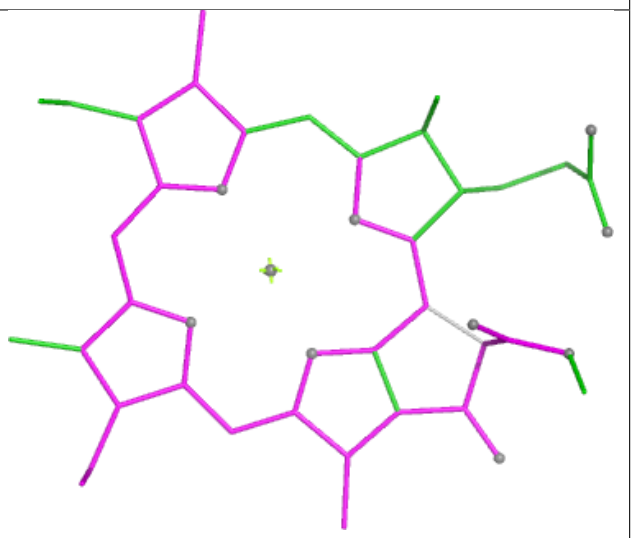


Rings

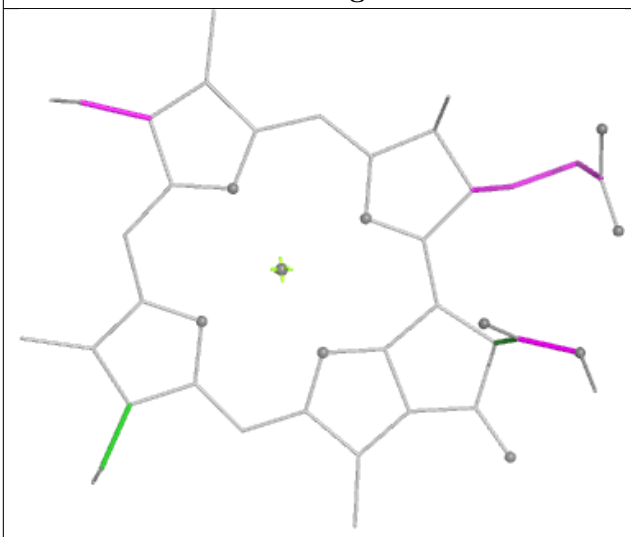
Ligand CLA r 310



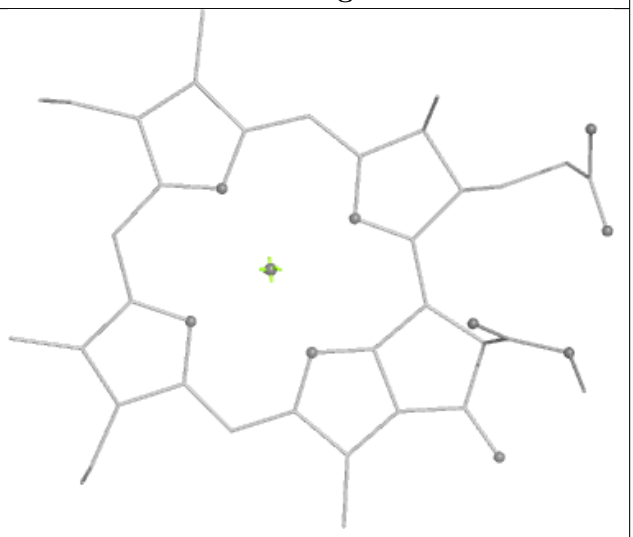
Bond lengths



Bond angles

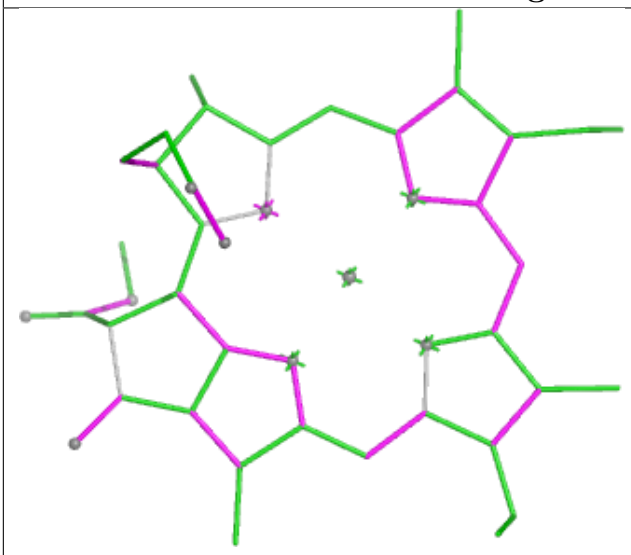


Torsions

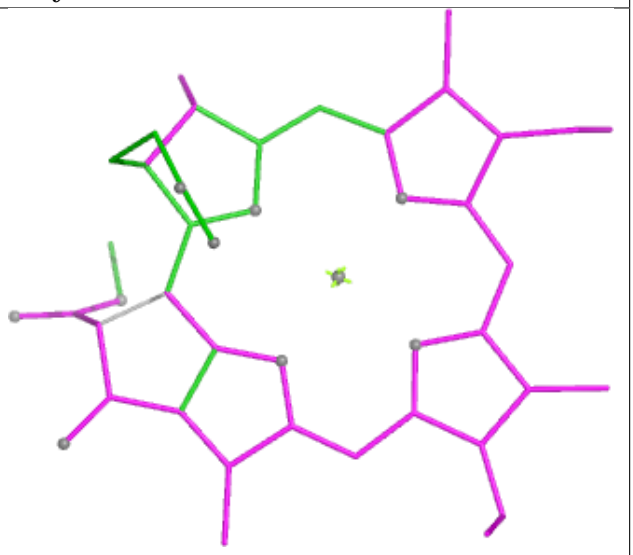


Rings

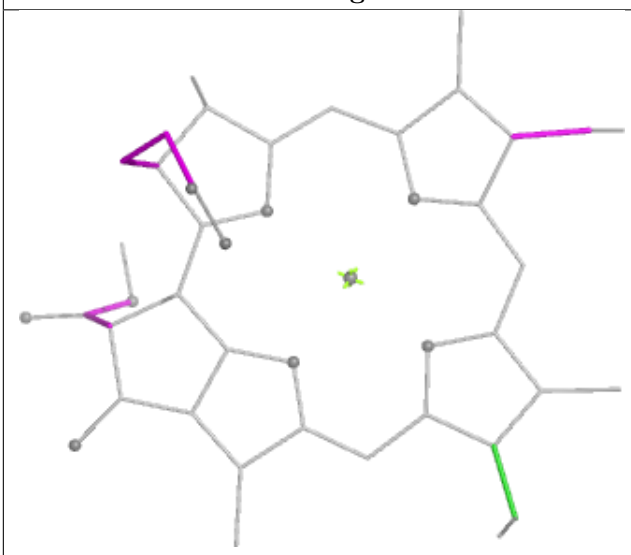
Ligand CLA y 602



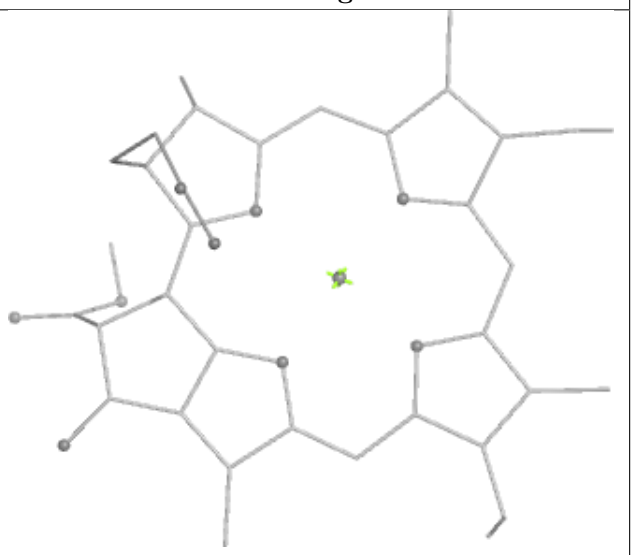
Bond lengths



Bond angles

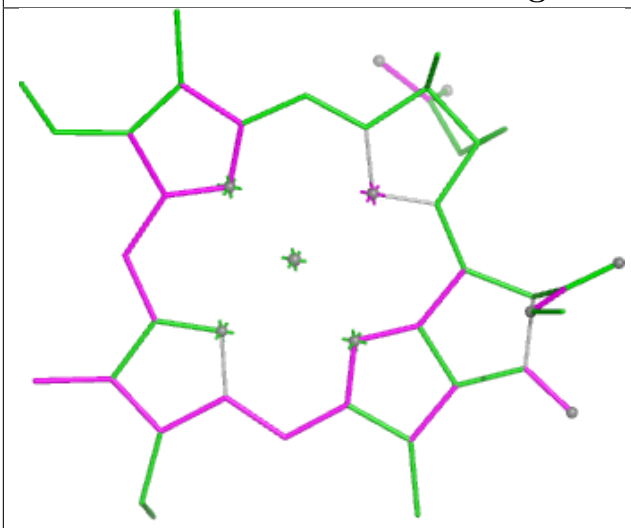


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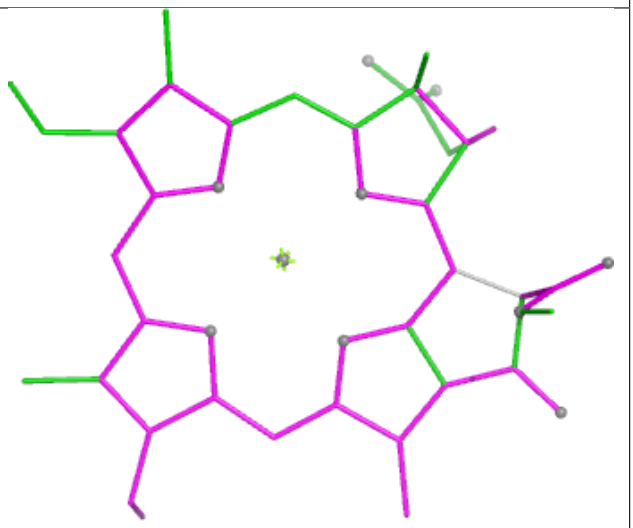


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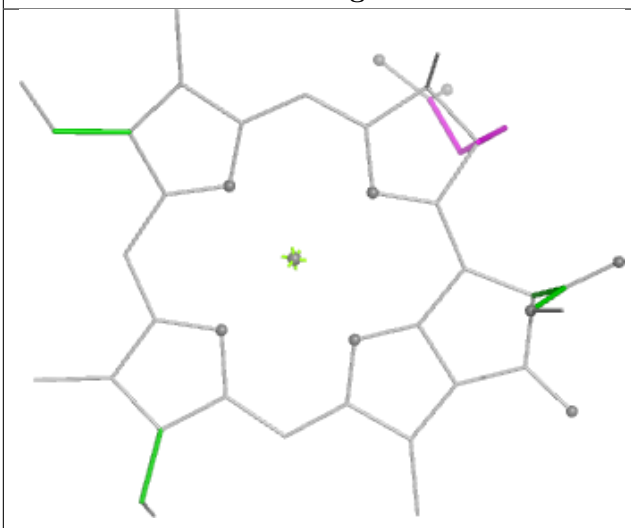
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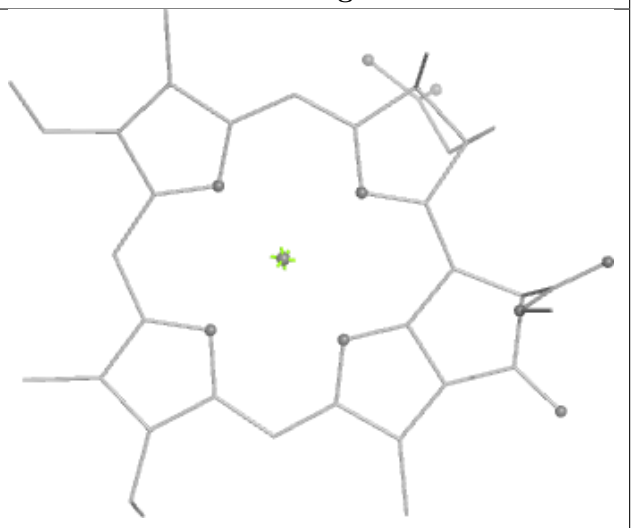
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Bond angles

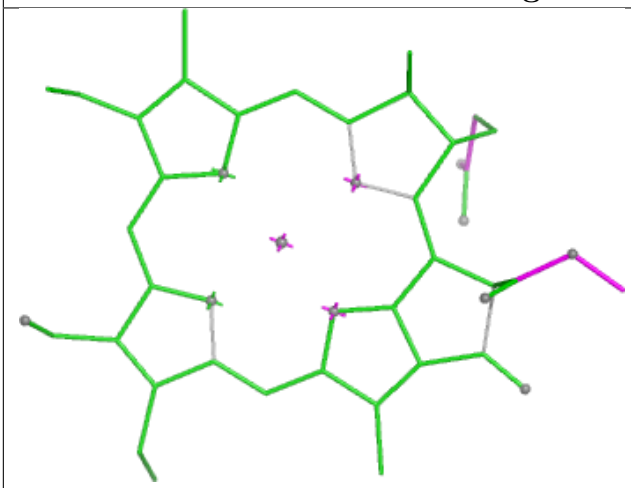


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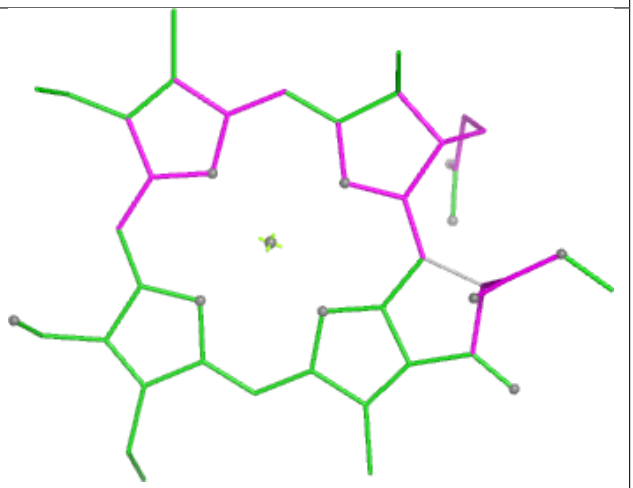


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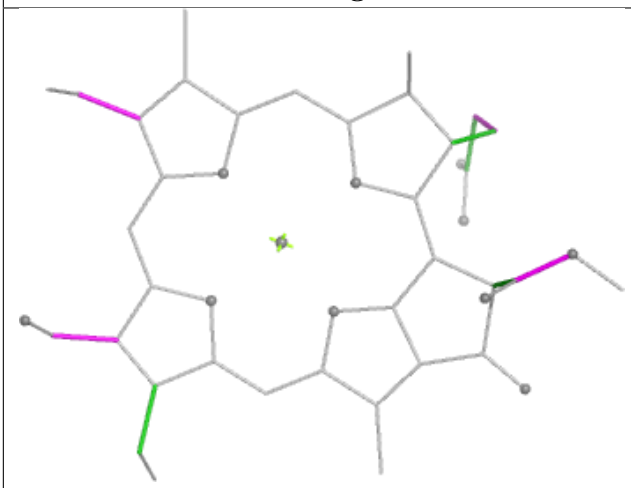
Ligand CHL N 607



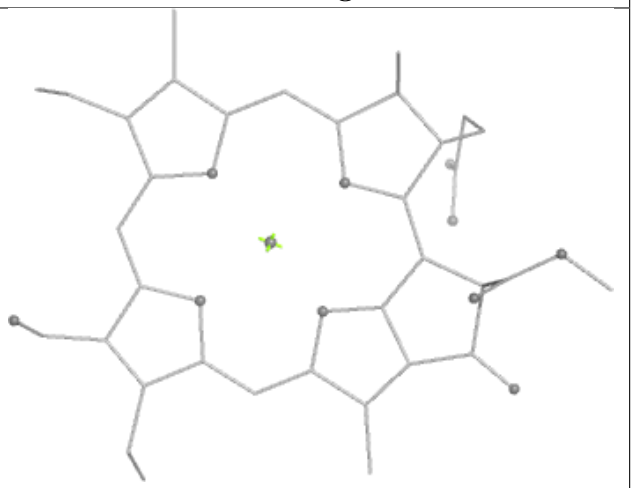
Bond lengths



Bond angles

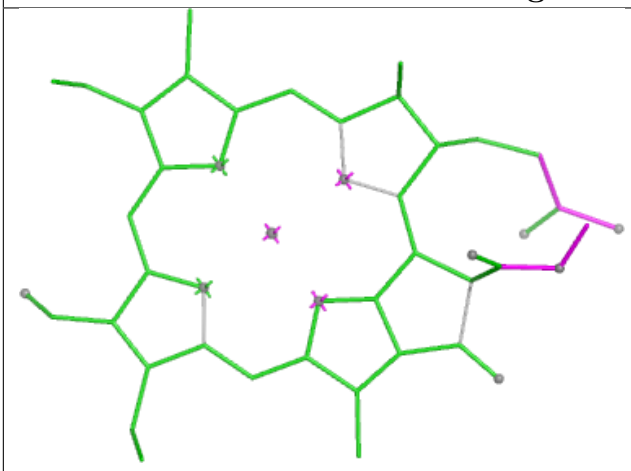


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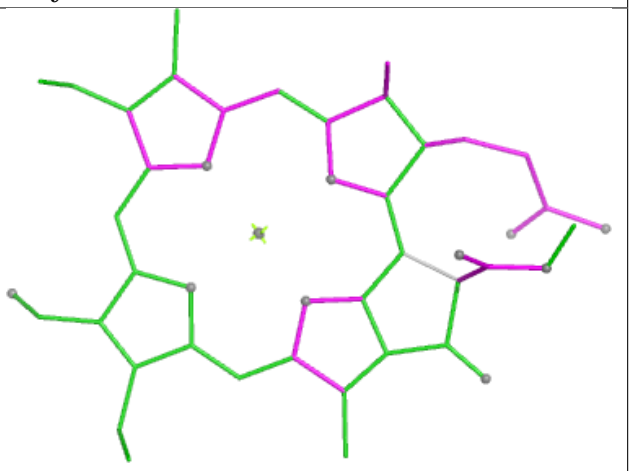


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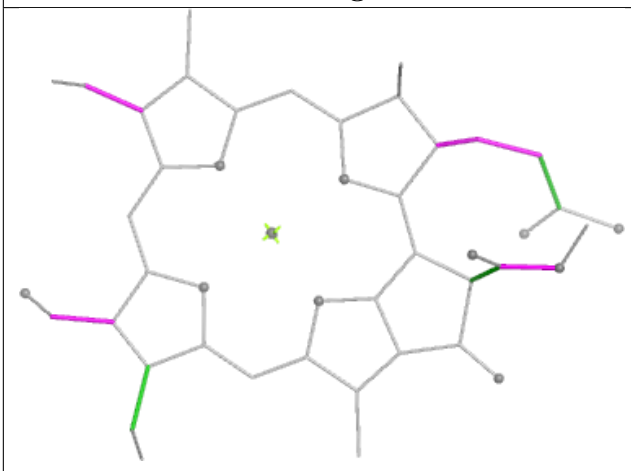
Ligand CHL y 601



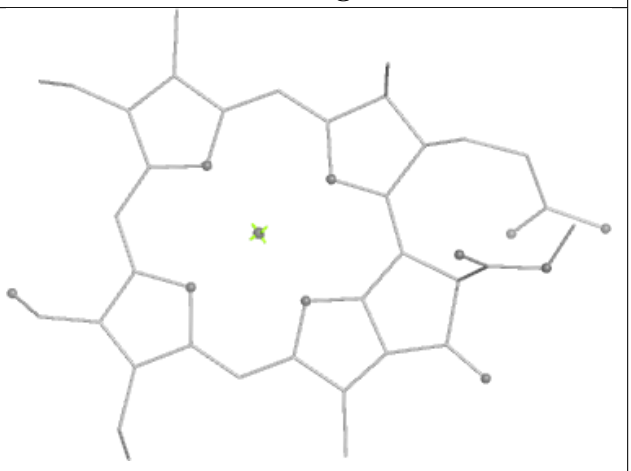
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Bond angles

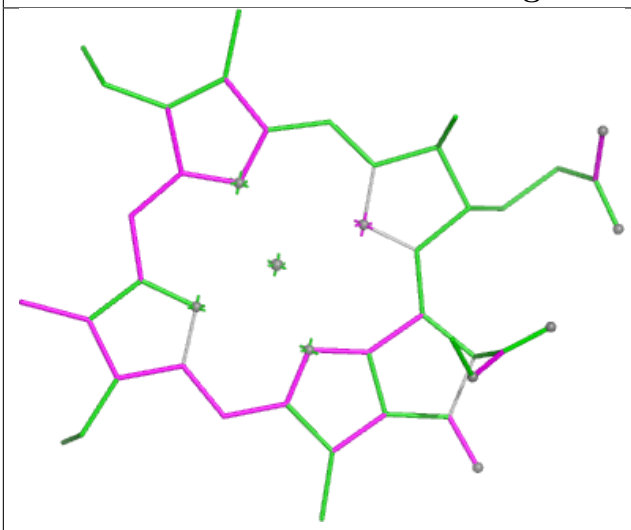


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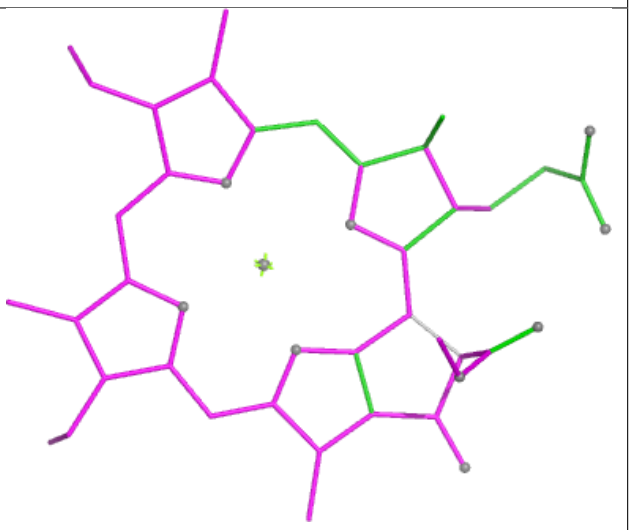


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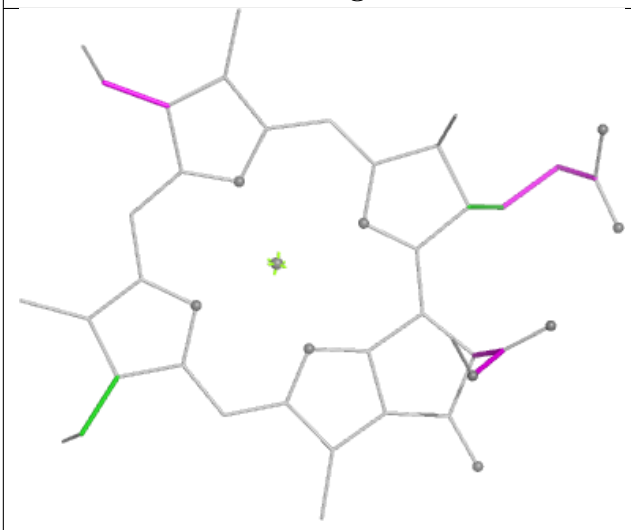
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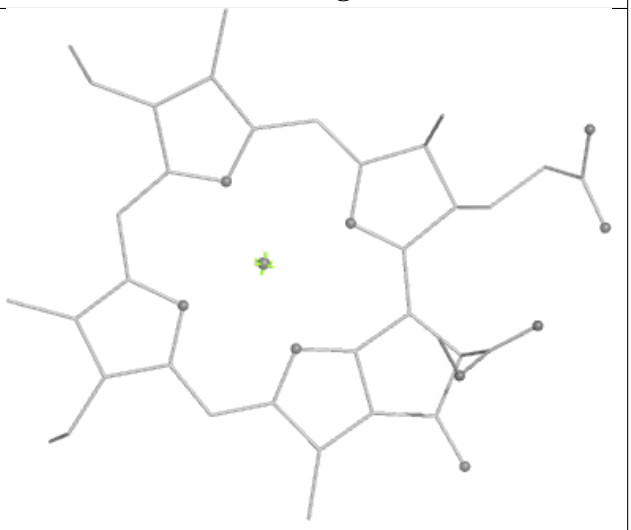
Bond lengths



Bond angles

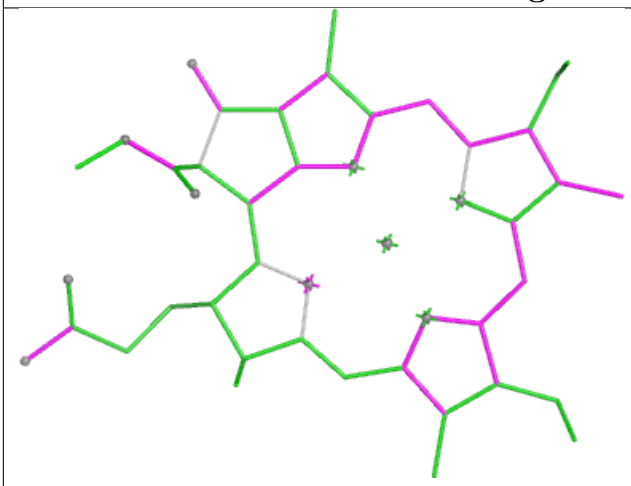


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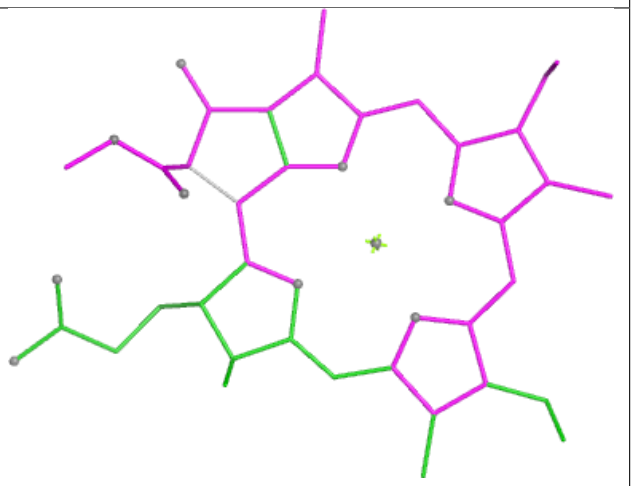


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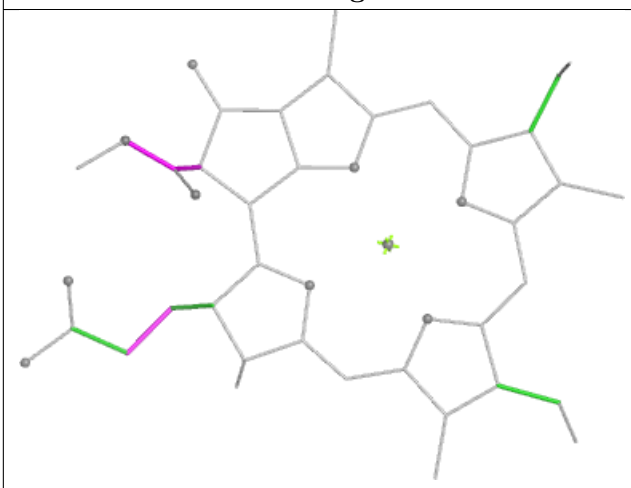
Ligand CLA 8 311



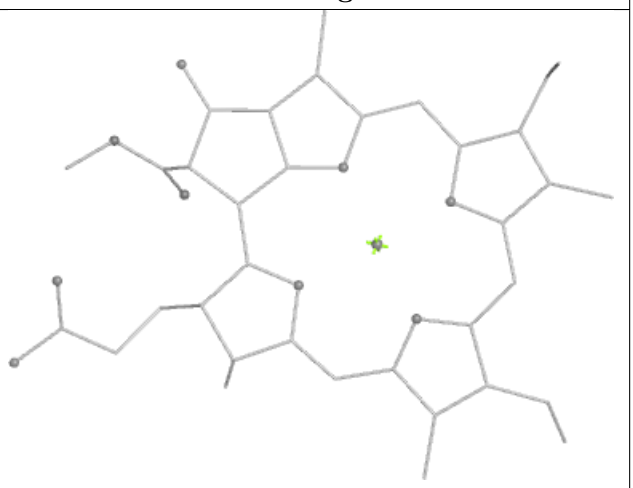
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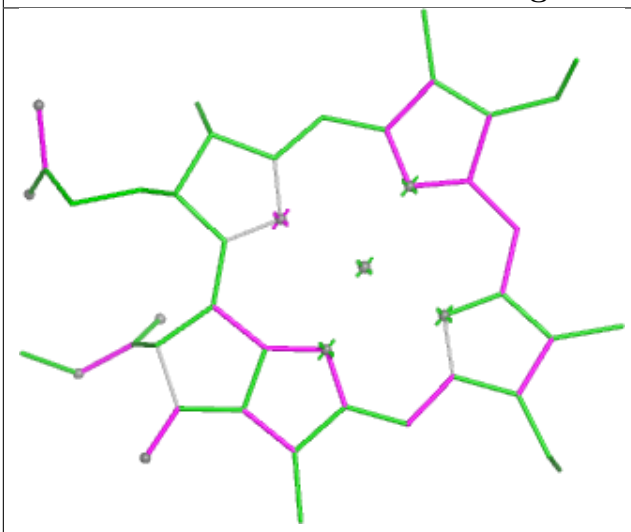


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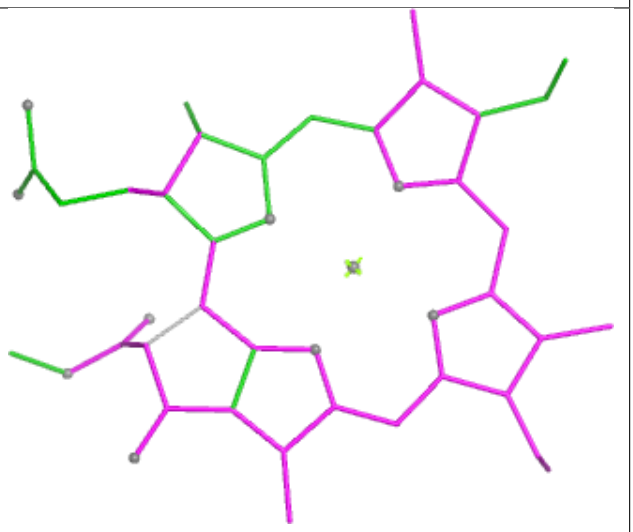


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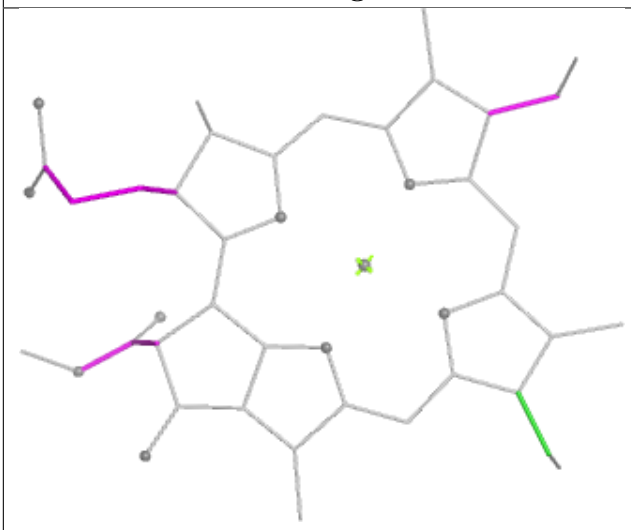
Ligand CLA r 309



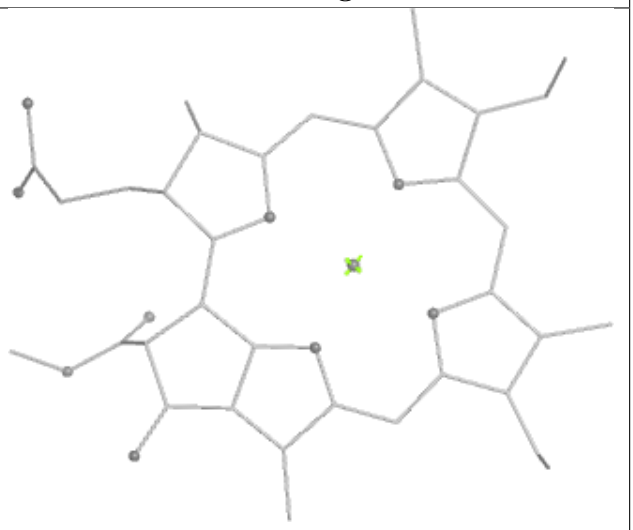
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Bond angles

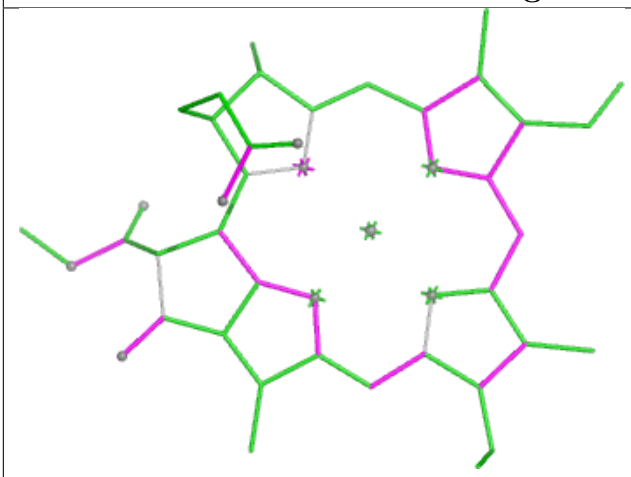


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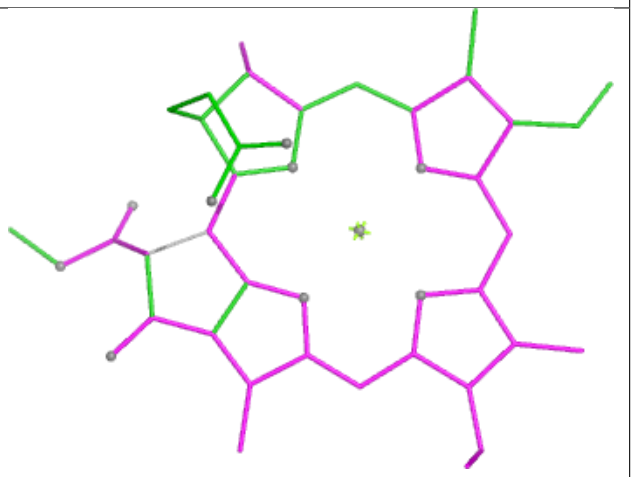


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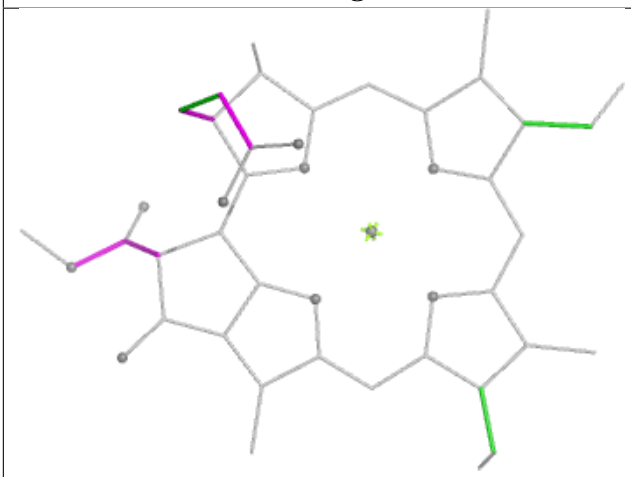
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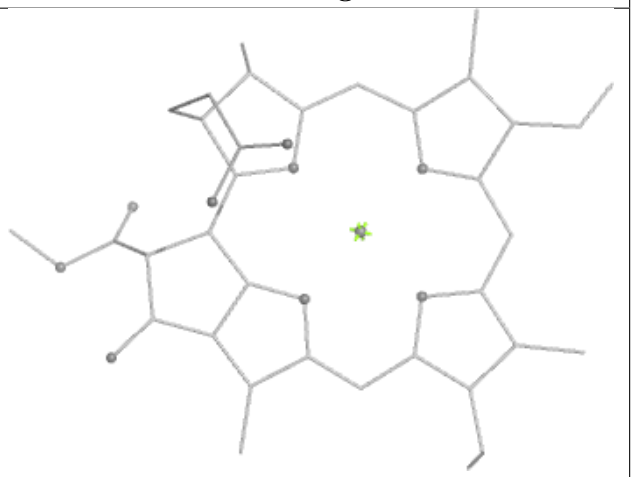
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Bond angles

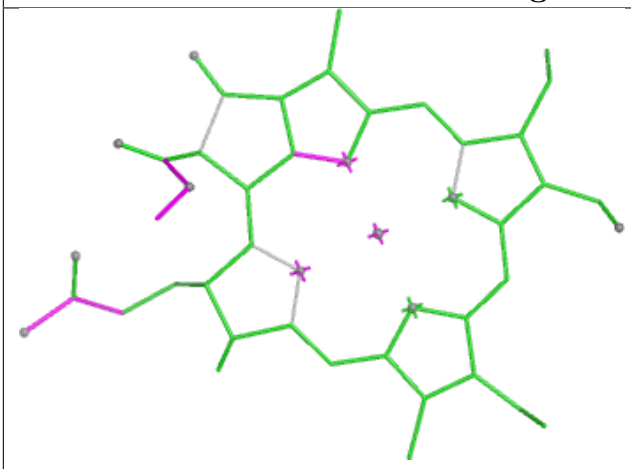


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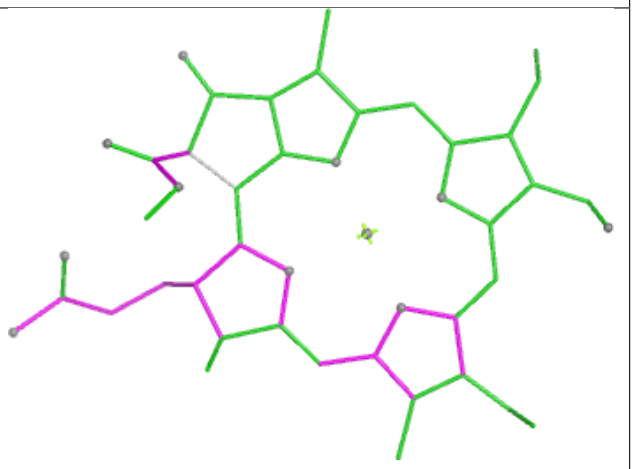


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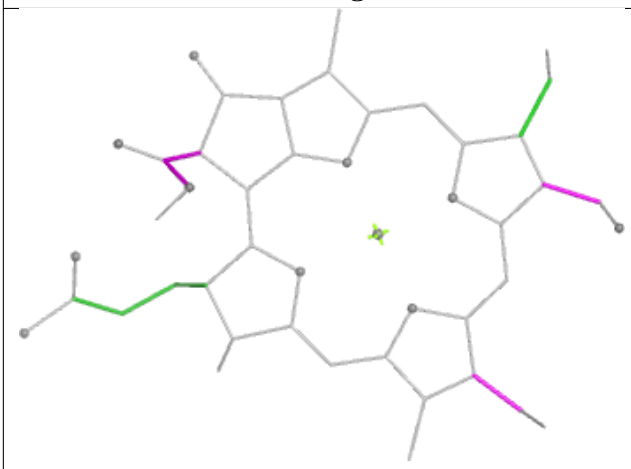
Ligand CHL s 302



Bond lengths



Bond angles

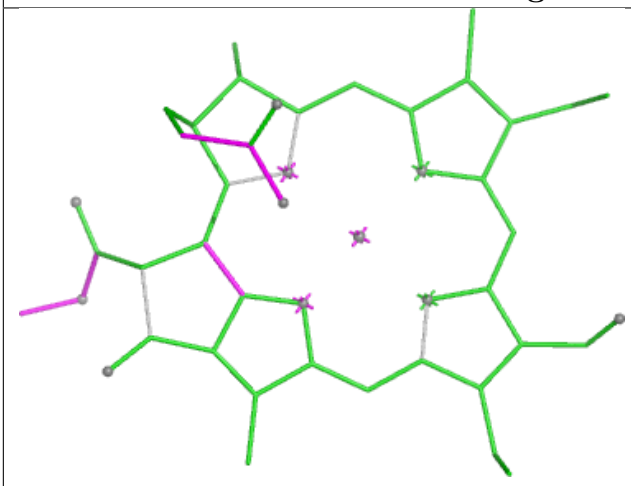


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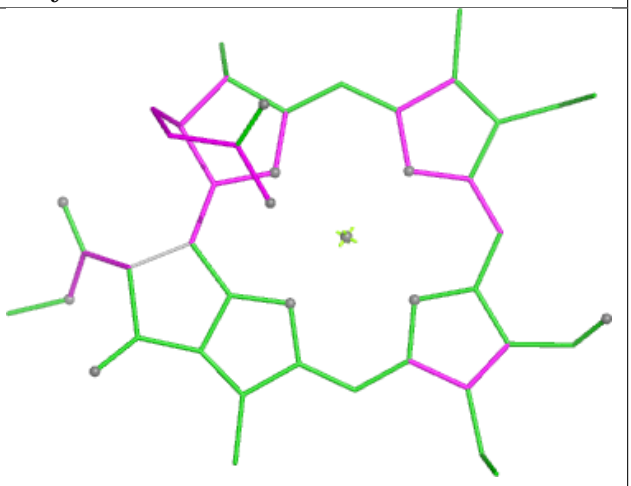


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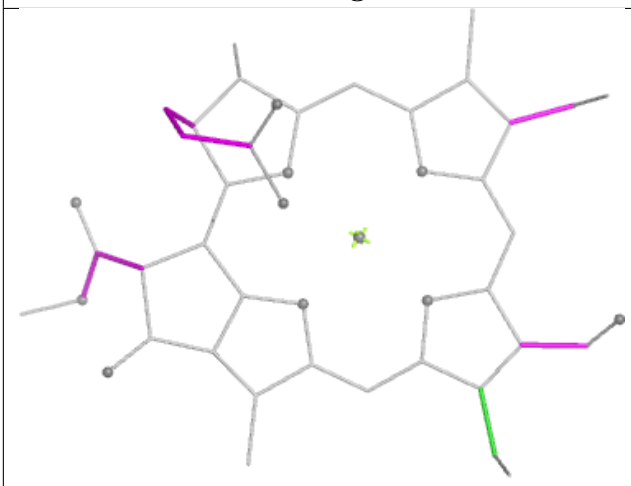
Ligand CHL y 609



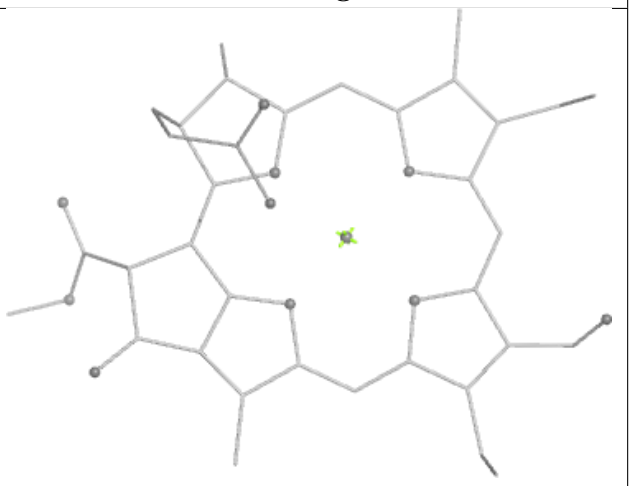
Bond lengths



Bond angles

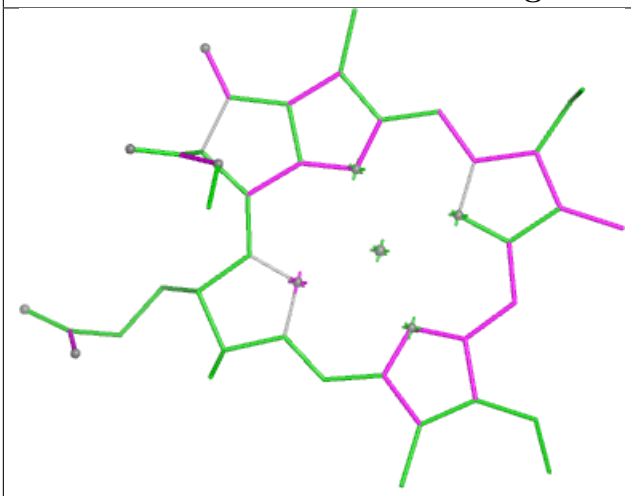


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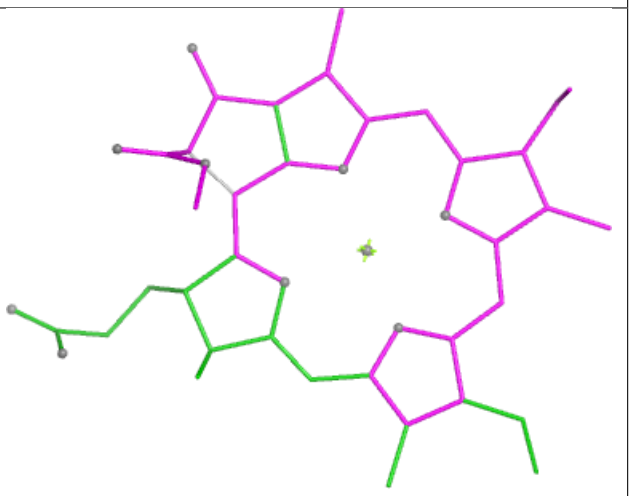


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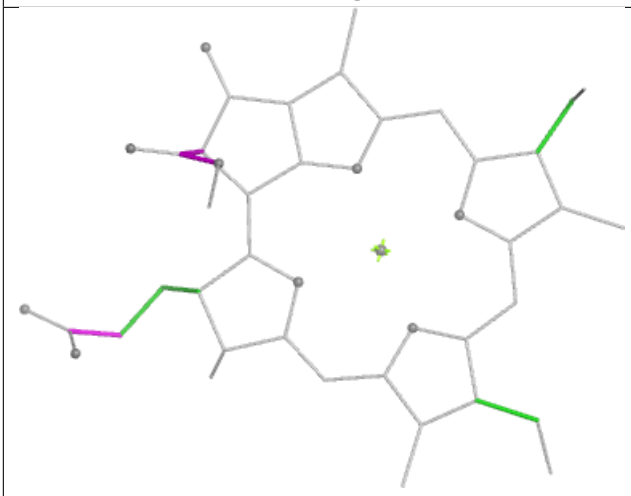
Ligand CLA C 510



Bond lengths



Bond angles

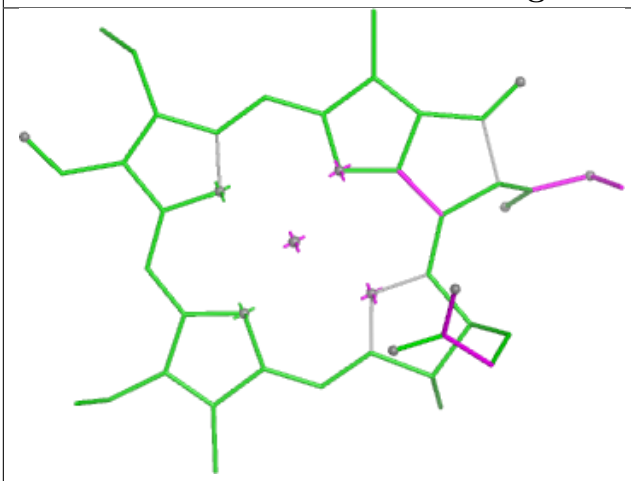


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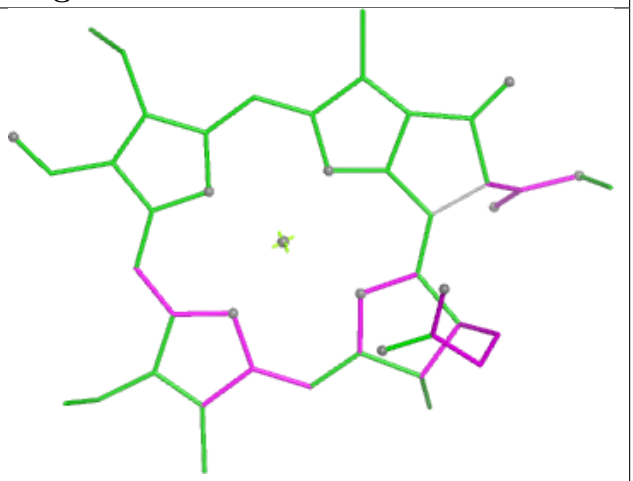


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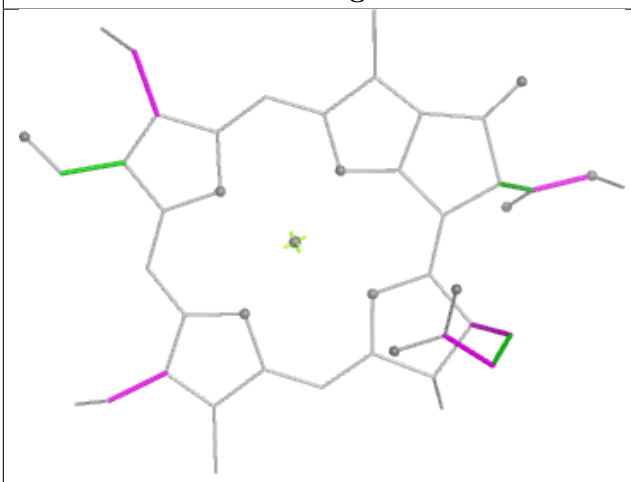
Ligand CHL g 606



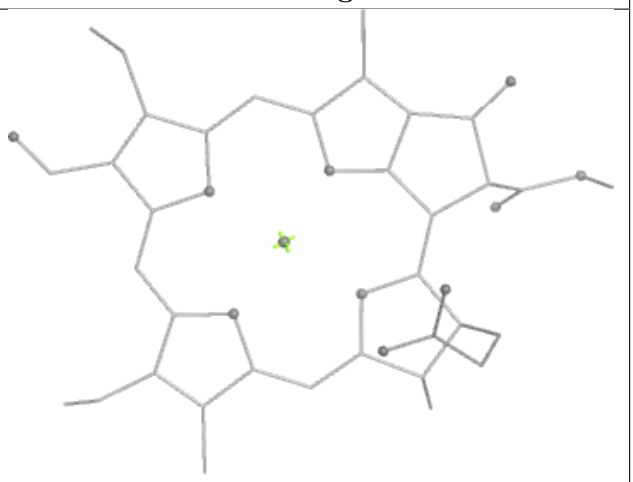
Bond lengths



Bond angles

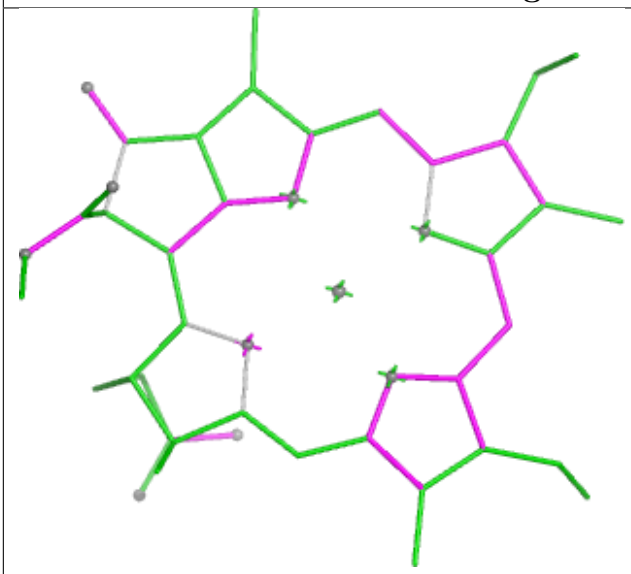


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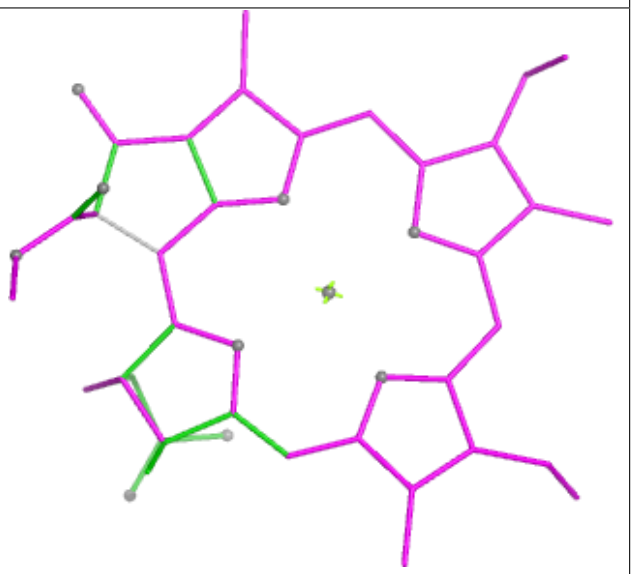


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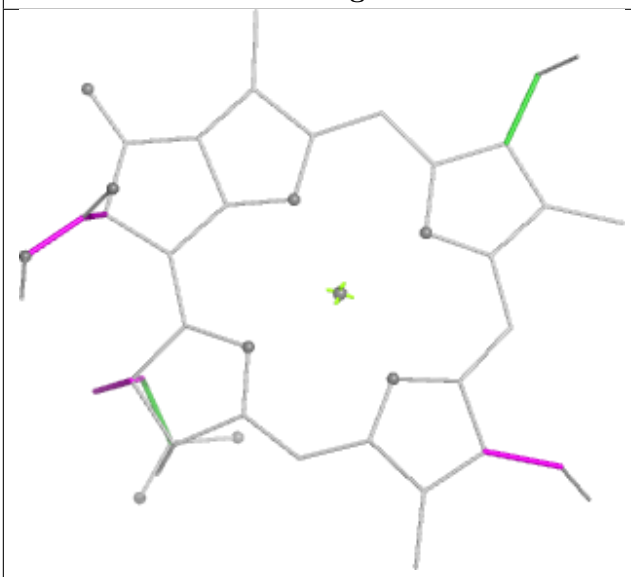
Ligand CLA D 401



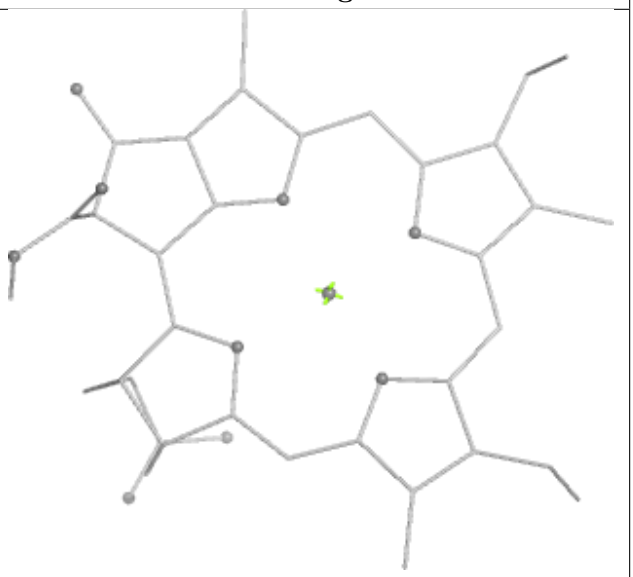
Bond lengths



Bond angles

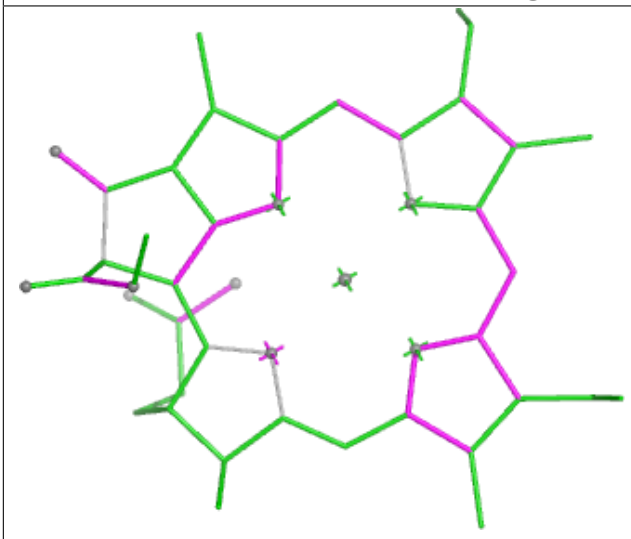


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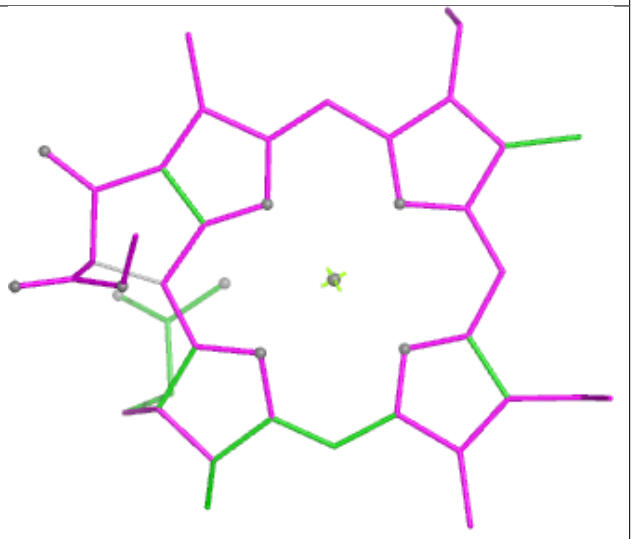


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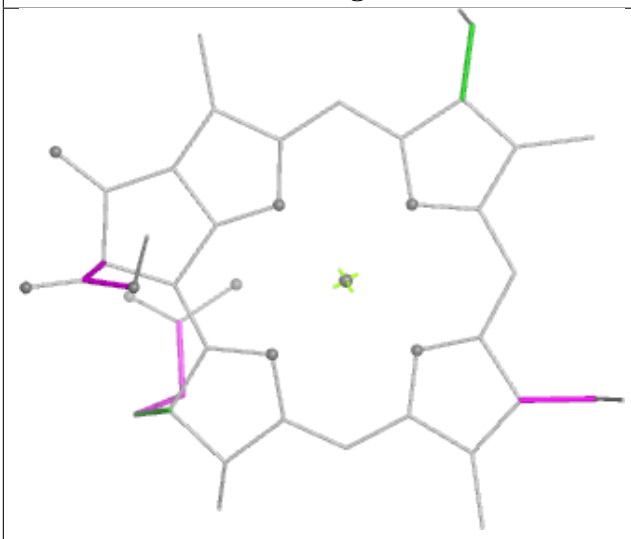
Ligand CLA C 502



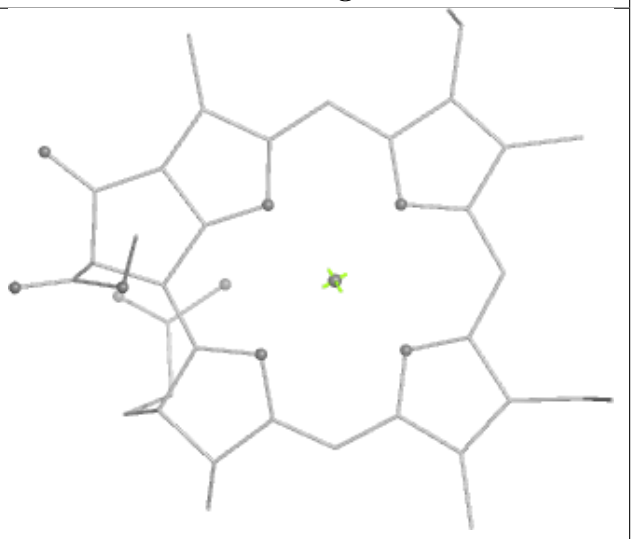
Bond lengths



Bond angles

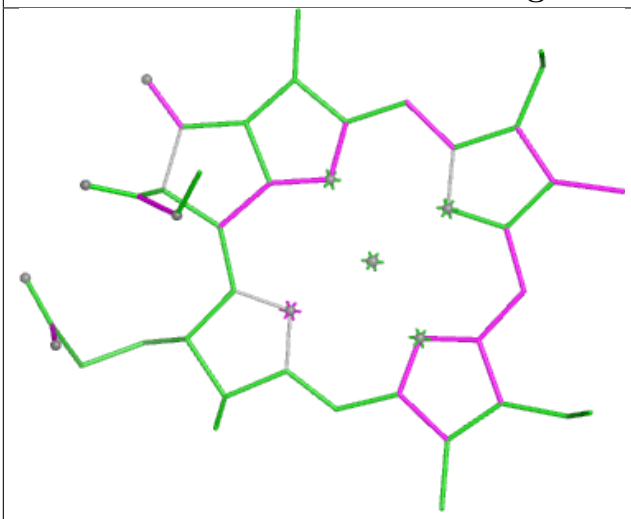


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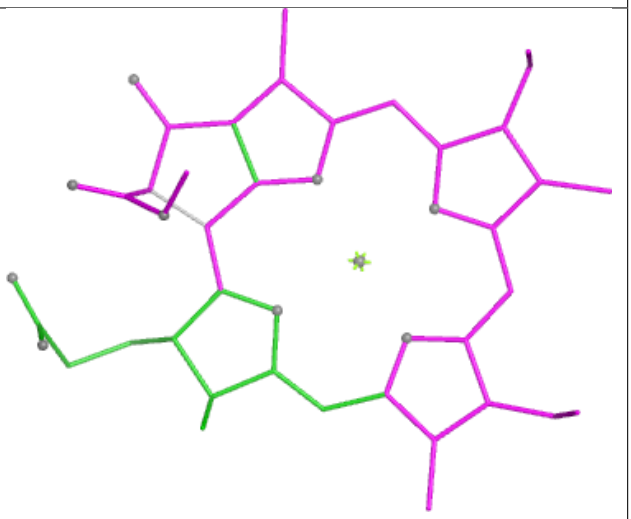


Rings

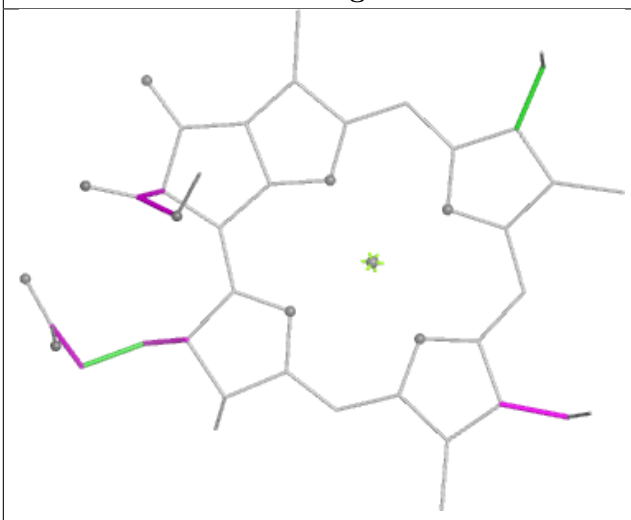
Ligand CLA n 612



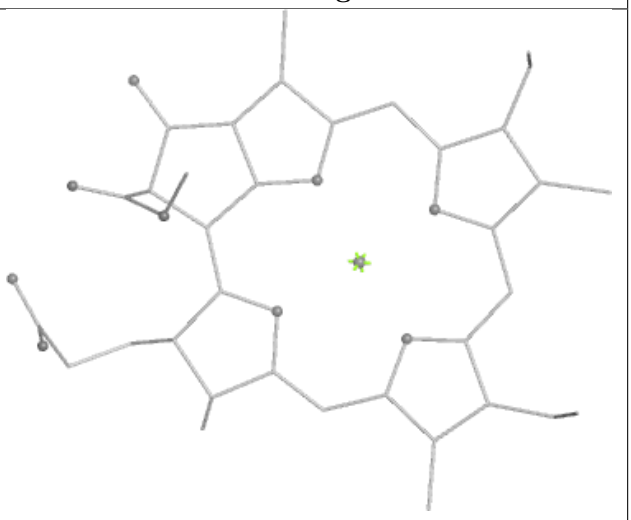
Bond lengths



Bond angles

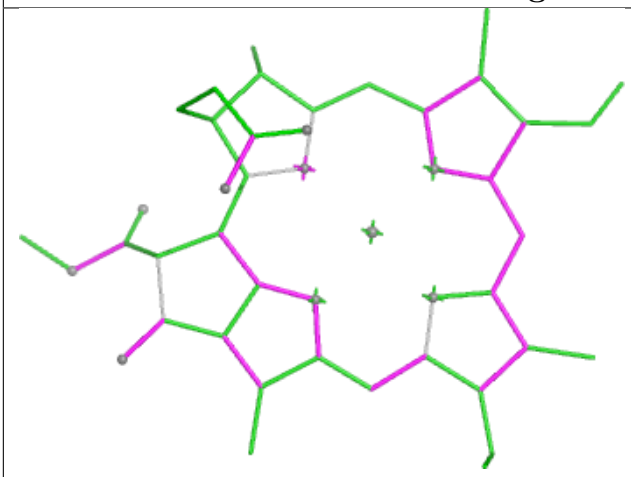


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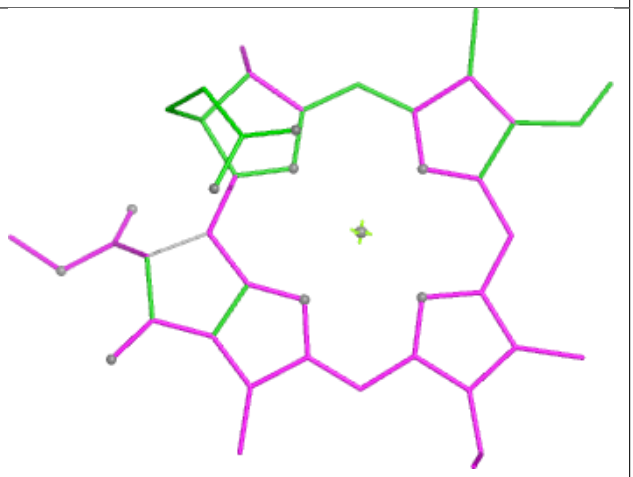


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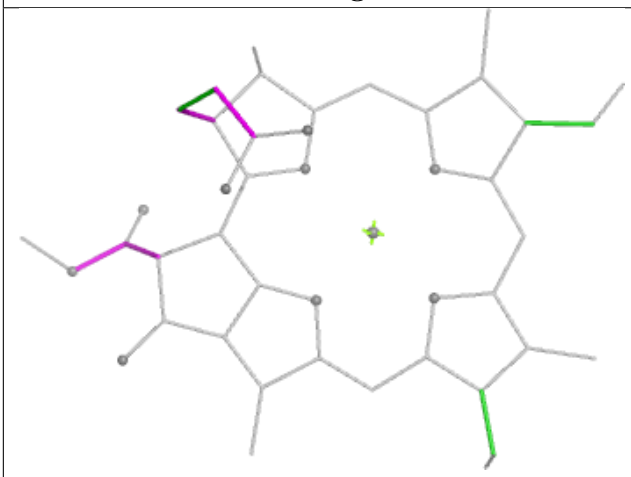
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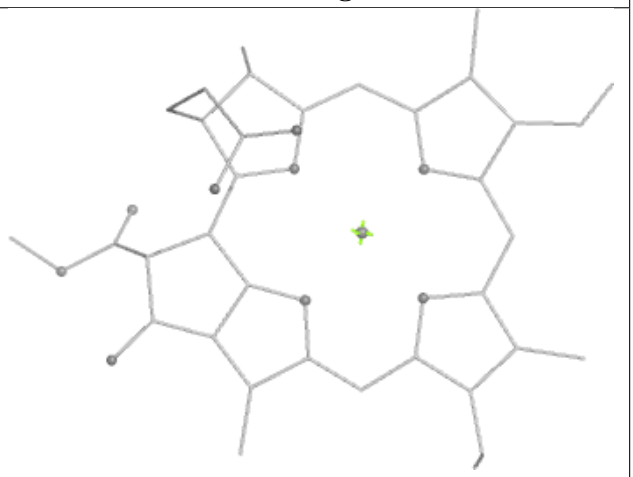
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Bond angles

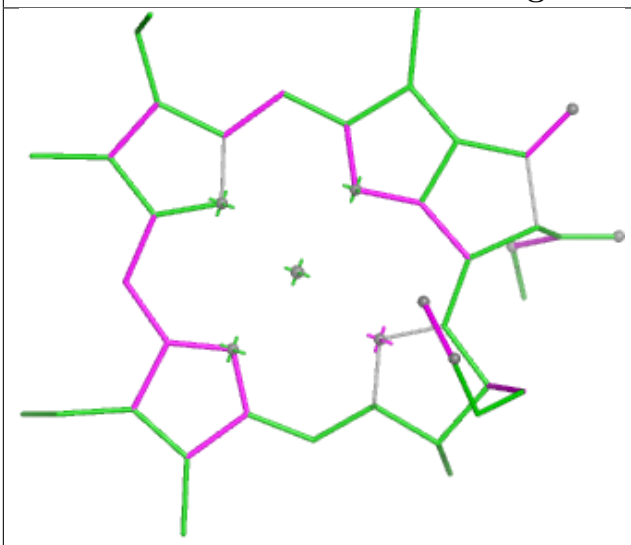


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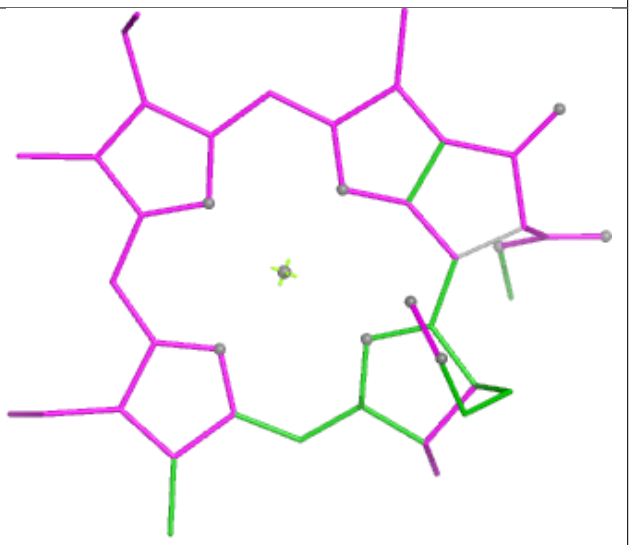


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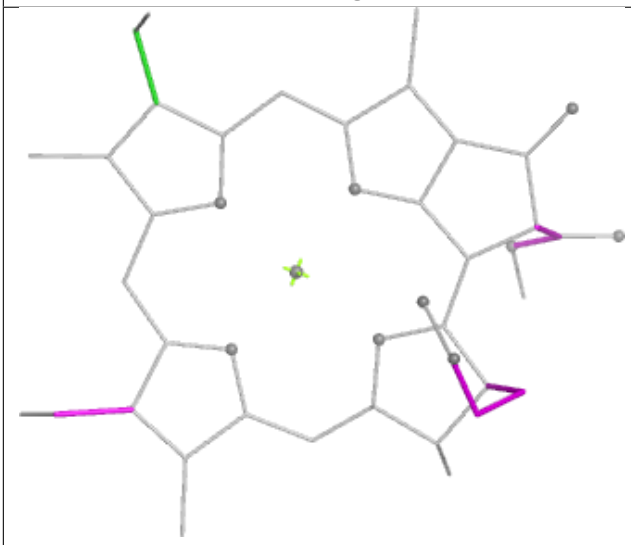
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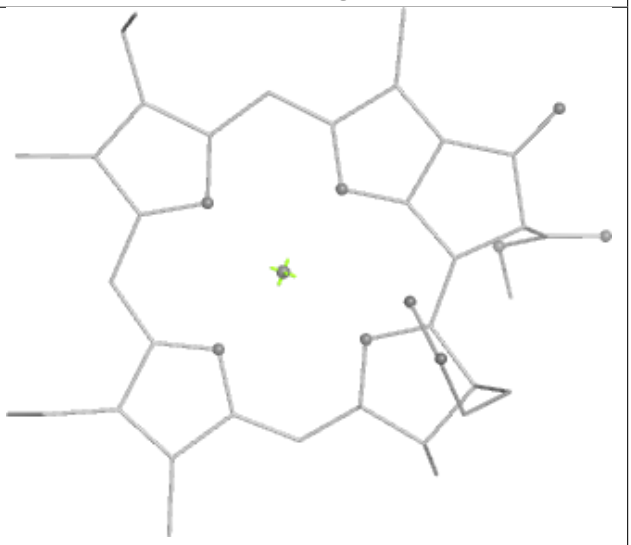
Bond lengths



Bond angles

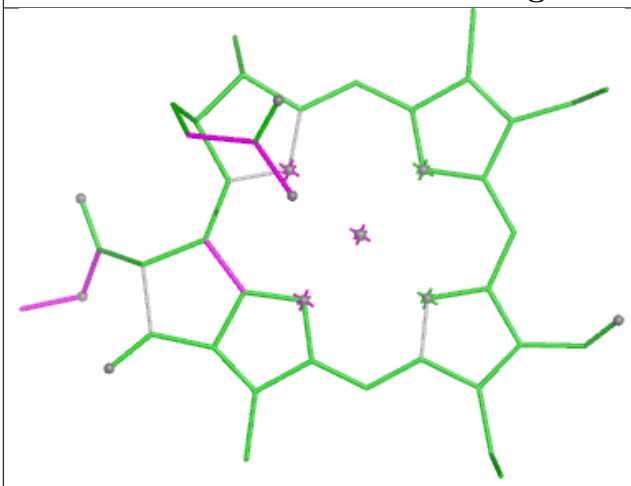


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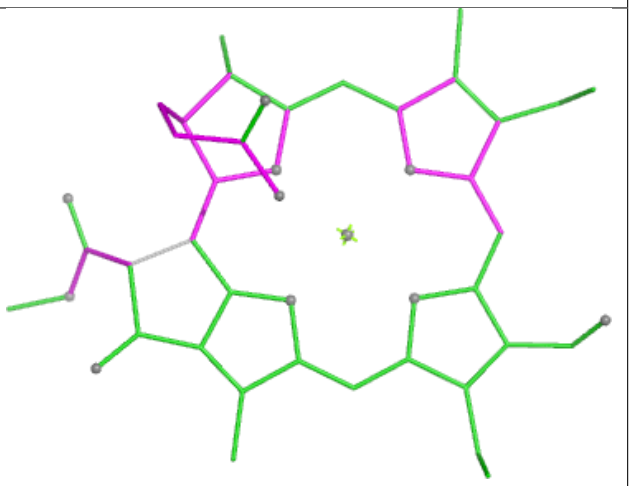


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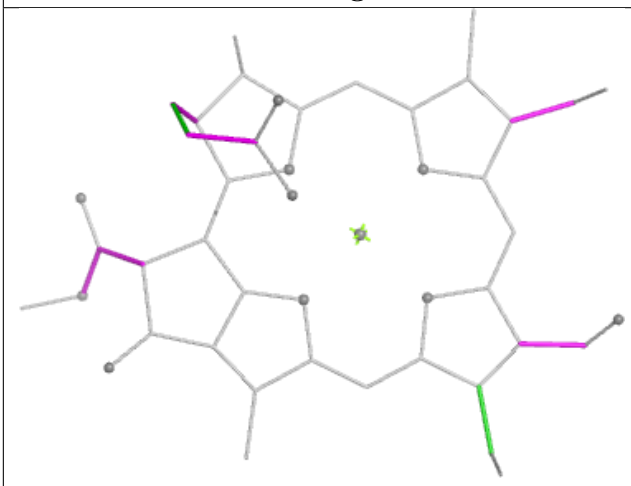
Ligand CHL 7 309



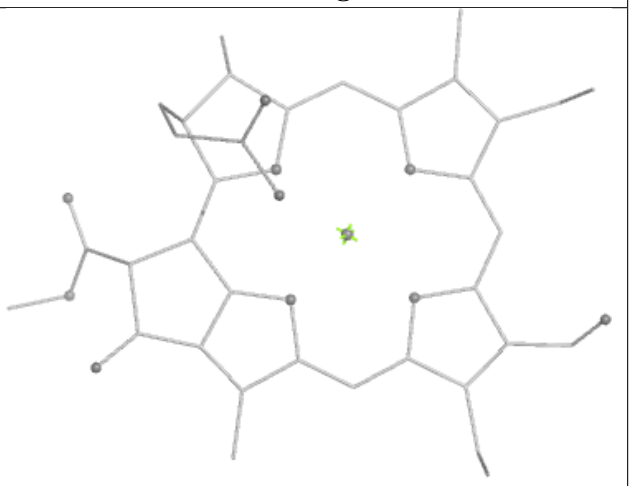
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Bond angles

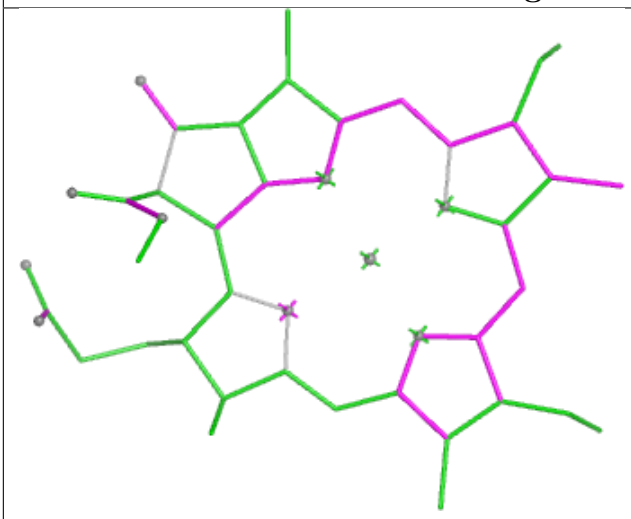


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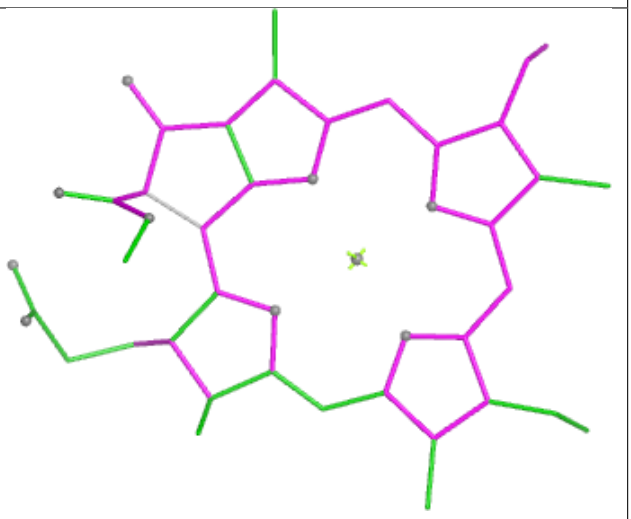


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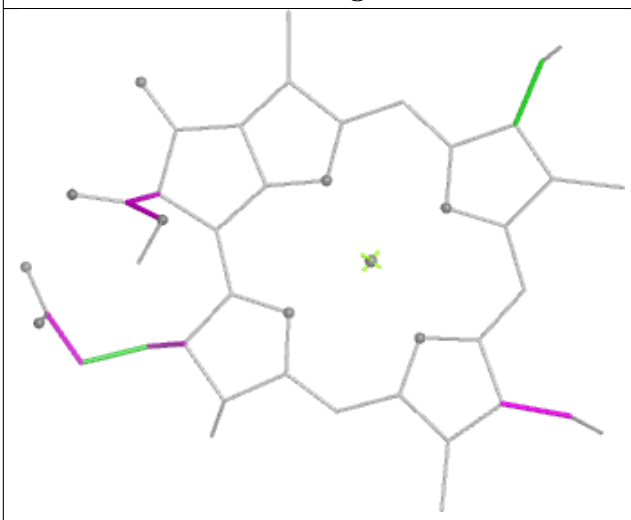
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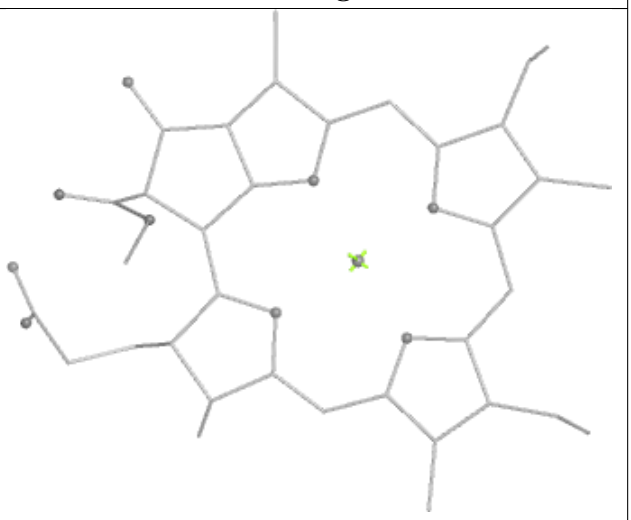
Bond lengths



Bond angles

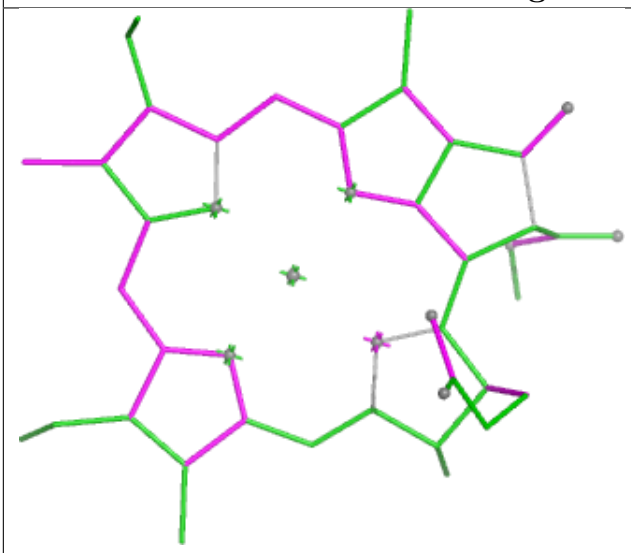


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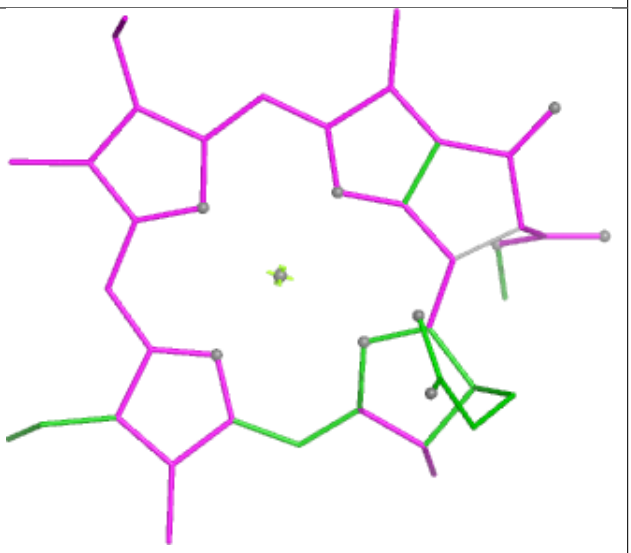


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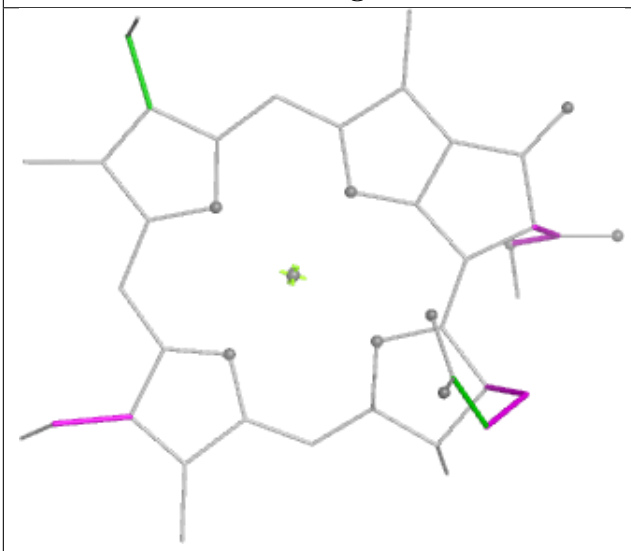
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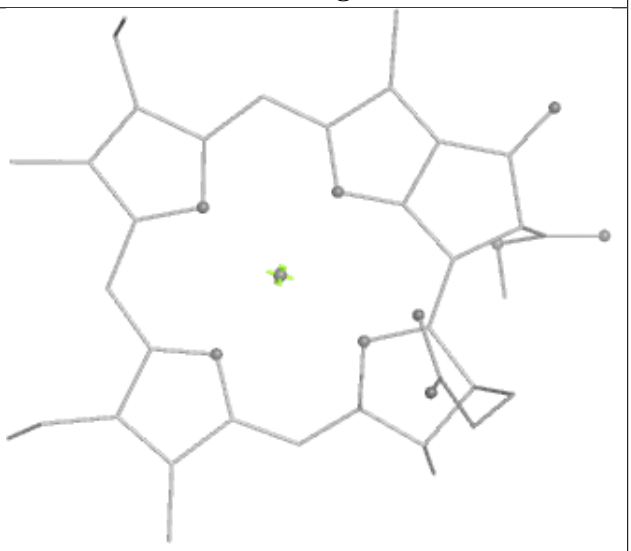
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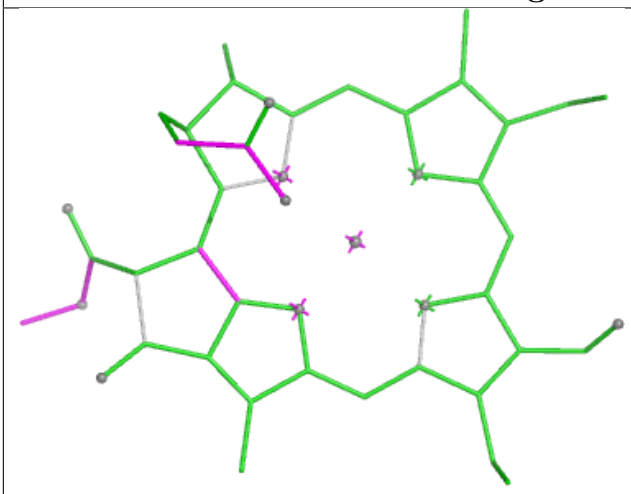


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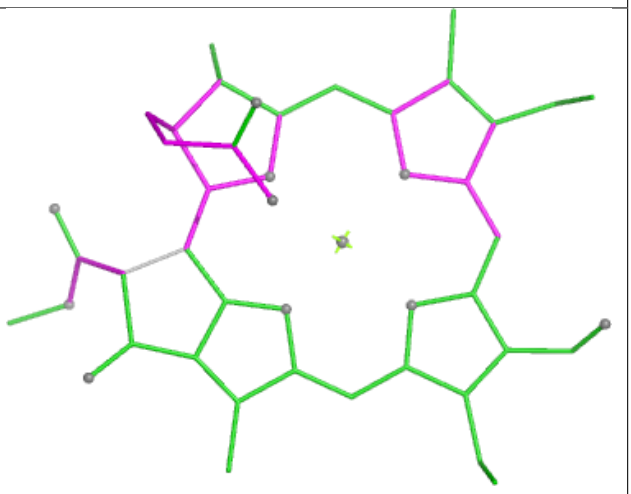


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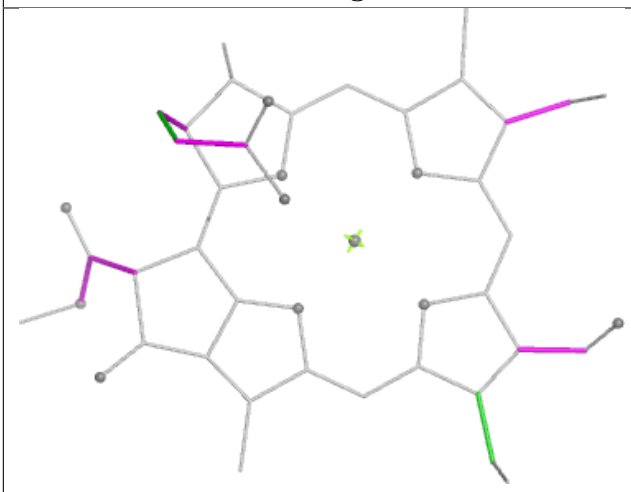
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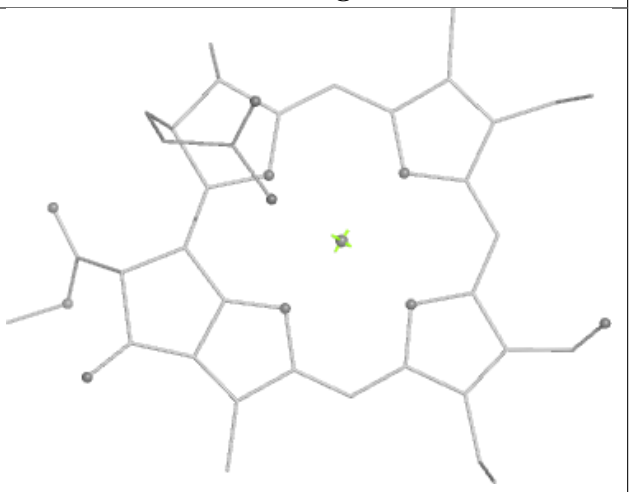
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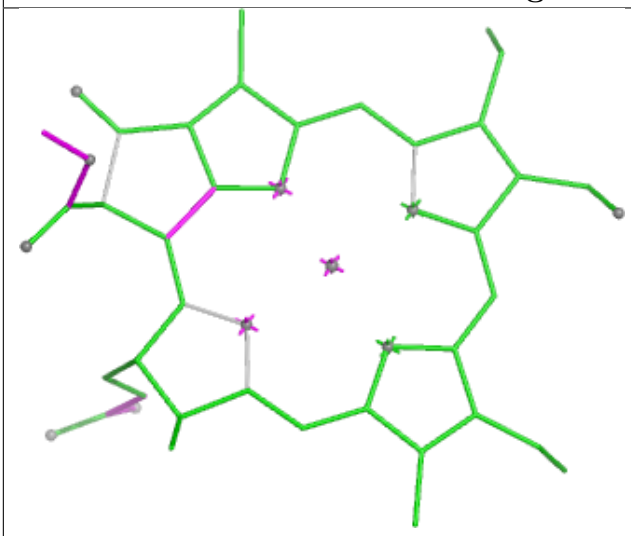


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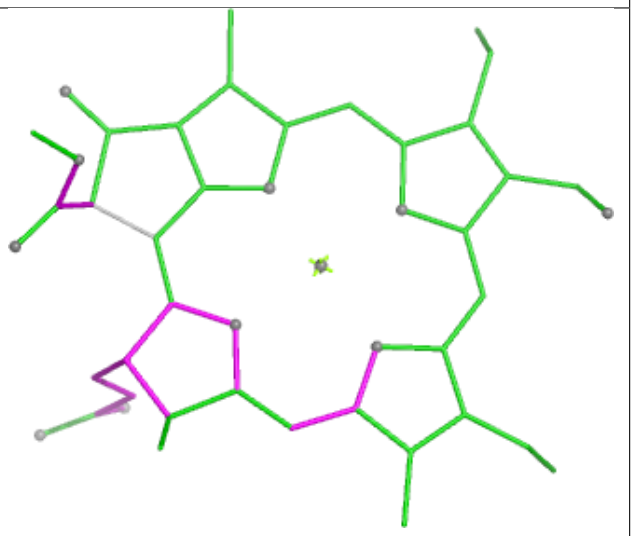


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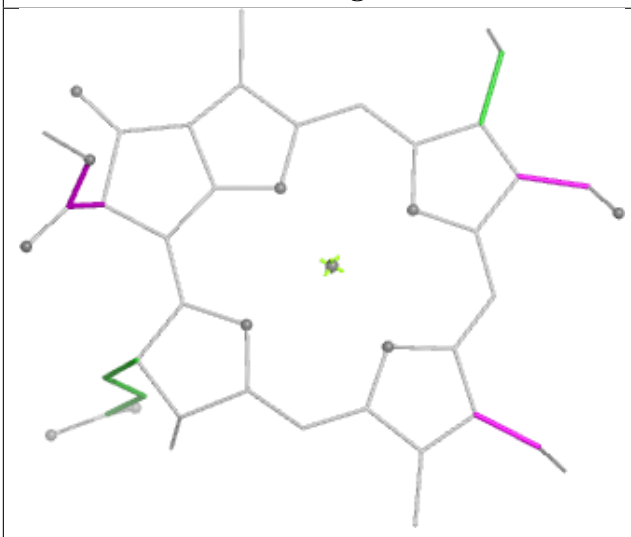
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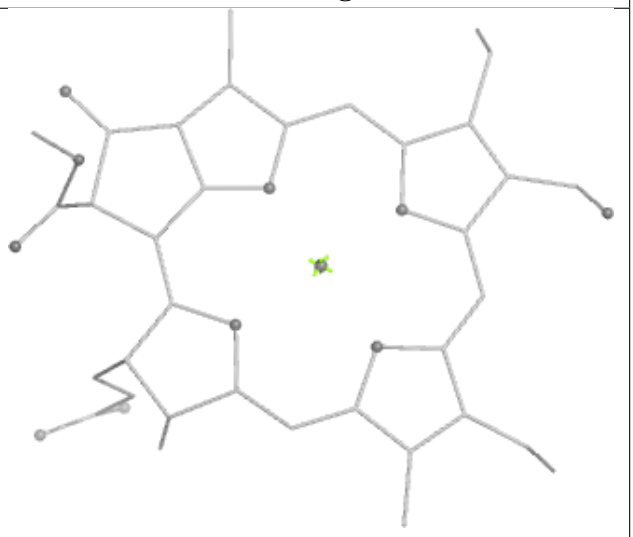
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Bond angles

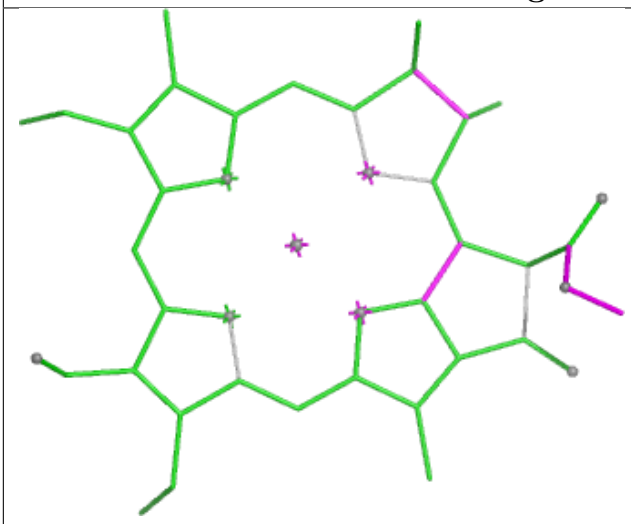


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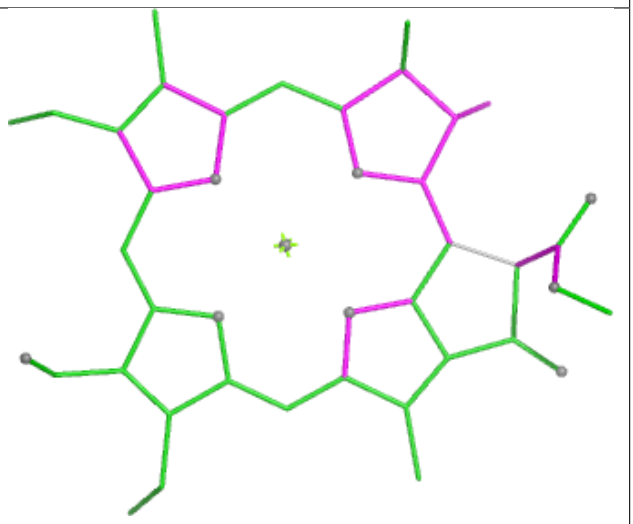


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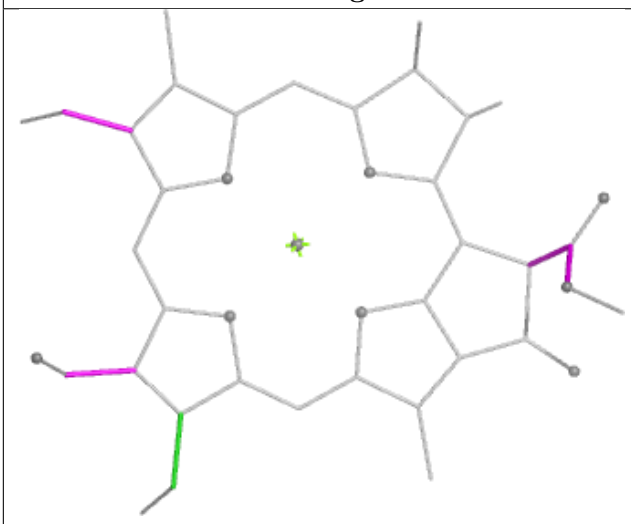
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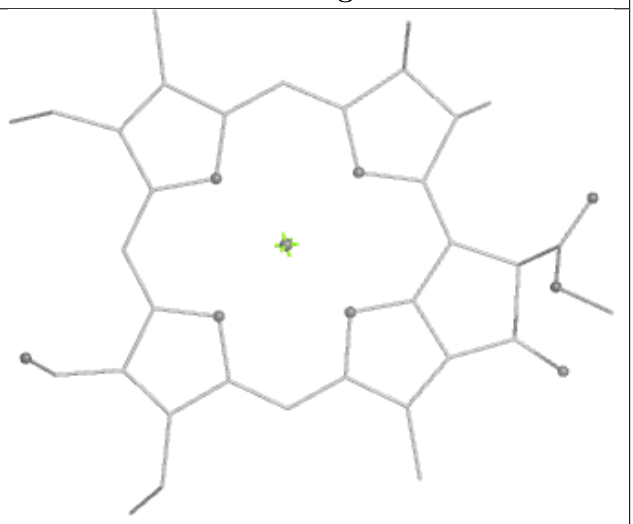
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Bond angles

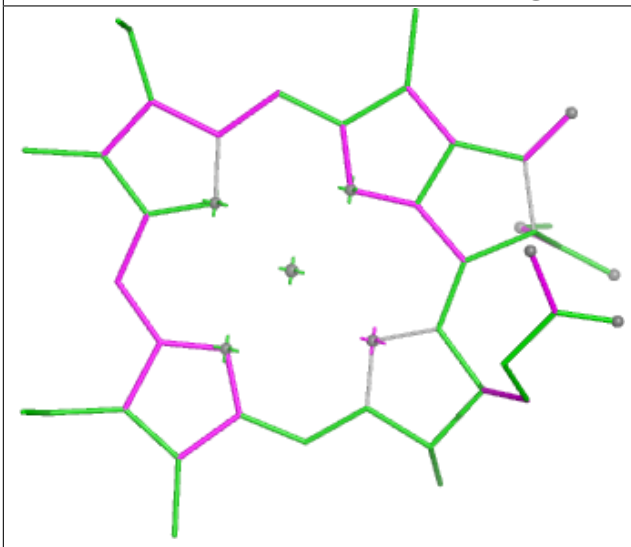


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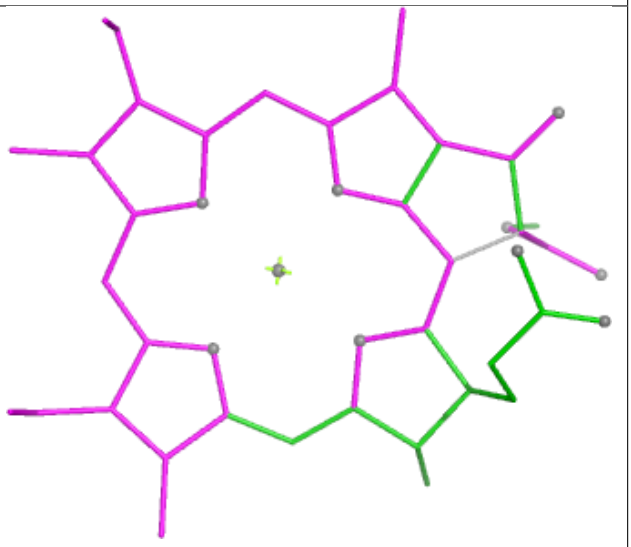


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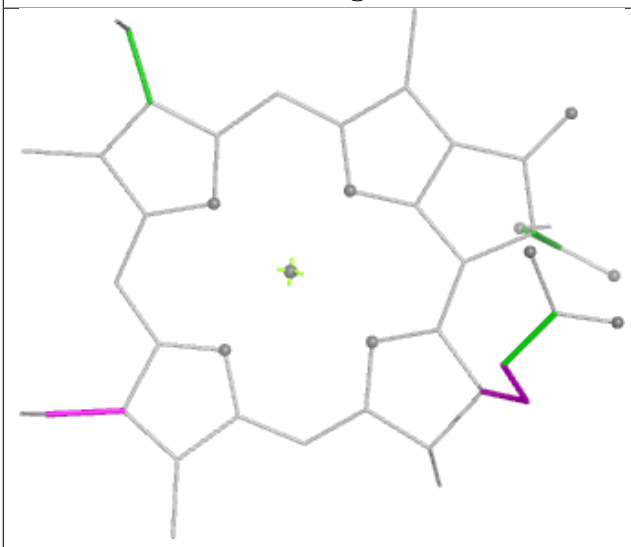
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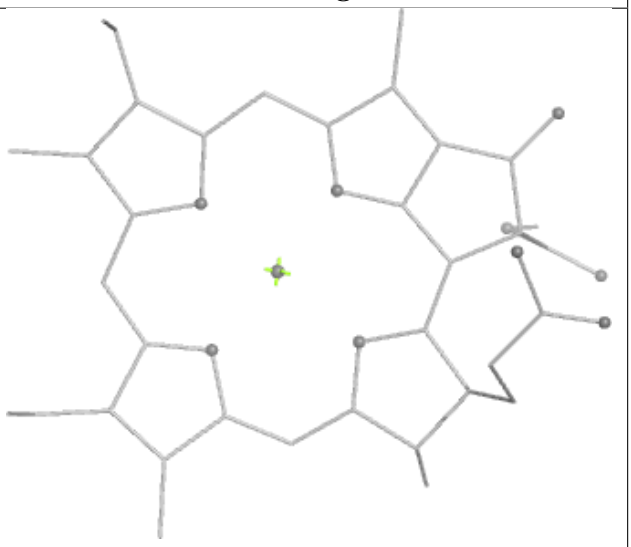
Bond lengths



Bond angles



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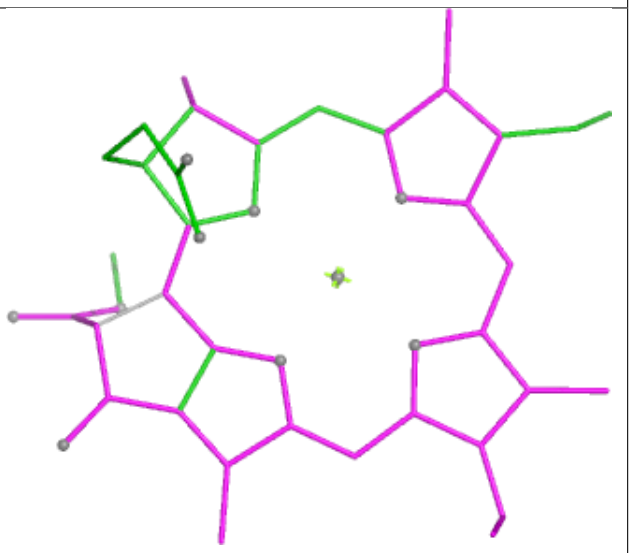


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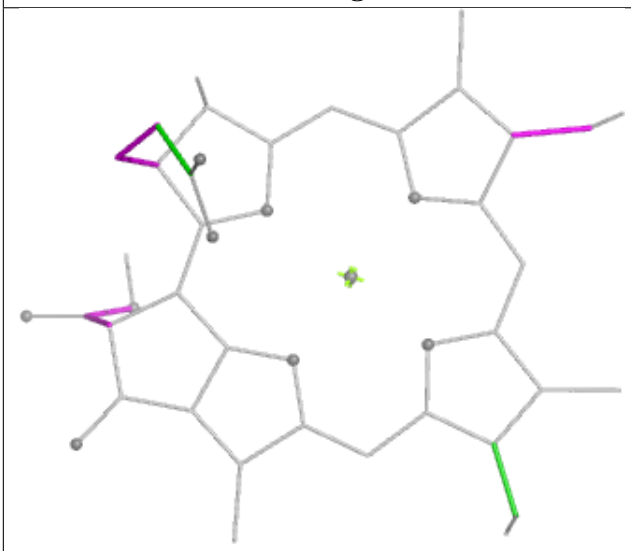
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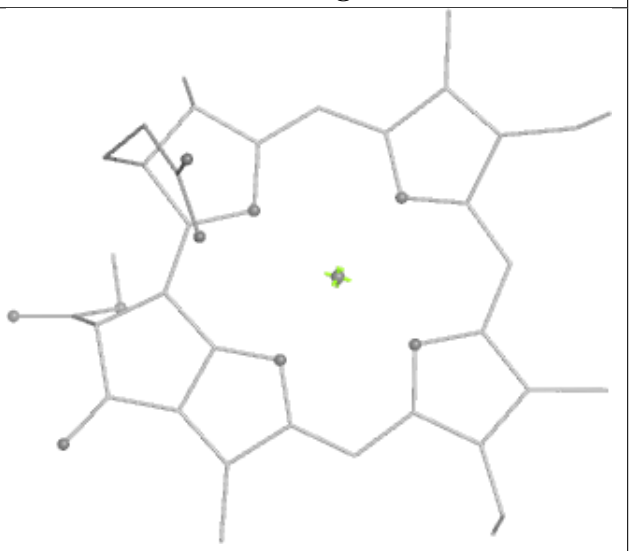
Bond lengths



Bond angles

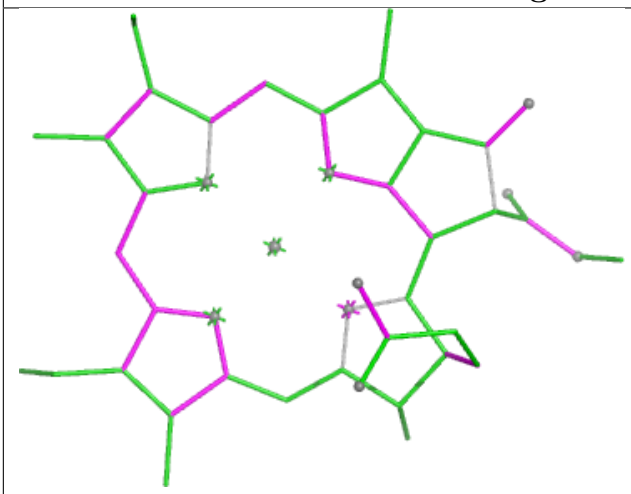


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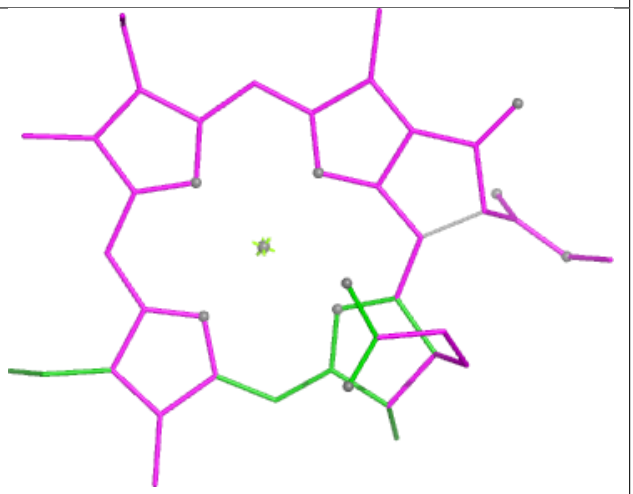


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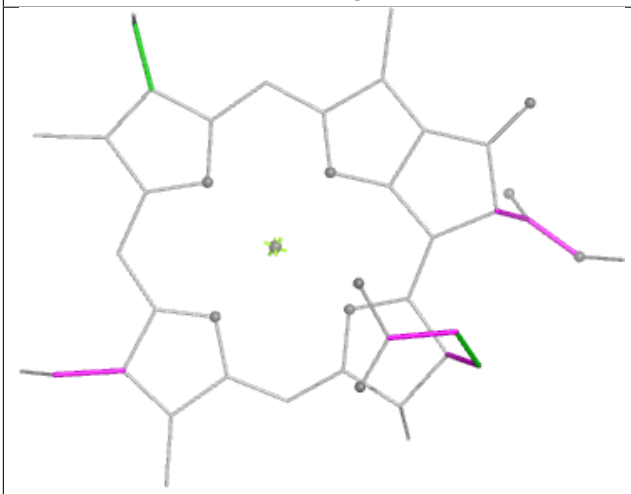
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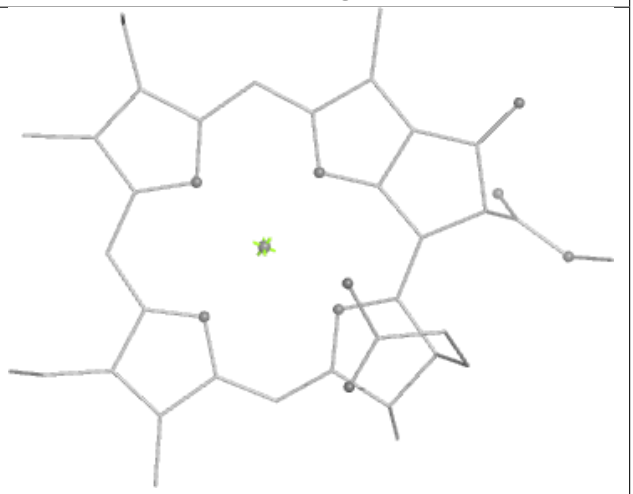
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Bond angles

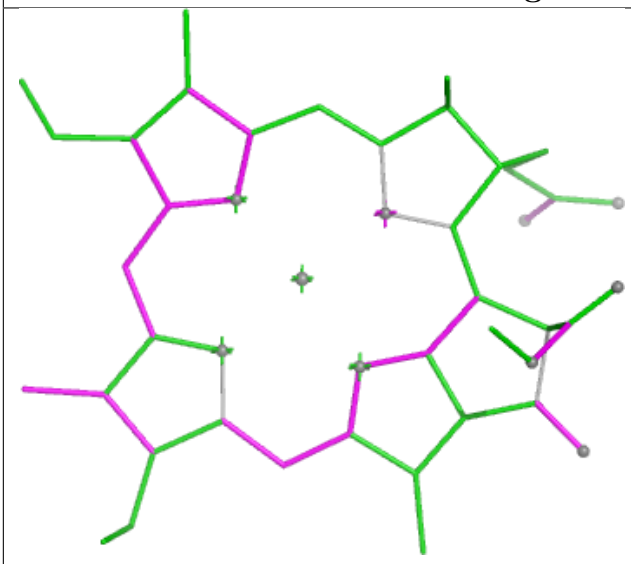


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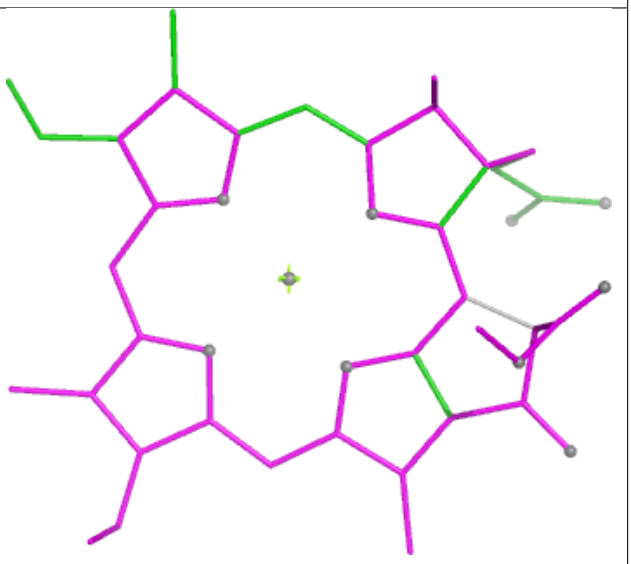


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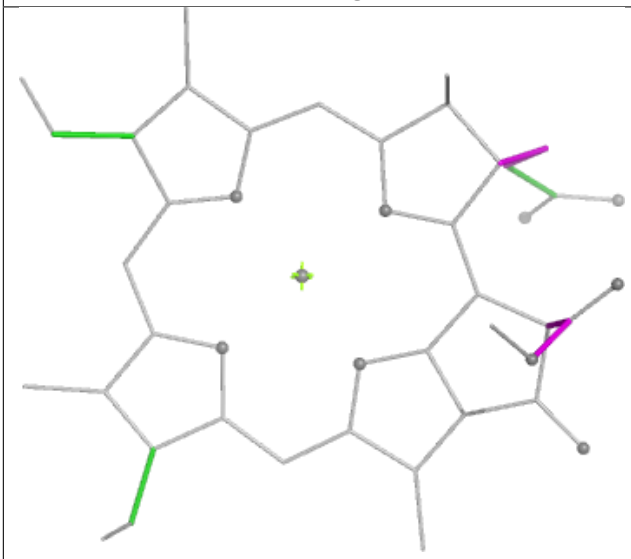
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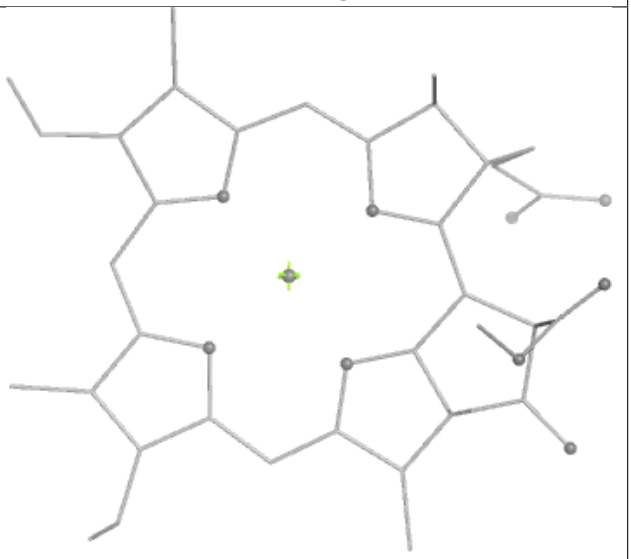
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Bond angles

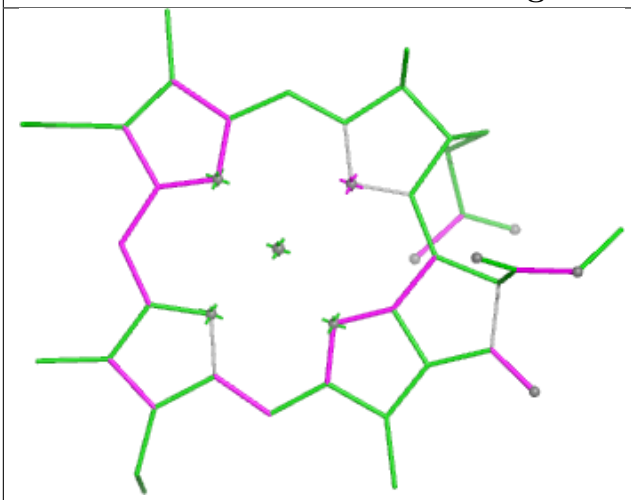


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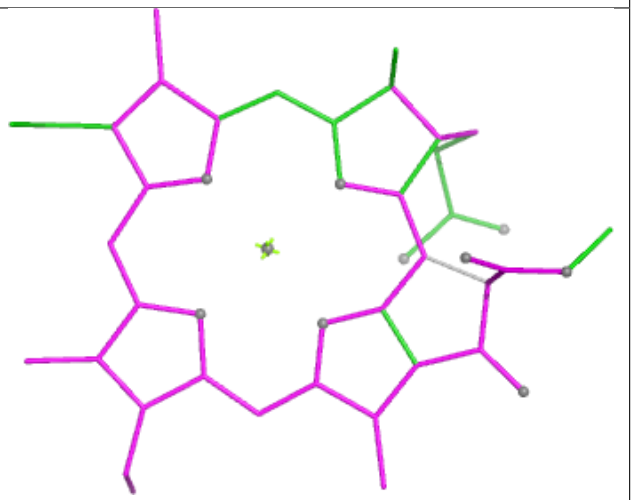


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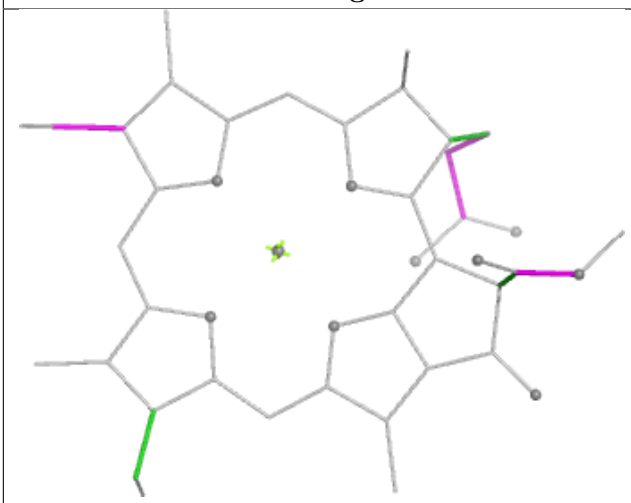
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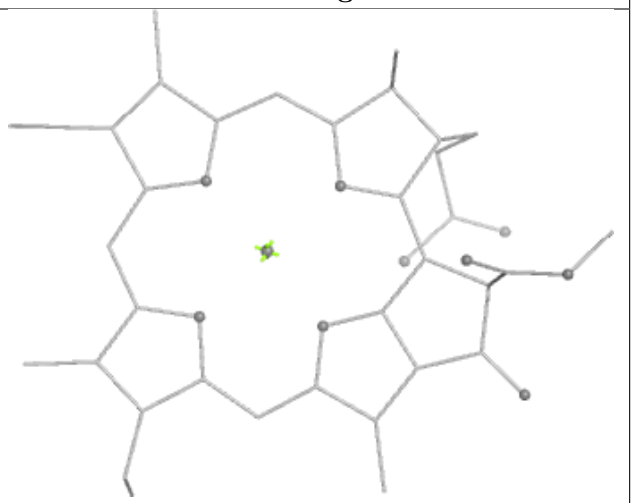
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Bond angles

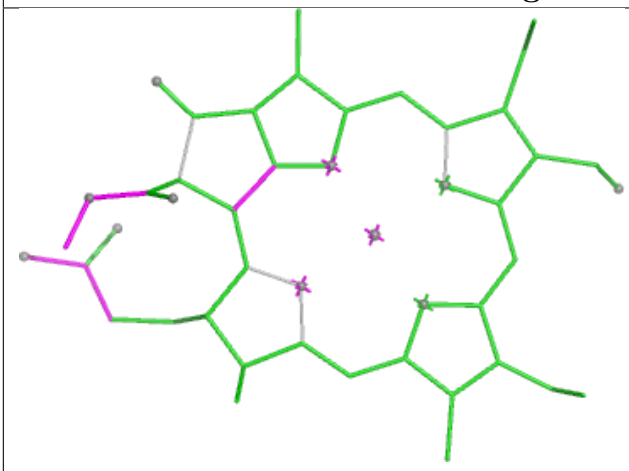


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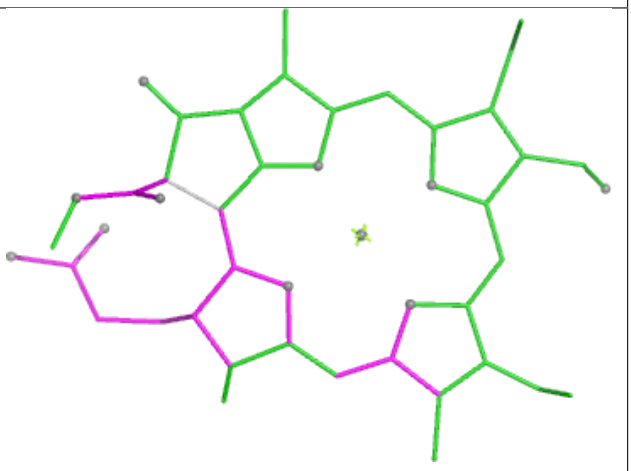


Rings

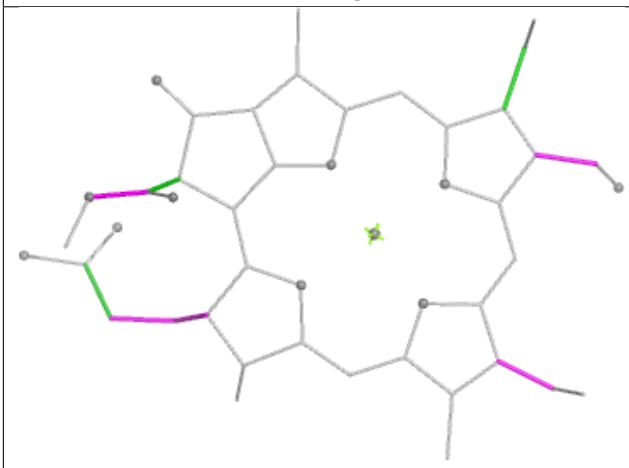
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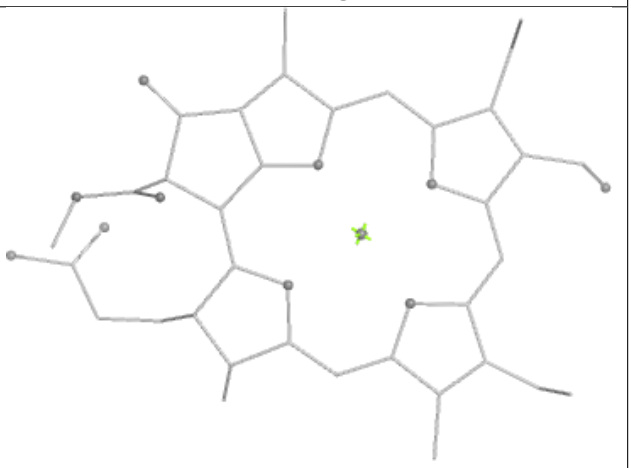
Bond lengths



Bond angles

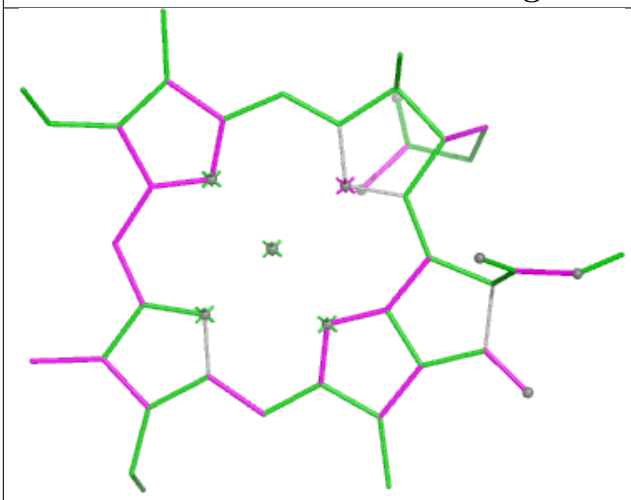


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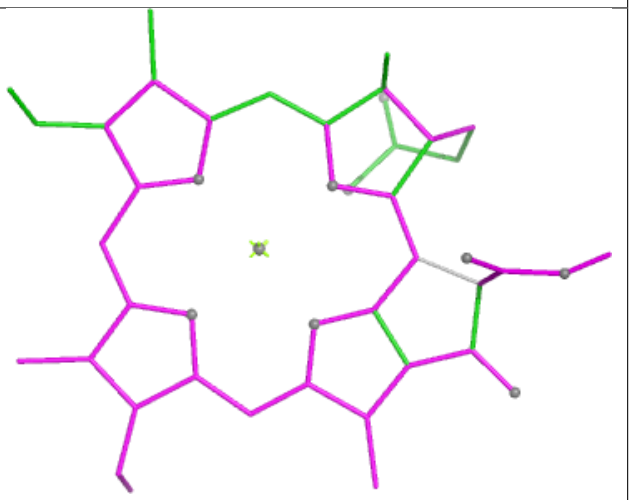


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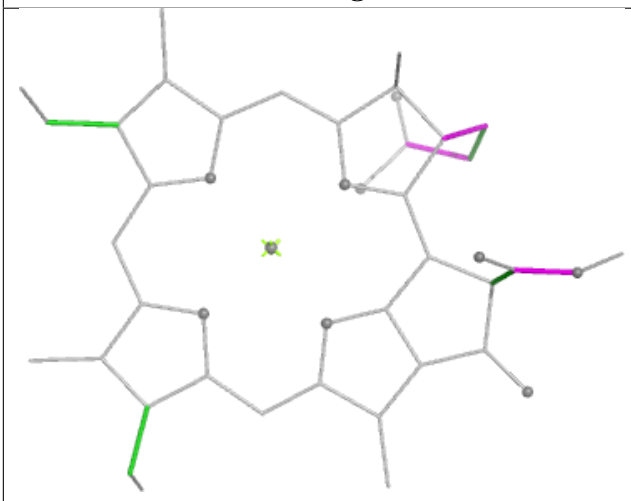
Ligand CLA G 614



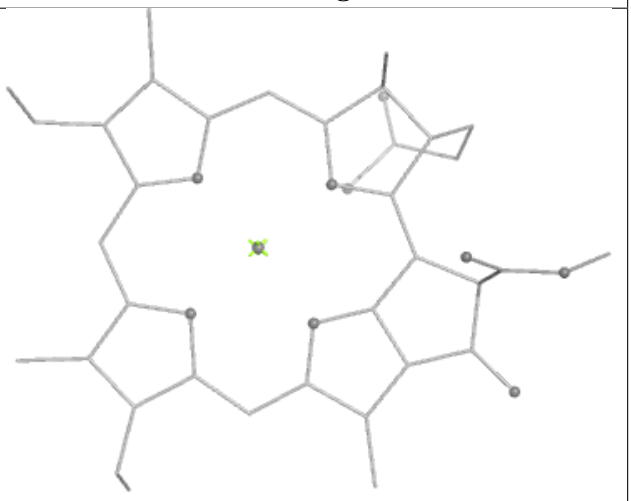
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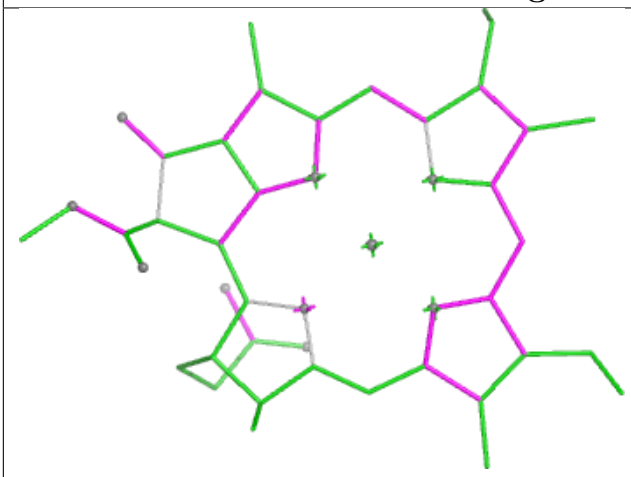


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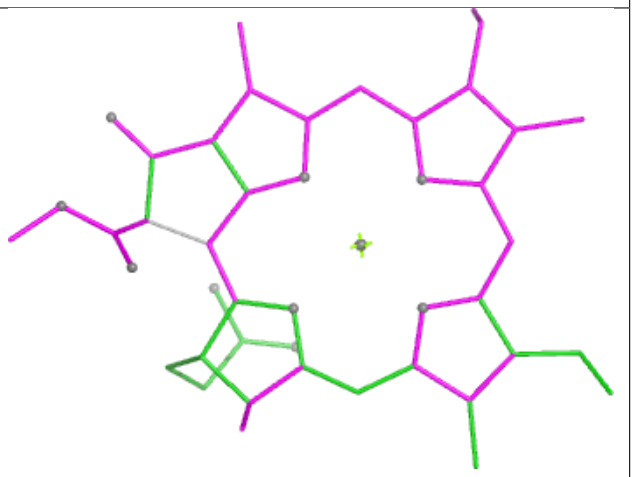


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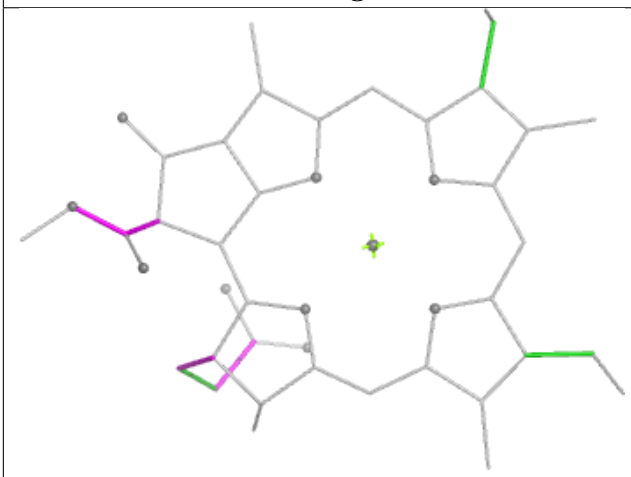
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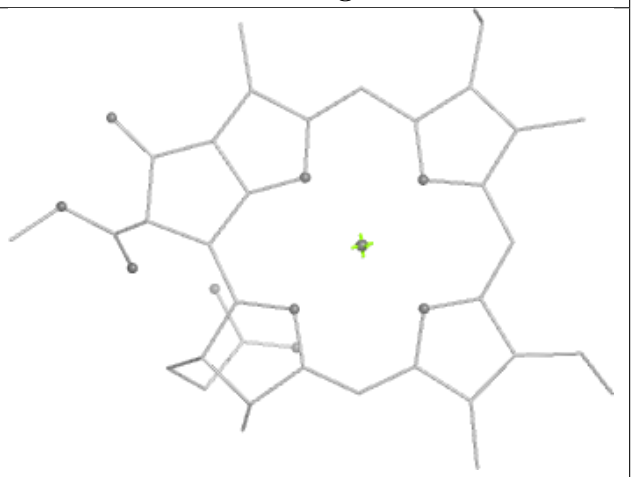
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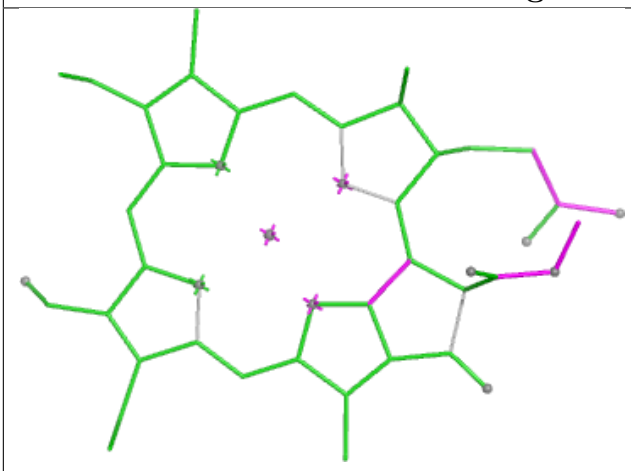


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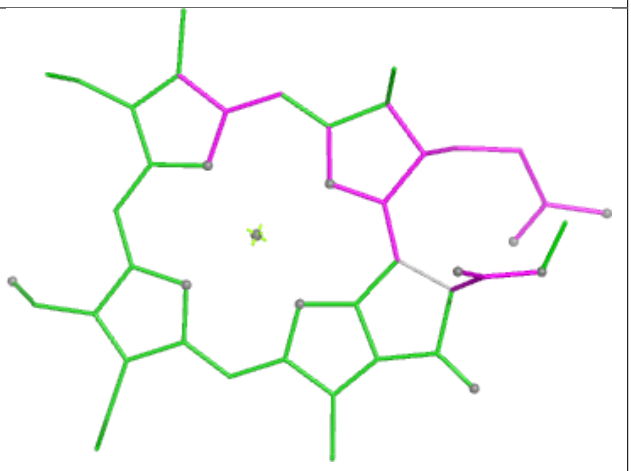


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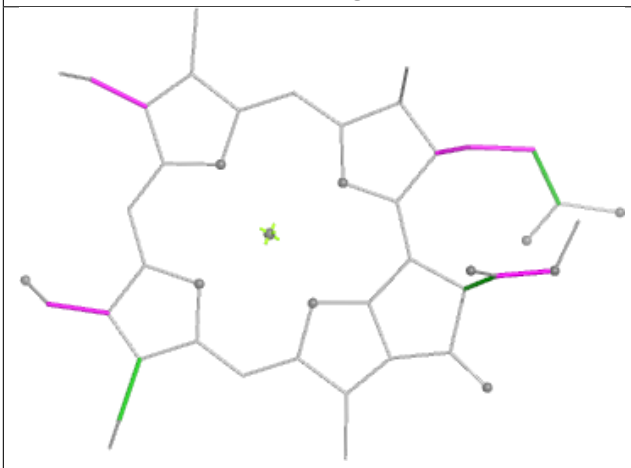
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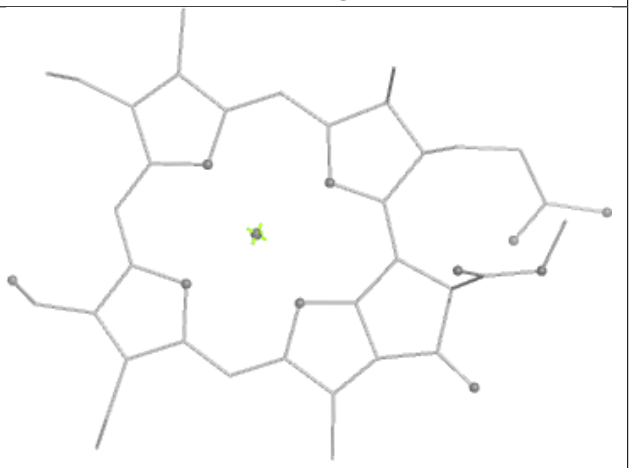
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Bond angles

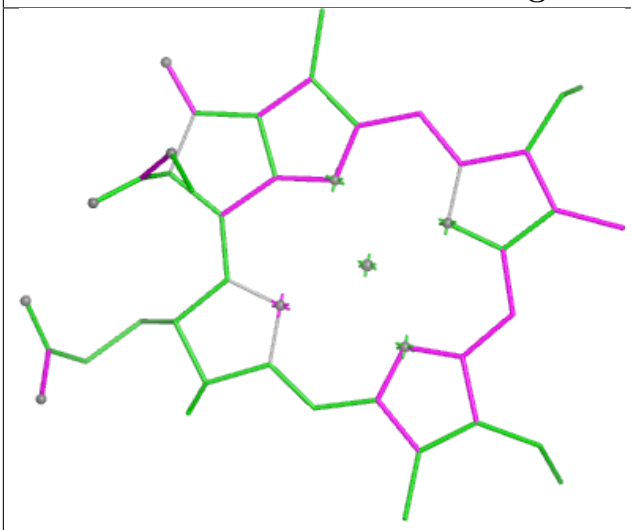


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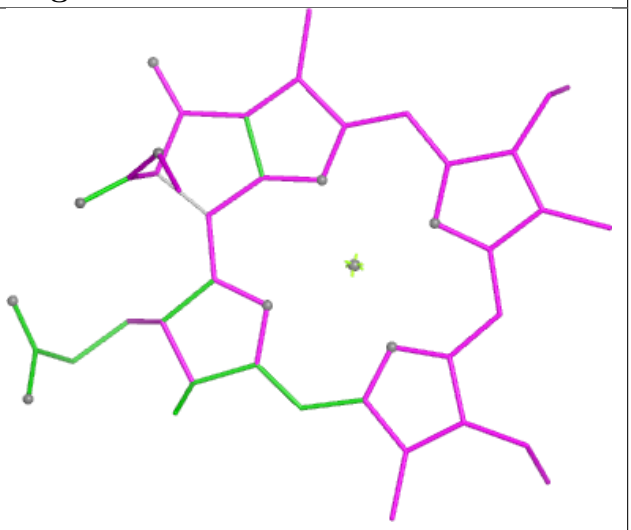


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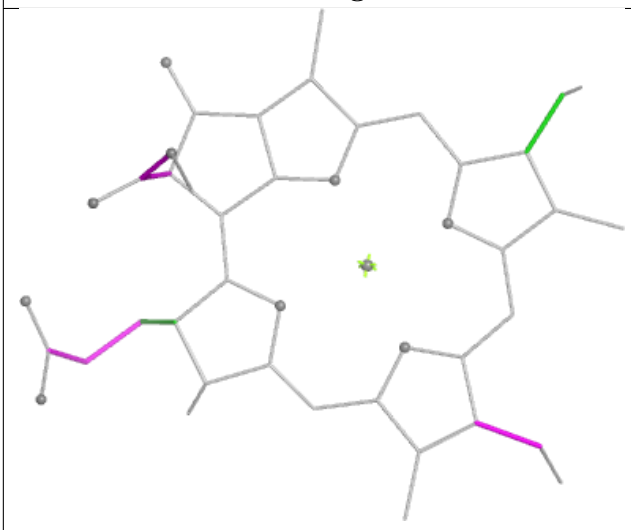
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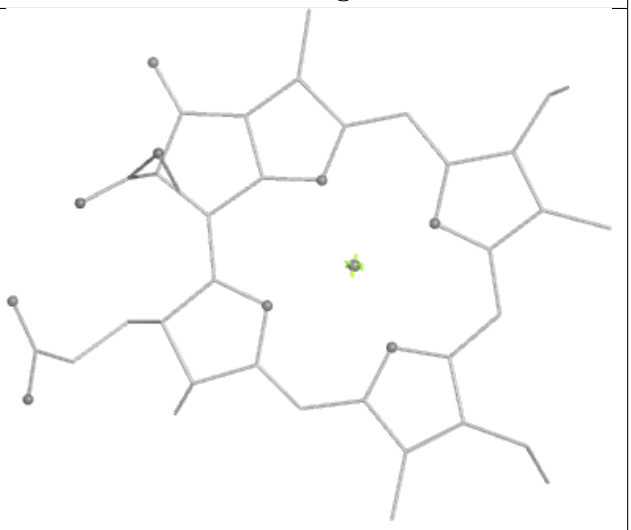
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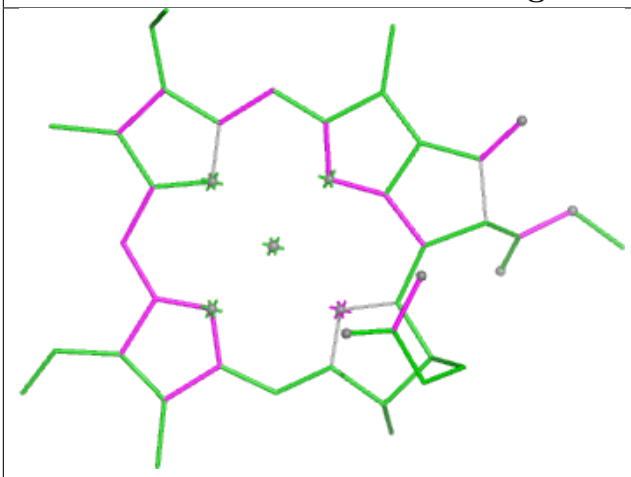


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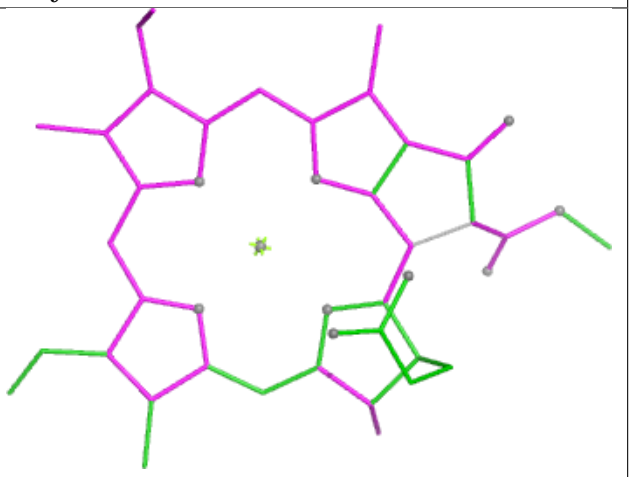


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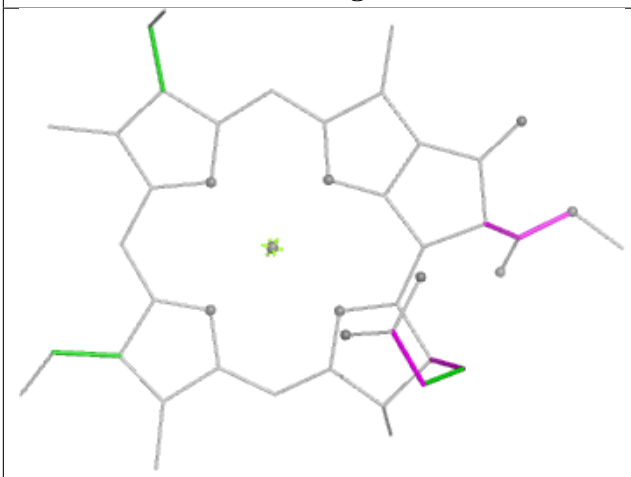
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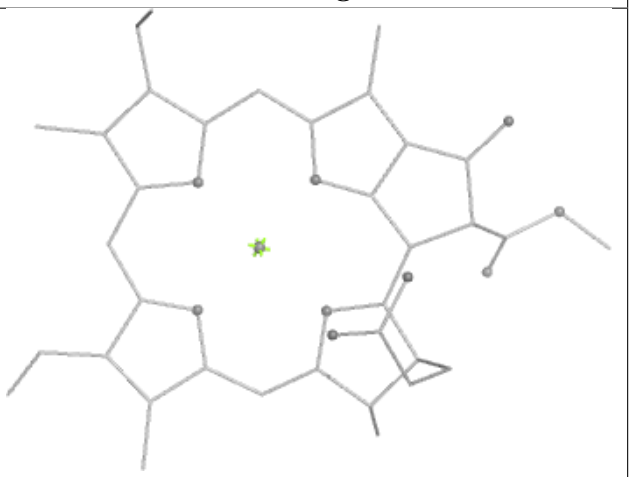
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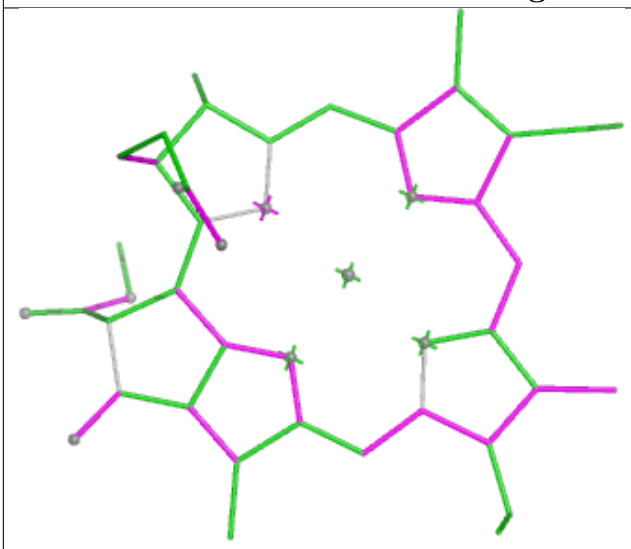


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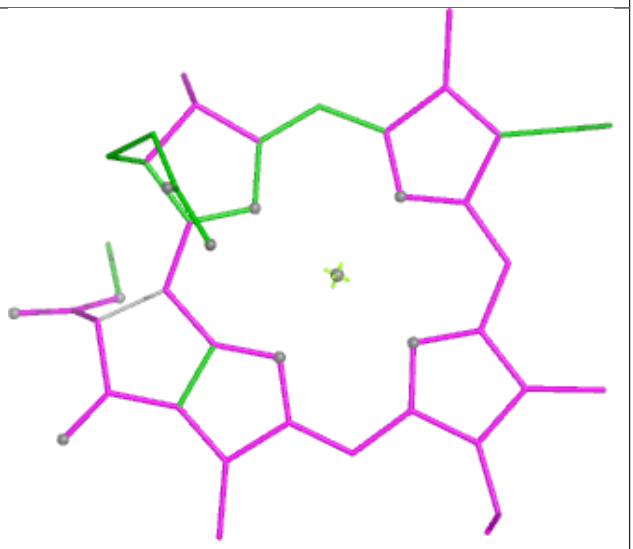


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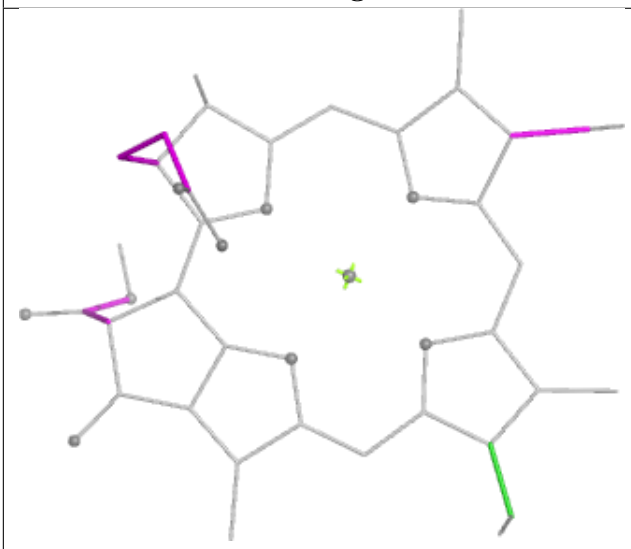
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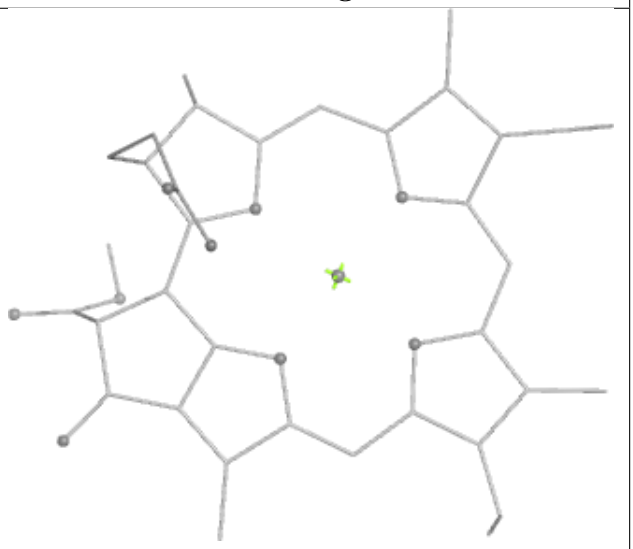
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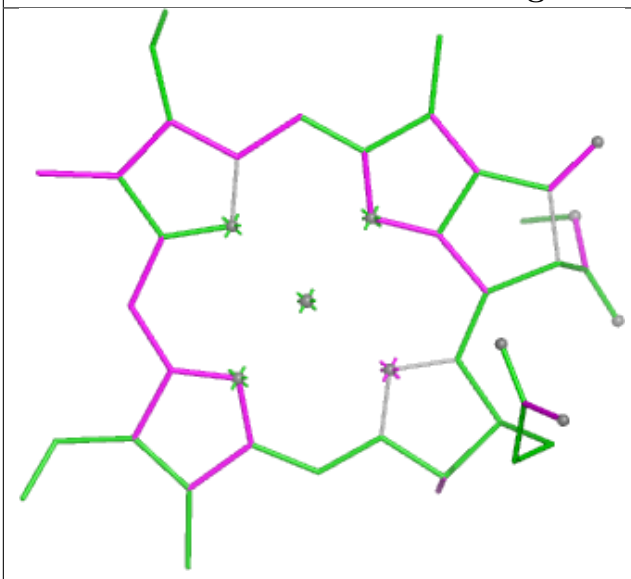


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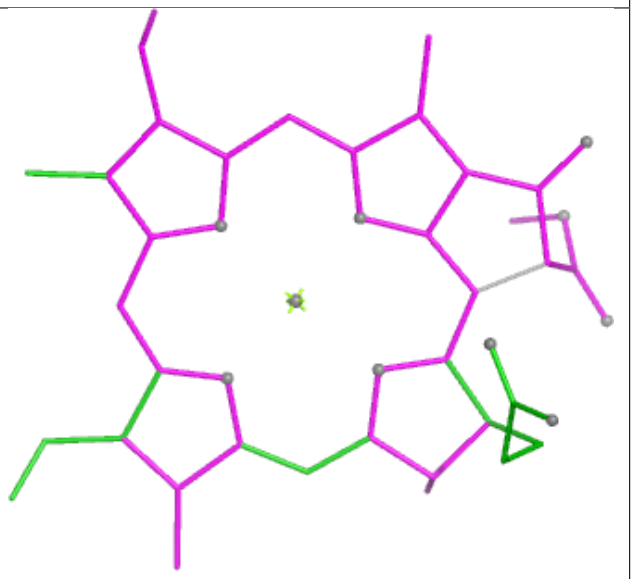


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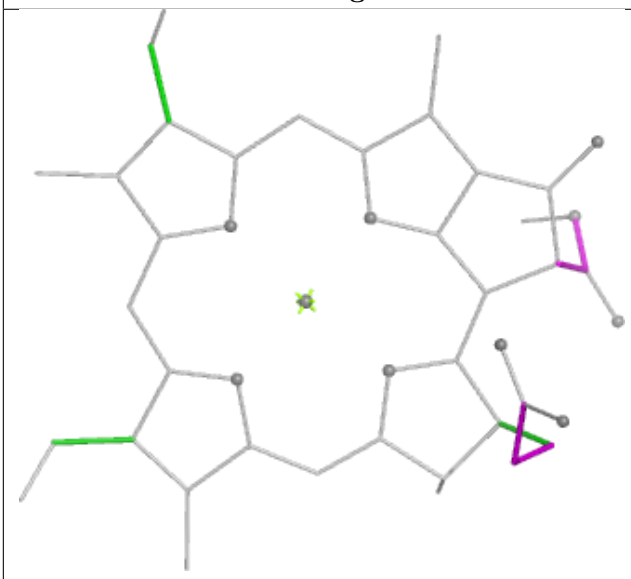
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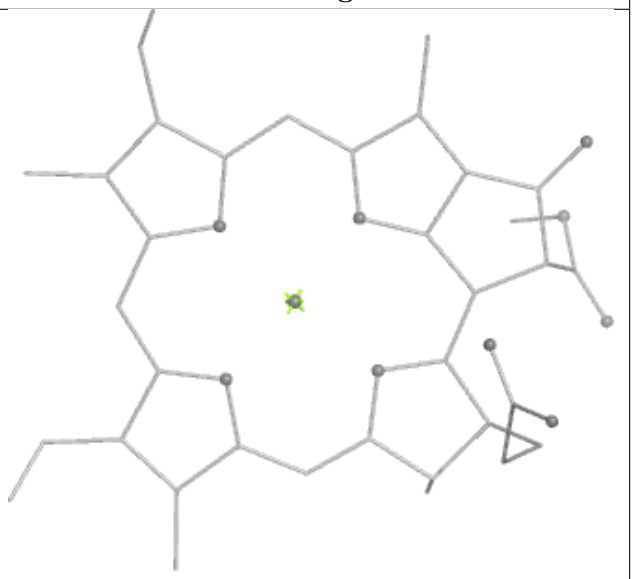
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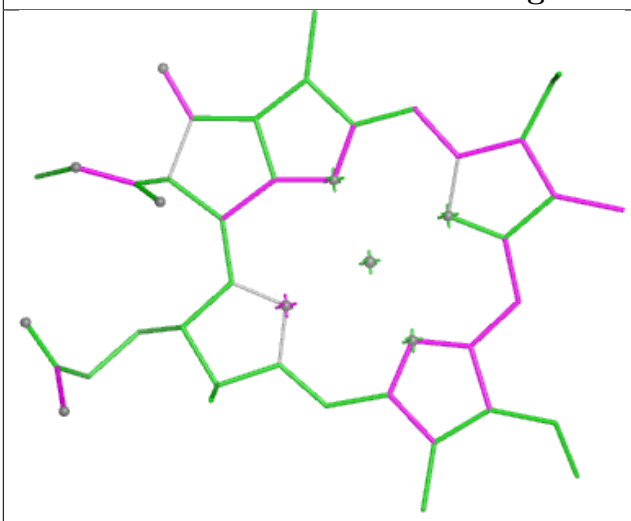


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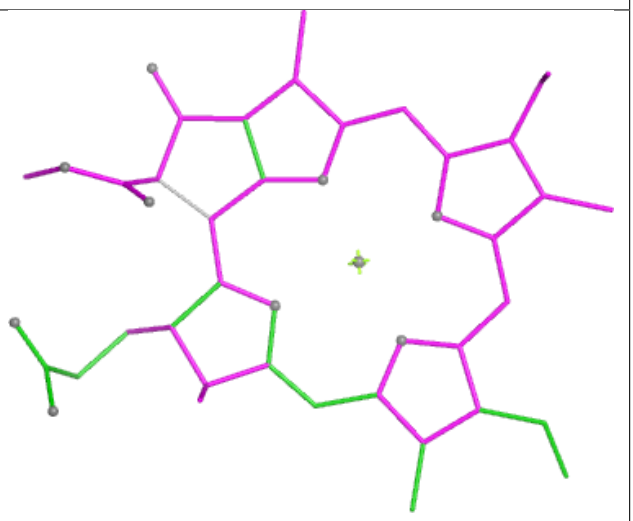


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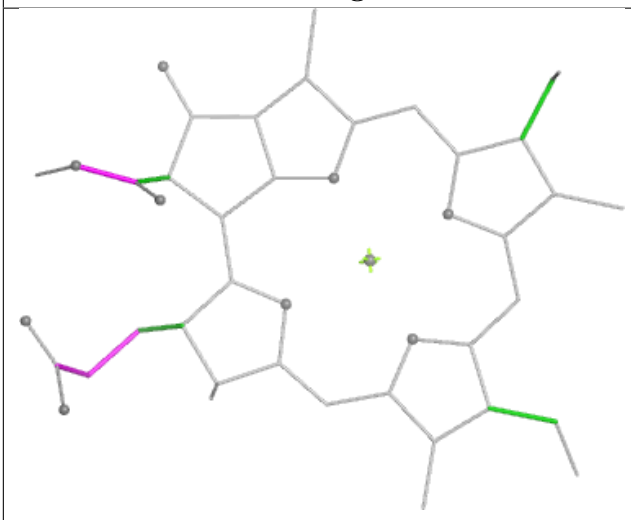
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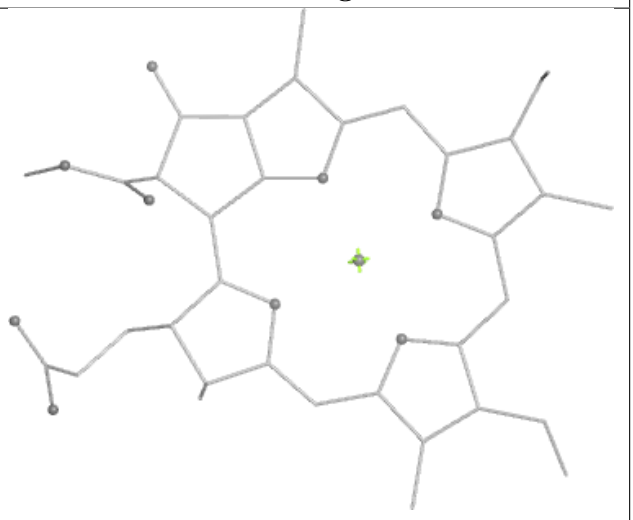
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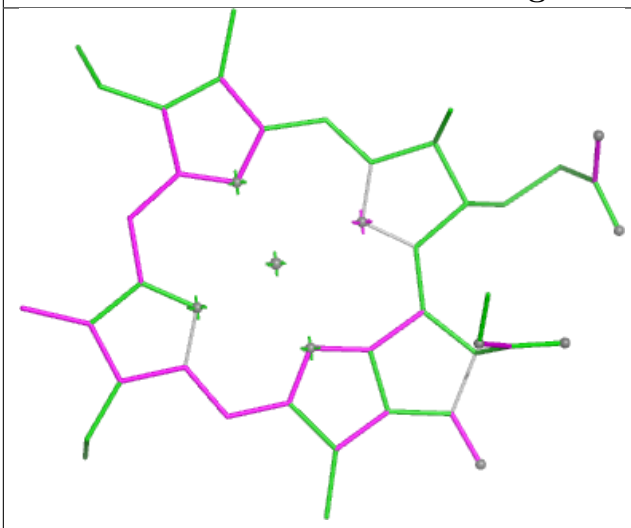


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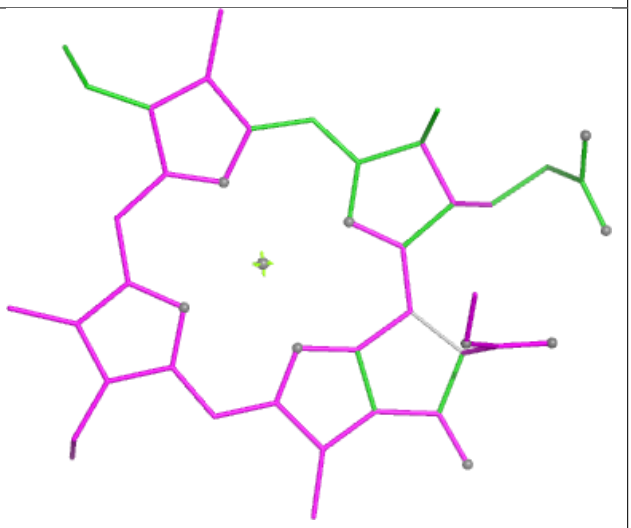


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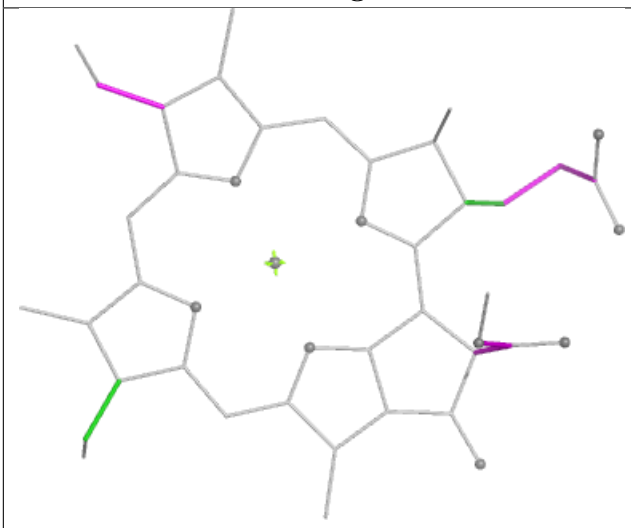
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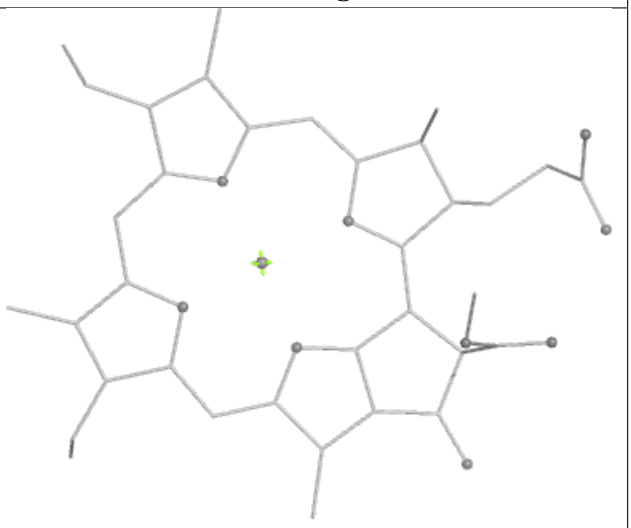
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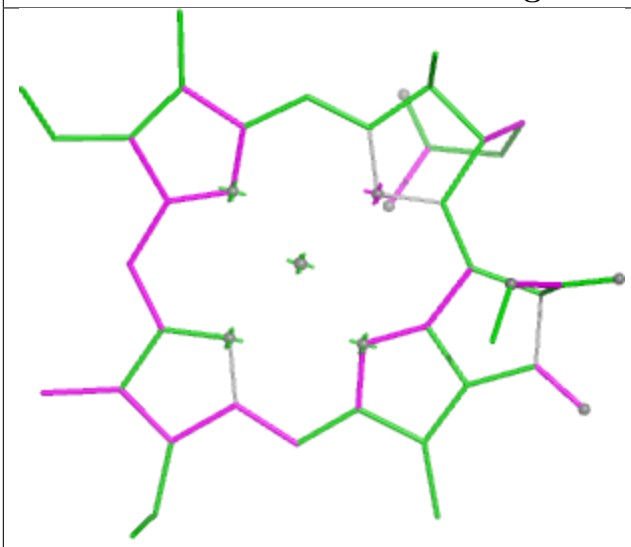


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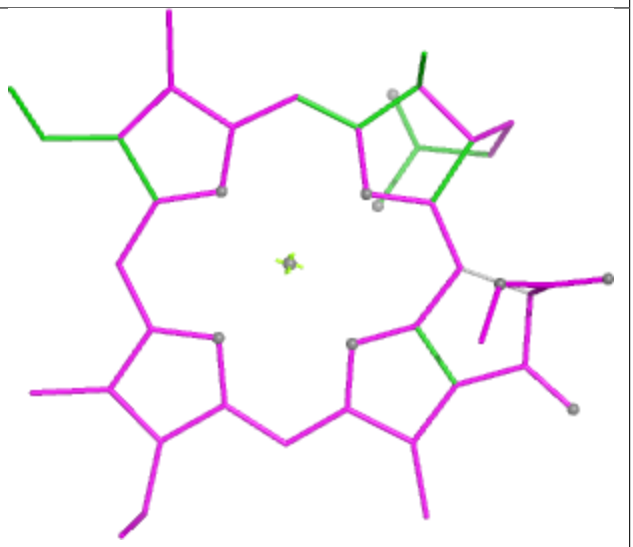


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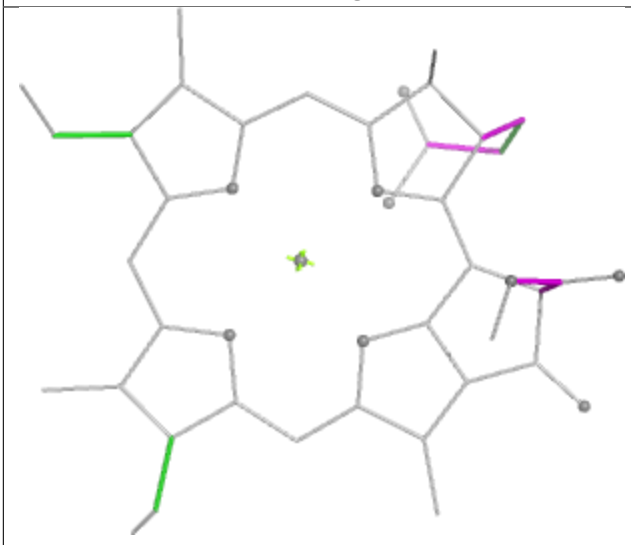
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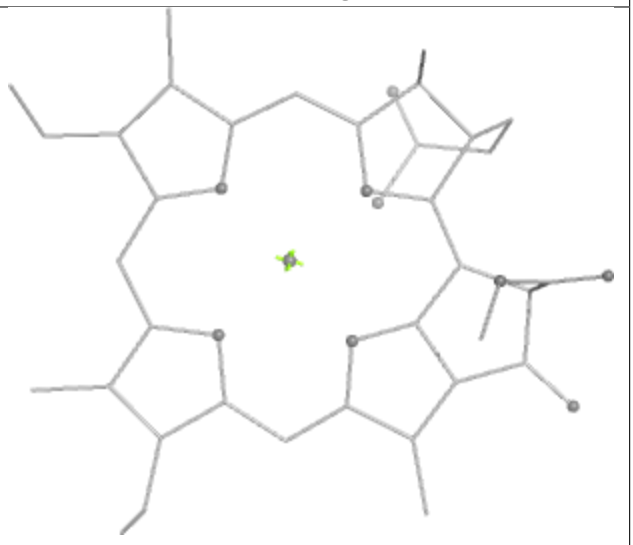
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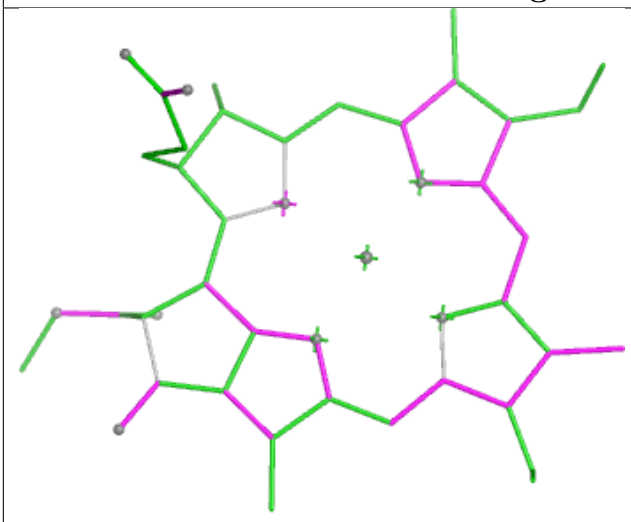


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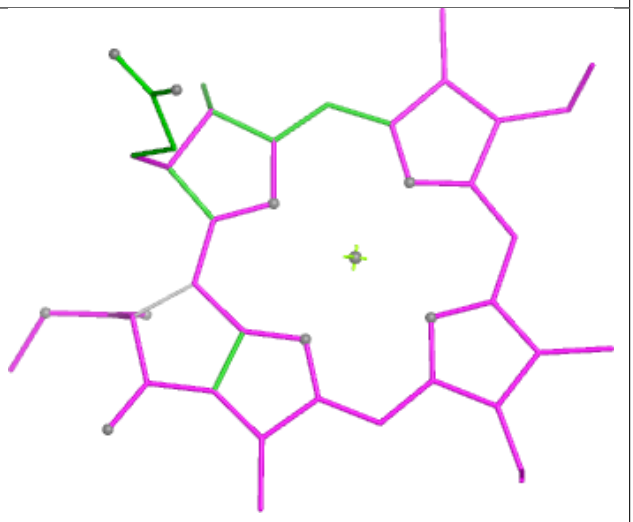


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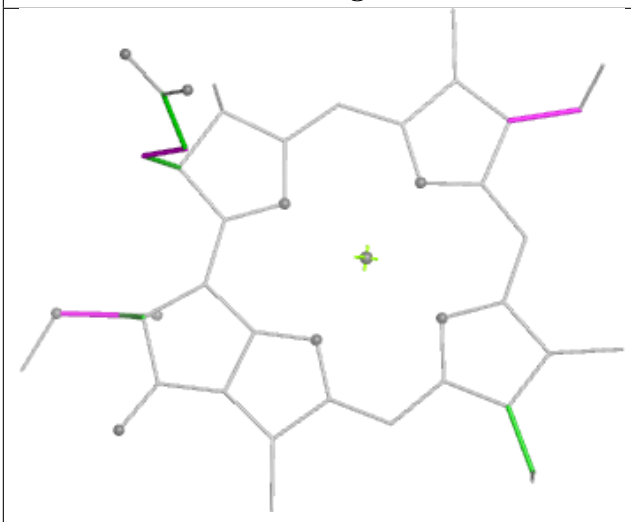
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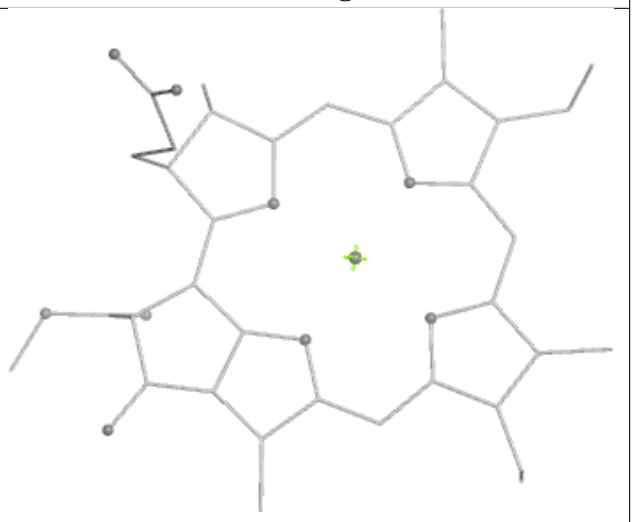
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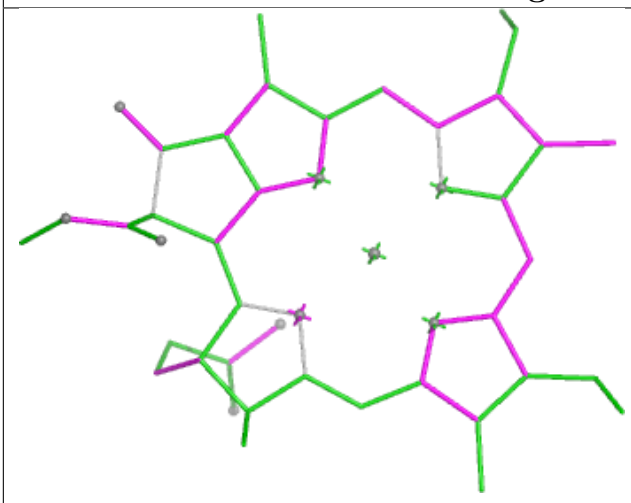


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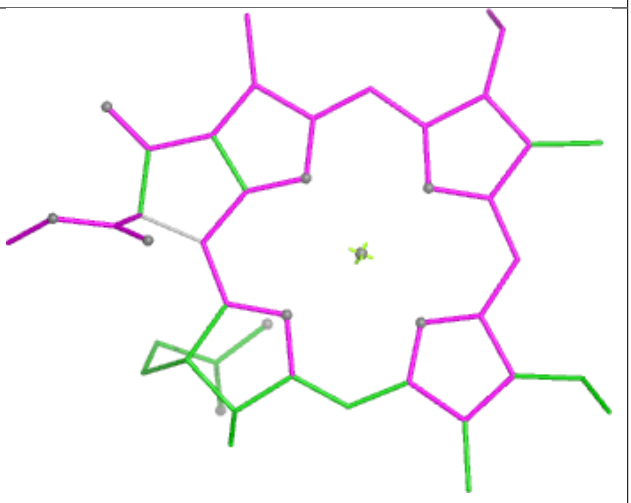


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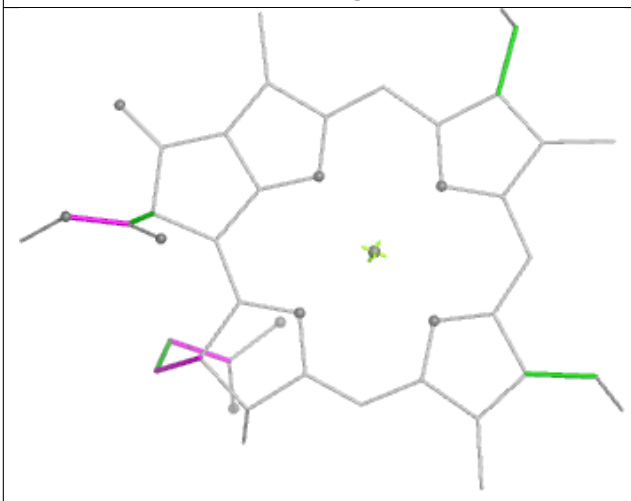
Ligand CLA 2 613



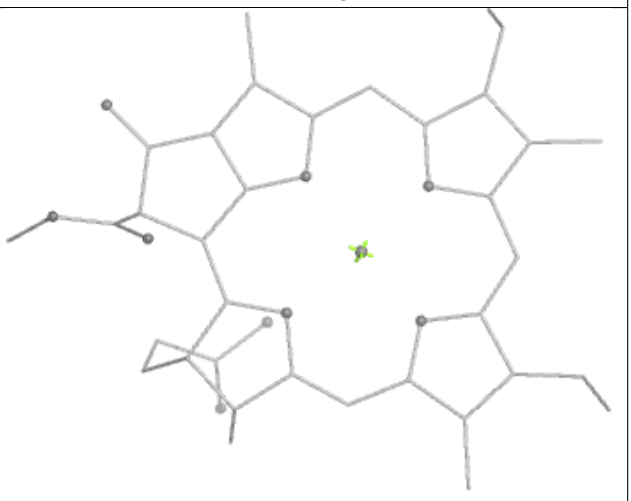
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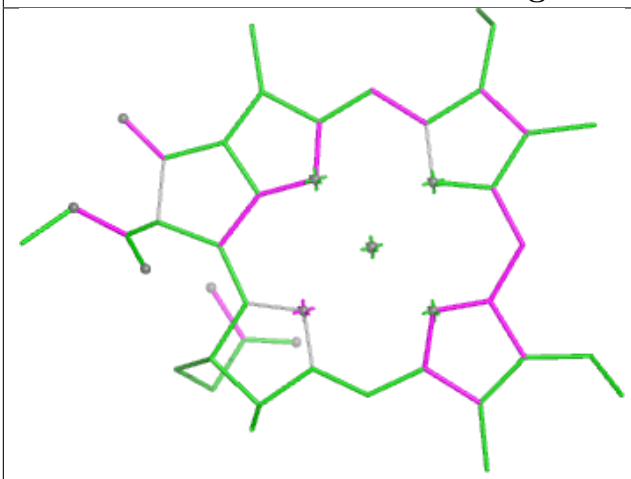


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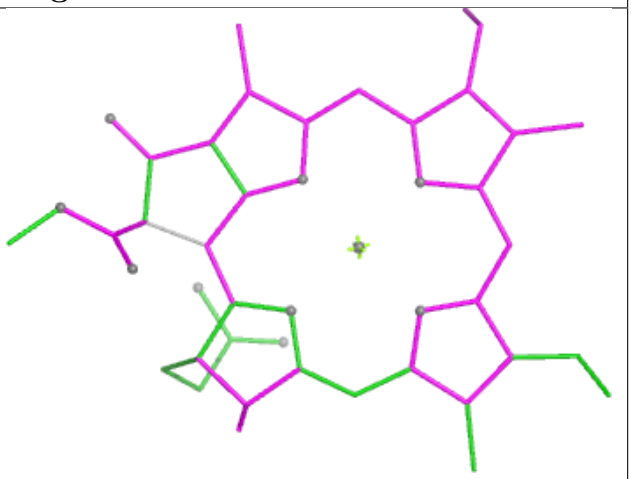


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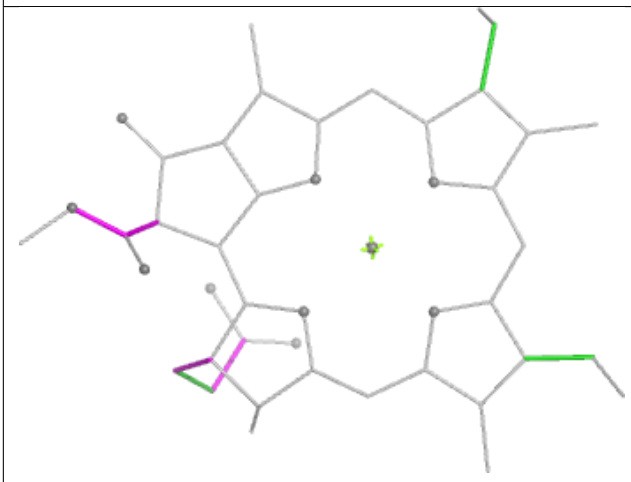
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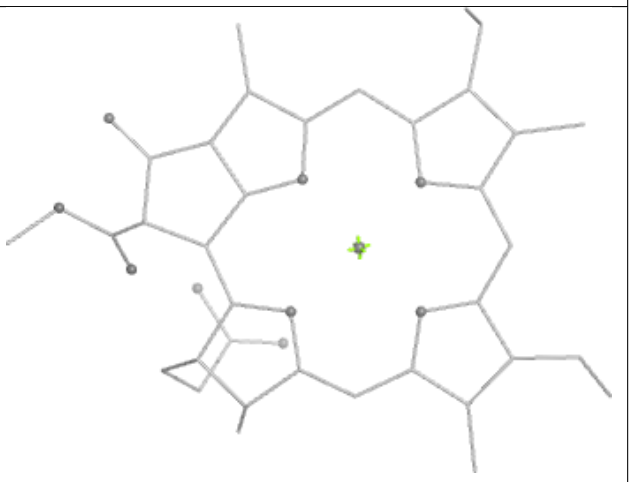
Bond lengths



Bond angles

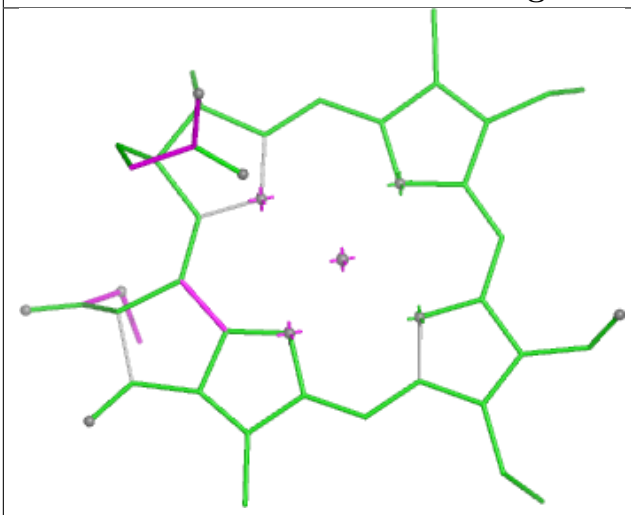


Torsions

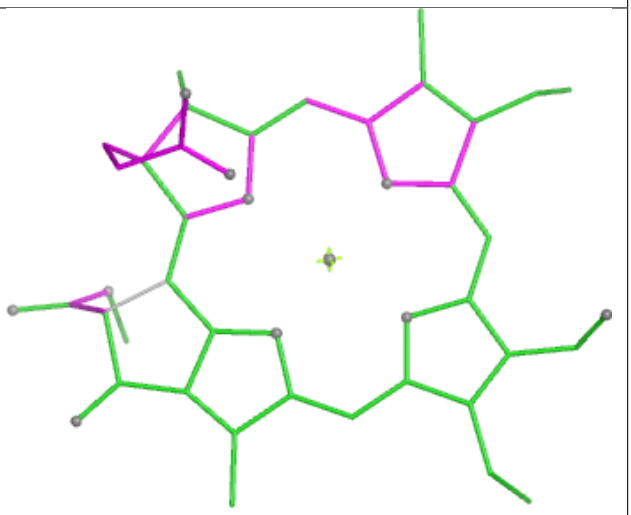


Rings

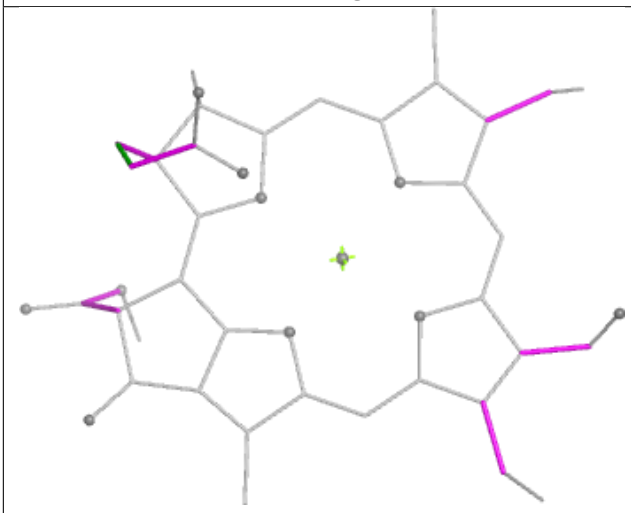
Ligand CHL 8 307



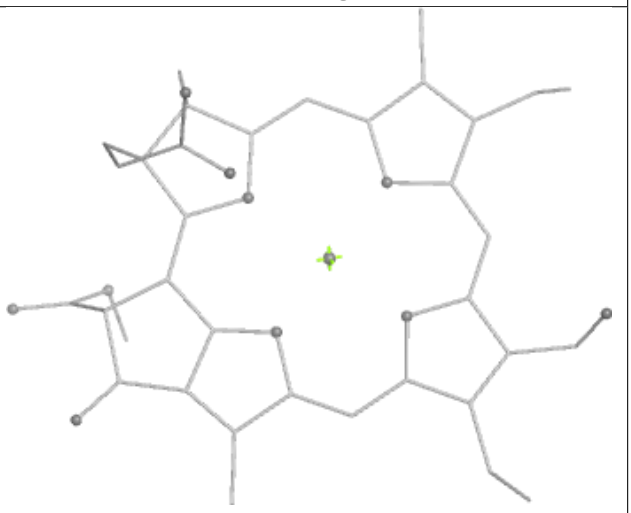
Bond lengths



Bond angles

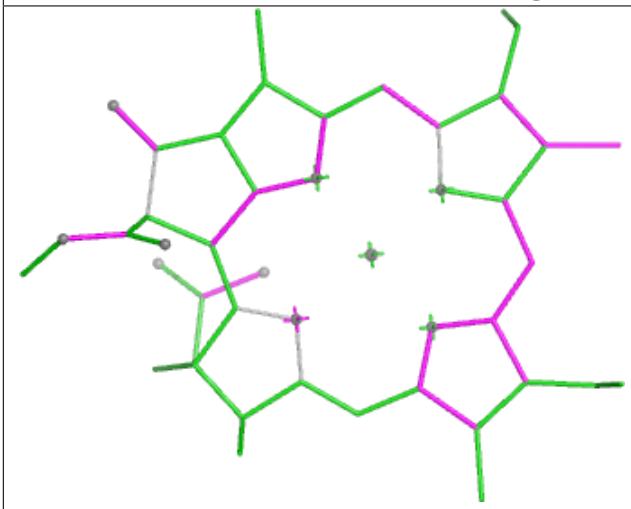


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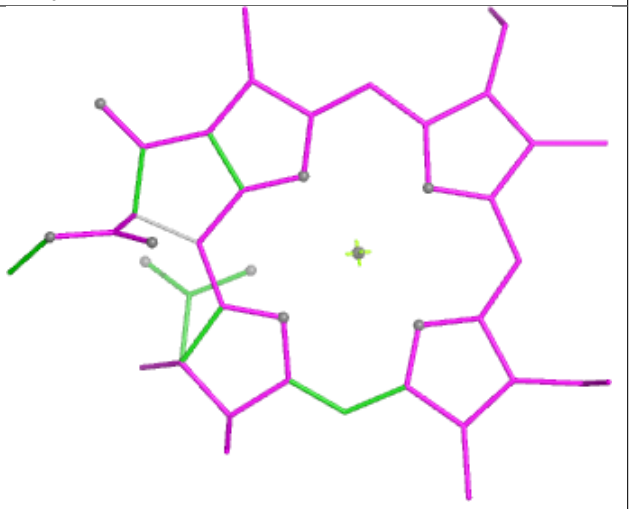


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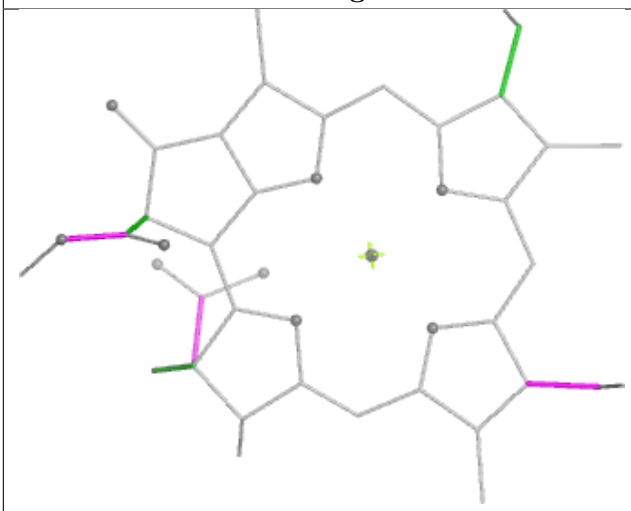
Ligand CLA y 613



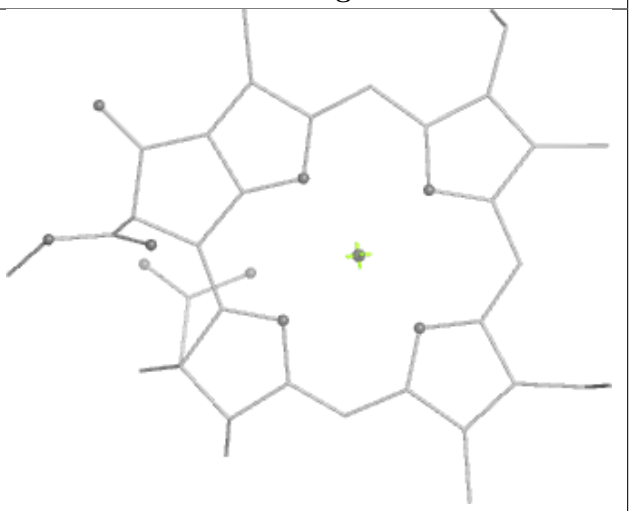
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Bond angles

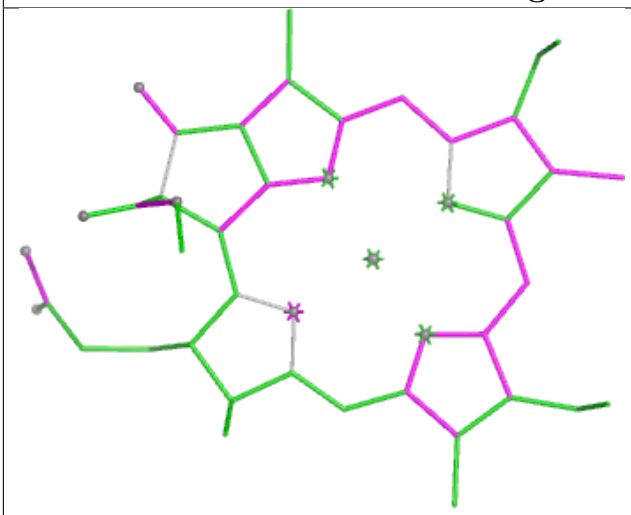


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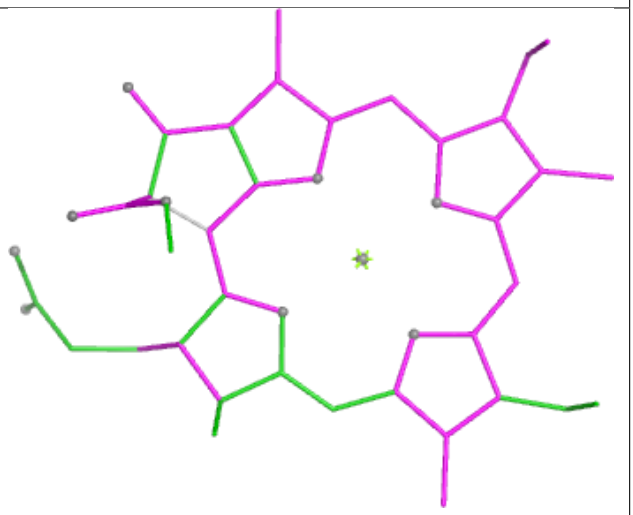


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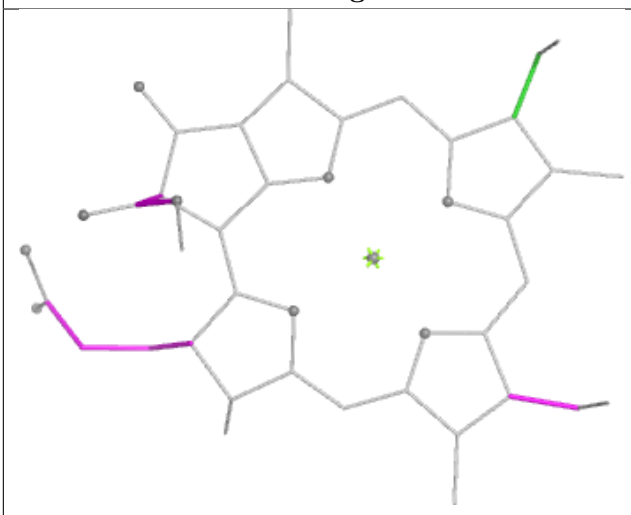
Ligand CLA 4 304



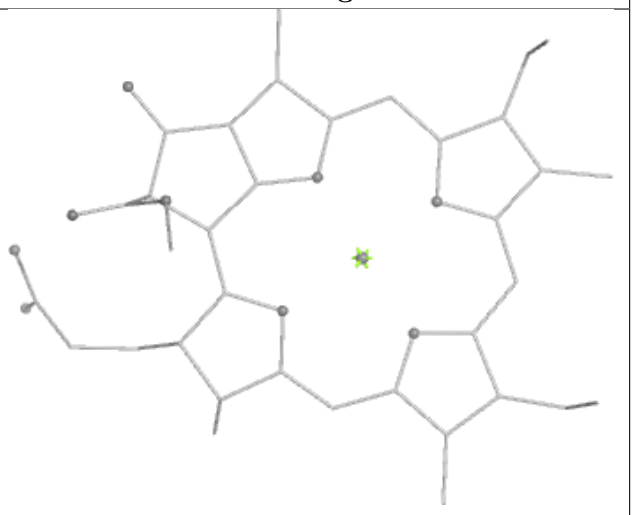
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Bond angles

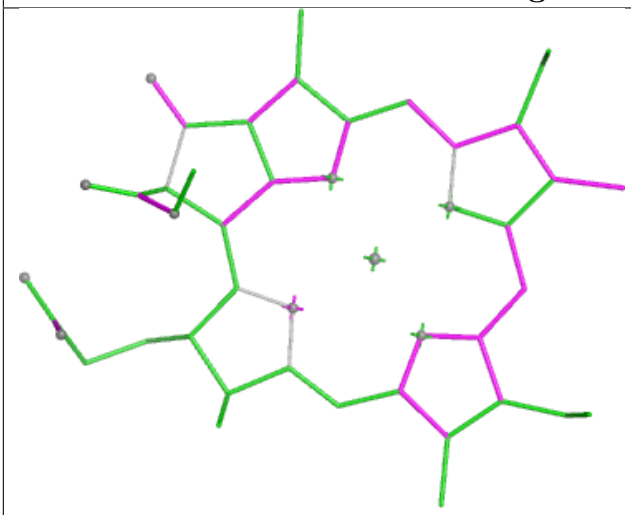


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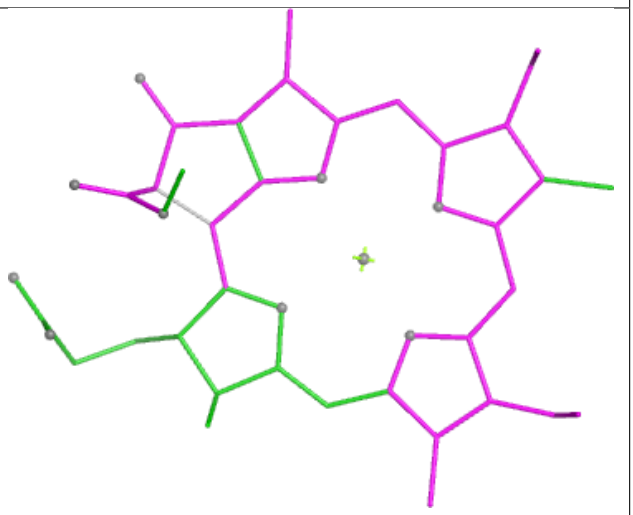


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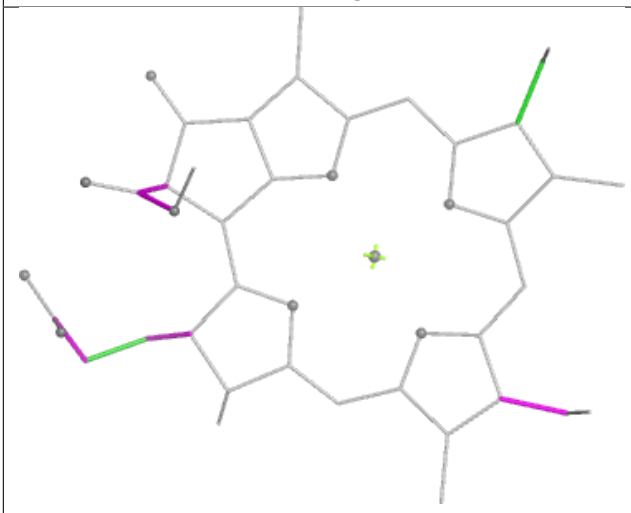
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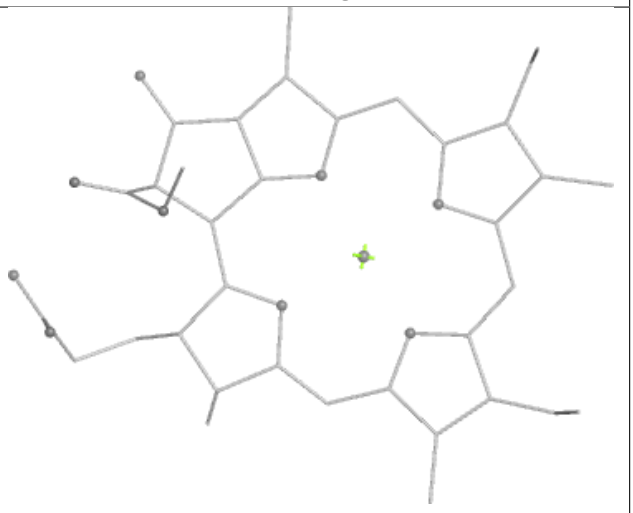
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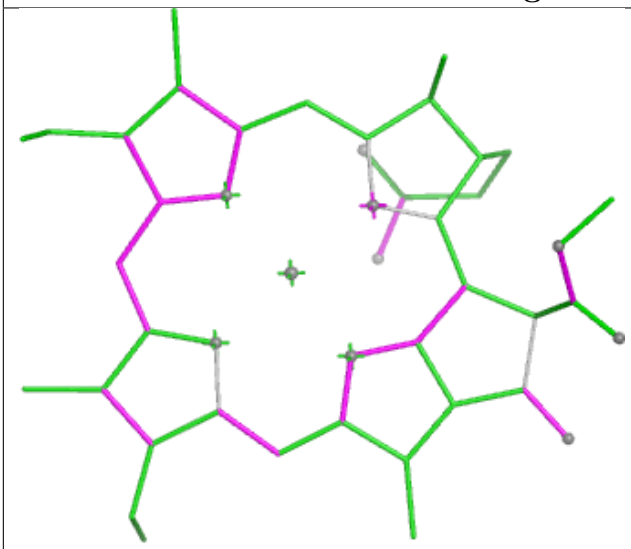


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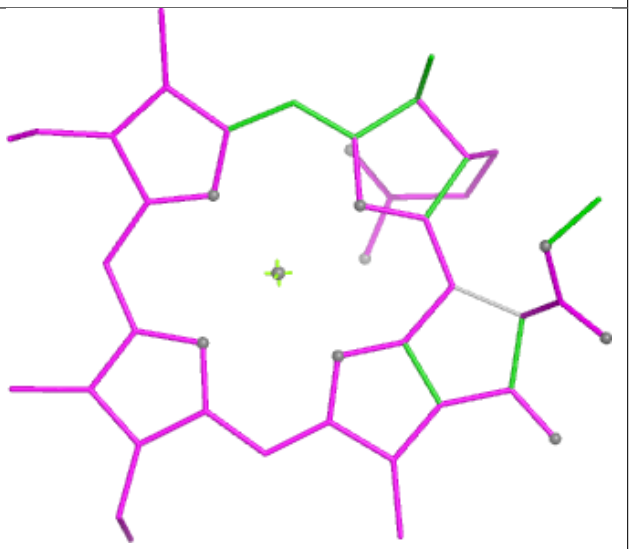


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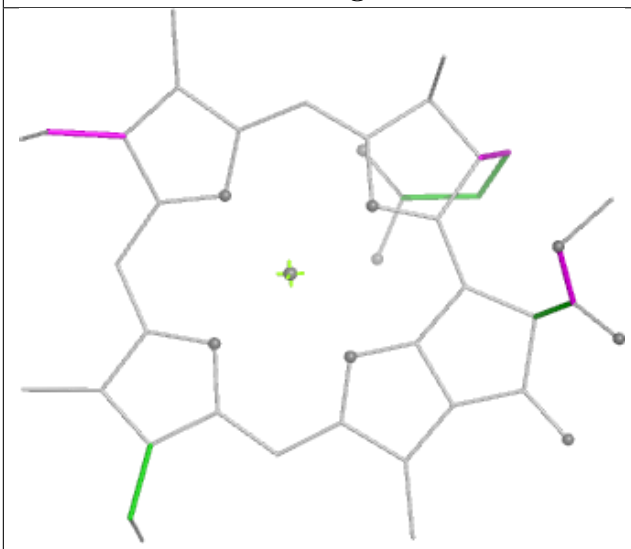
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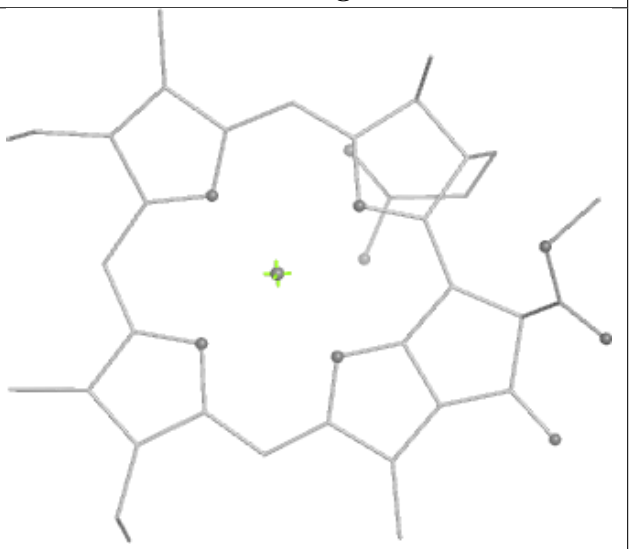
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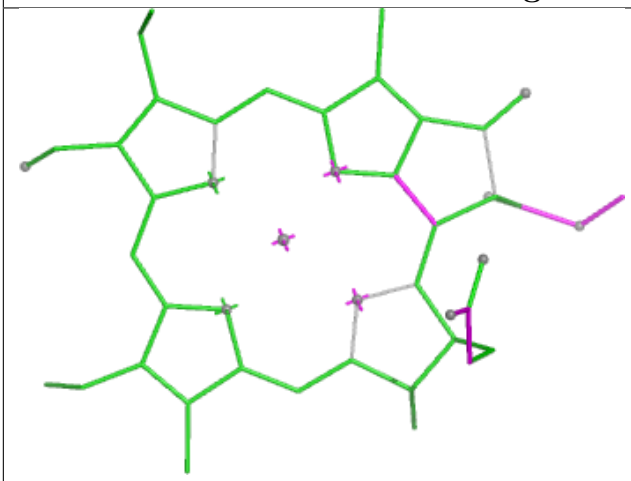


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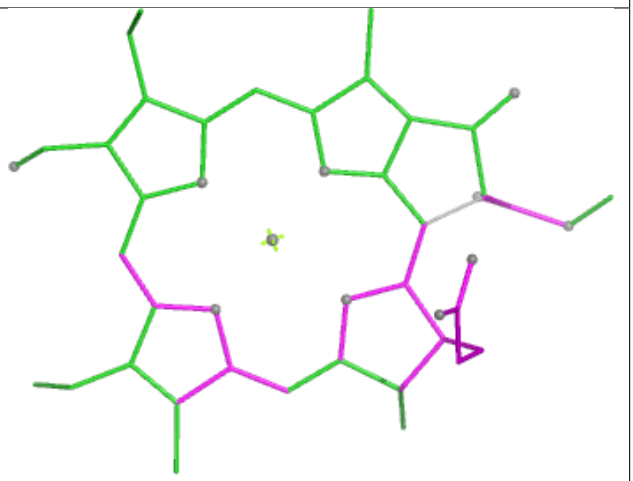


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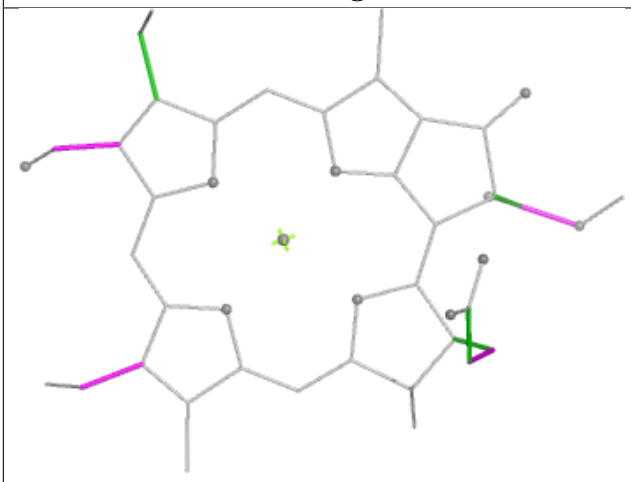
Ligand CHL Y 607



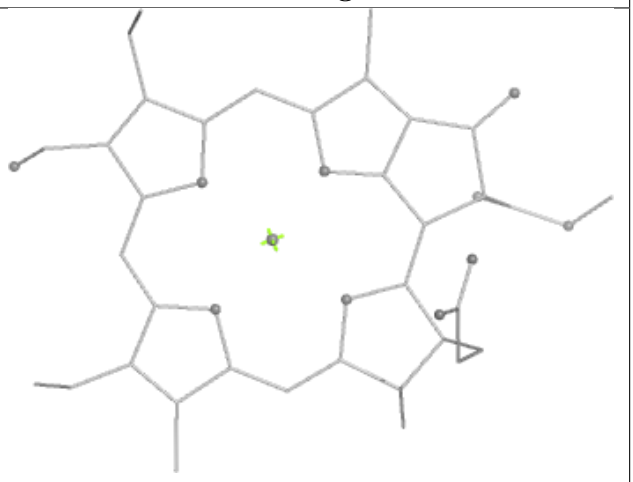
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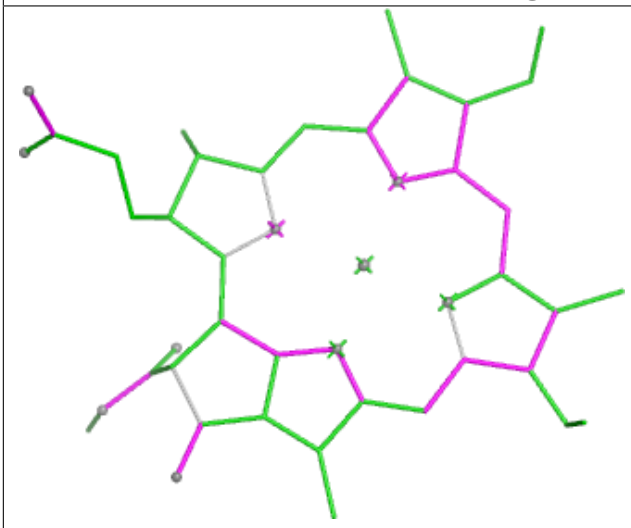
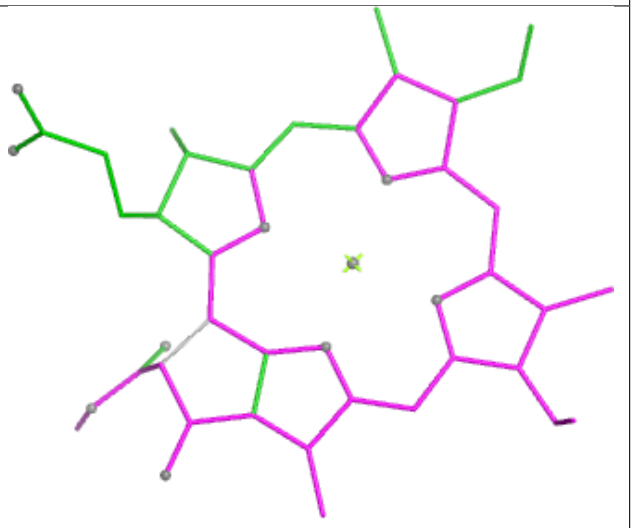
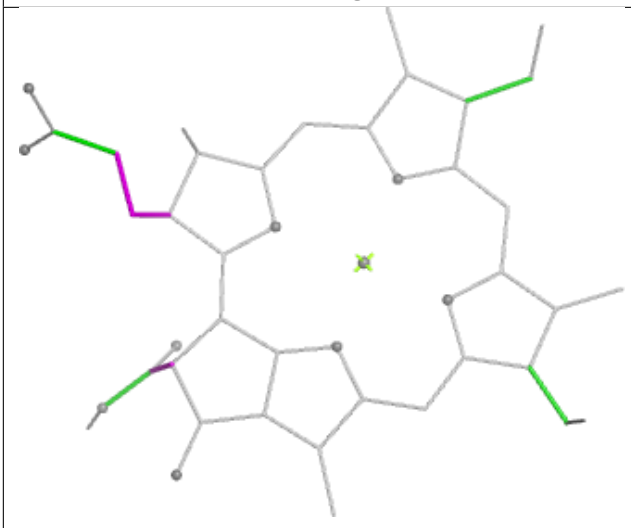
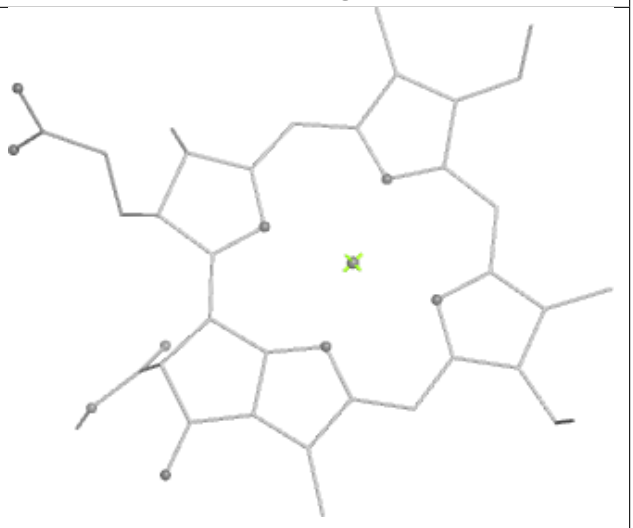
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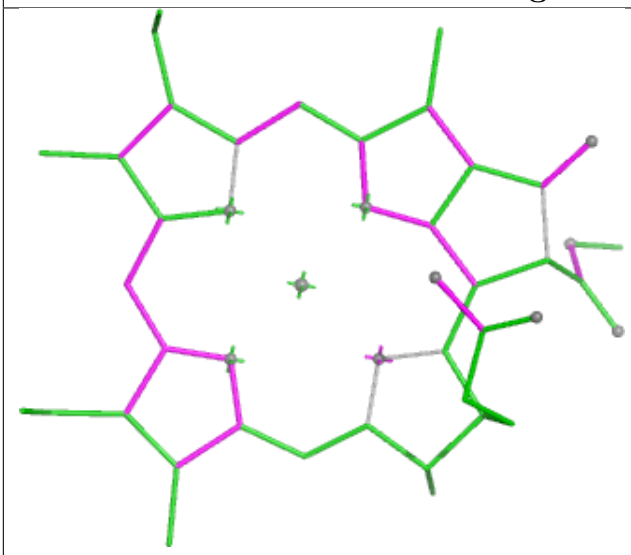
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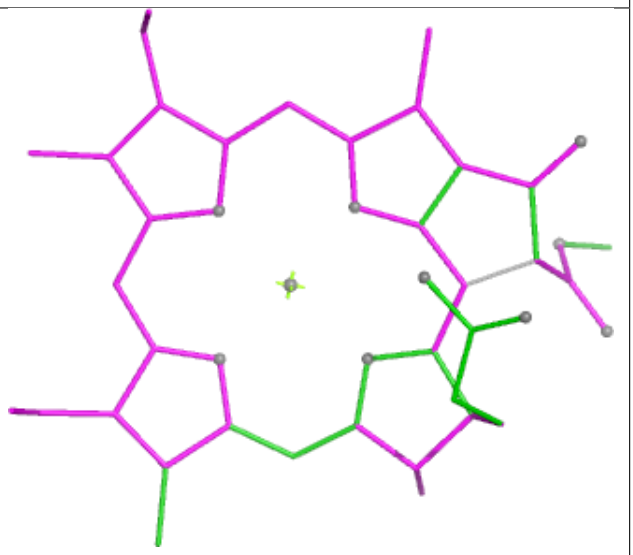
Rings

Ligand CLA A 405	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

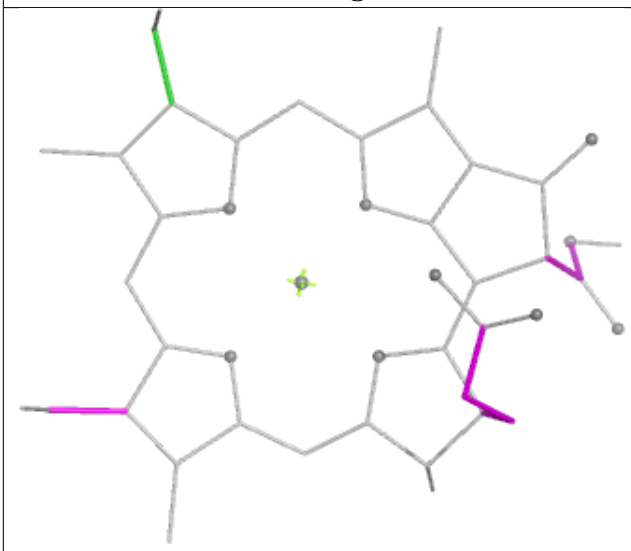
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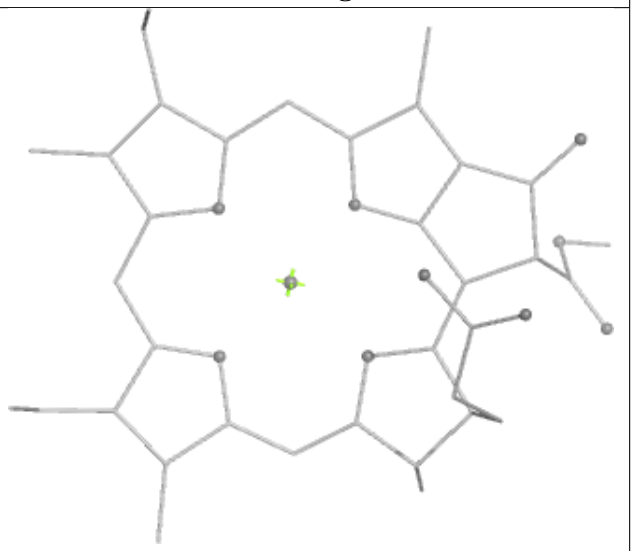
Bond lengths



Bond angles

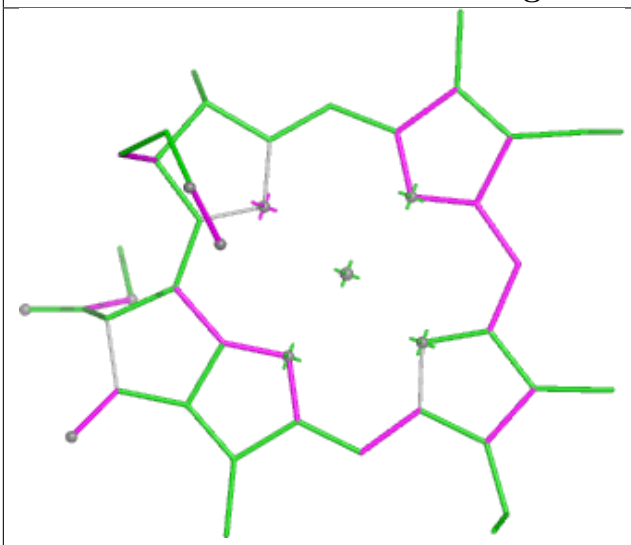


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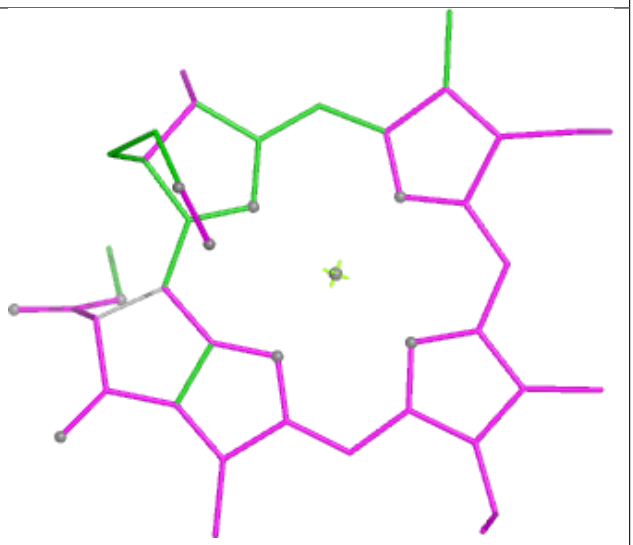


Rings

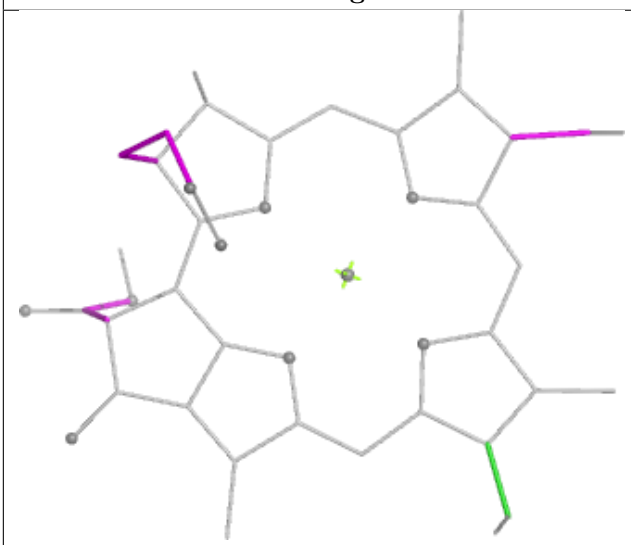
Ligand CLA N 602



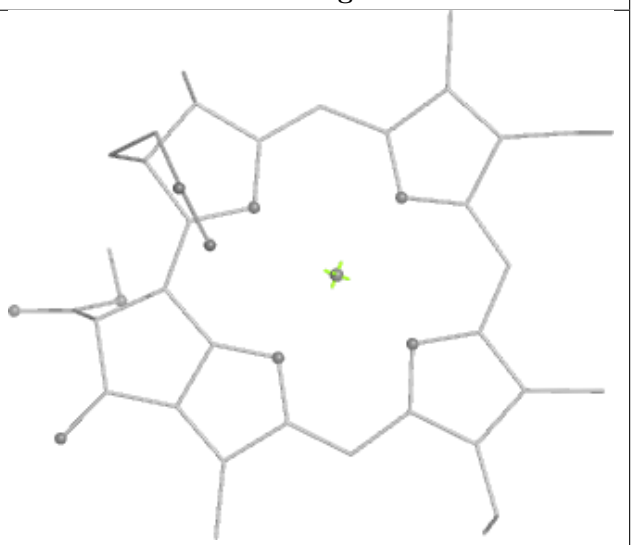
Bond lengths



Bond angles

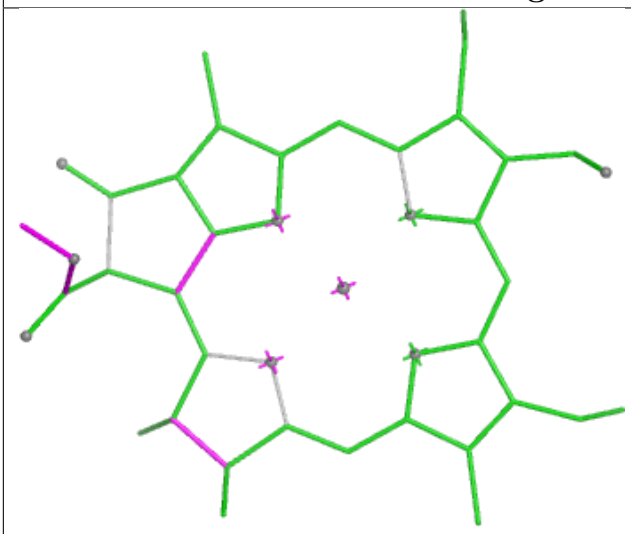


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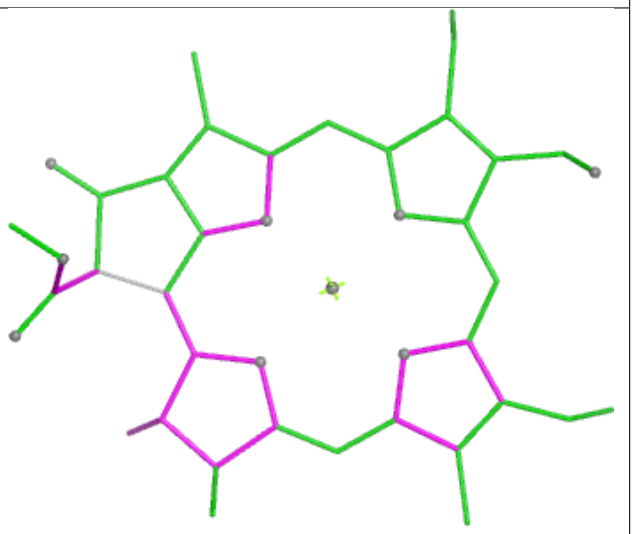


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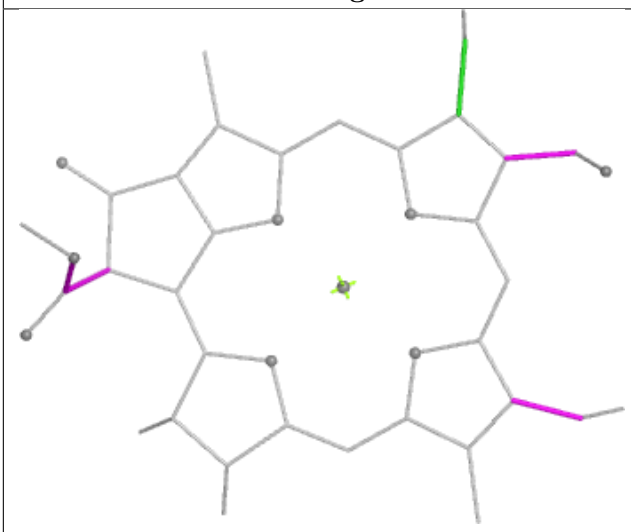
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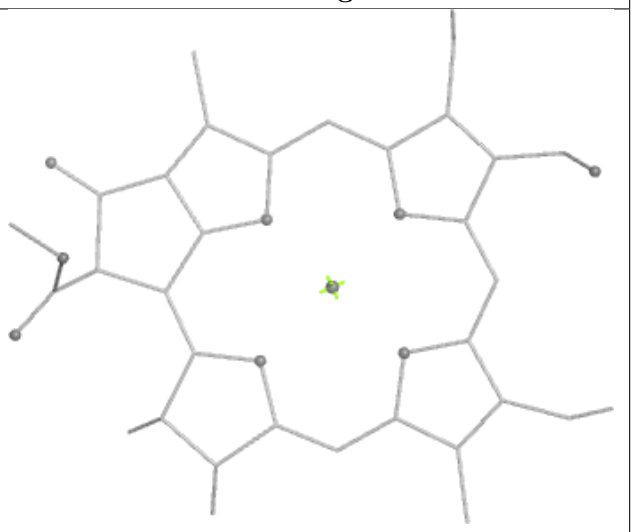
Bond lengths



Bond angles

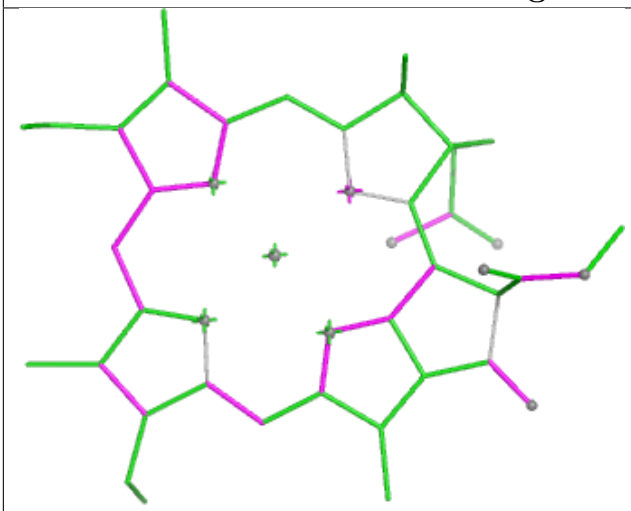


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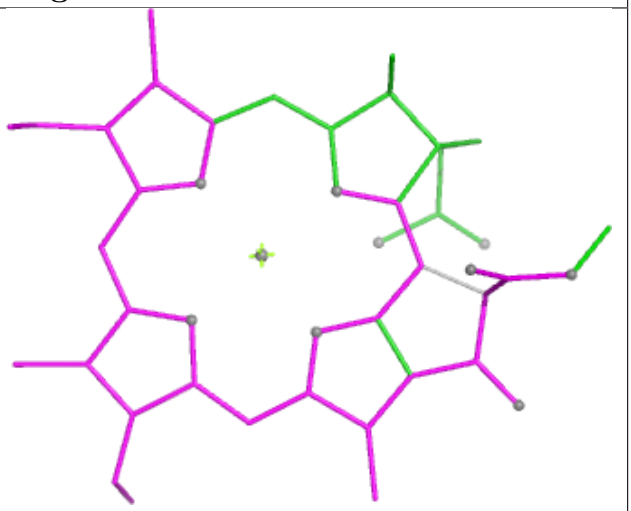


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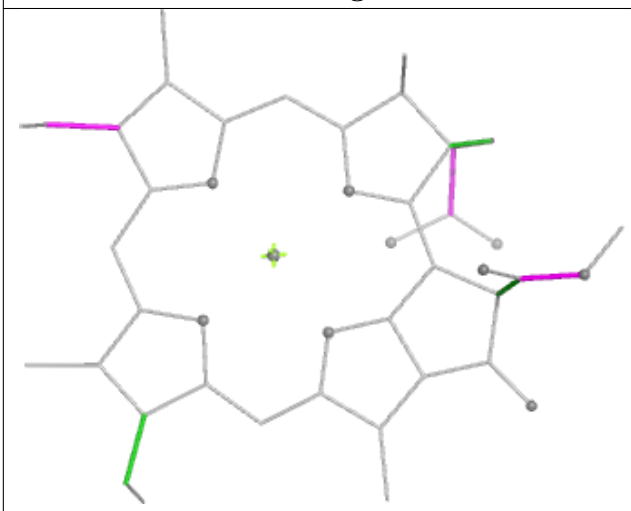
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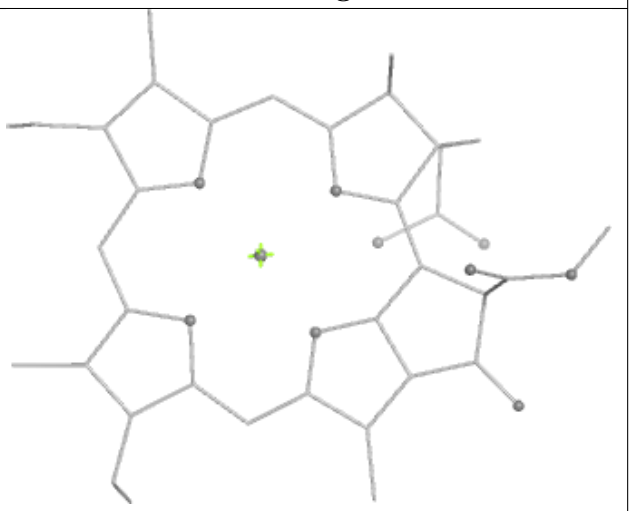
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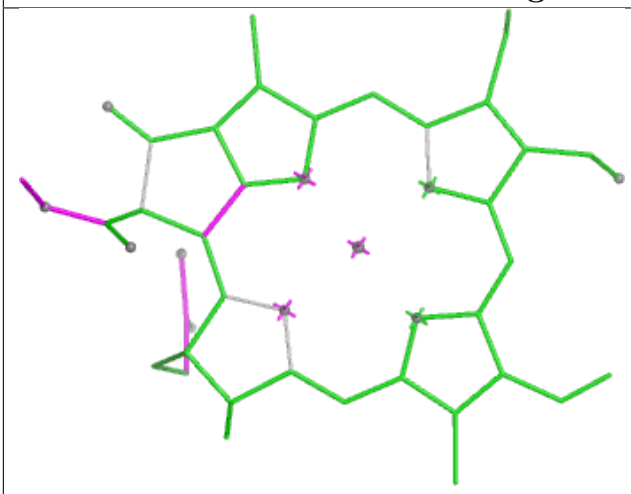


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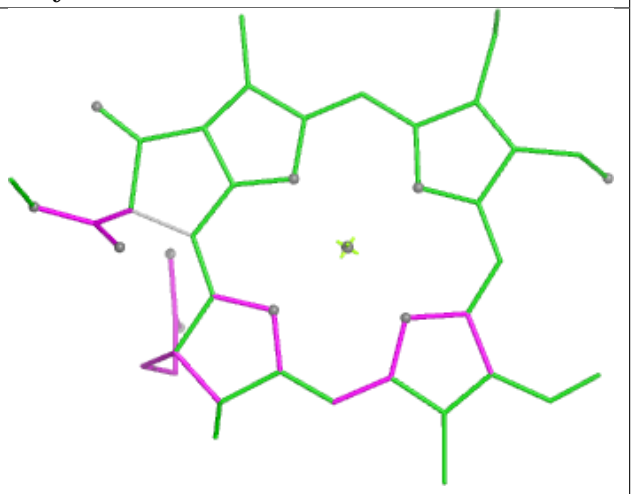


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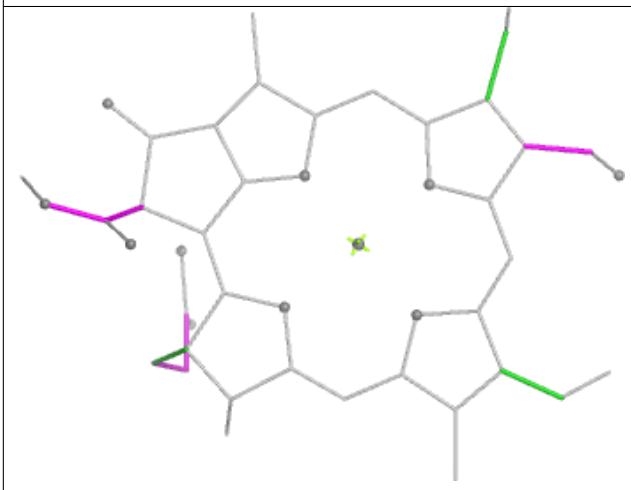
Ligand CHL y 608



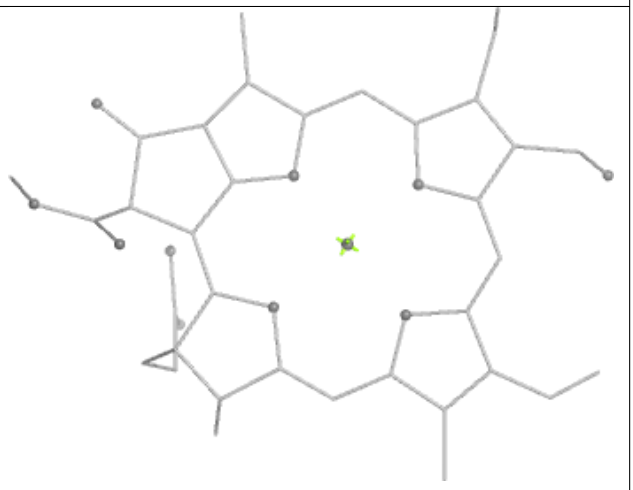
Bond lengths



Bond angles

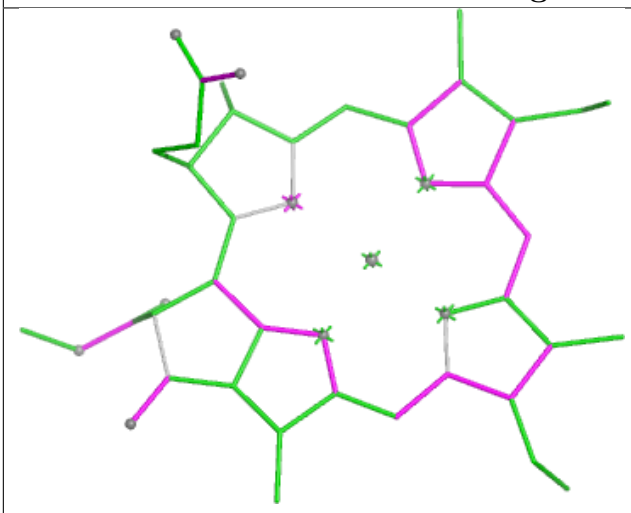


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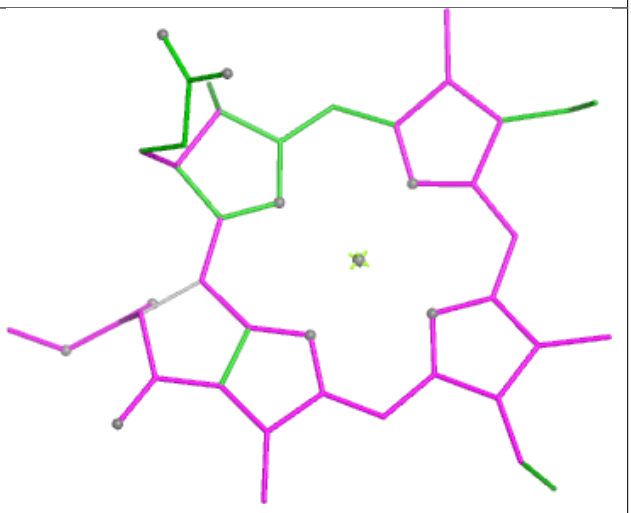


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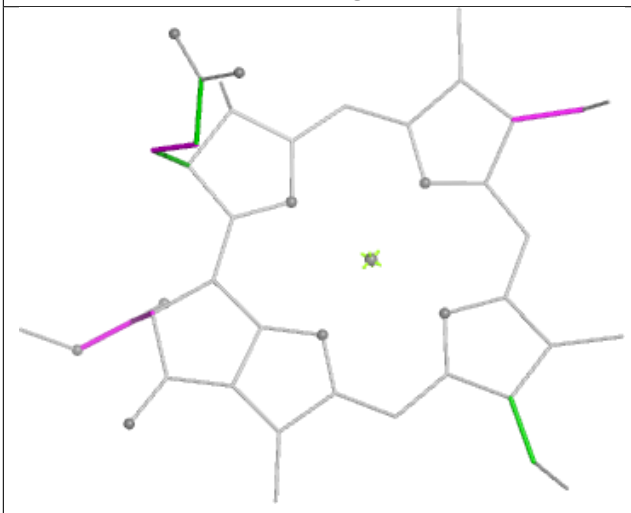
Ligand CLA s 309



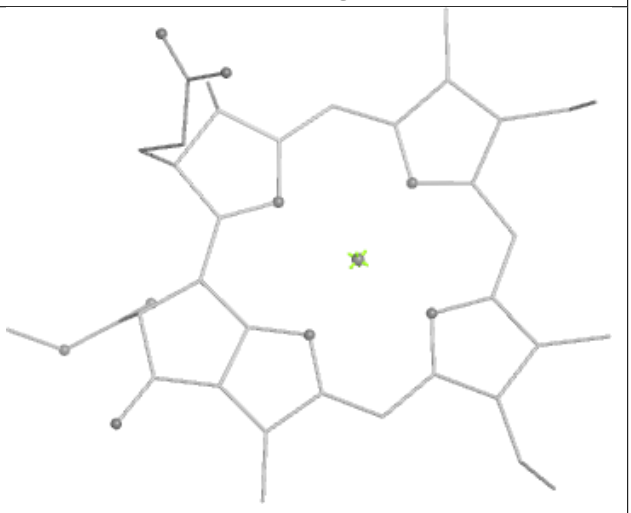
Bond lengths



Bond angles

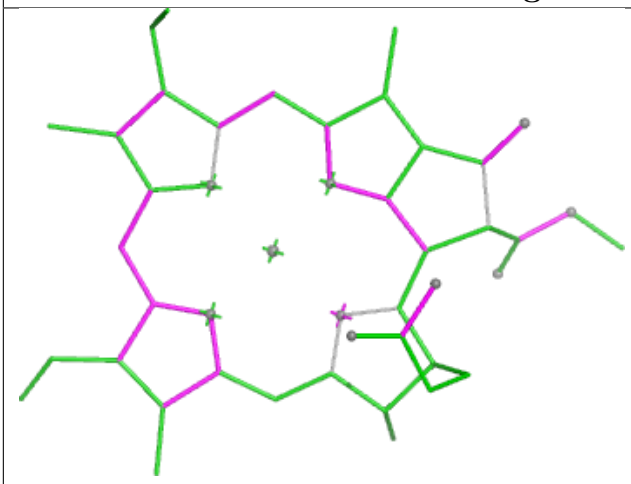


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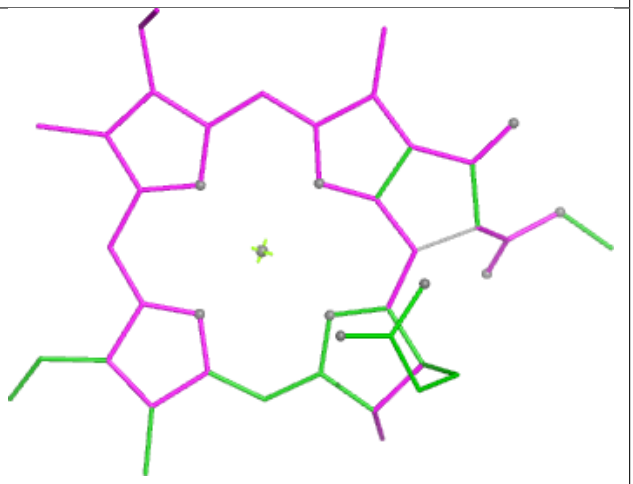


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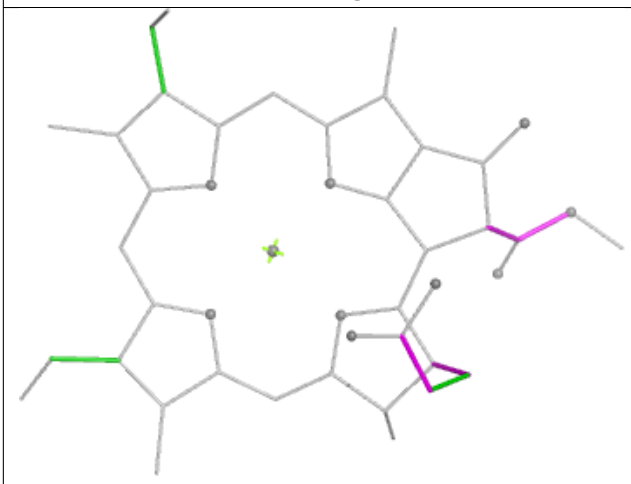
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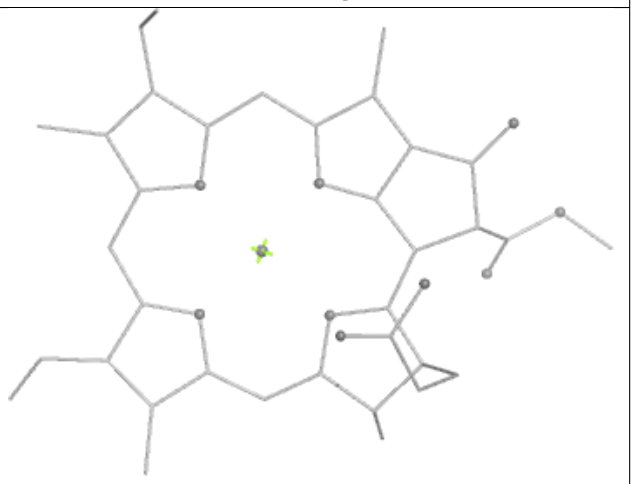
Bond lengths



Bond angles

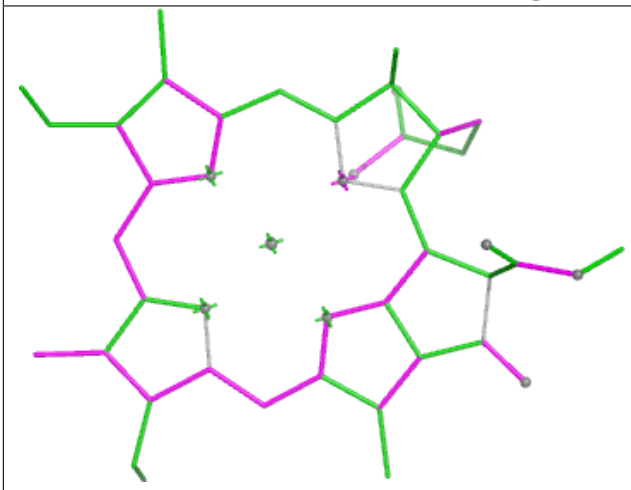


Torsions

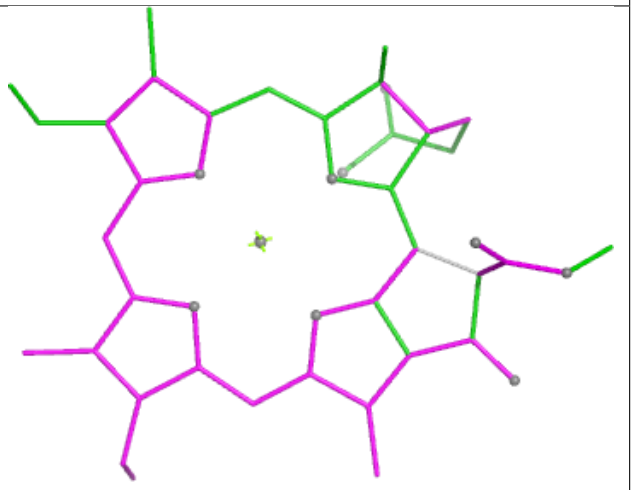


Rings

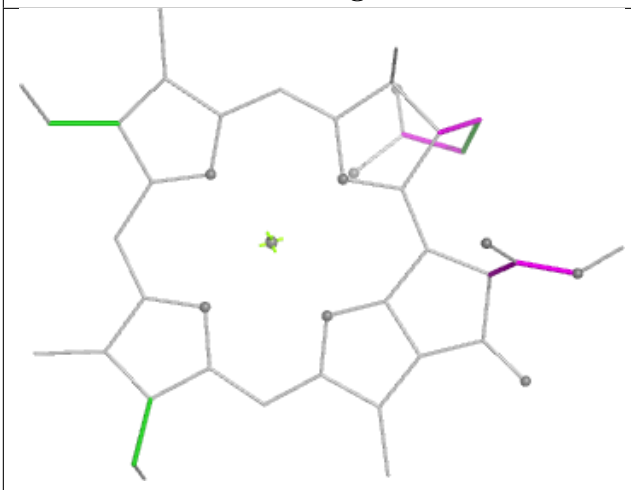
Ligand CLA n 614



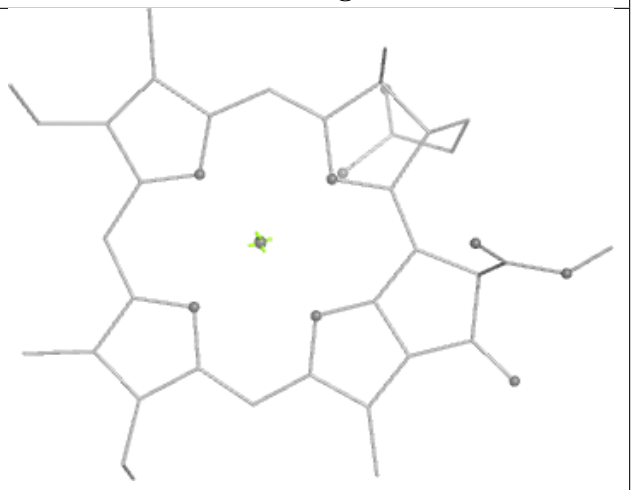
Bond lengths



Bond angles

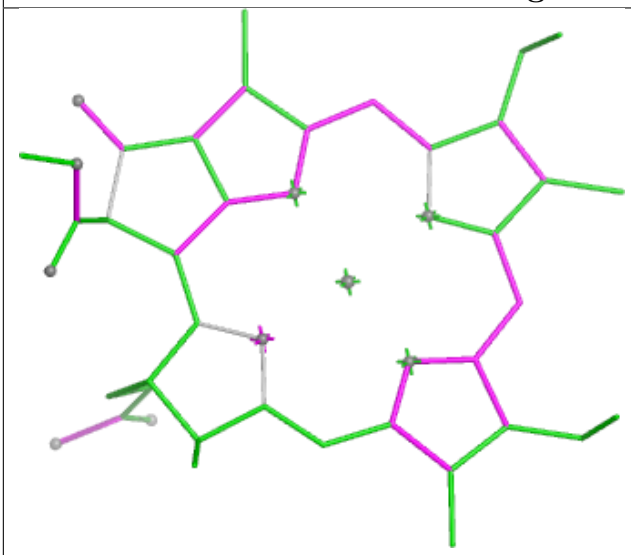


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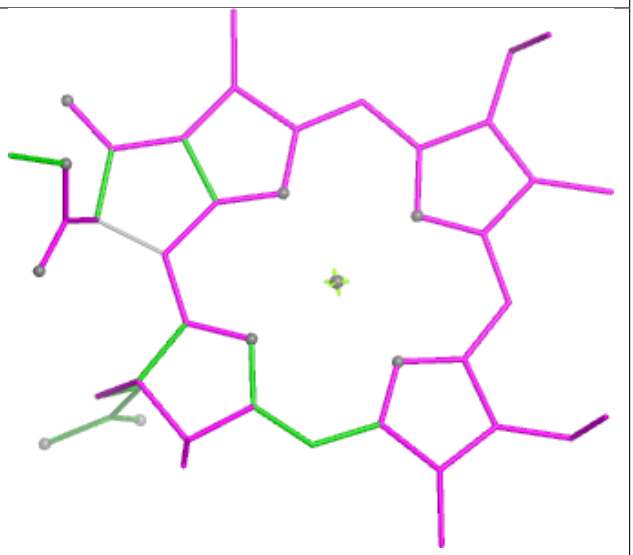


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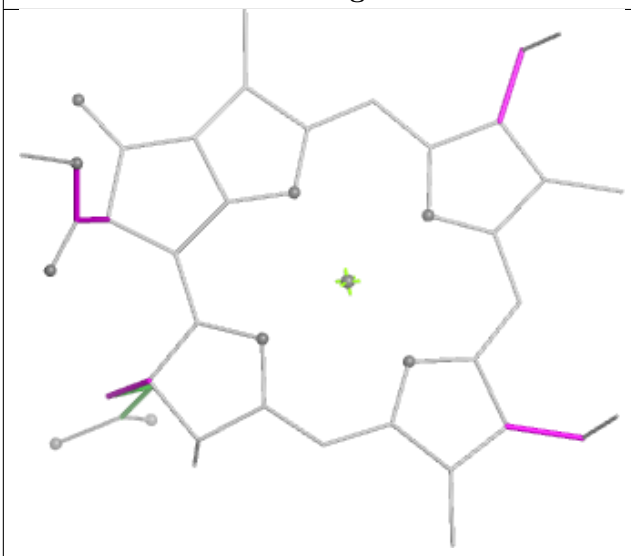
Ligand CLA b 604



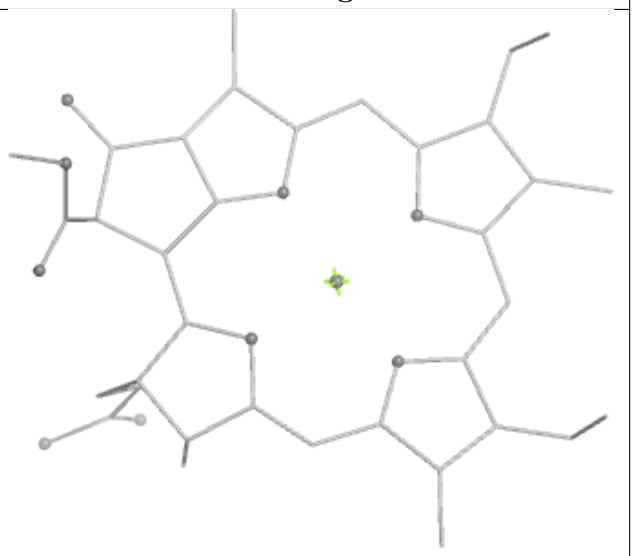
Bond lengths



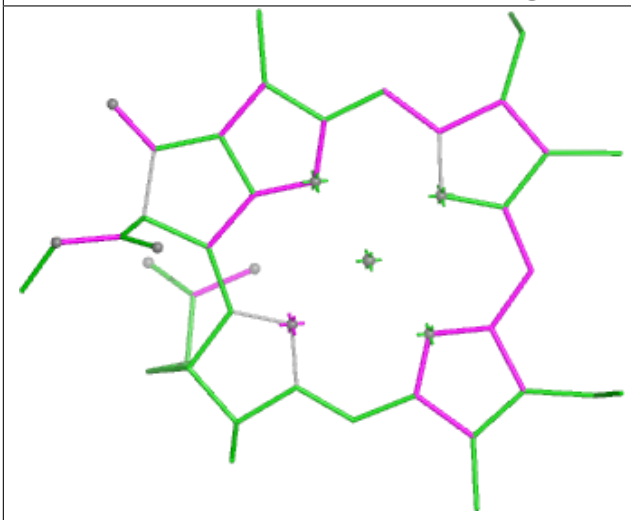
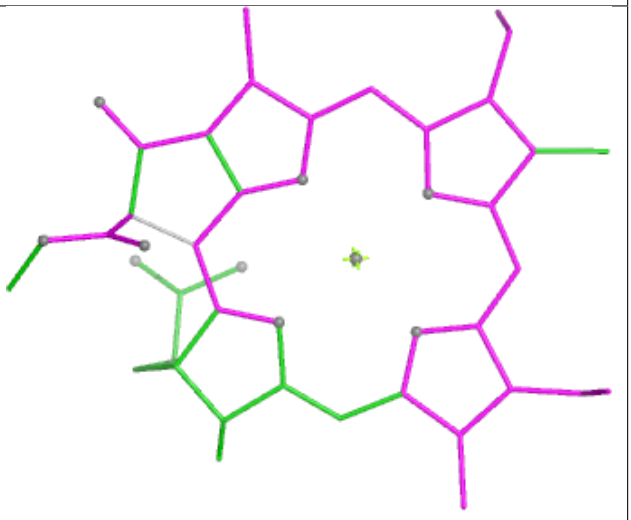
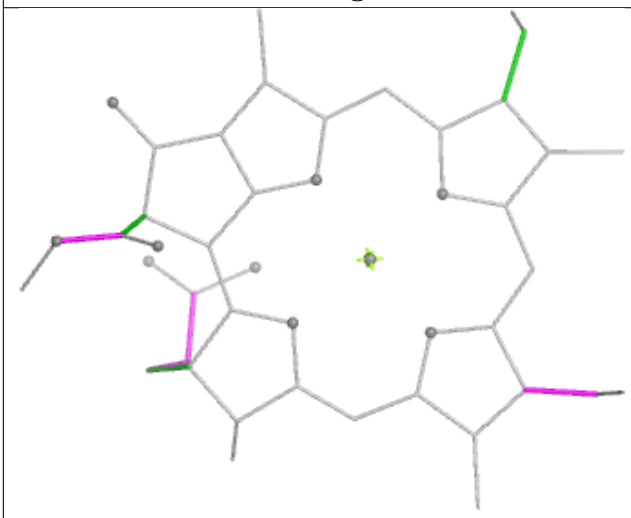
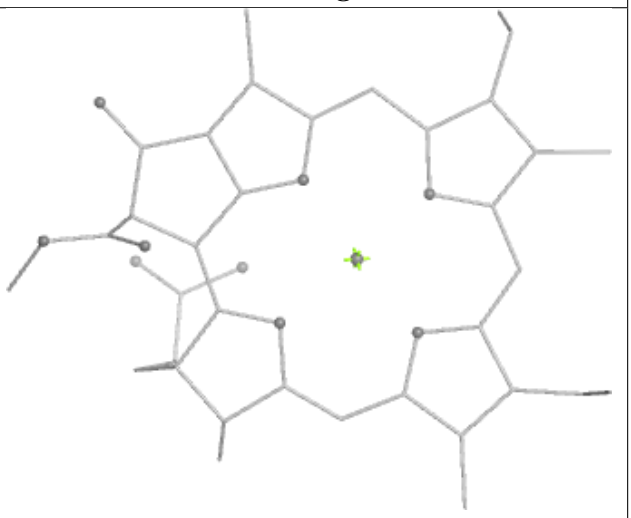
Bond angles



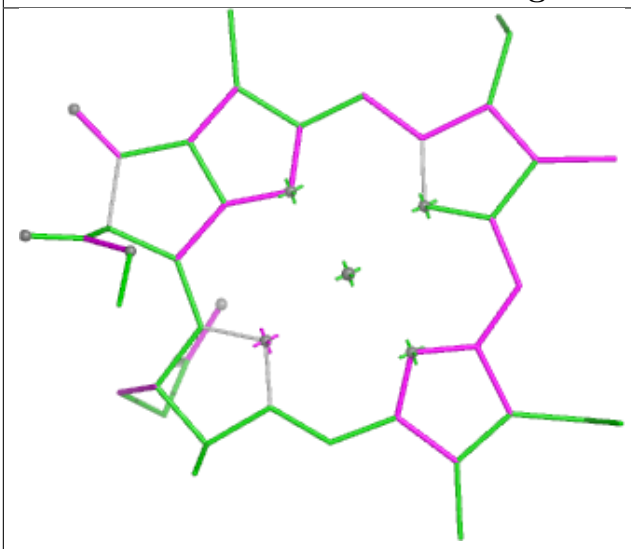
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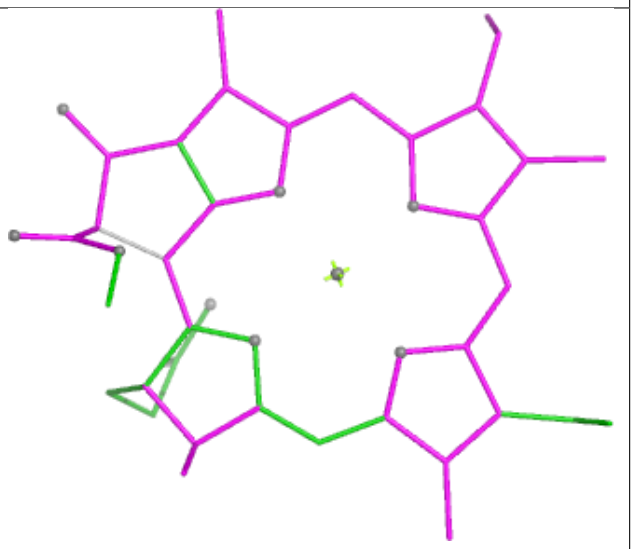
Rings

Ligand CLA N 613	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

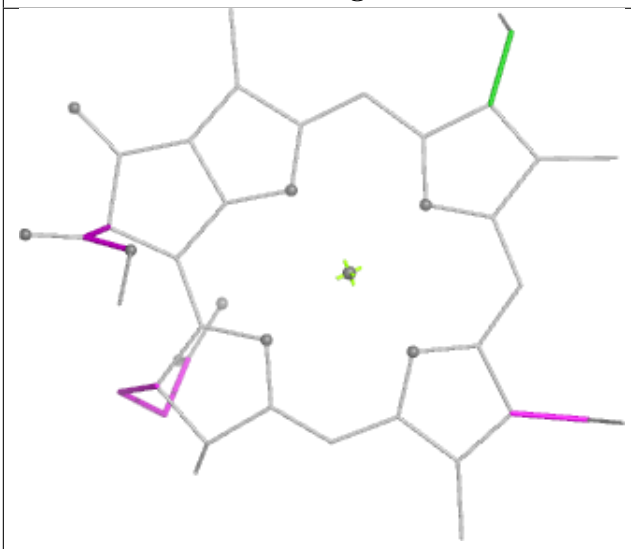
Ligand CLA 7 303



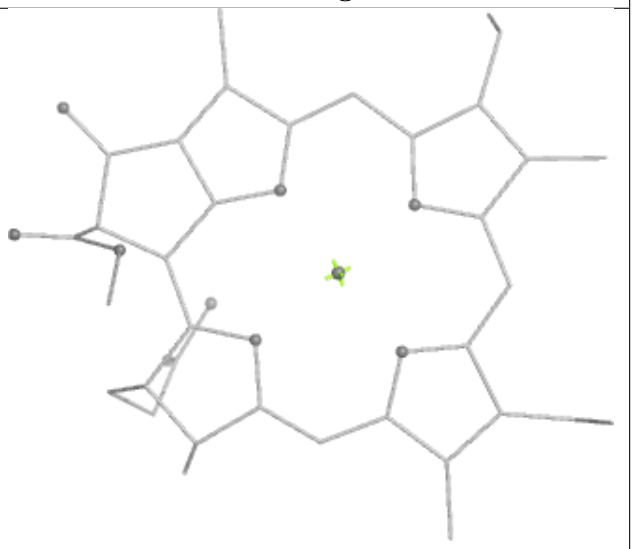
Bond lengths



Bond angles

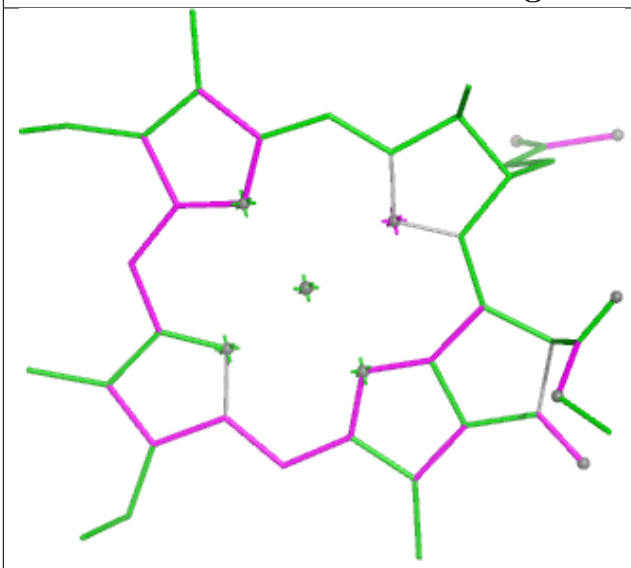


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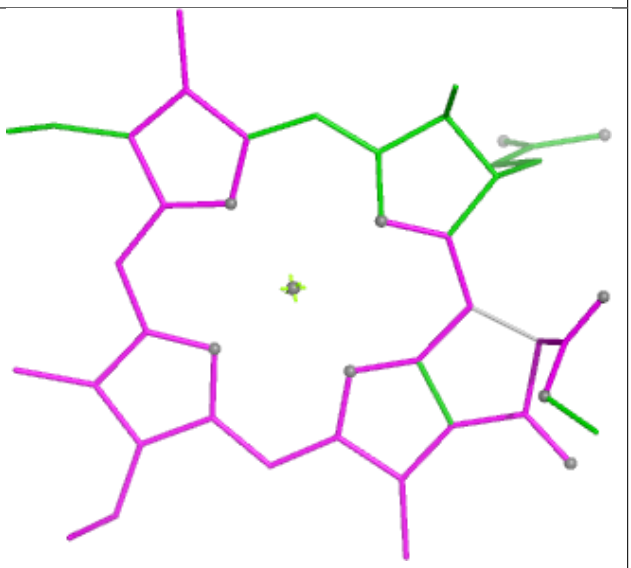


Rings

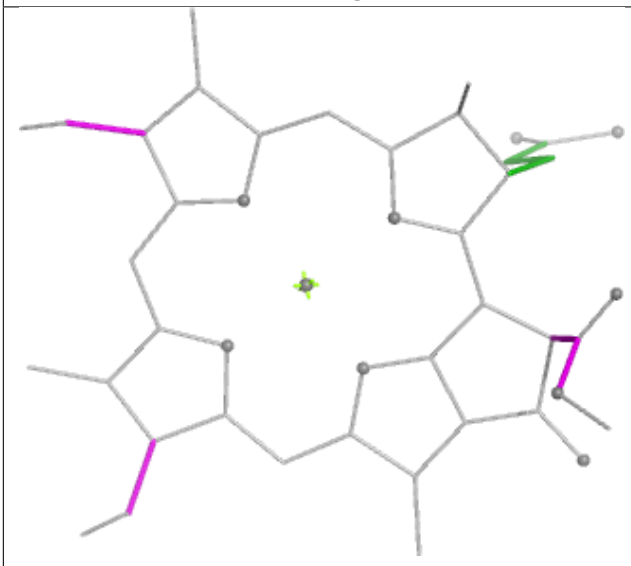
Ligand CLA B 604



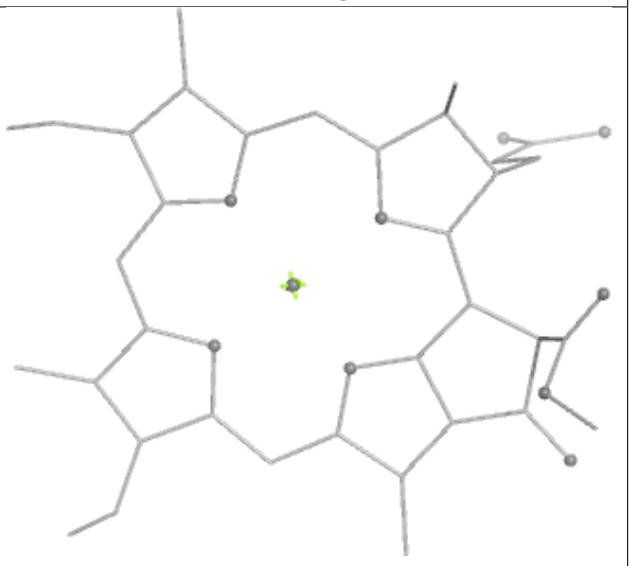
Bond lengths



Bond angles

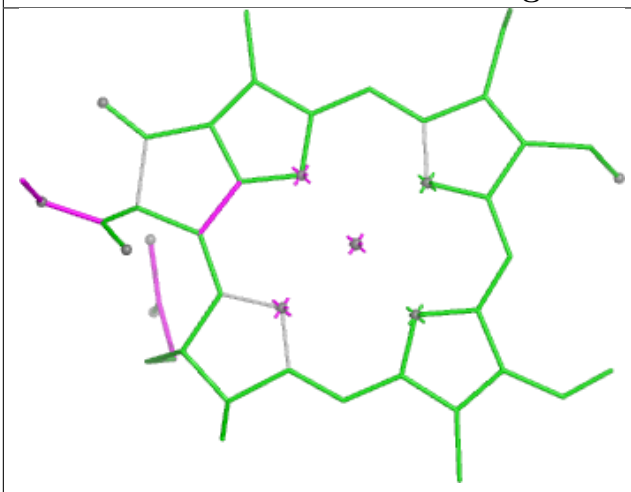


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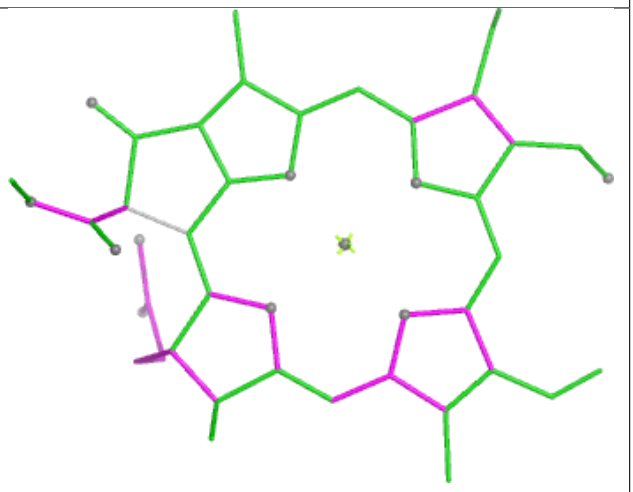


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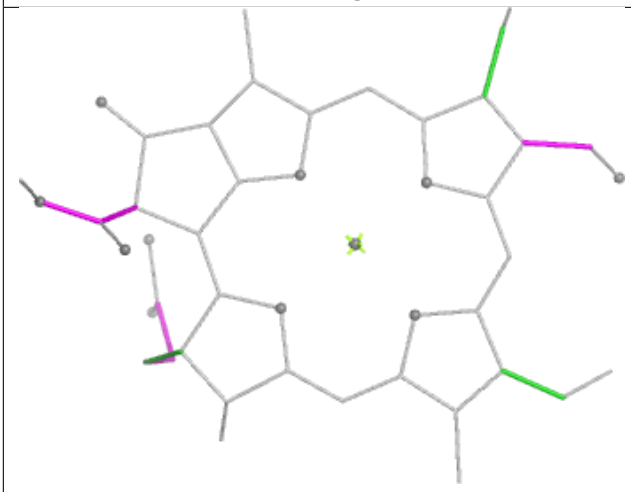
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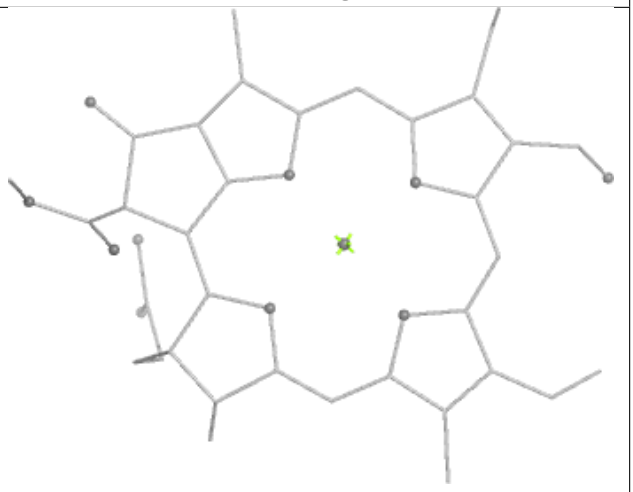
Bond lengths



Bond angles

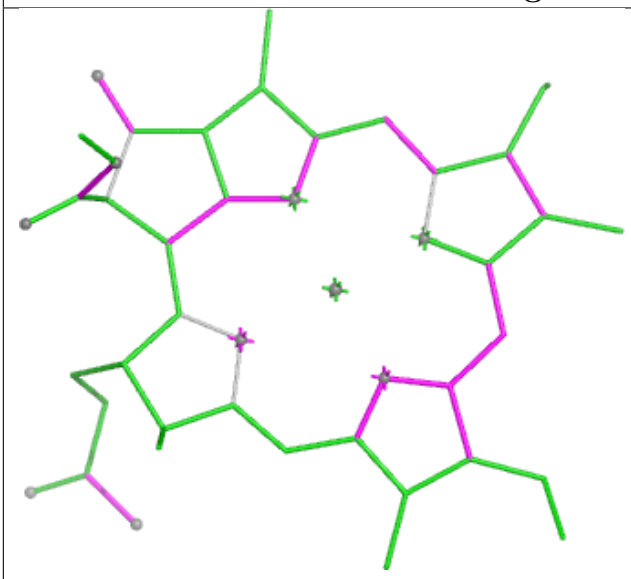


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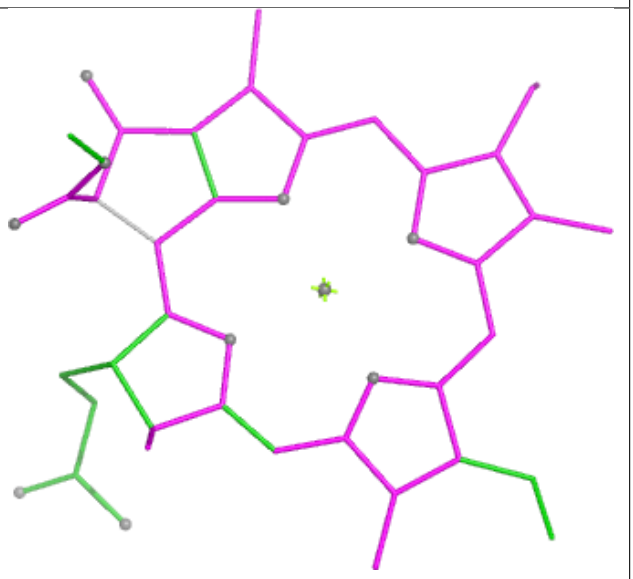


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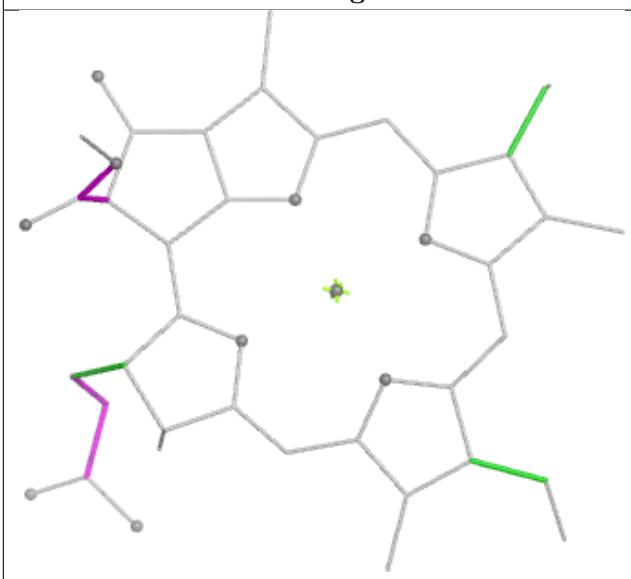
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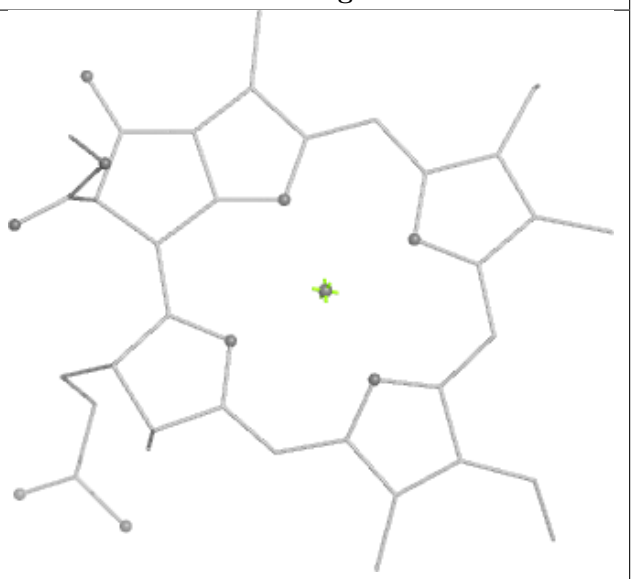
Bond lengths



Bond angles

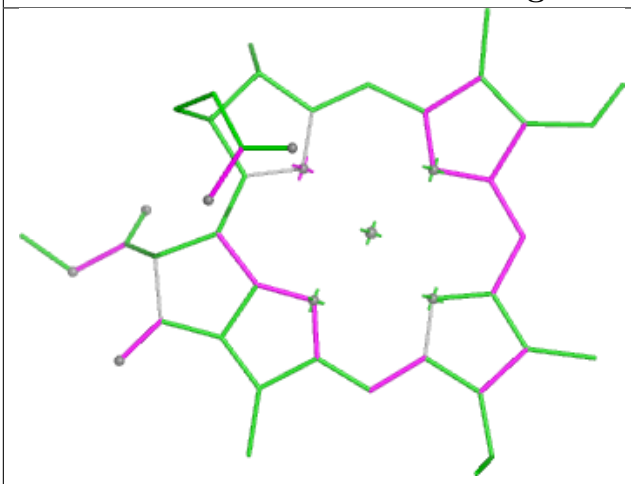


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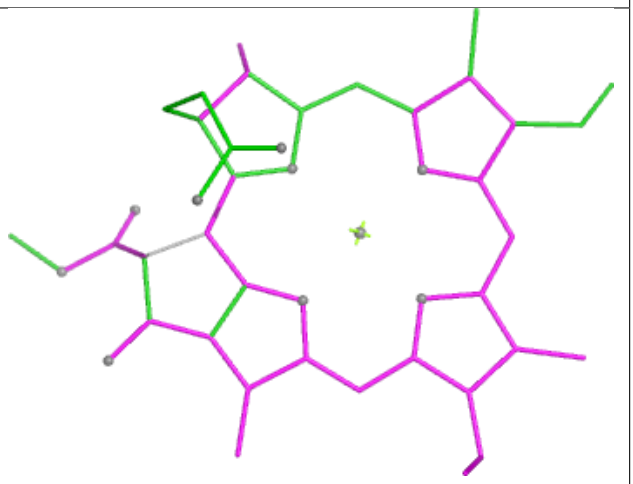


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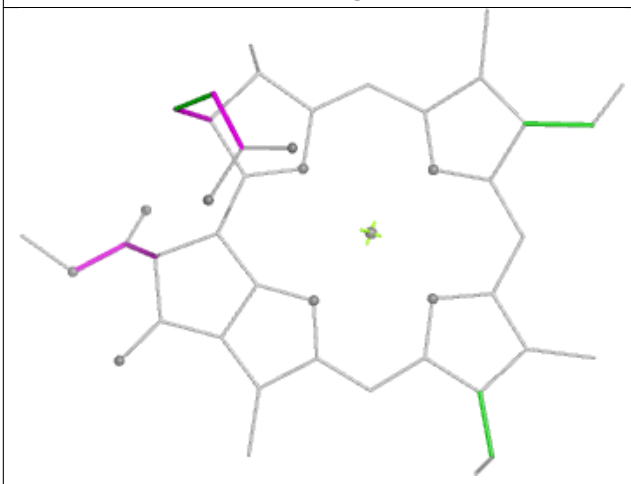
Ligand CLA n 610



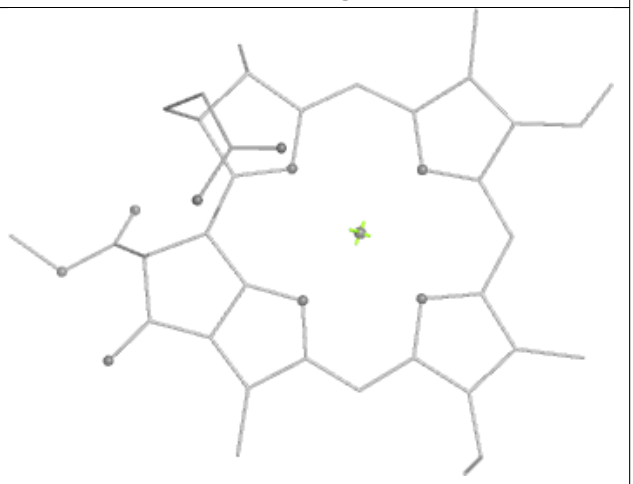
Bond lengths



Bond angles

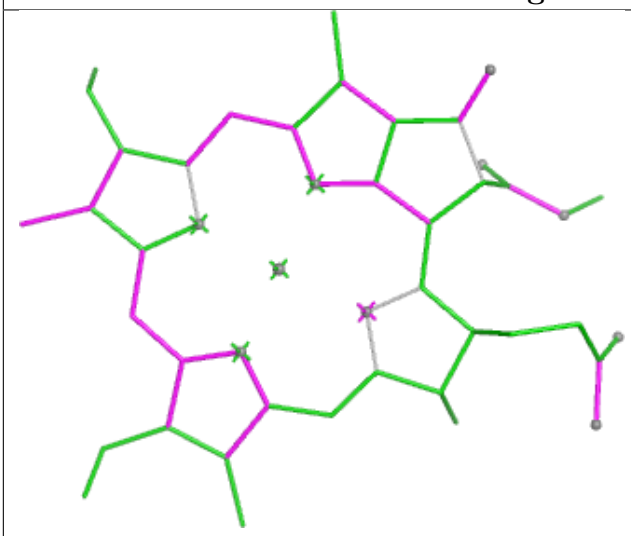


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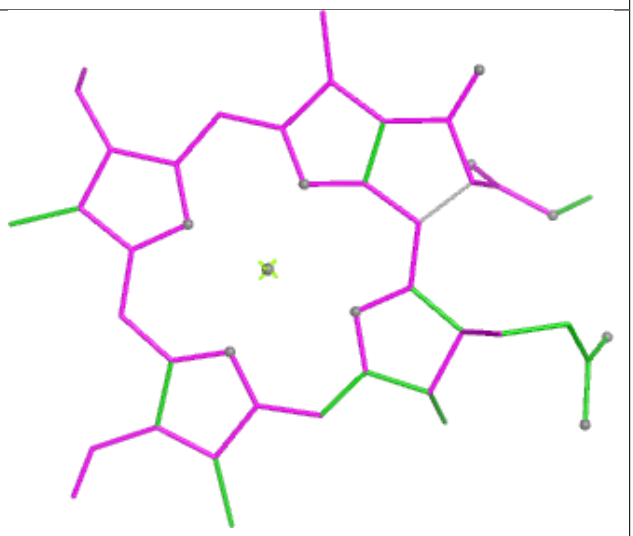


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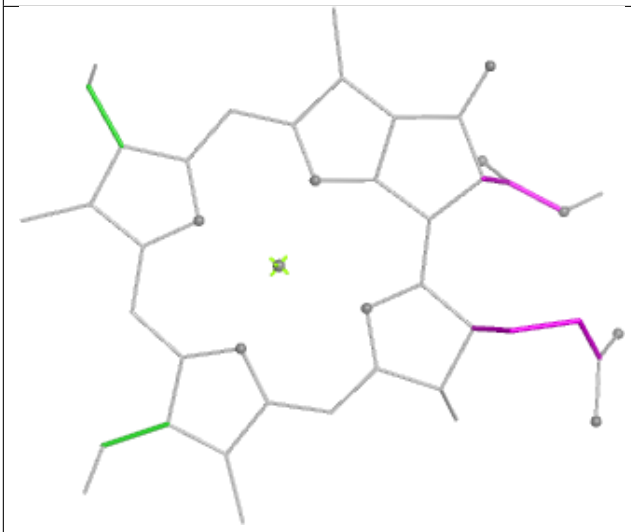
Ligand CLA b 615



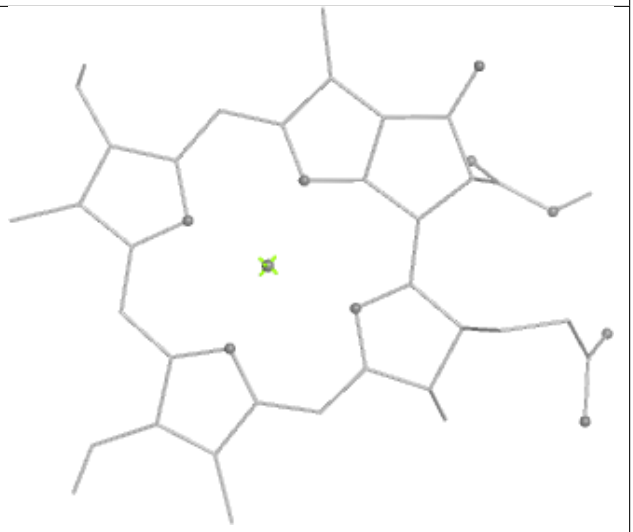
Bond lengths



Bond angles

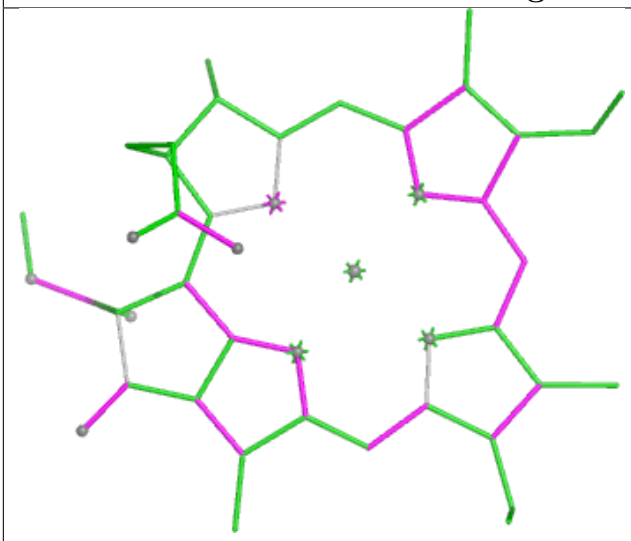


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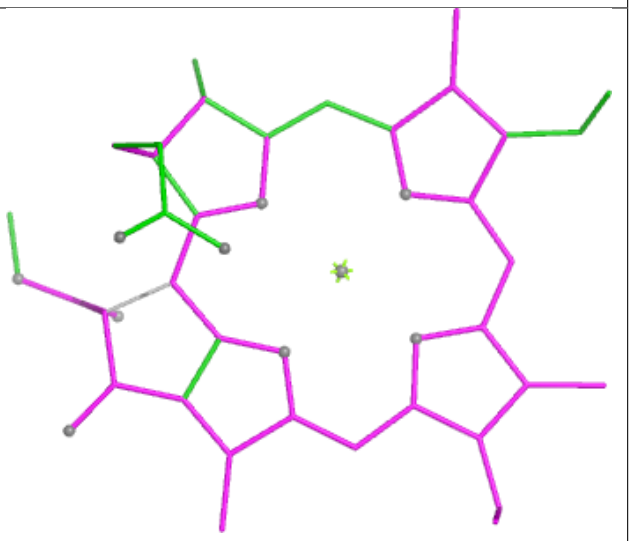


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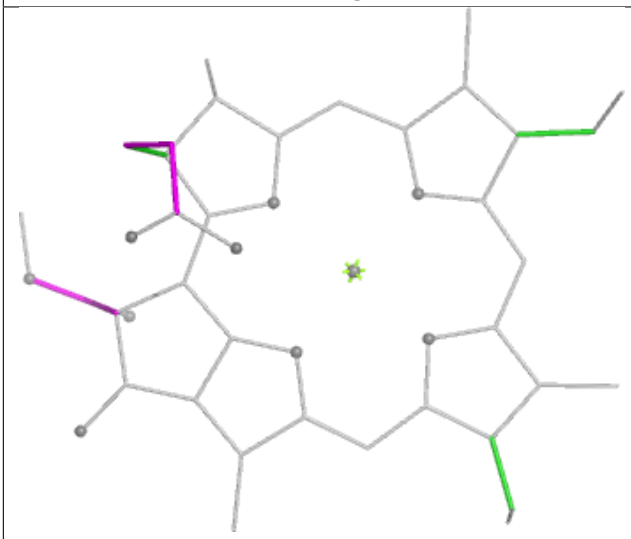
Ligand CLA n 611



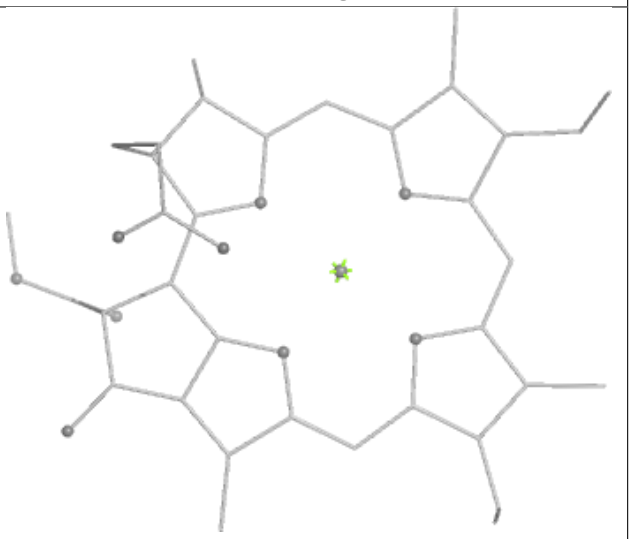
Bond lengths



Bond angles

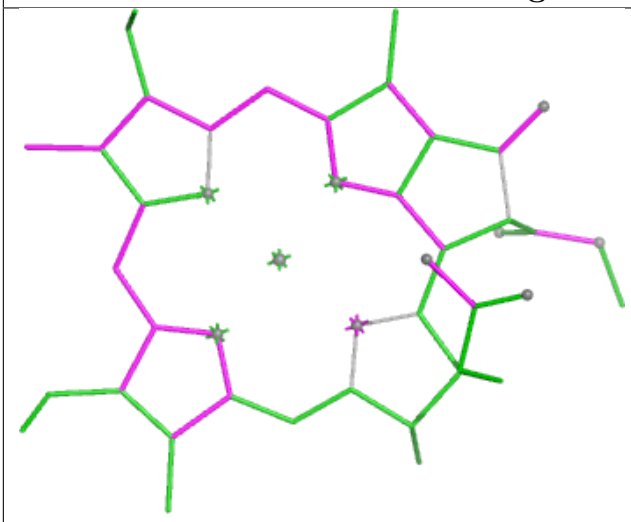


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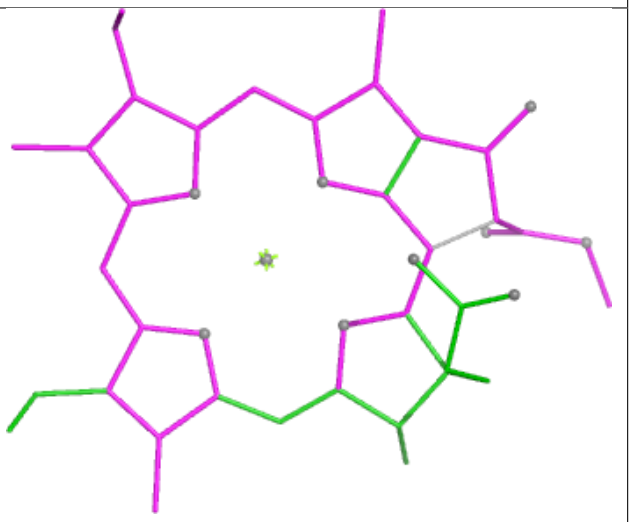


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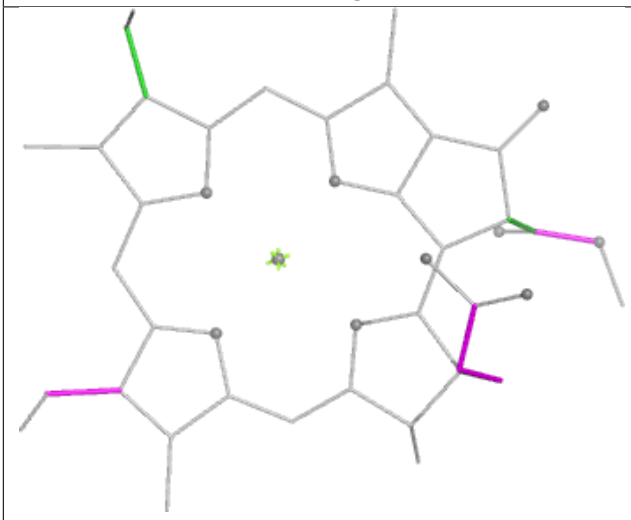
Ligand CLA 7 311



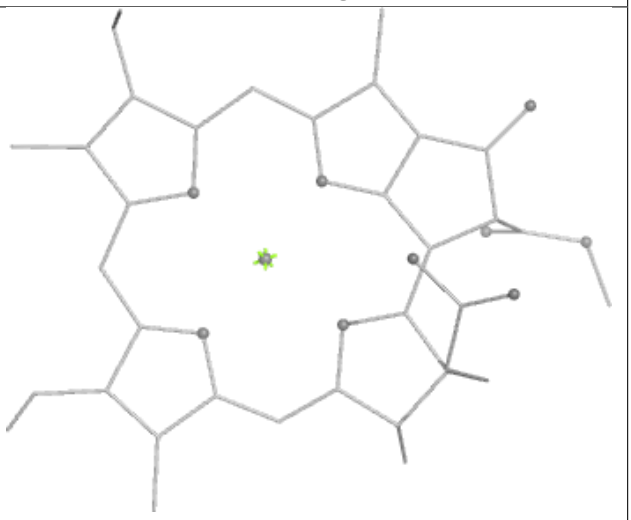
Bond lengths



Bond angles

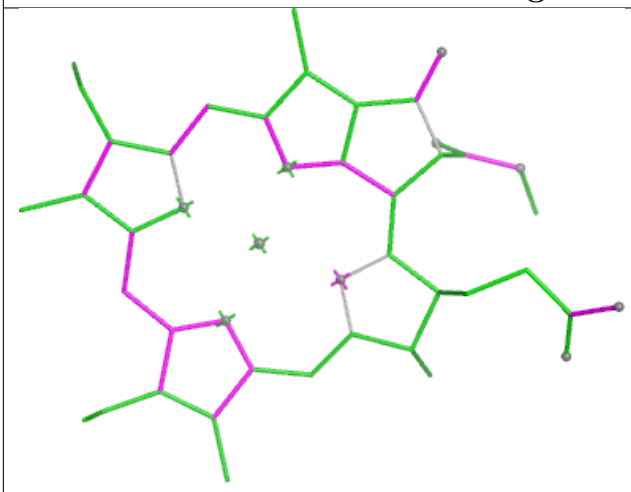


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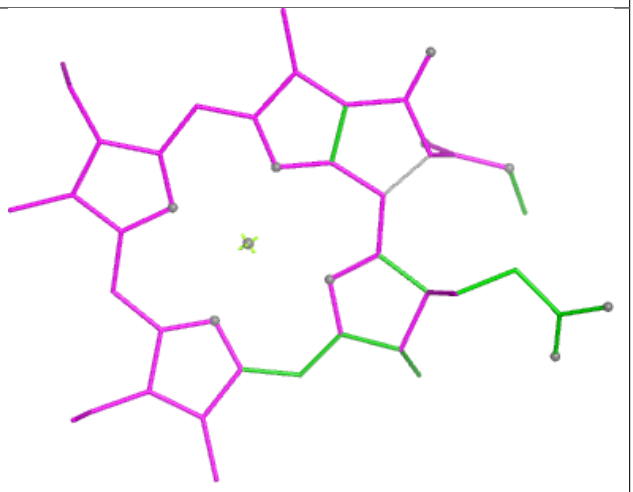


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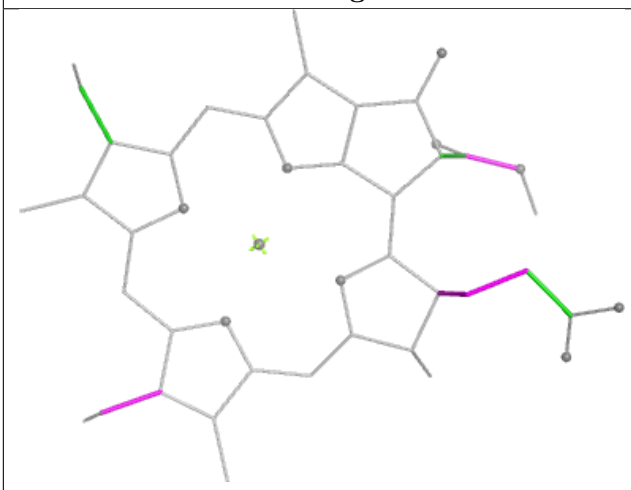
Ligand CLA b 602



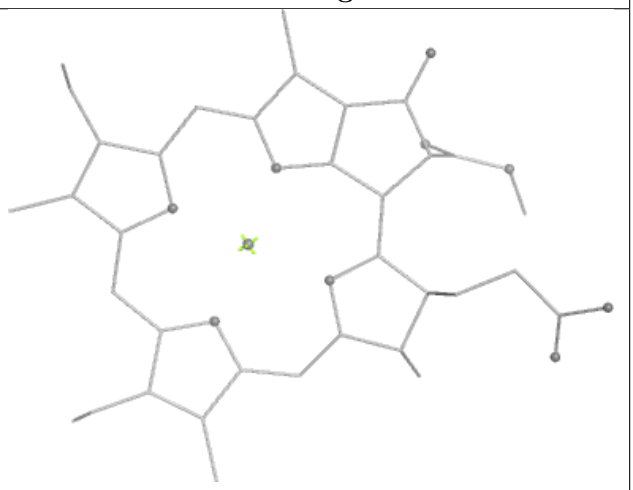
Bond lengths



Bond angles

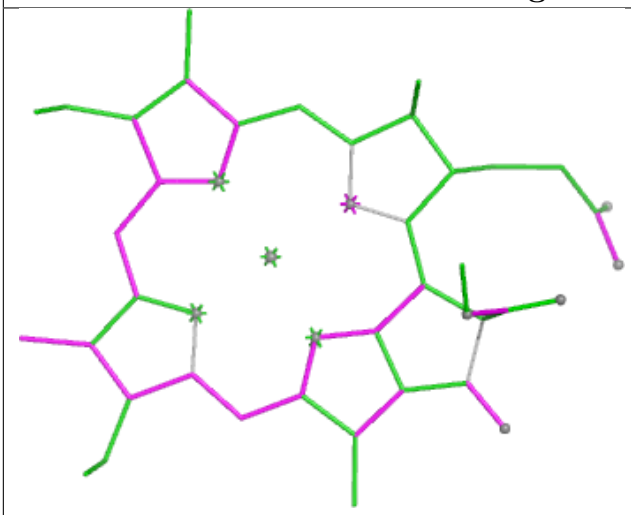


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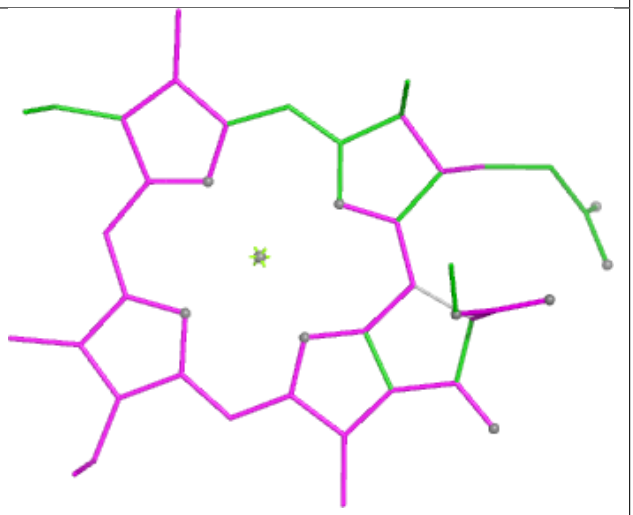


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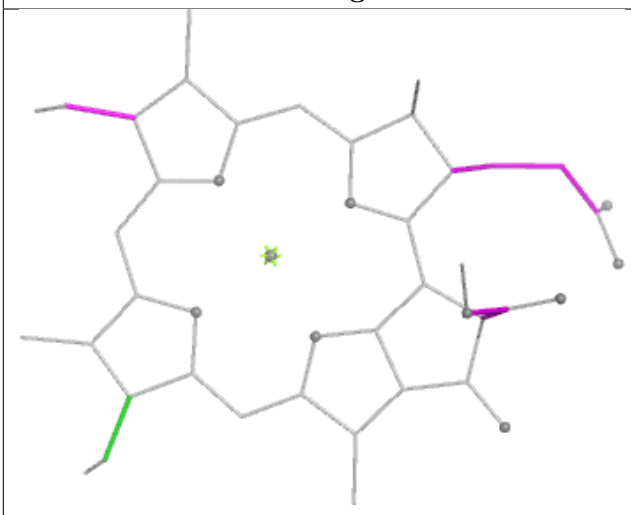
Ligand CLA 8 304



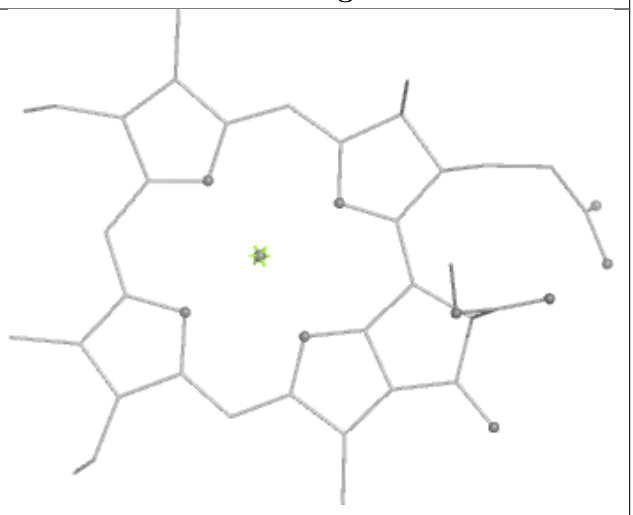
Bond lengths



Bond angles

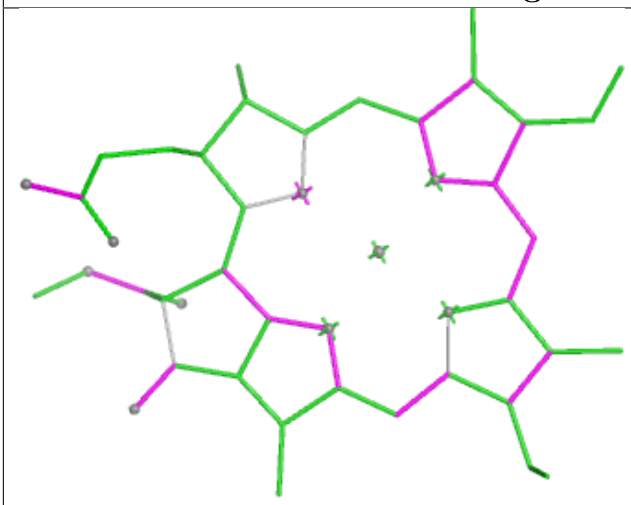


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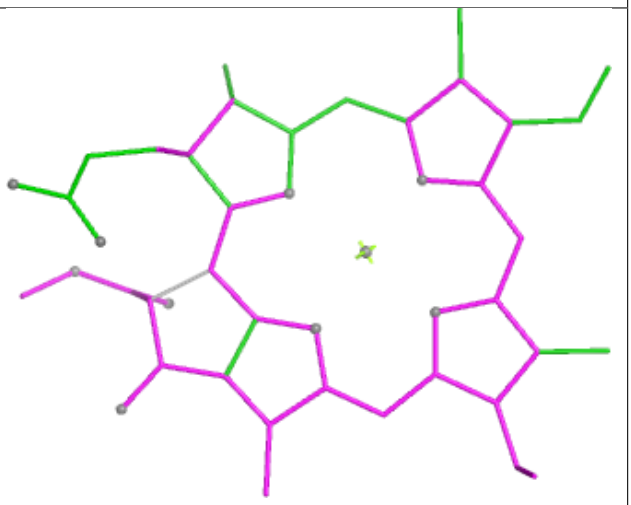


Rings

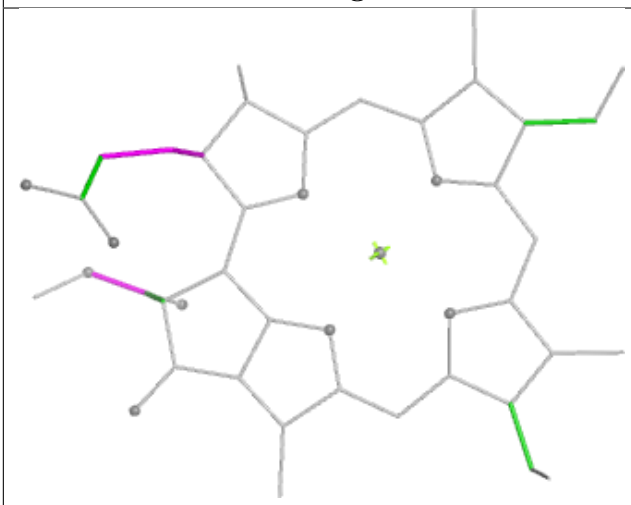
Ligand CLA A 402



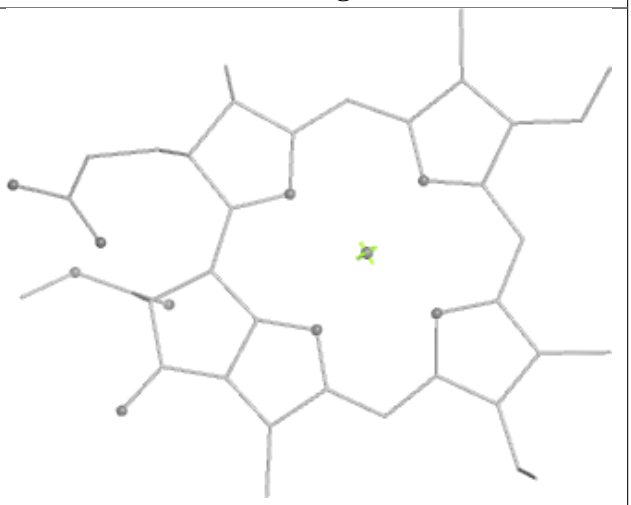
Bond lengths



Bond angles

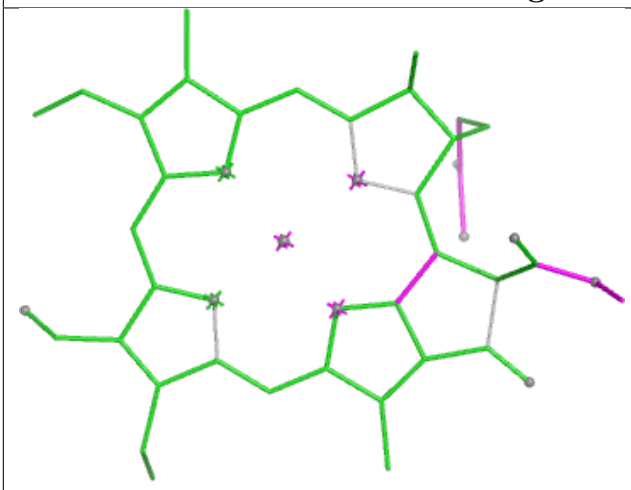


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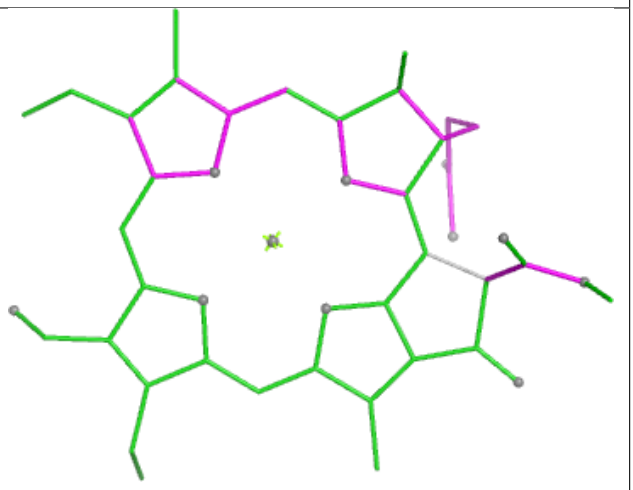


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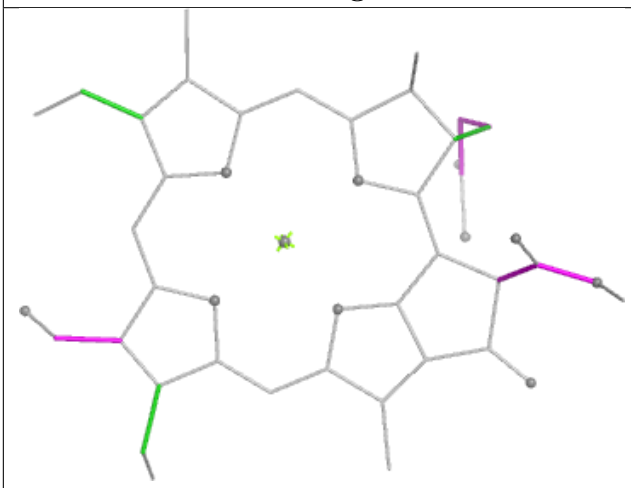
Ligand CHL 5 608



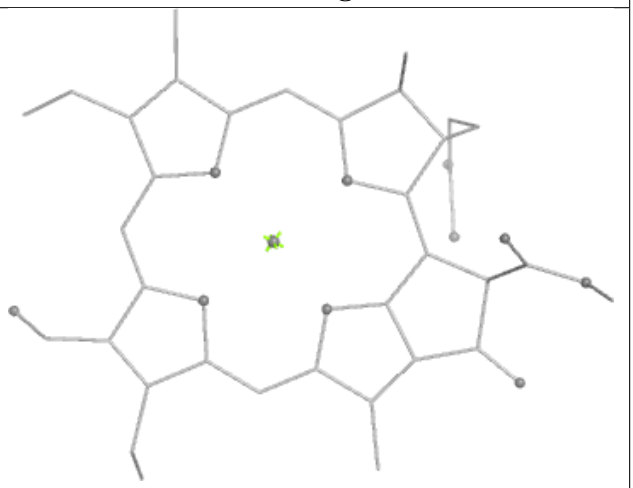
Bond lengths



Bond angles

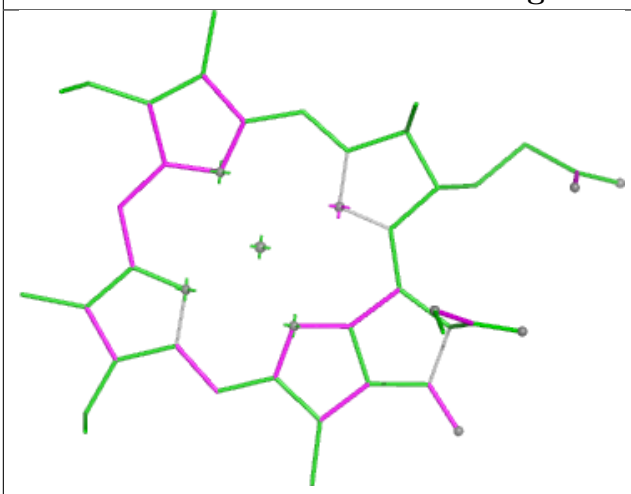


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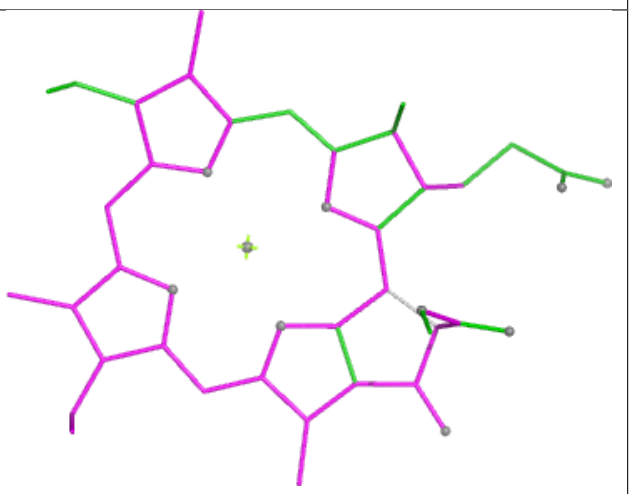


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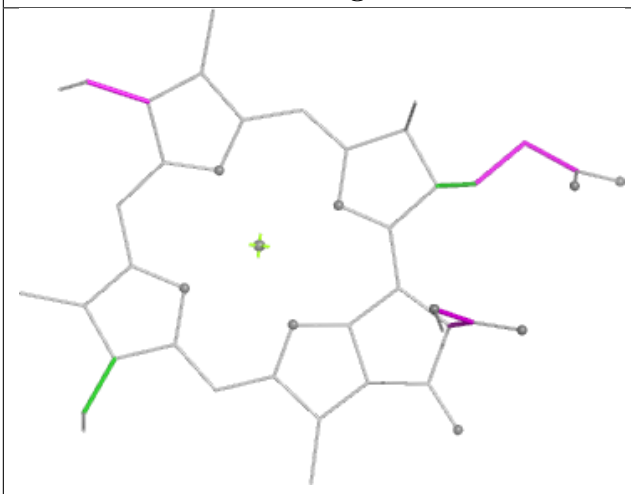
Ligand CLA S 304



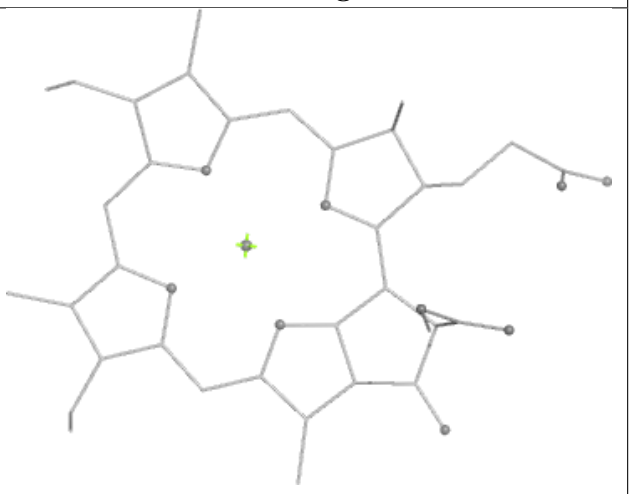
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Bond angles

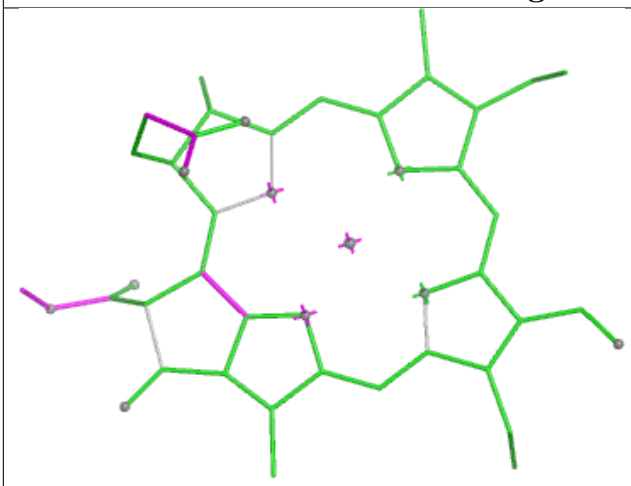


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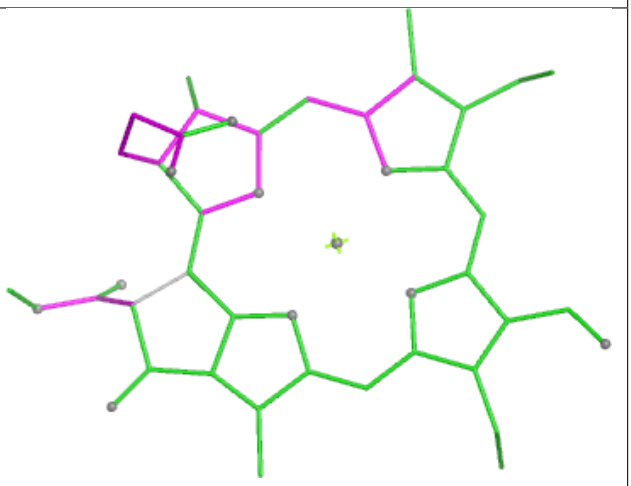


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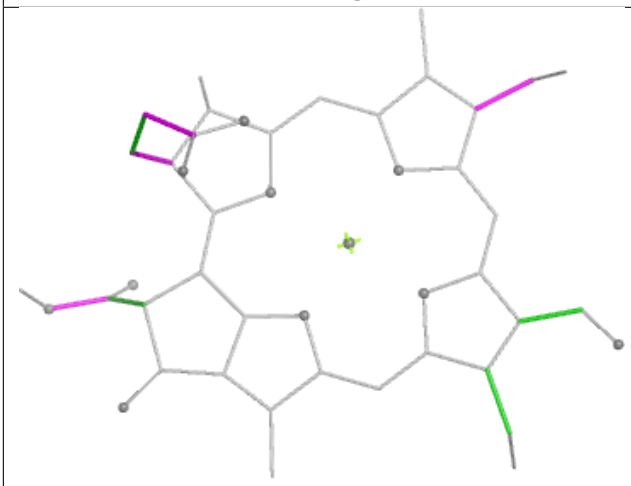
Ligand CHL 7 307



Bond lengths



Bond angles

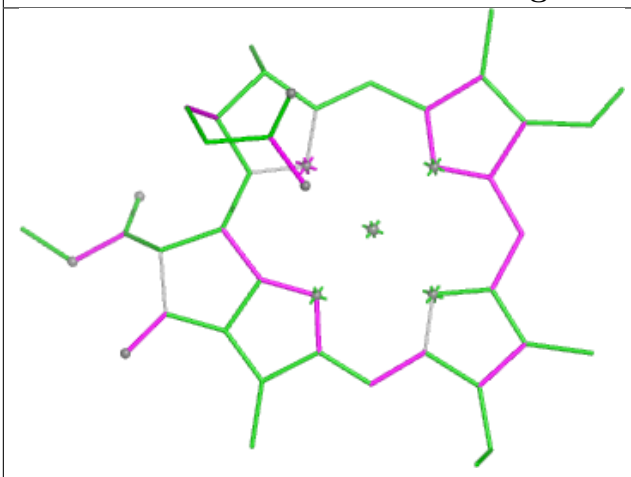


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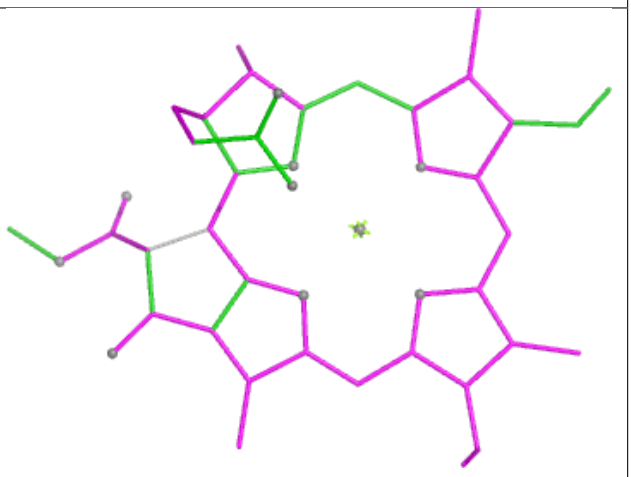


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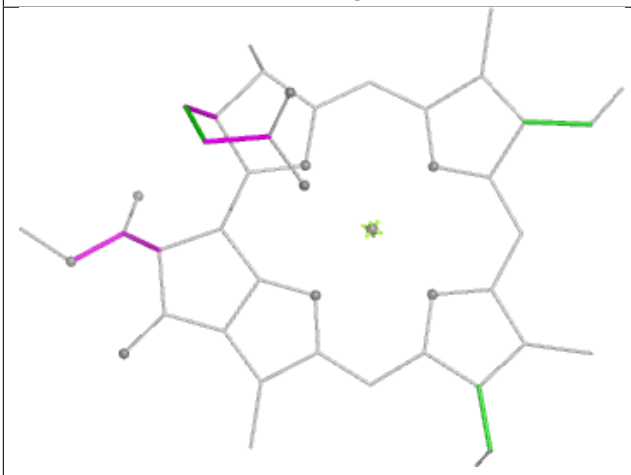
Ligand CLA r 308



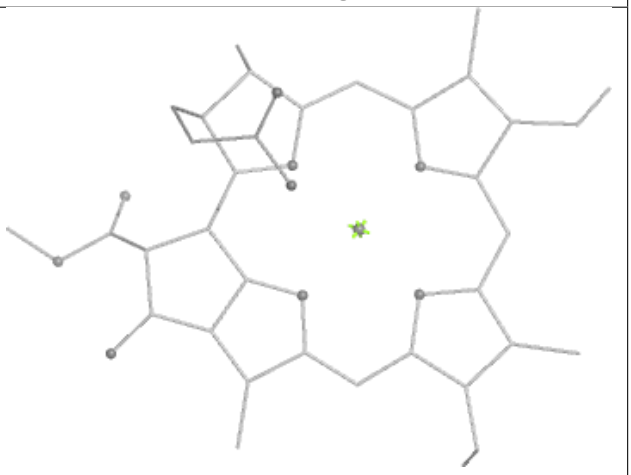
Bond lengths



Bond angles

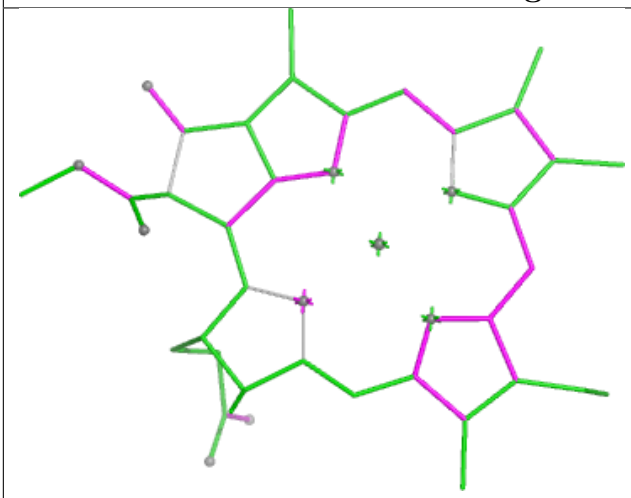


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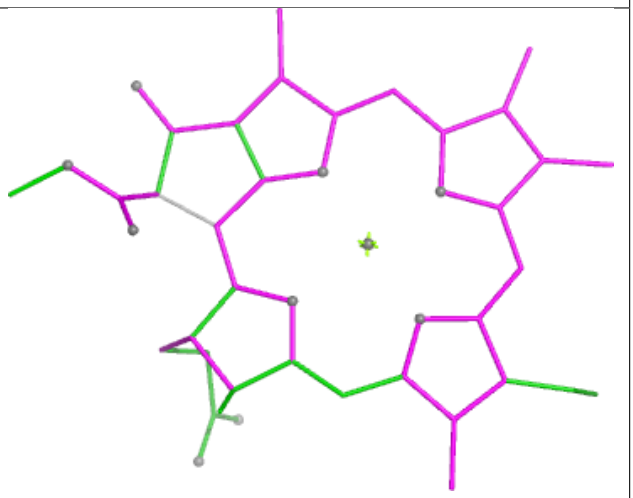


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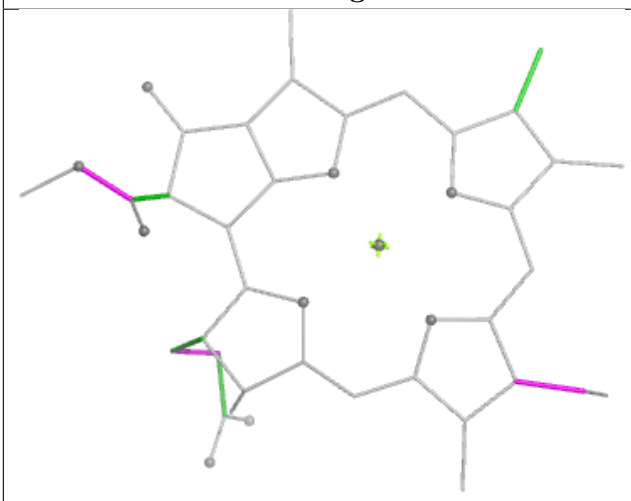
Ligand CLA B 606



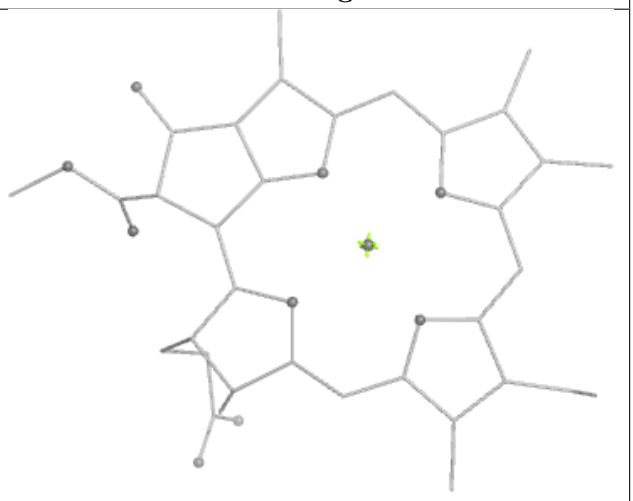
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Bond angles

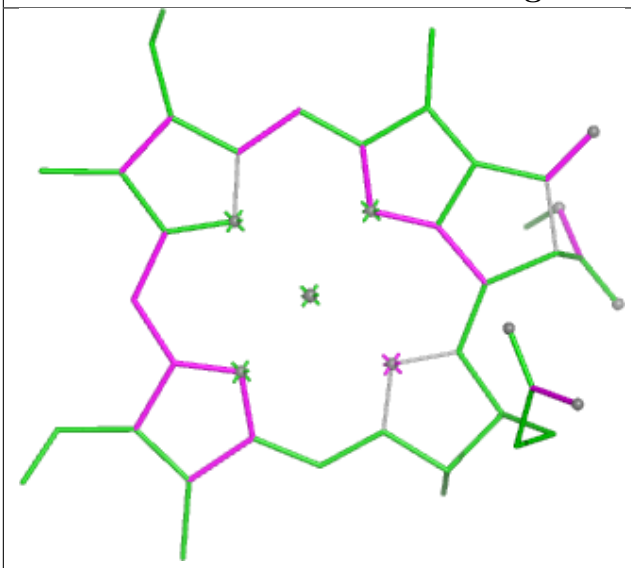


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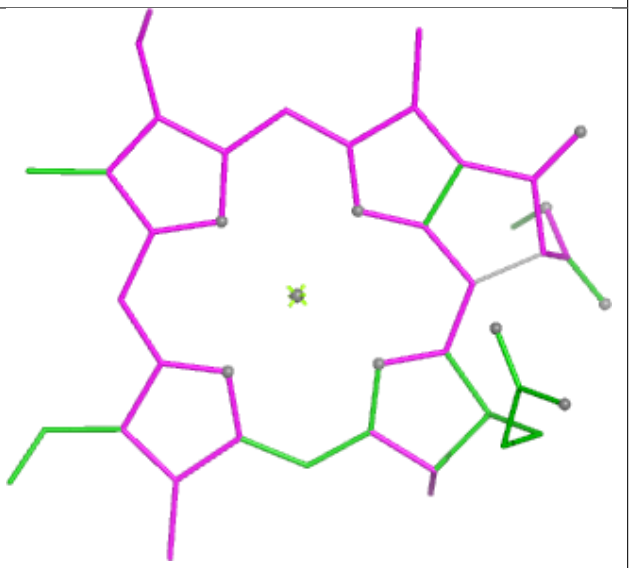


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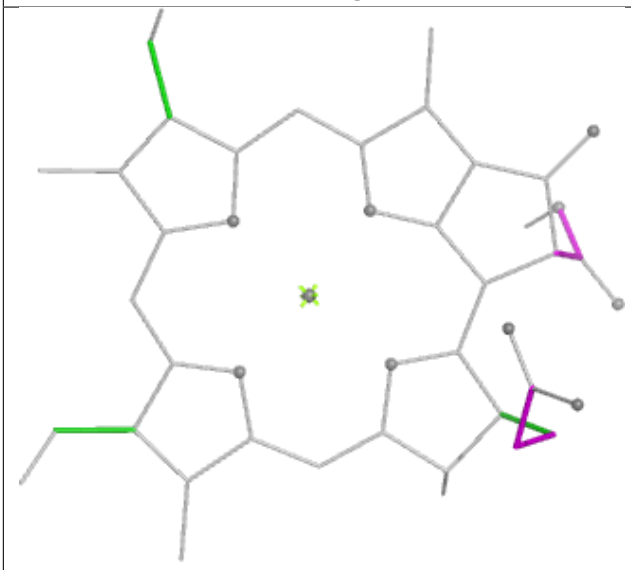
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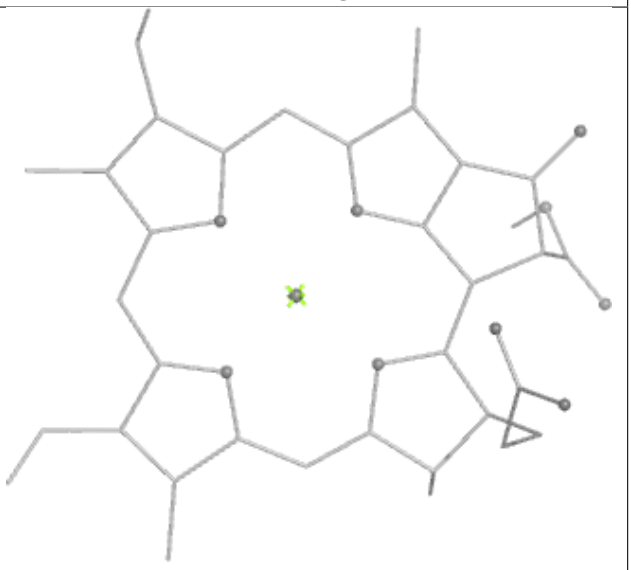
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Bond angles

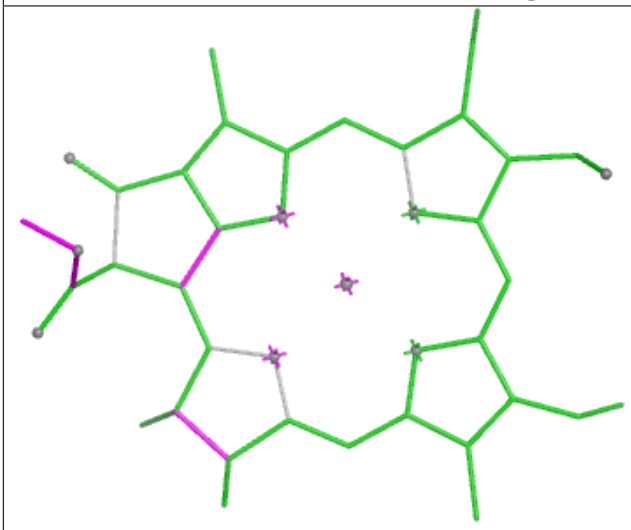


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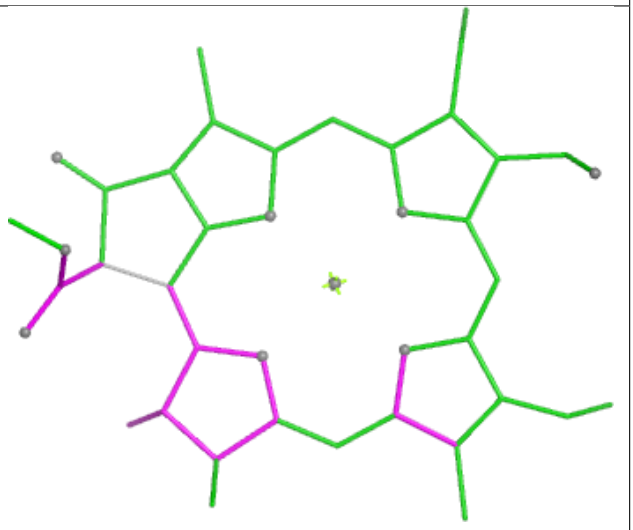


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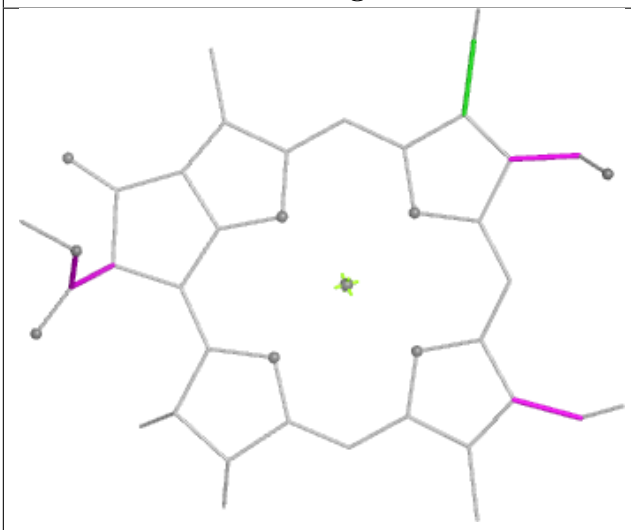
Ligand CHL G 605



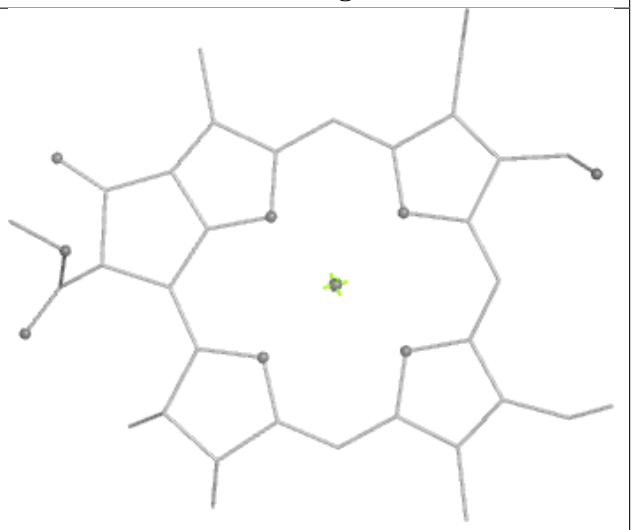
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Bond angles

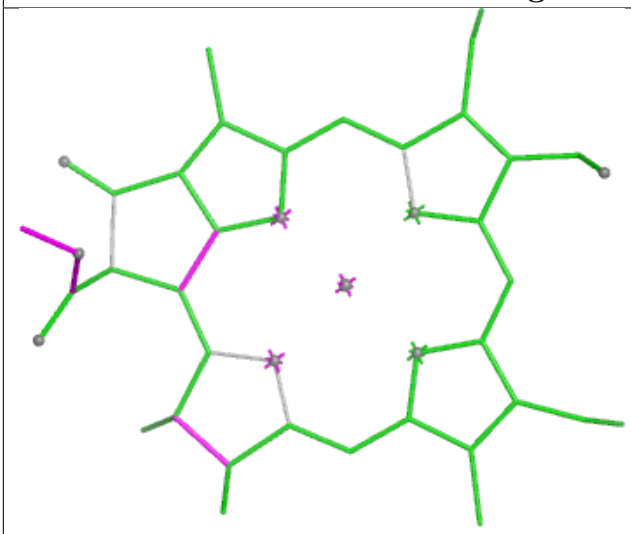


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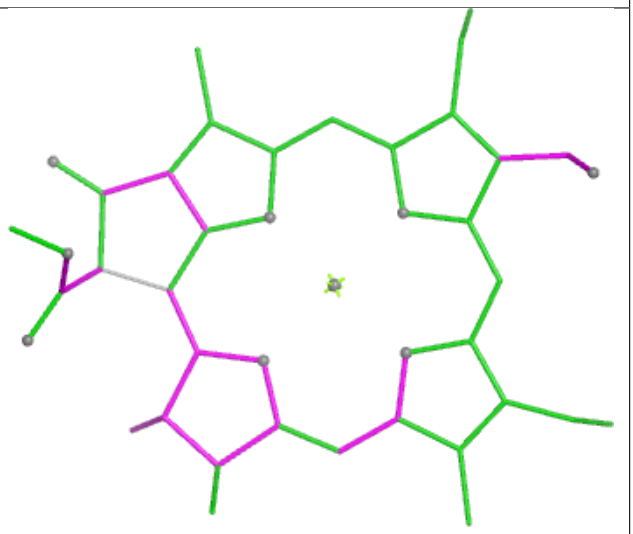


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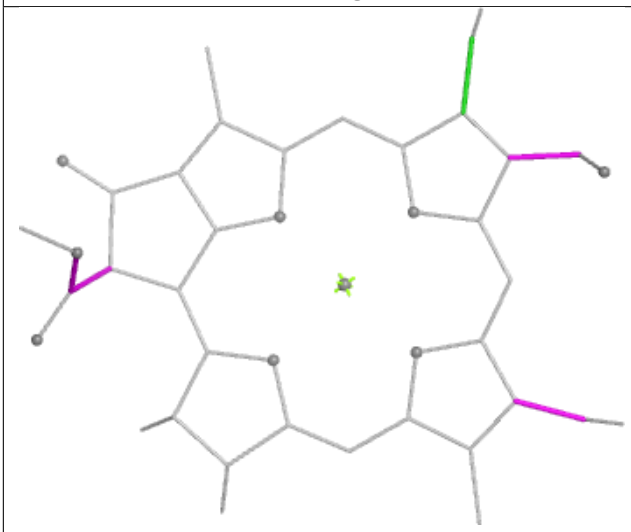
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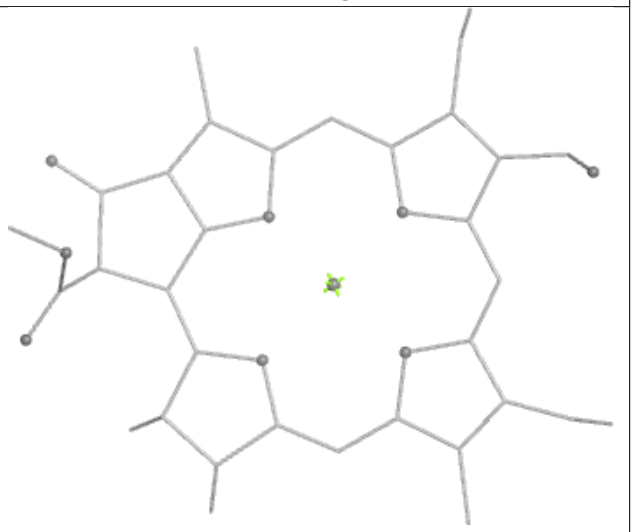
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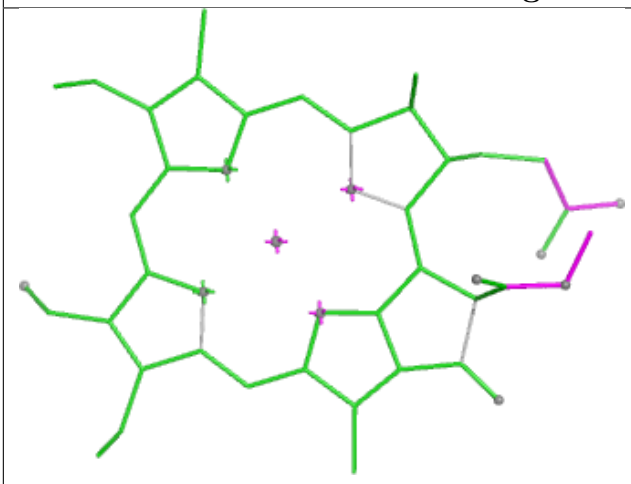


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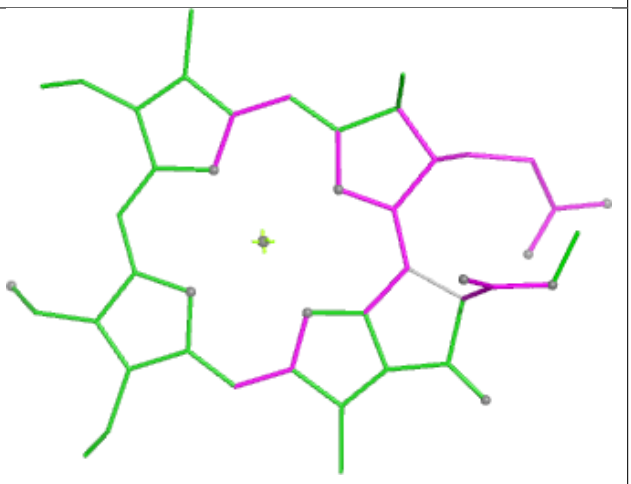


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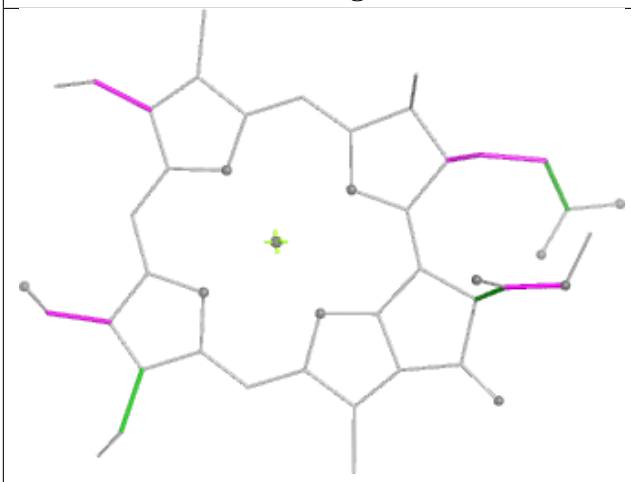
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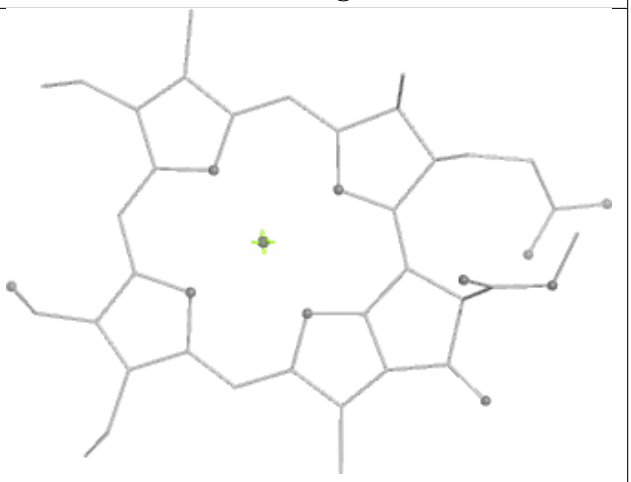
Bond lengths



Bond angles

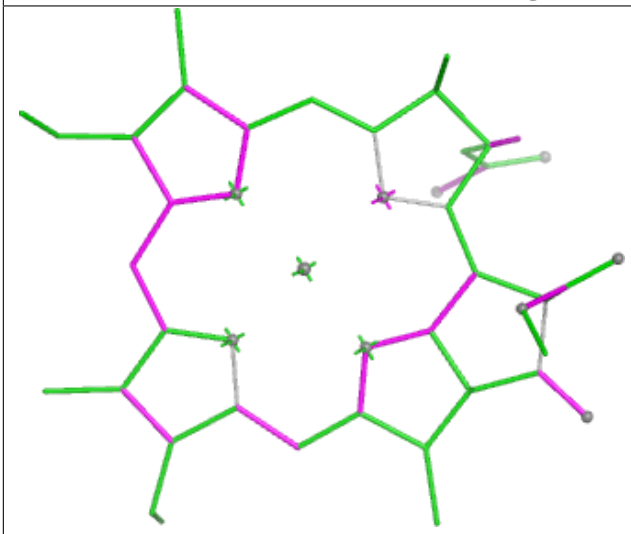


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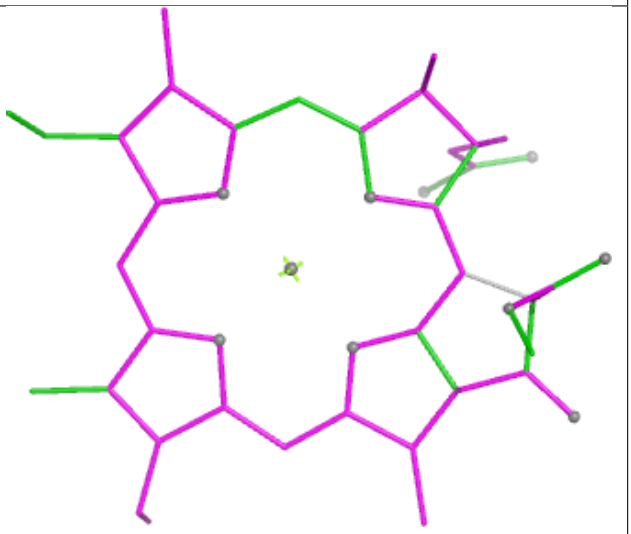


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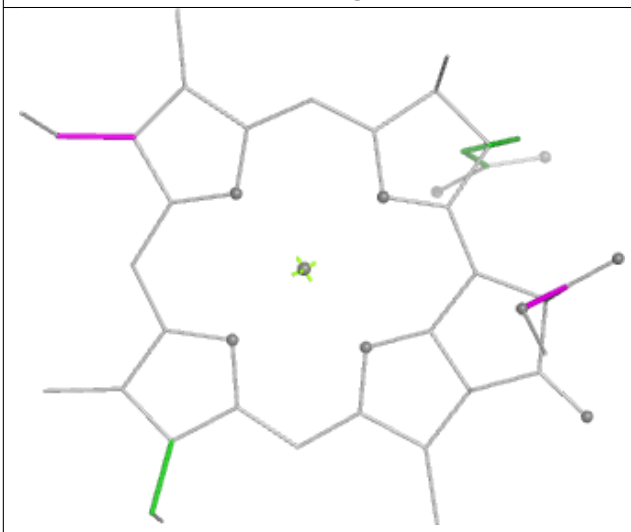
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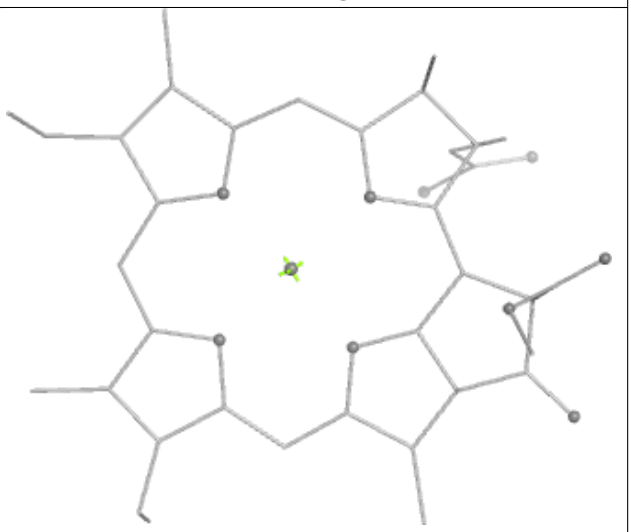
Bond lengths



Bond angles

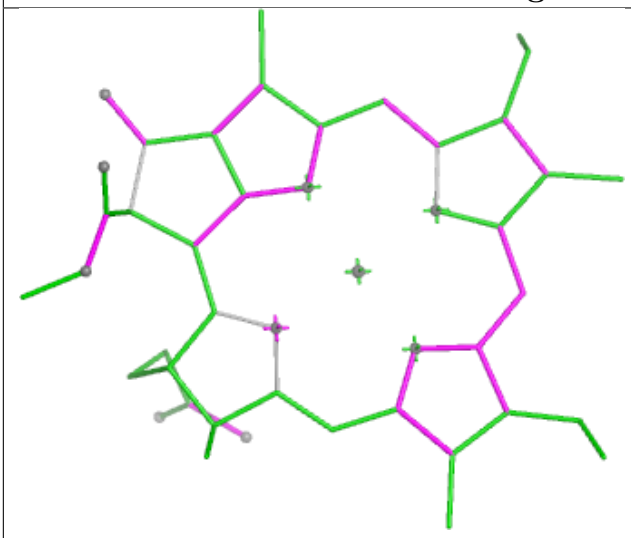


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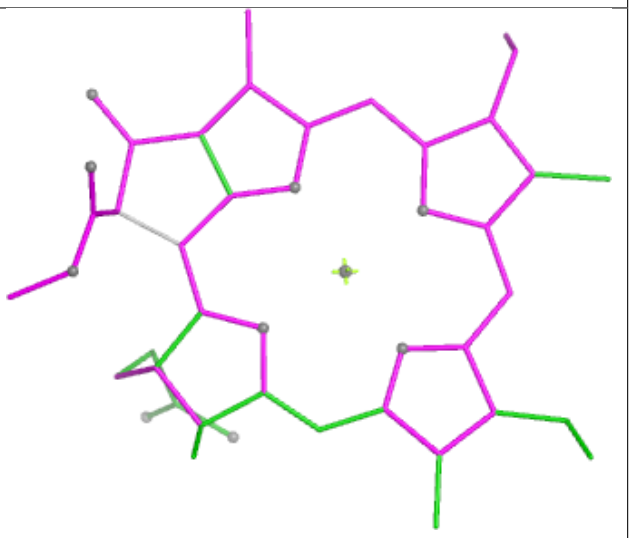


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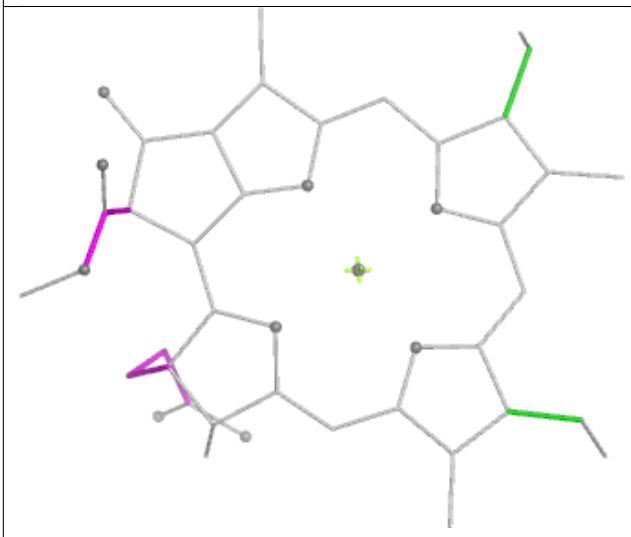
Ligand CLA S 305



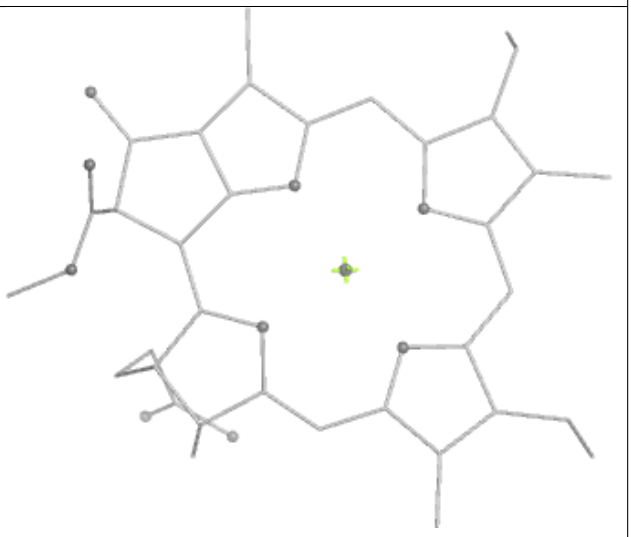
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Bond angles

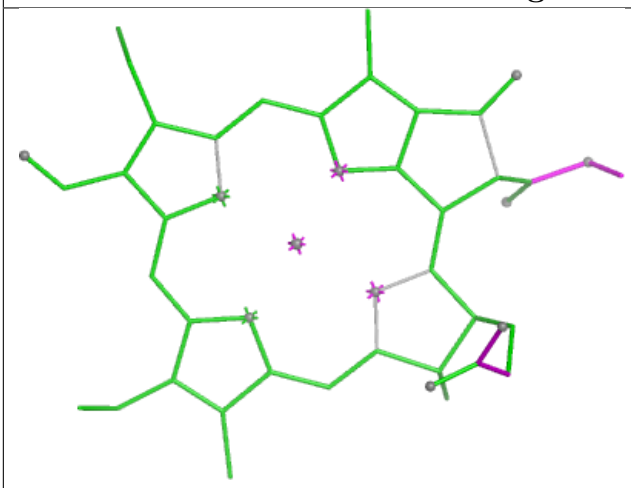


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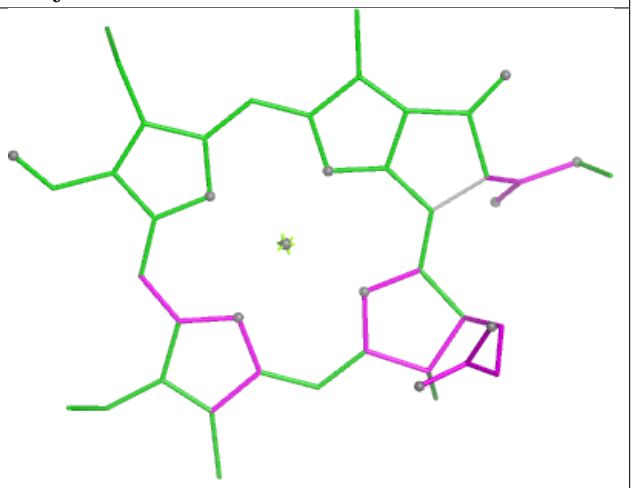


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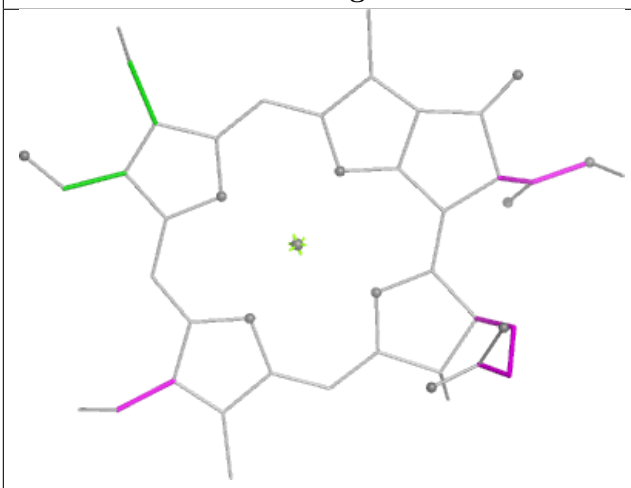
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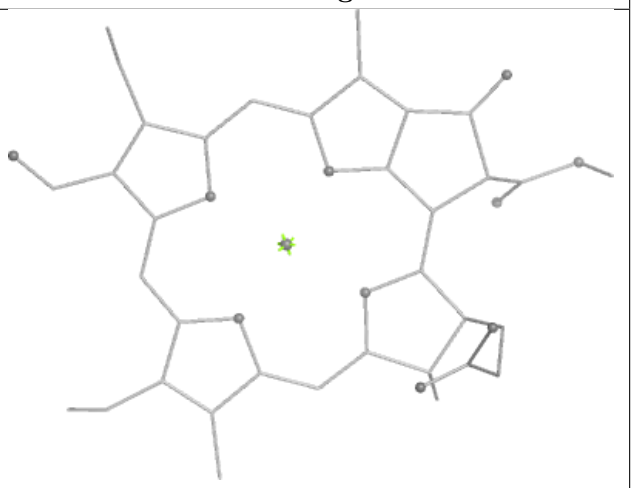
Bond lengths



Bond angles

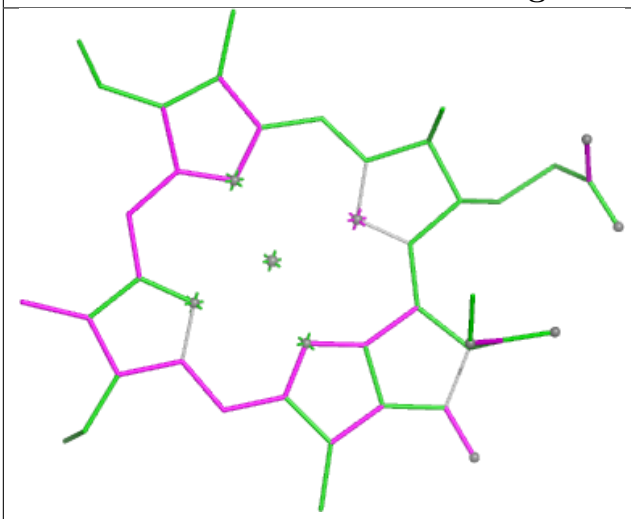


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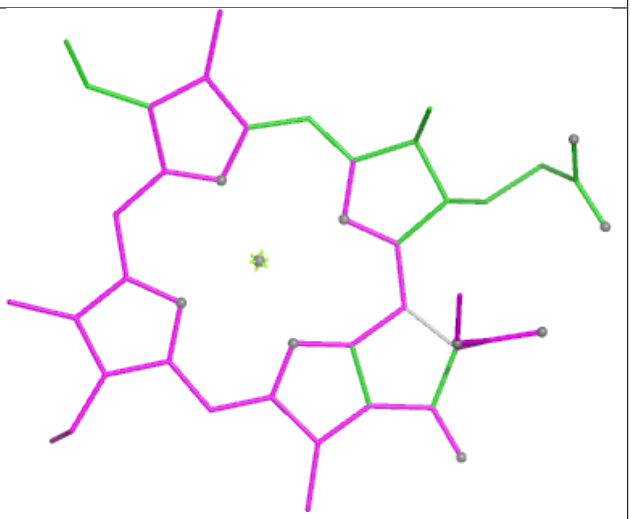


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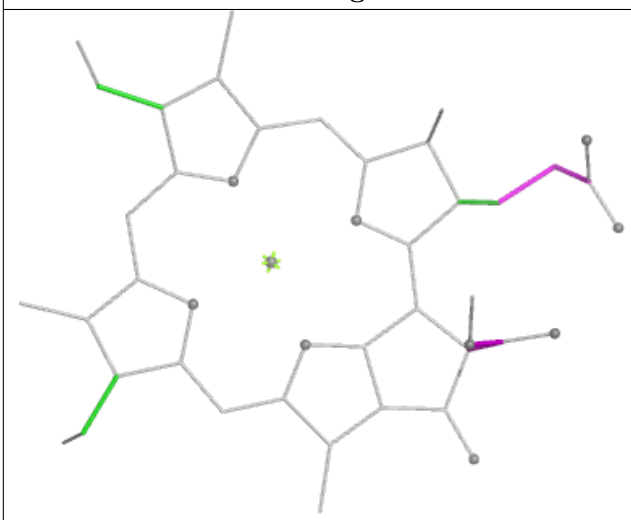
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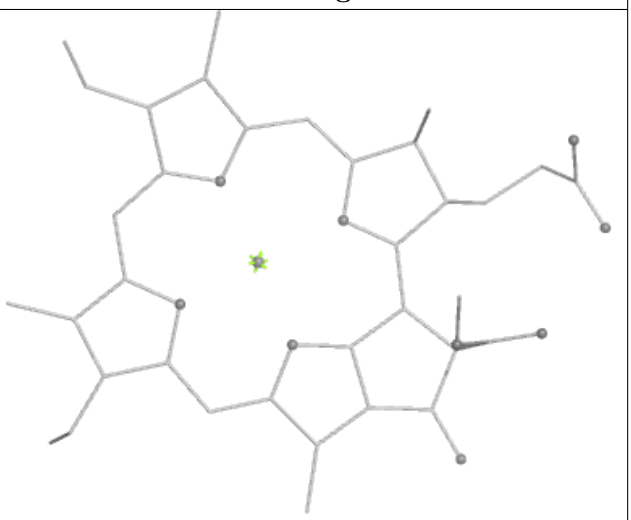
Bond lengths



Bond angles

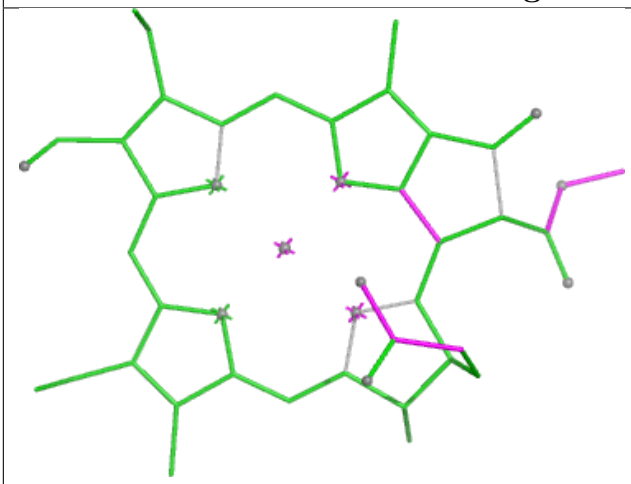


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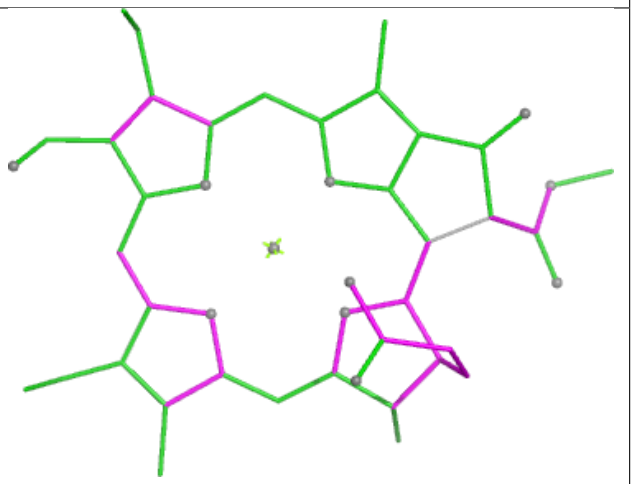


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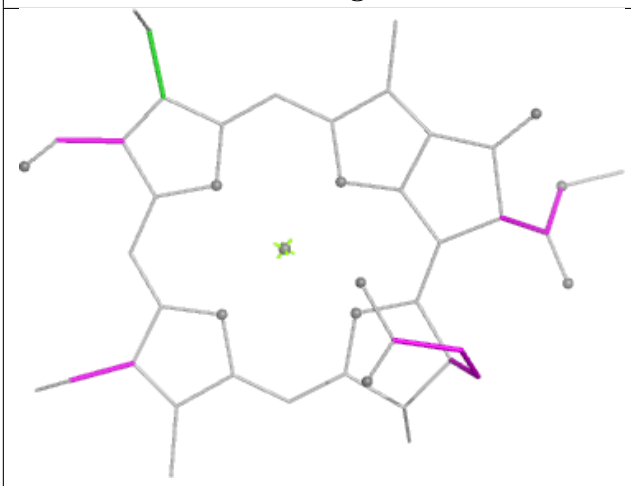
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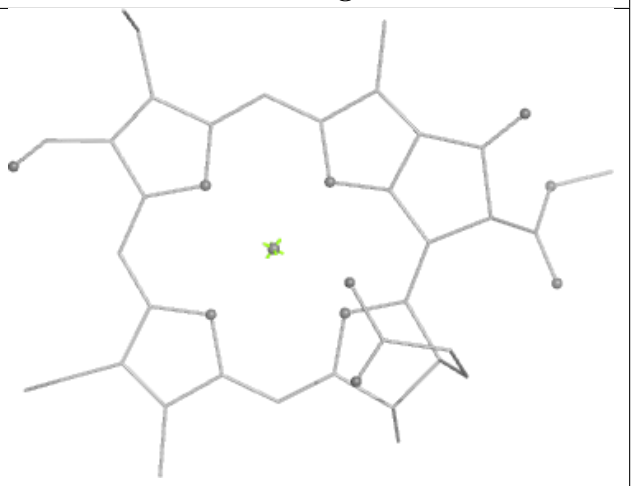
Bond lengths



Bond angles

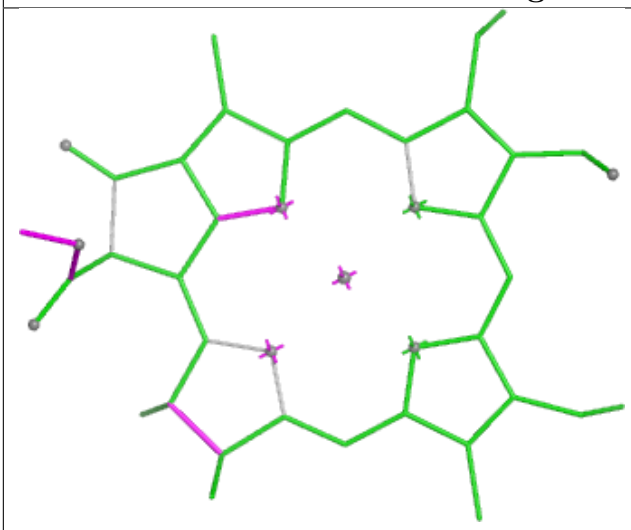


Torsions

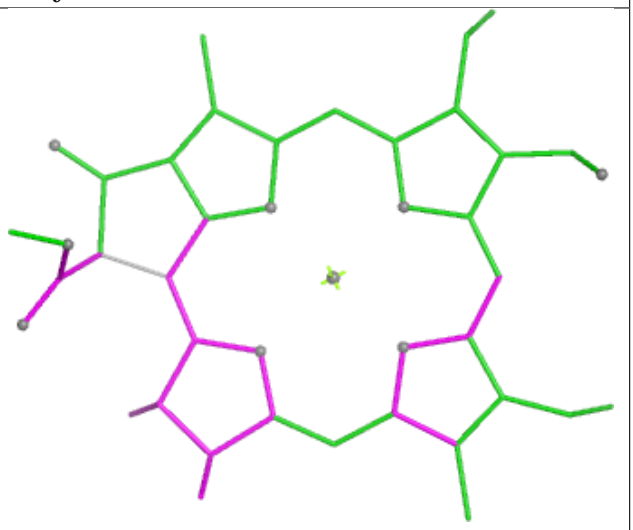


Rings

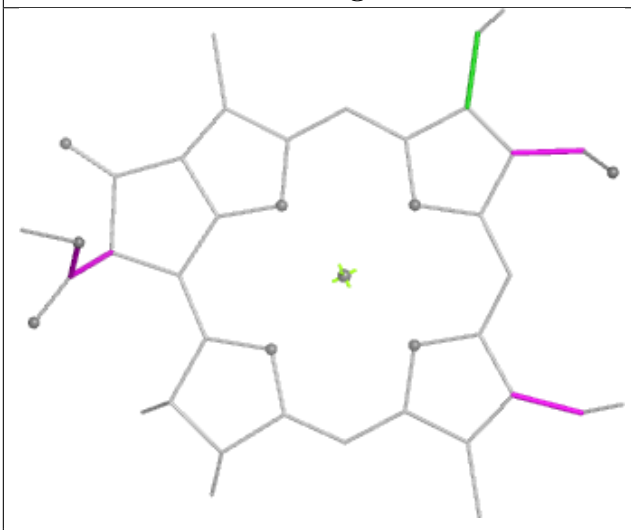
Ligand CHL y 605



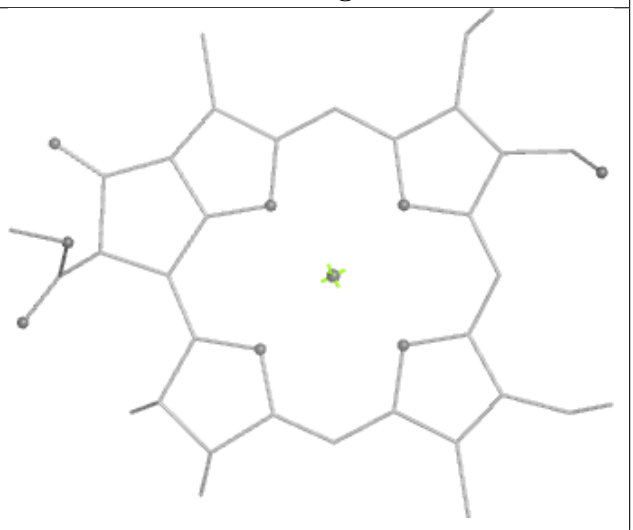
Bond lengths



Bond angles

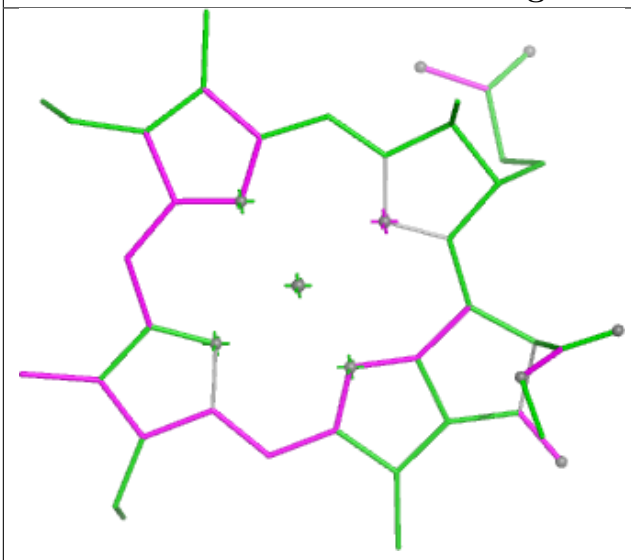


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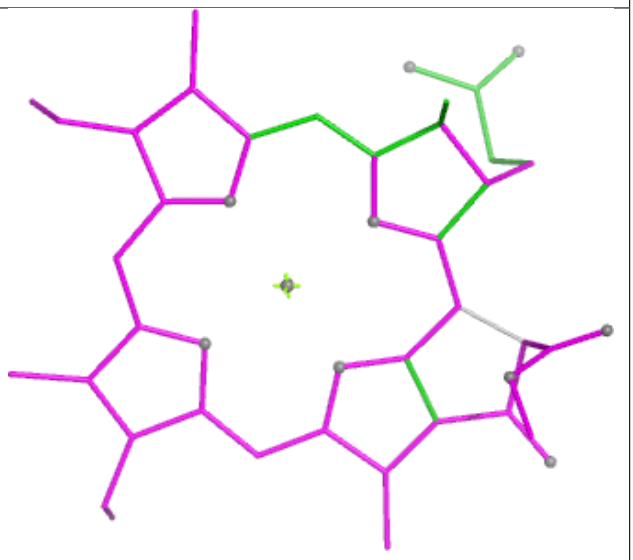


Rings

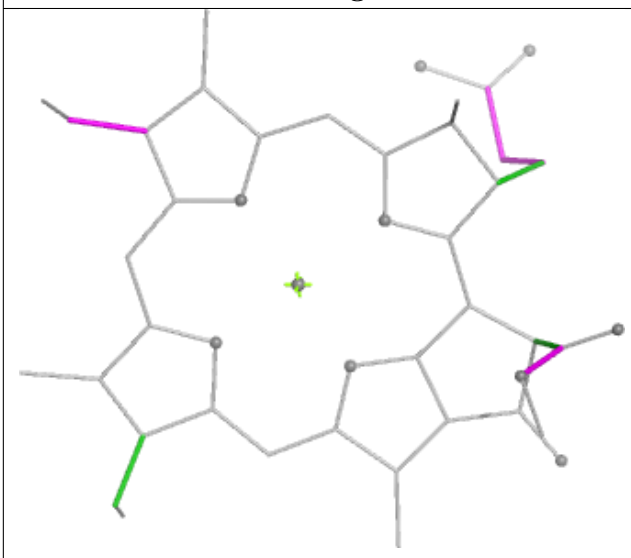
Ligand CLA b 603



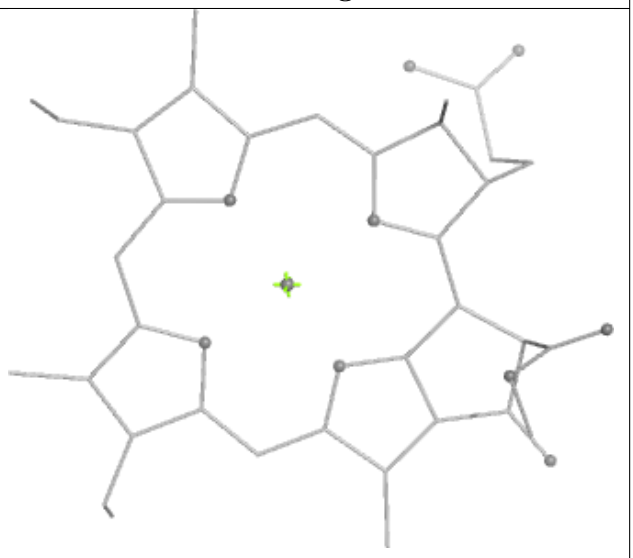
Bond lengths



Bond angles

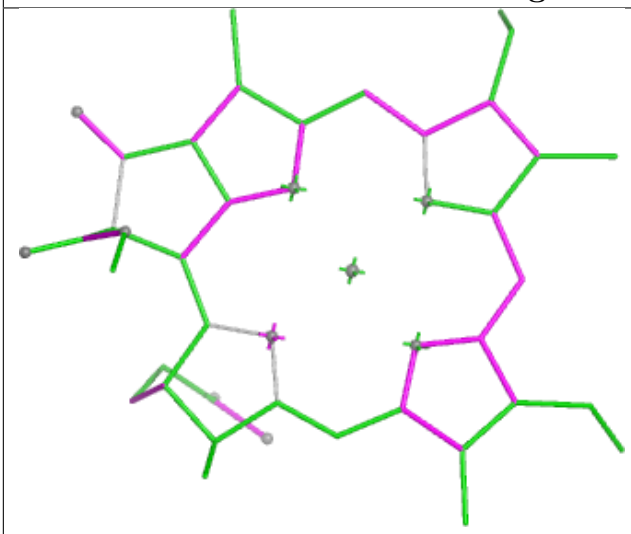


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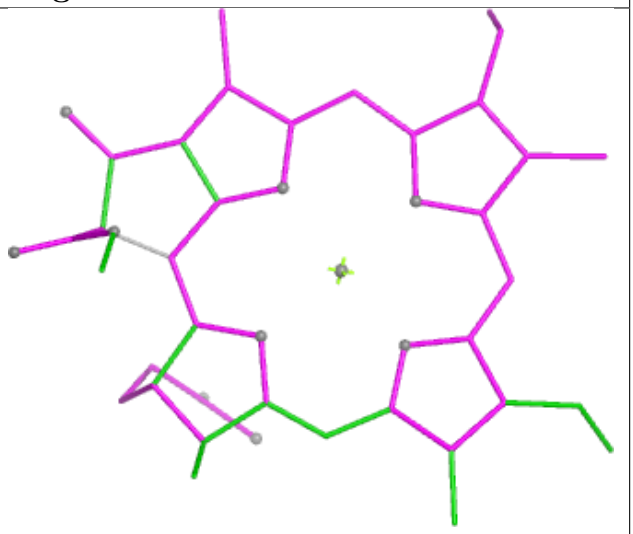


Rings

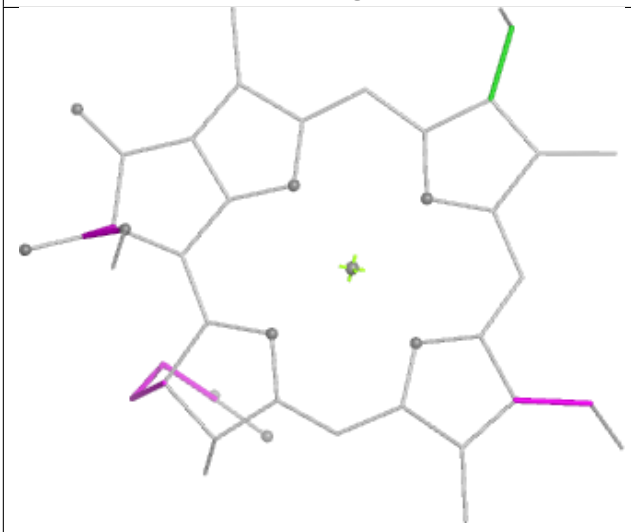
Ligand CLA g 604



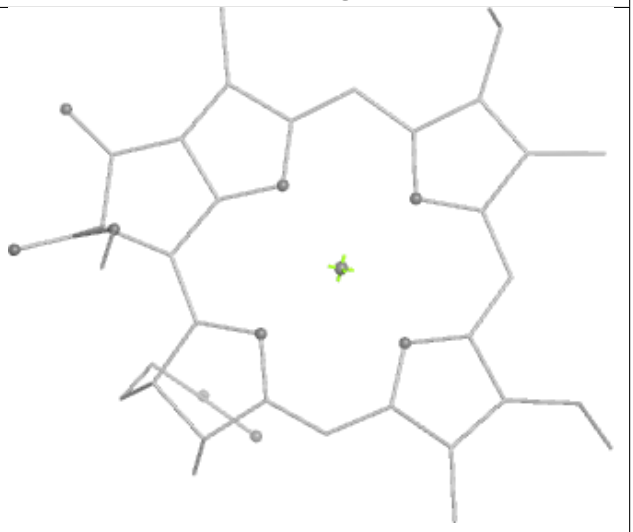
Bond lengths



Bond angles

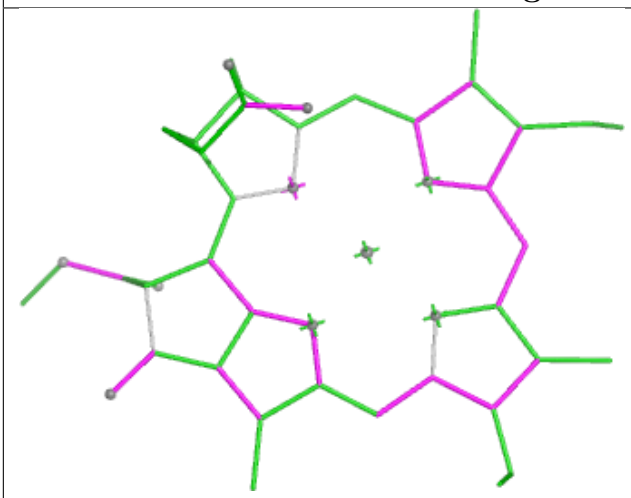


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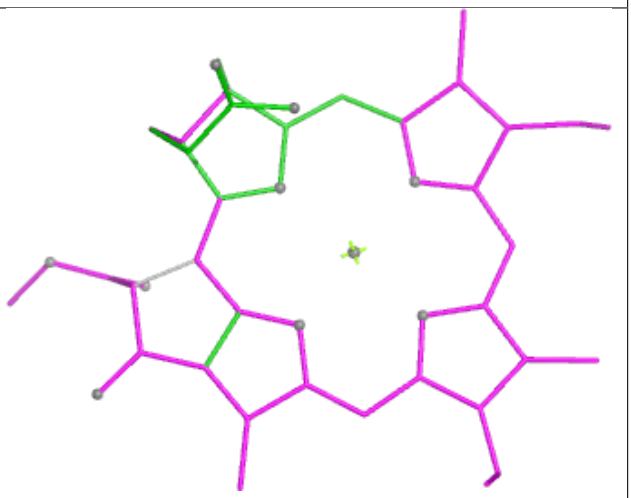


Rings

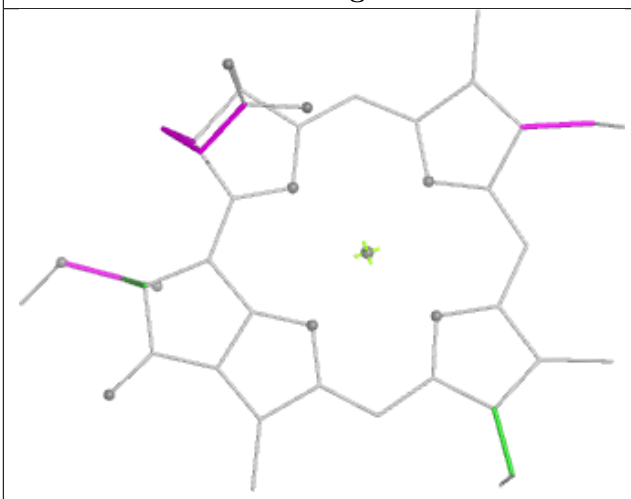
Ligand CLA D 404



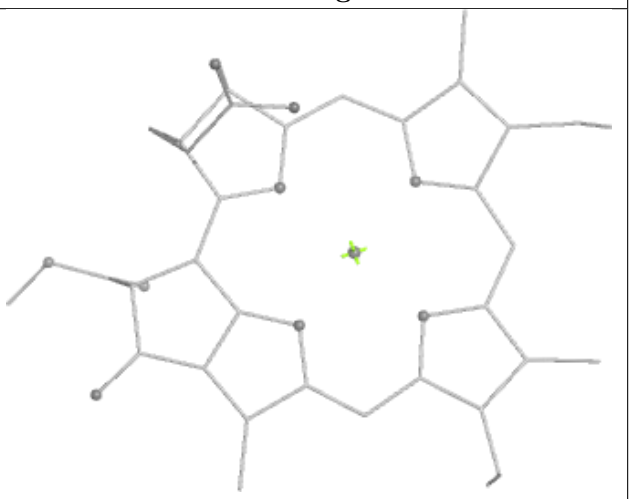
Bond lengths



Bond angles

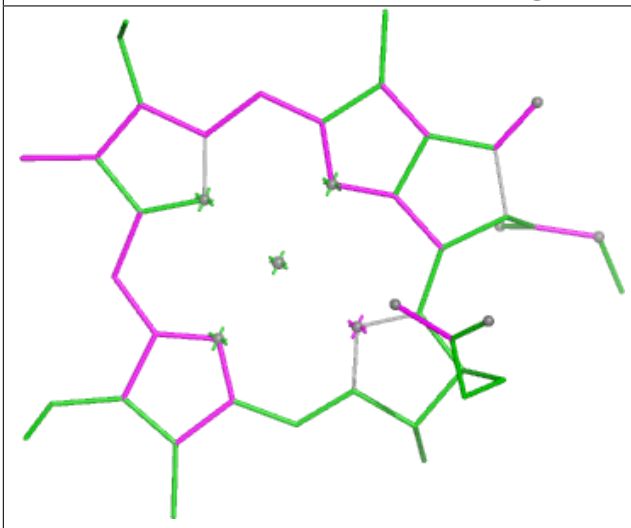


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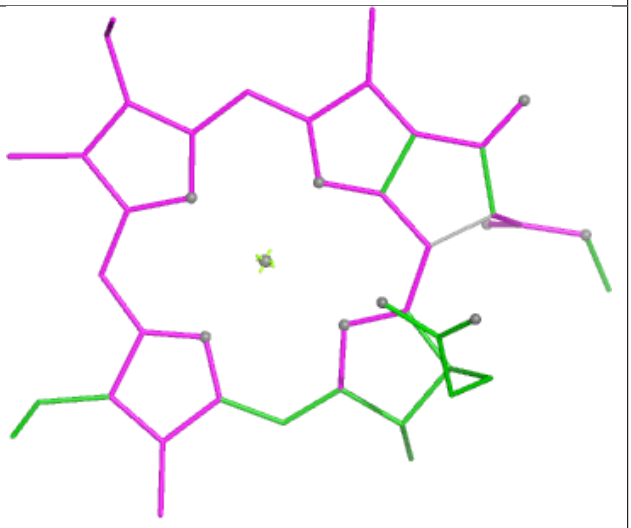


Rings

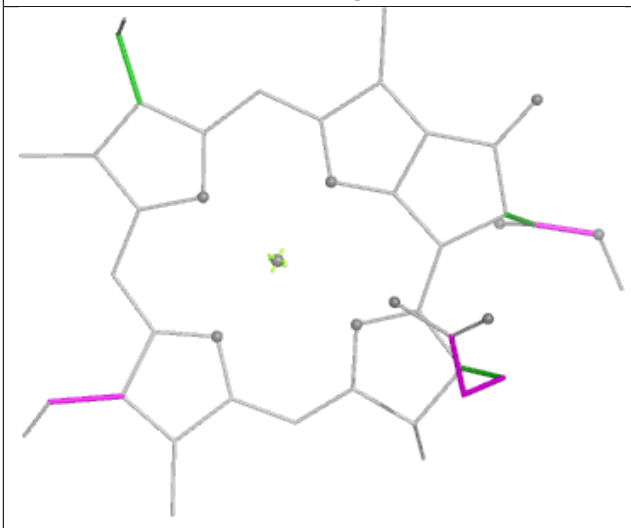
Ligand CLA 5 611



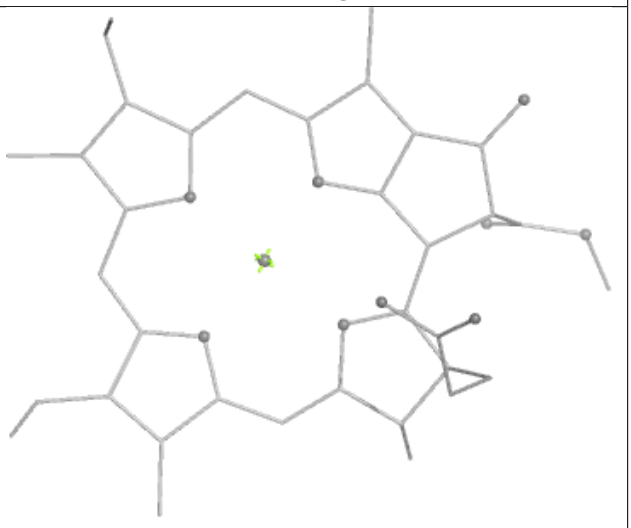
Bond lengths



Bond angles

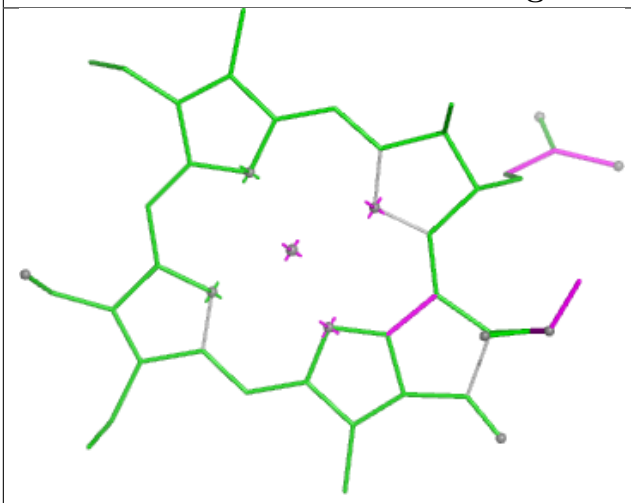


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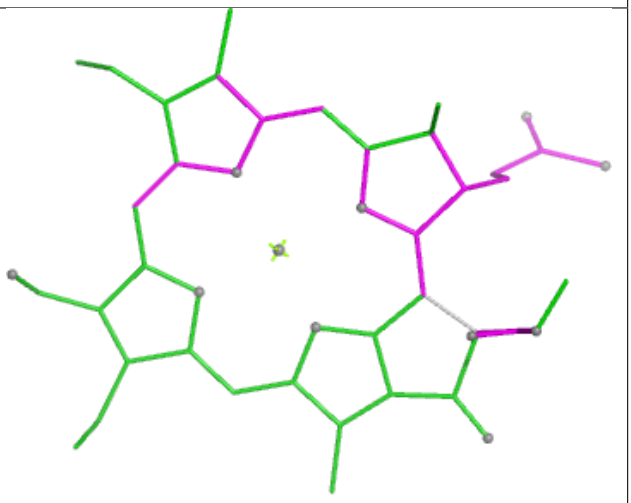


Rings

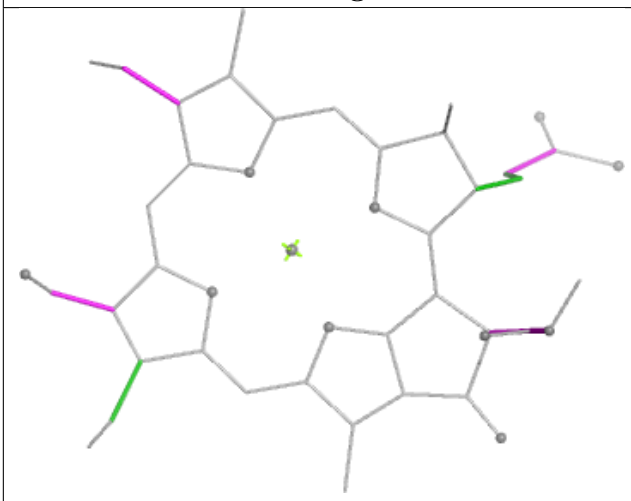
Ligand CHL S 307



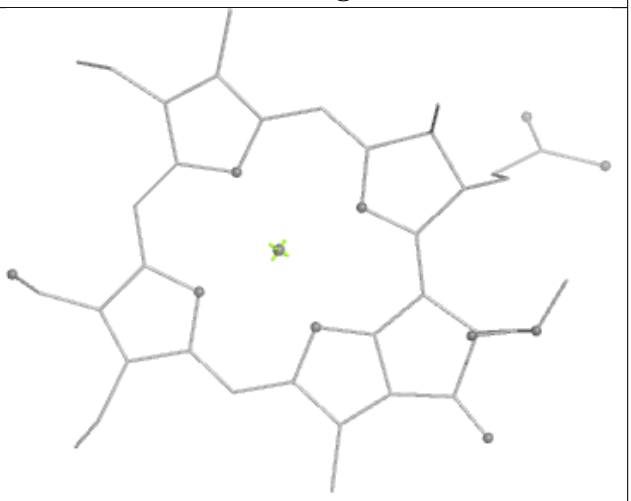
Bond lengths



Bond angles

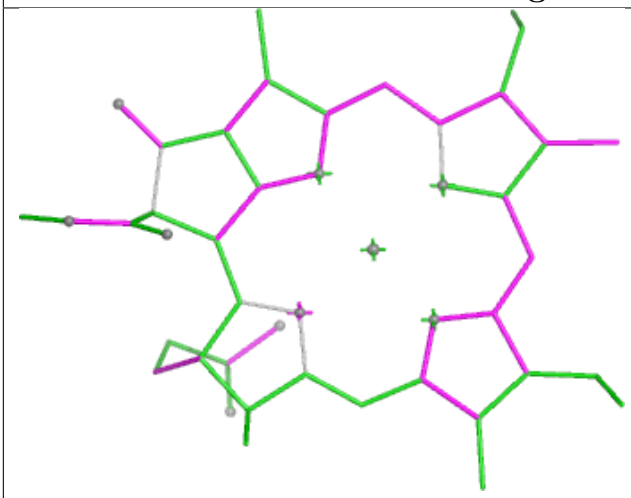


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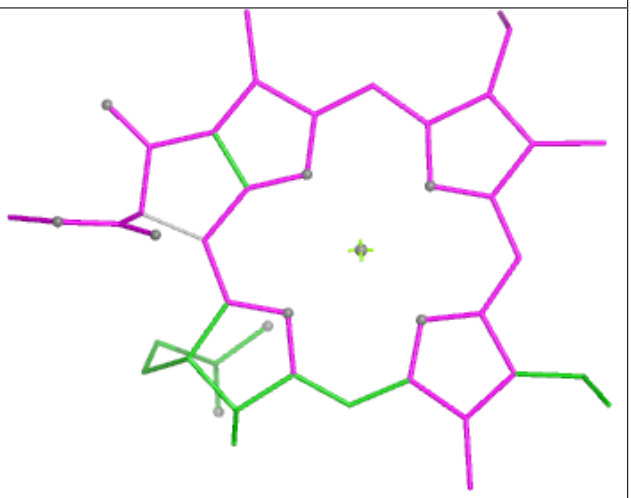


Rings

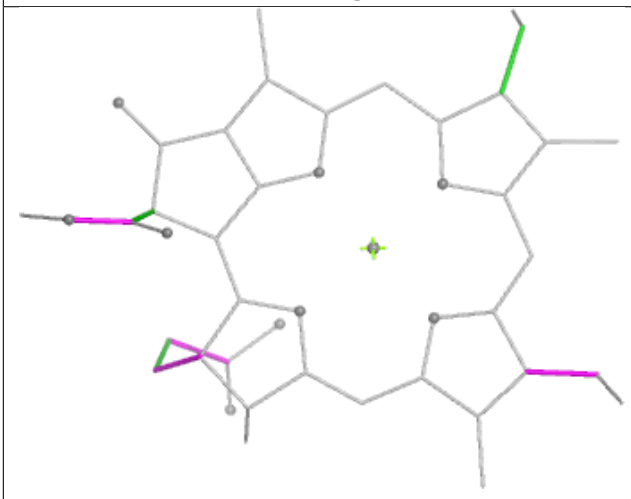
Ligand CLA 5 614



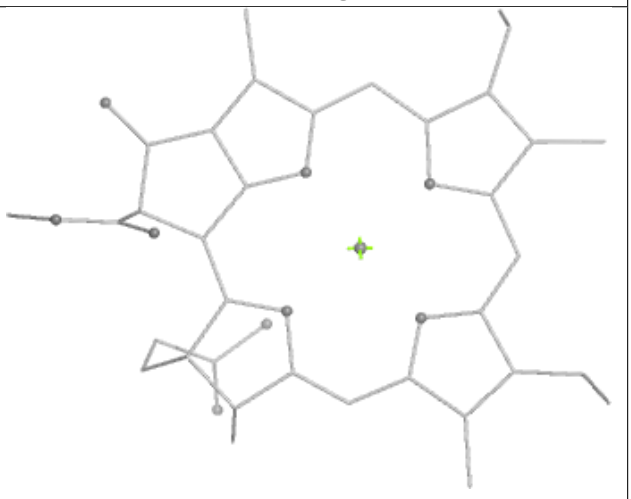
Bond lengths



Bond angles

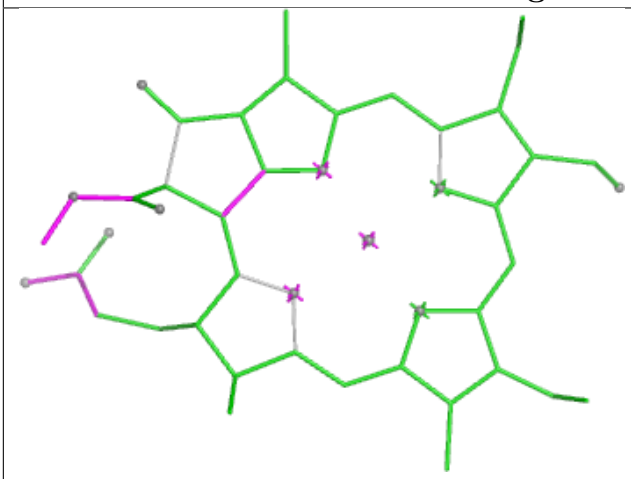


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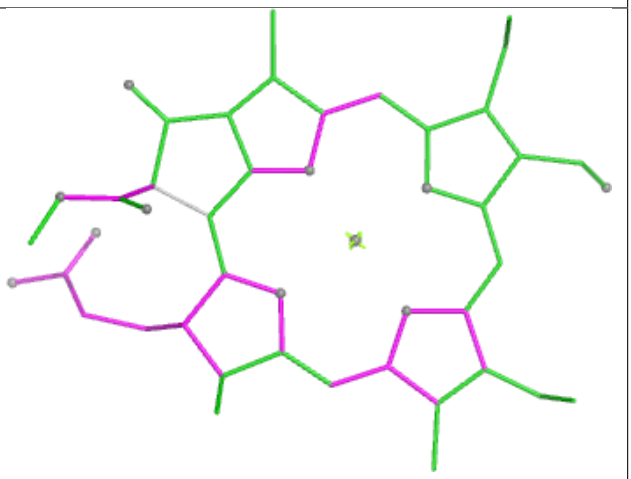


Rings

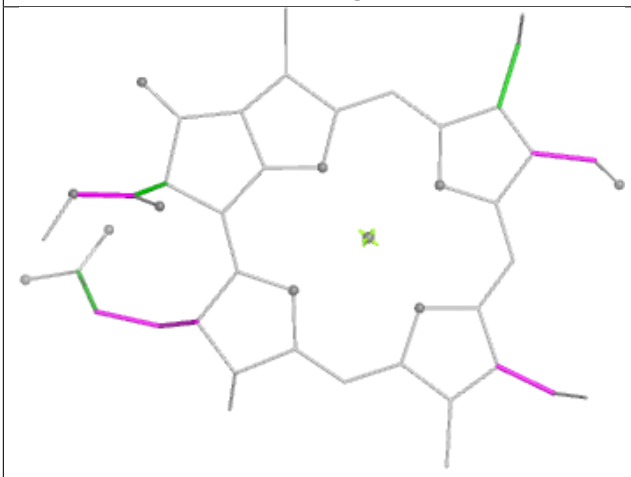
Ligand CHL 5 601



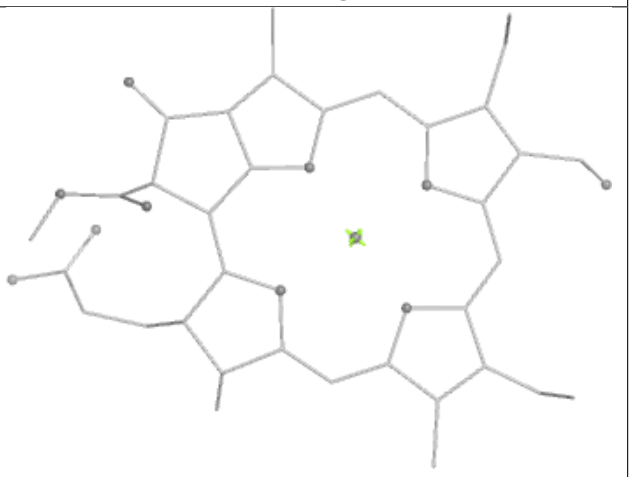
Bond lengths



Bond angles

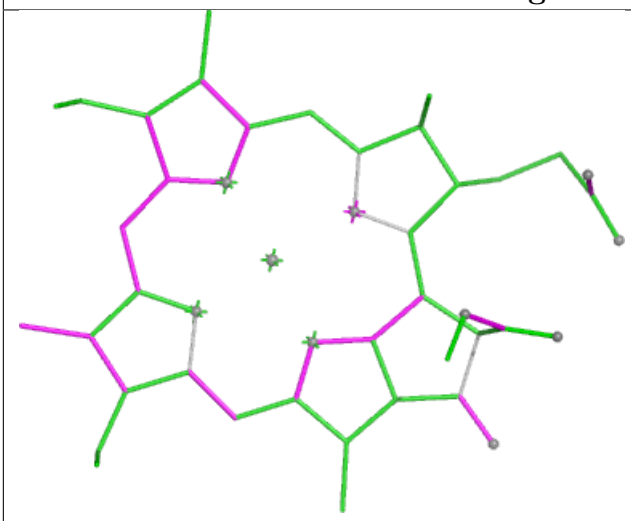


Torsions

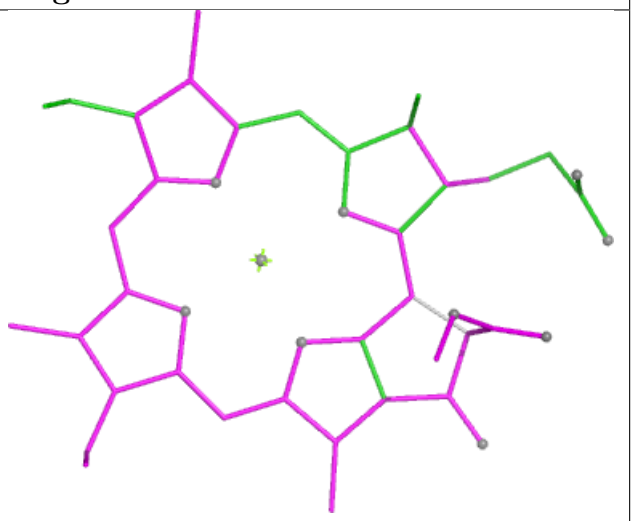


Rings

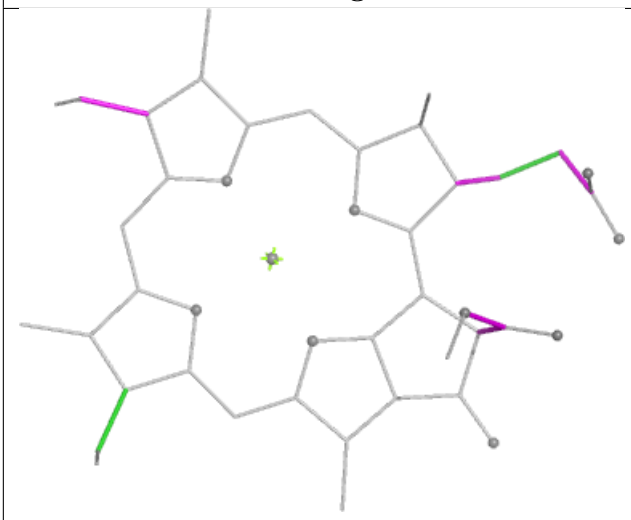
Ligand CLA g 612



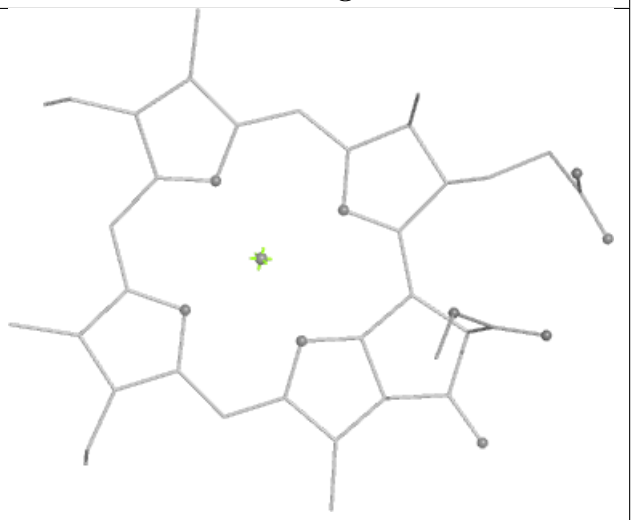
Bond lengths



Bond angles

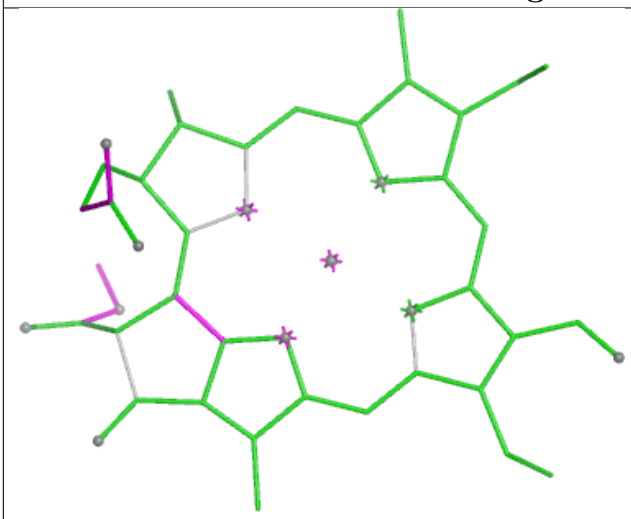


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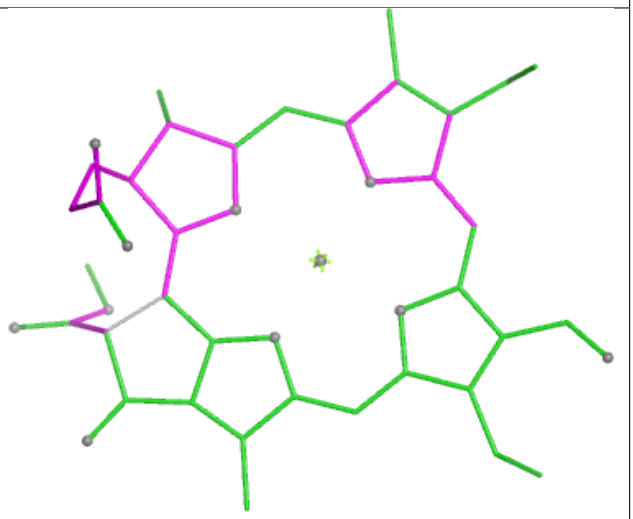


Rings

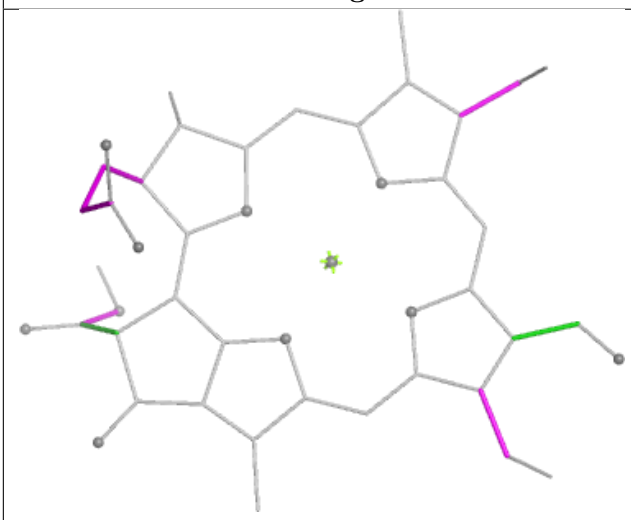
Ligand CHL S 306



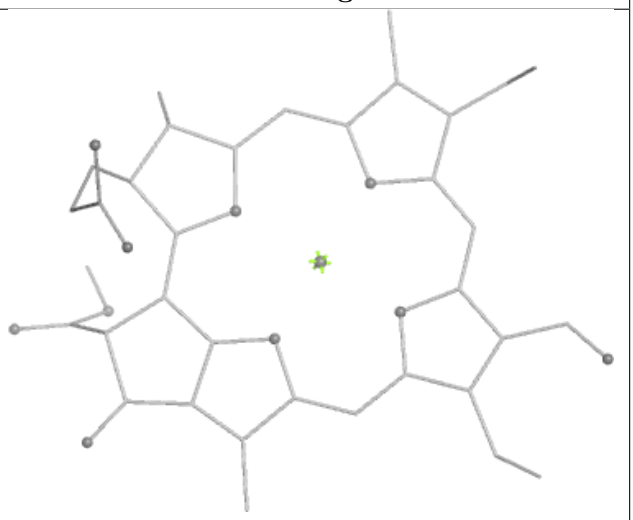
Bond lengths



Bond angles



Torsions

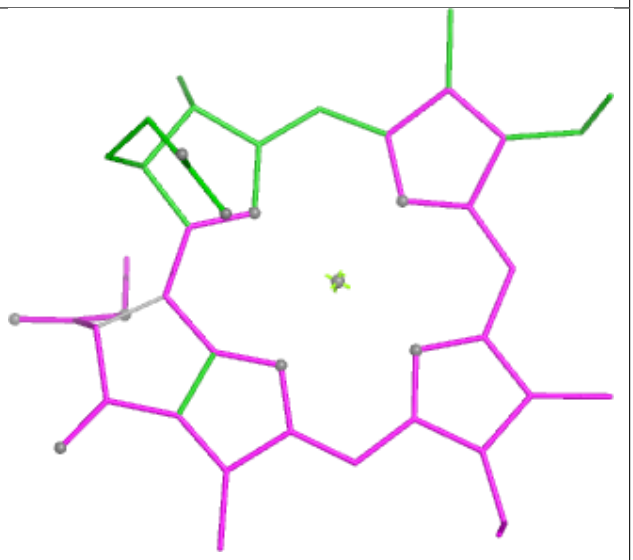


Rings

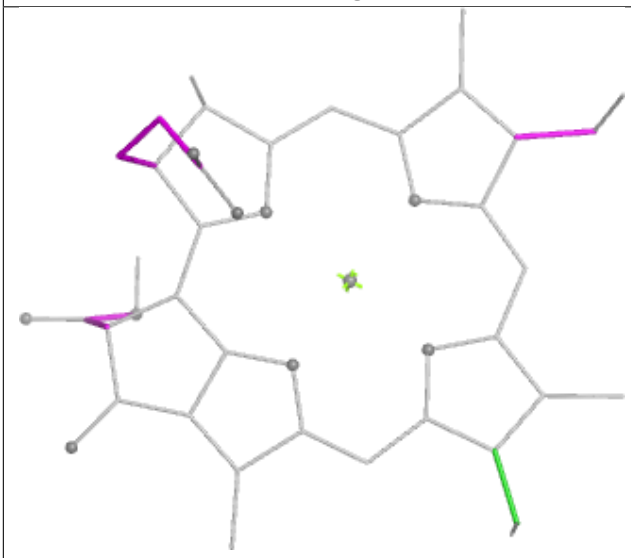
Ligand CLA S 303



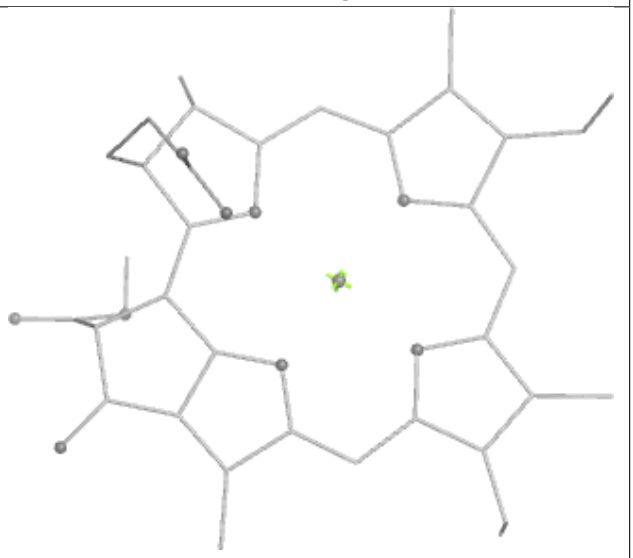
Bond lengths



Bond angles

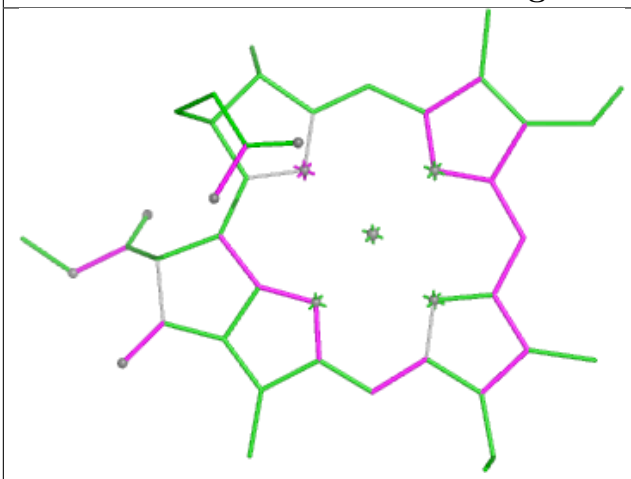


Torsions

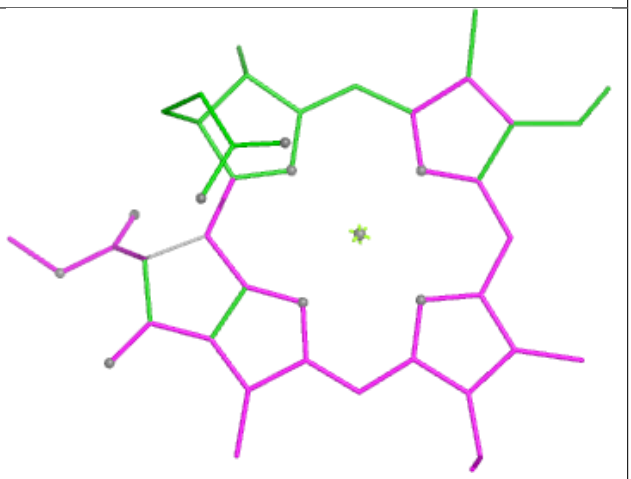


Rings

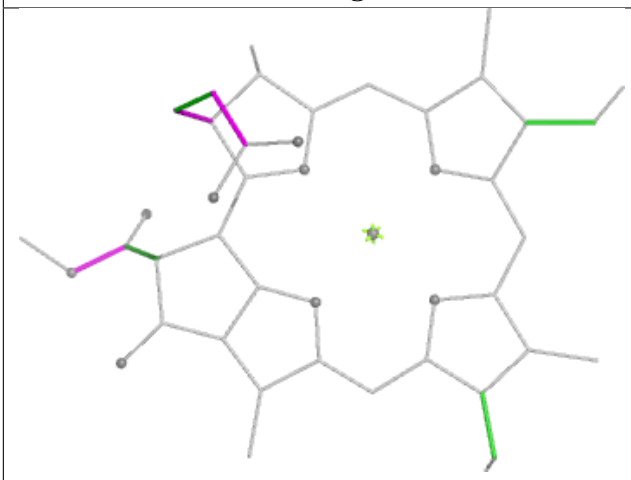
Ligand CLA 6 609



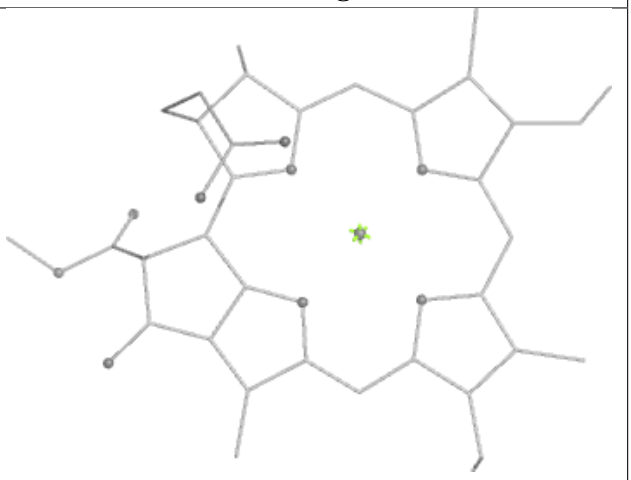
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

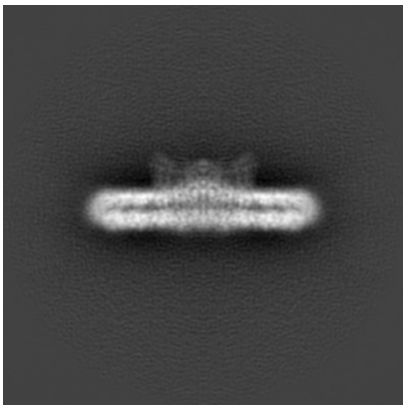
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3491. These allow visual inspection of the internal detail of the map and identification of artifacts.

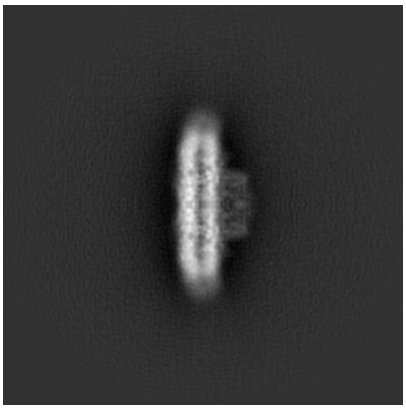
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

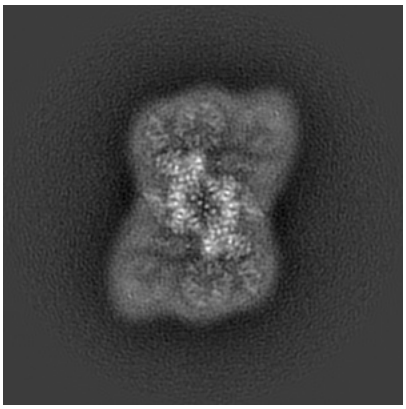
6.1.1 Primary map



X

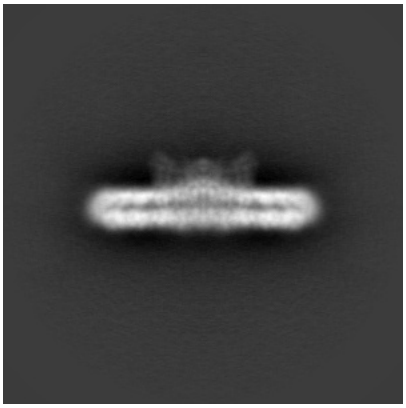


Y

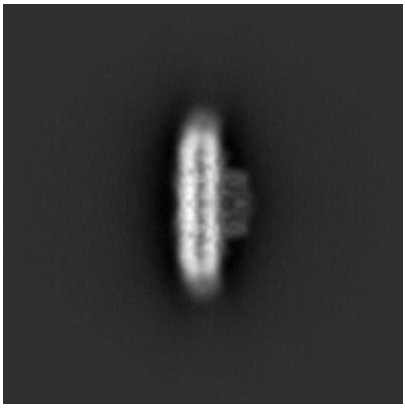


Z

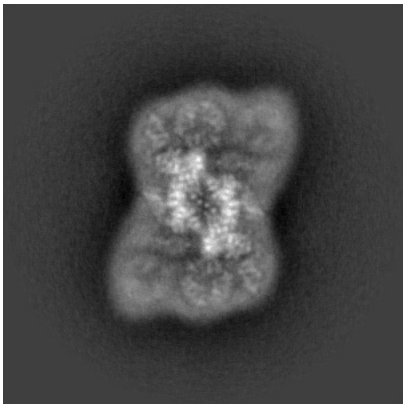
6.1.2 Raw map



X



Y

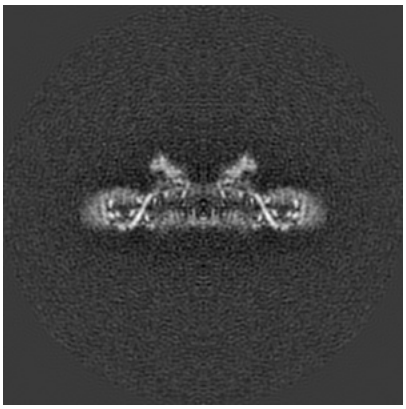


Z

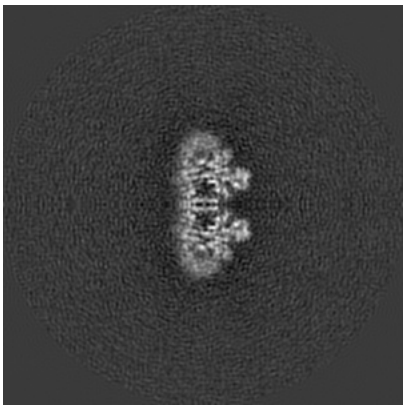
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

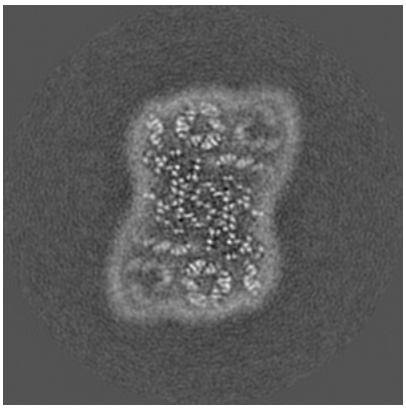
6.2.1 Primary map



X Index: 234

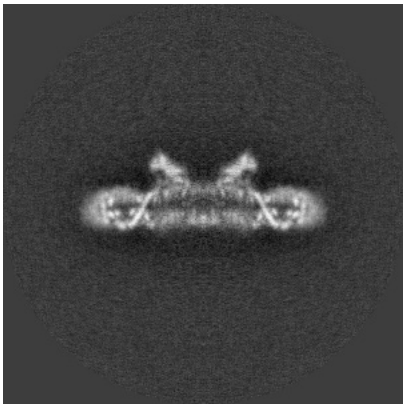


Y Index: 234

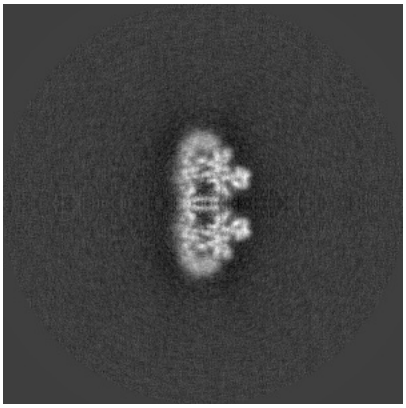


Z Index: 234

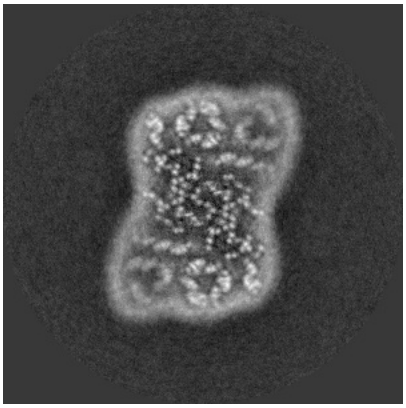
6.2.2 Raw map



X Index: 234



Y Index: 234

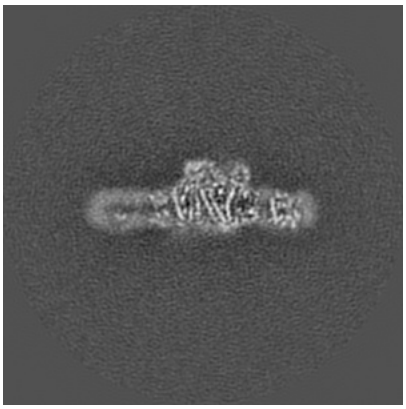


Z Index: 234

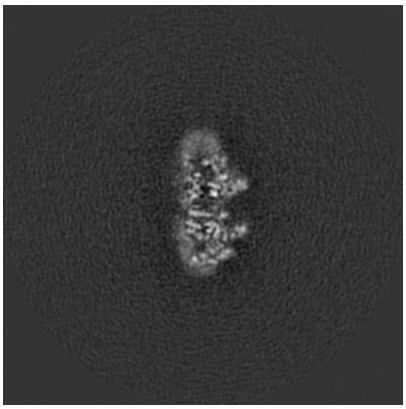
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

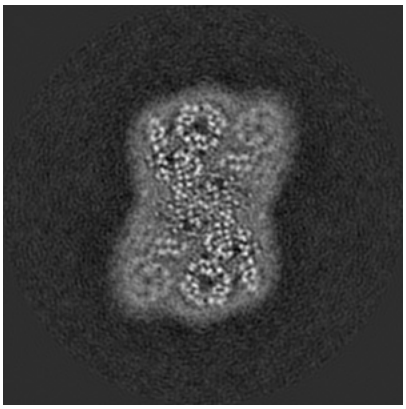
6.3.1 Primary map



X Index: 208

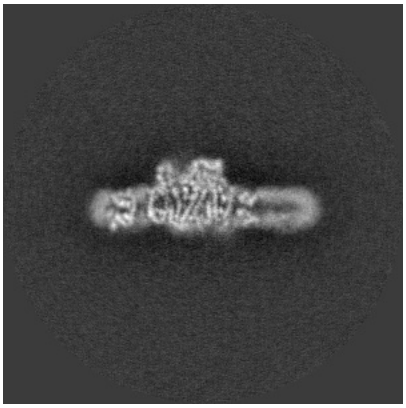


Y Index: 243

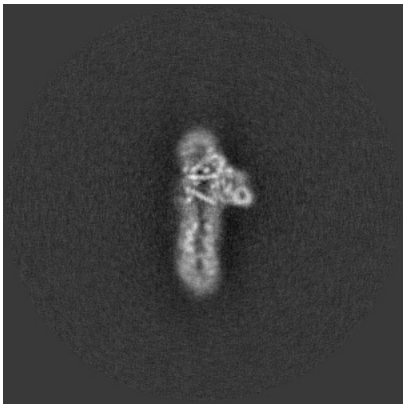


Z Index: 218

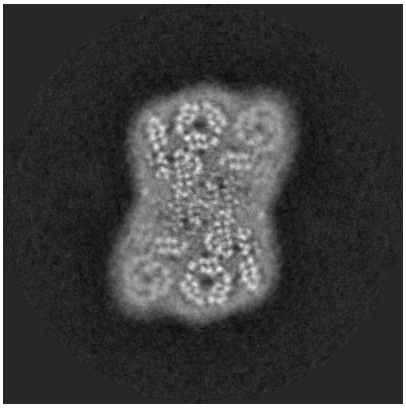
6.3.2 Raw map



X Index: 262



Y Index: 190

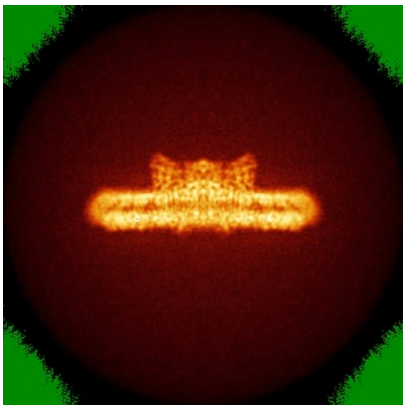


Z Index: 218

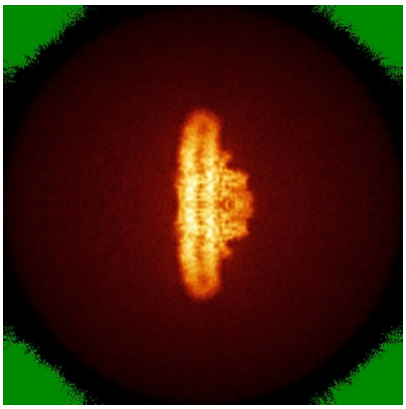
The images above show the largest variance slices of the map in three orthogonal directions.

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

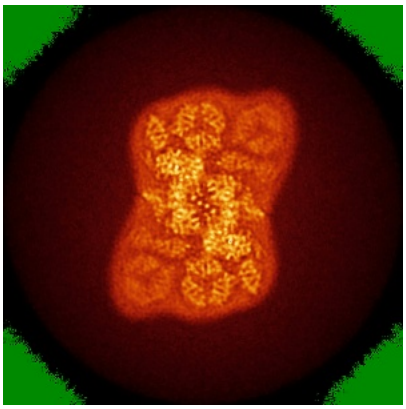
6.4.1 Primary map



X

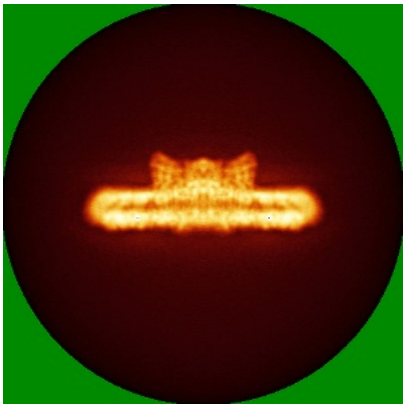


Y

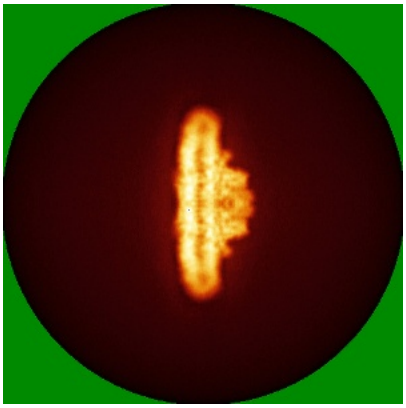


Z

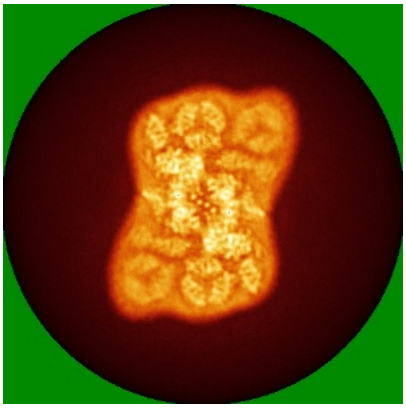
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

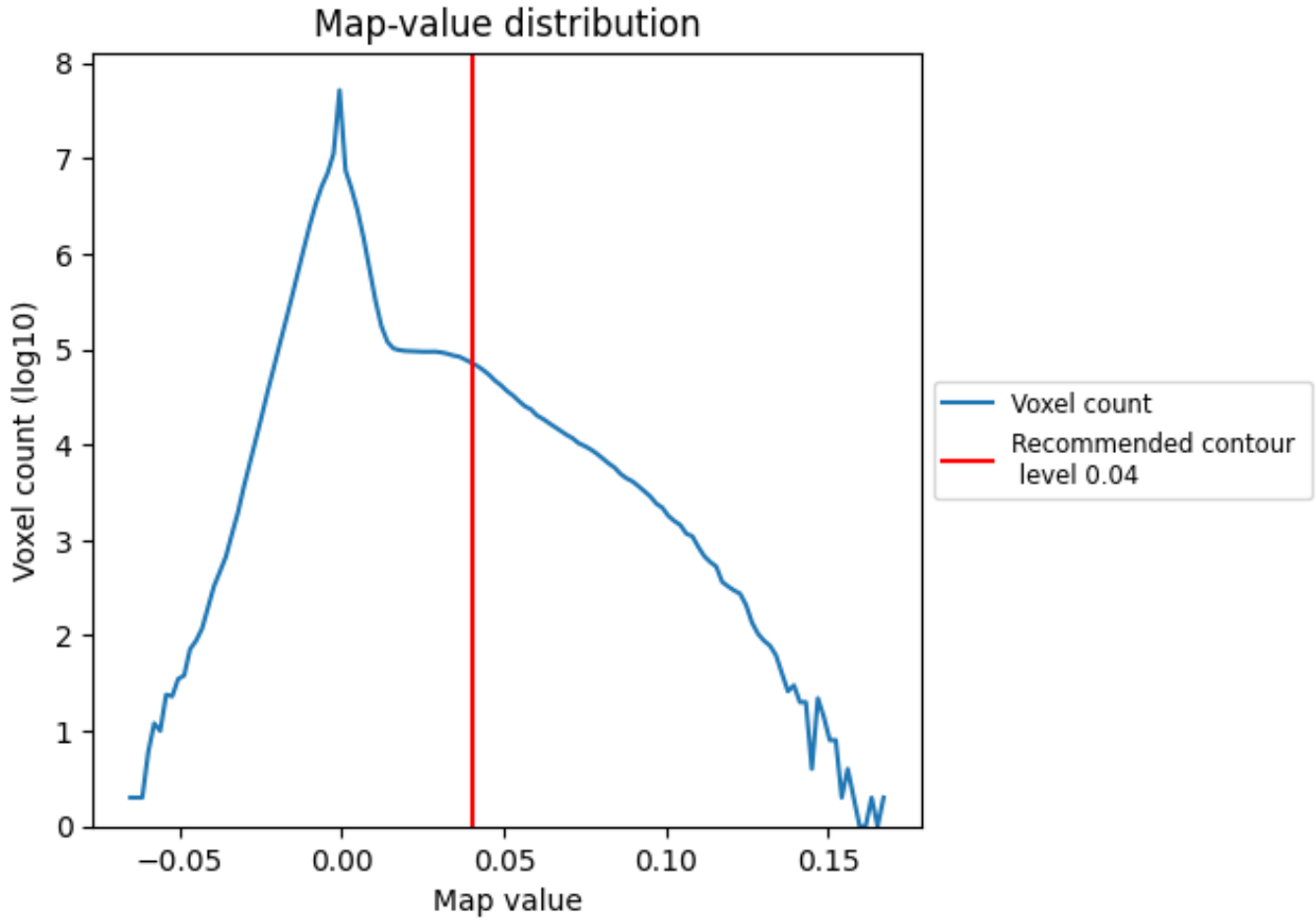
6.6 Mask visualisation (i)

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

7 Map analysis

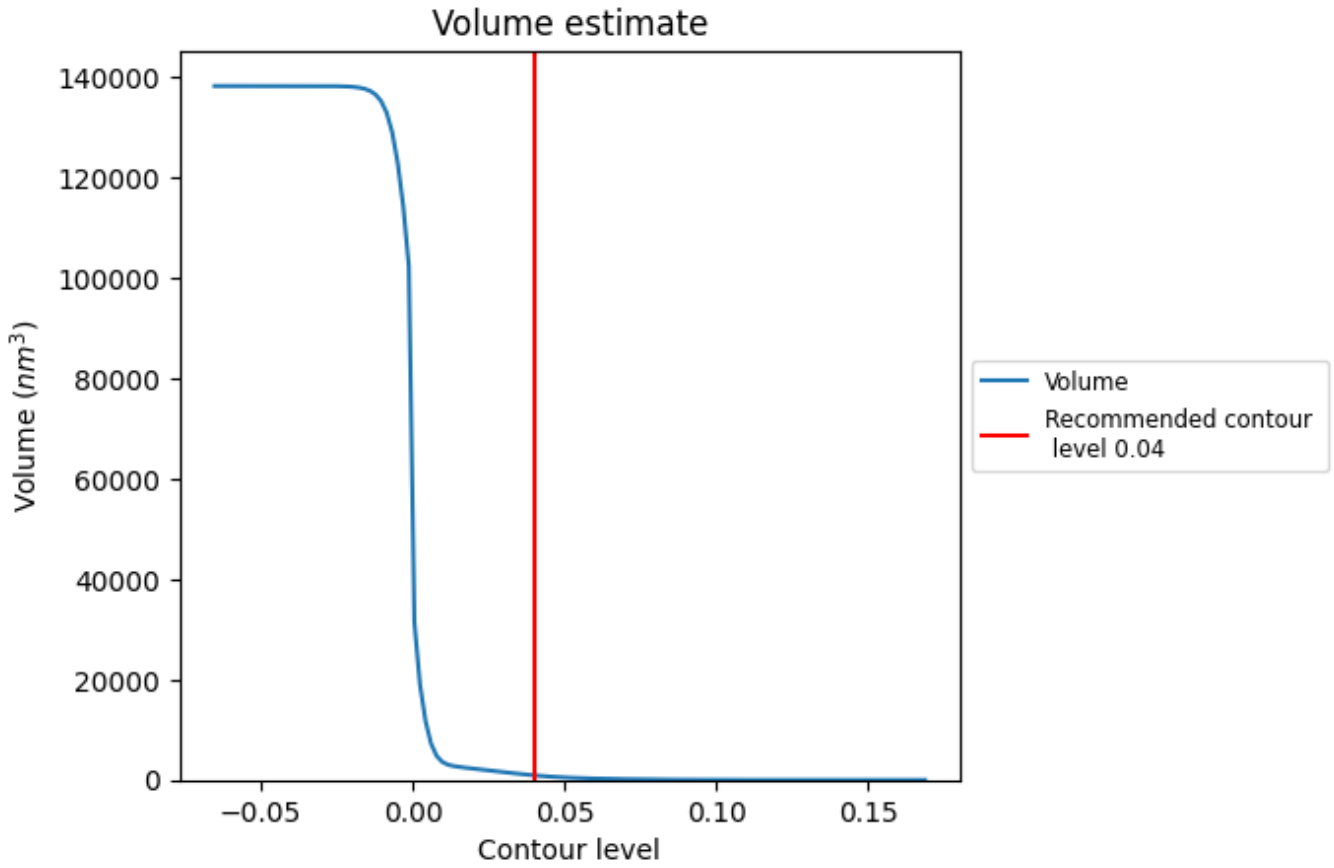
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

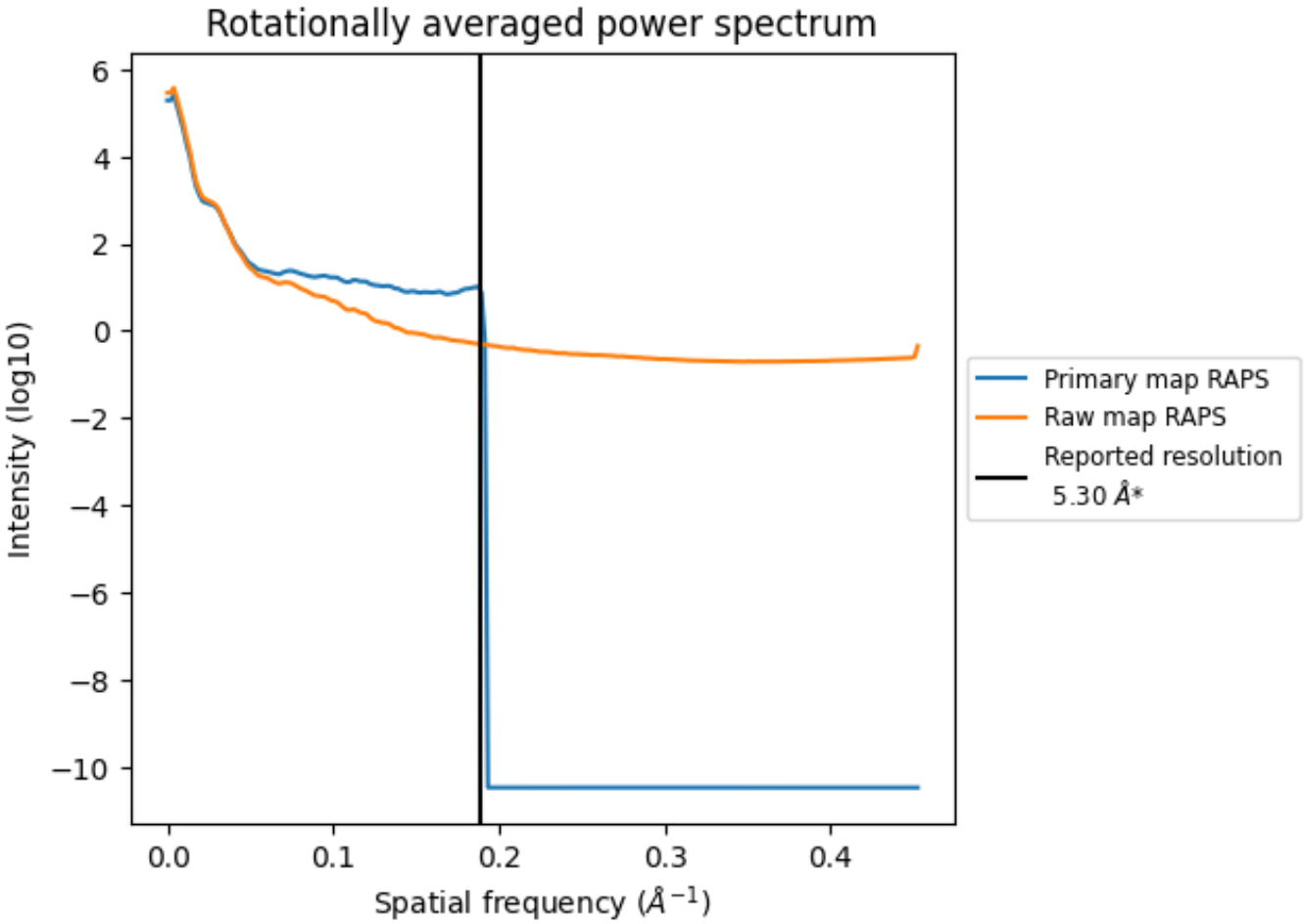
7.2 Volume estimate



The volume at the recommended contour level is 930 nm^3; this corresponds to an approximate mass of 840 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)

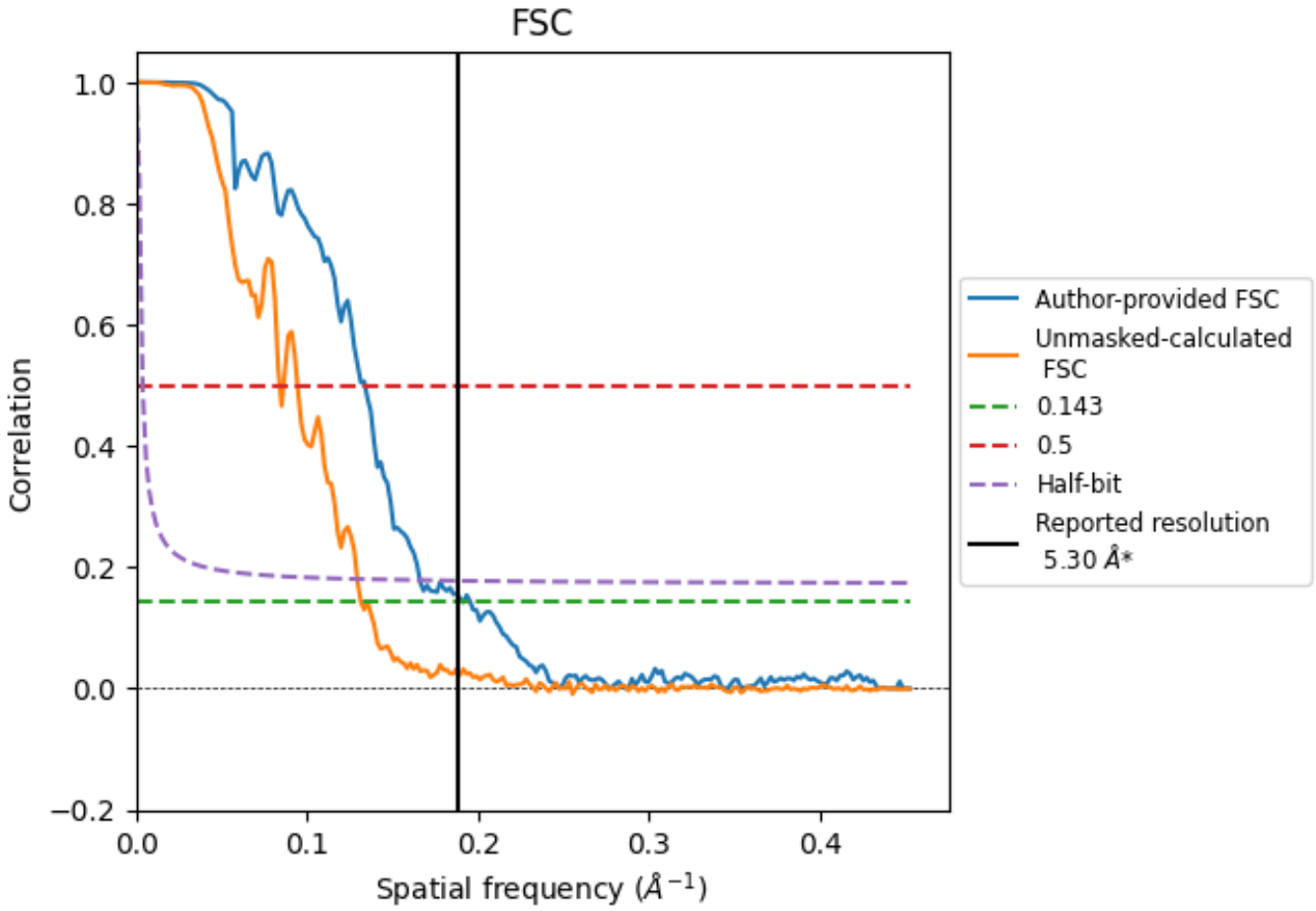


*Reported resolution corresponds to spatial frequency of 0.189 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.189 Å^{-1}

8.2 Resolution estimates (i)

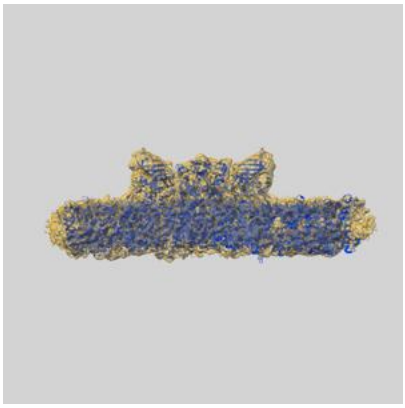
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	5.23	7.47	6.02
Unmasked-calculated*	7.60	11.90	7.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.60 differs from the reported value 5.3 by more than 10 %

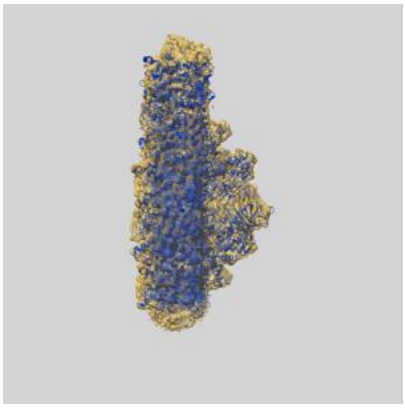
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3491 and PDB model 5MDX. Per-residue inclusion information can be found in section 3 on page 28.

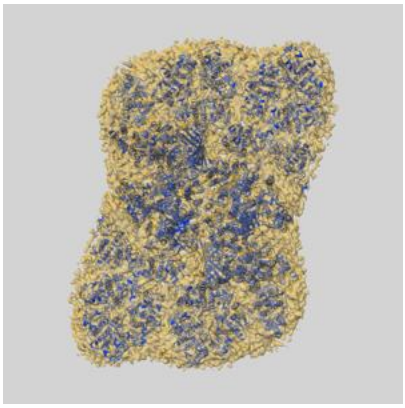
9.1 Map-model overlay



X



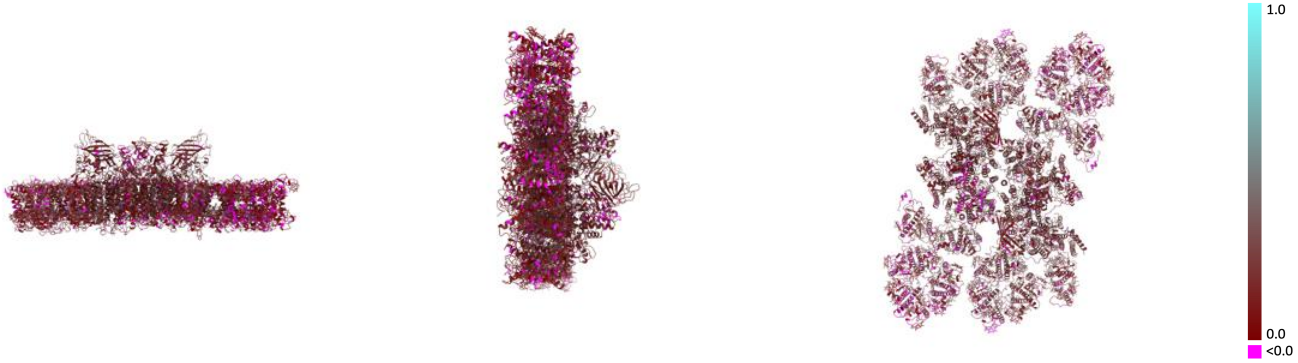
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

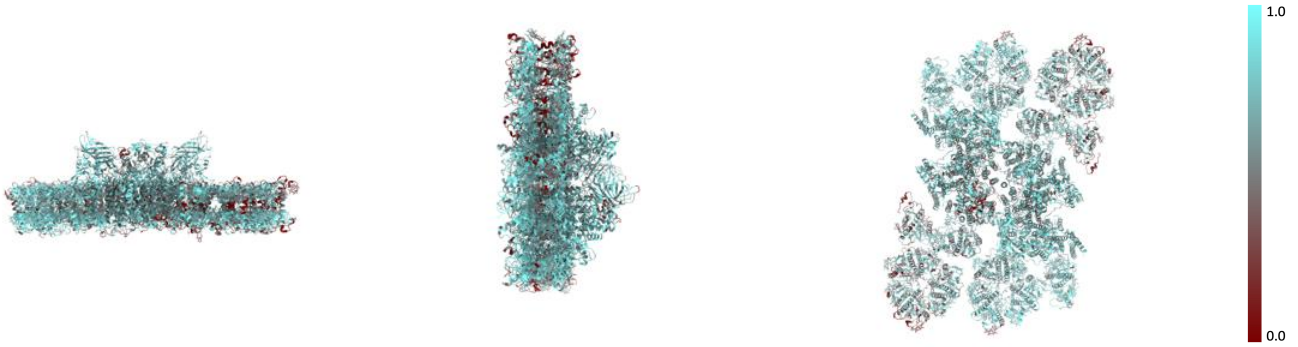
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

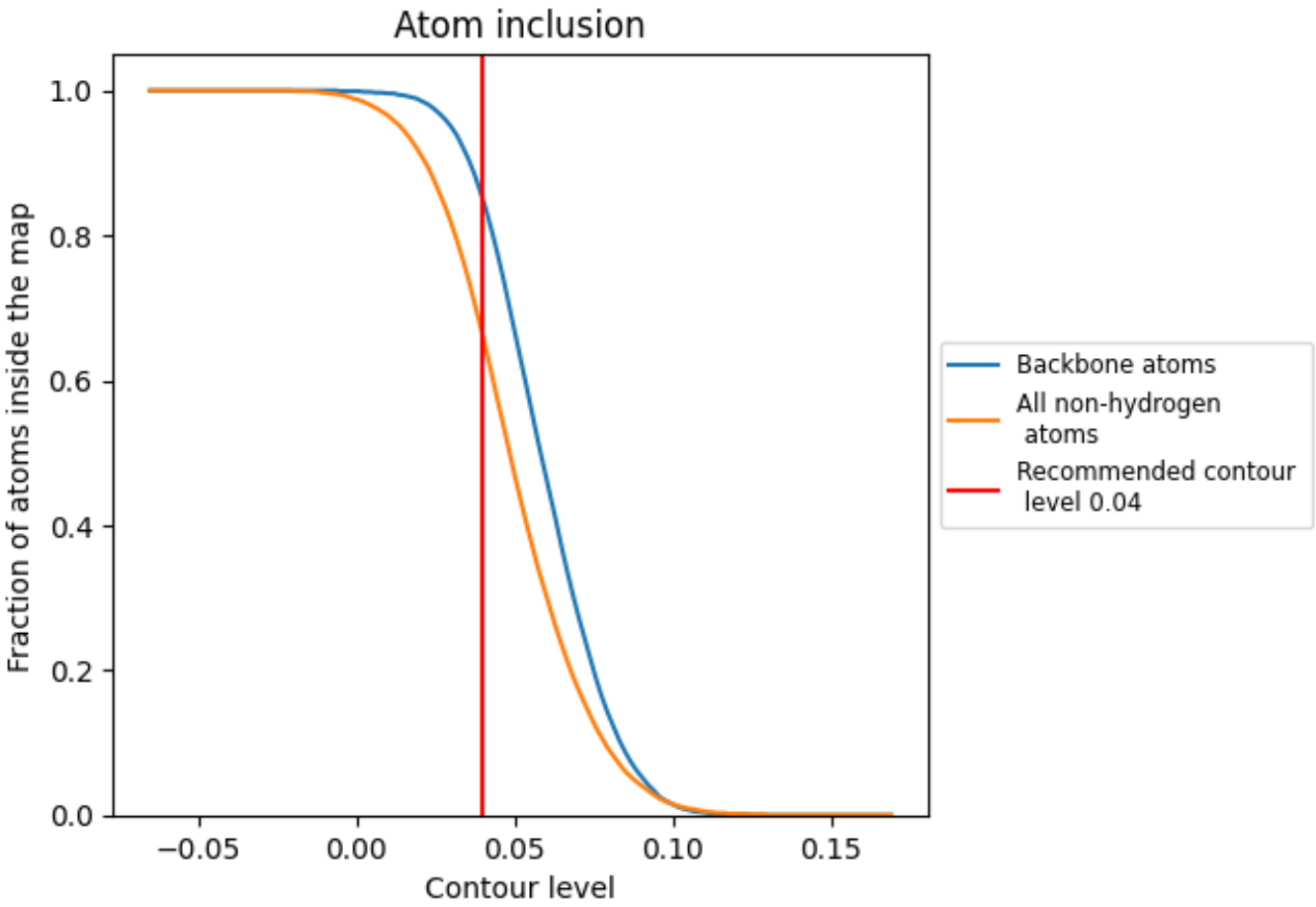
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6600	0.1630
1	0.6190	0.1070
2	0.5790	0.1060
3	0.5530	0.0770
4	0.5170	0.1150
5	0.6190	0.1080
6	0.5790	0.1060
7	0.5530	0.0780
8	0.5170	0.1160
A	0.6300	0.2030
B	0.6970	0.1970
C	0.7380	0.2150
D	0.6570	0.2030
E	0.7040	0.1680
F	0.7210	0.1220
G	0.7100	0.1470
H	0.7060	0.2160
I	0.5870	0.1790
K	0.6740	0.2180
L	0.6330	0.1940
M	0.5870	0.1950
N	0.7540	0.1700
O	0.7250	0.2070
R	0.6530	0.1620
S	0.7370	0.1660
T	0.5420	0.1940
W	0.6510	0.2050
X	0.6060	0.1600
Y	0.7030	0.1760
Z	0.6690	0.1580
a	0.6500	0.2110
b	0.5830	0.1220
c	0.7460	0.2260
d	0.6660	0.2030
e	0.7250	0.1830



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Chain	Atom inclusion	Q-score
f	0.6850	0.1790
g	0.7100	0.1450
h	0.6610	0.1880
i	0.5800	0.1780
k	0.6910	0.2100
l	0.6230	0.1810
m	0.5560	0.1770
n	0.7540	0.1690
o	0.7000	0.1850
r	0.6530	0.1610
s	0.7370	0.1640
t	0.5420	0.2050
w	0.6270	0.2140
x	0.5750	0.1480
y	0.7030	0.1760
z	0.6730	0.1730