Full wwPDB EM Validation Report

Oct 18, 2023 – 05:14 PM JST

PDB ID	:	8IML
EMDB ID	:	EMD-35568
Title	:	Rs2I-Rs2II, Rs1I-Rs1II, RbI-RbII cylinder in cyanobacterial phycobilisome from Anthocerotibacter panamensis (Cluster D)
Authors	:	Wang, C.H.; Yang, C.H.; Wu, H.Y.; Jiang, H.W.; Ho, M.C.; Ho, M.Y.
Deposited on	:	2023-03-07
Resolution	:	2.74 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:

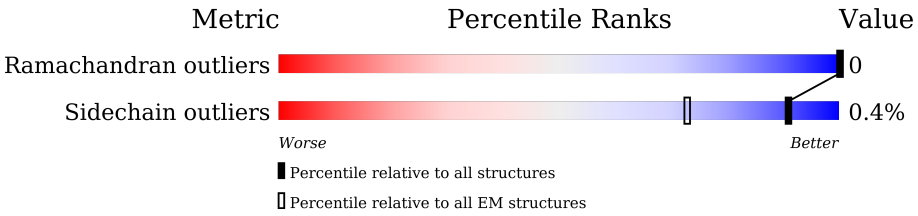
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.74 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	3	531	97%
2	A	163	20% 99%
2	B	163	5% 99%
2	C	163	12% 99%
2	D	163	99%
2	E	163	99%
2	F	163	99%
2	N	163	52% 99%
2	O	163	99%

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Mol	Chain	Length	Quality of chain
2	P	163	7% 99%
2	Q	163	99%
2	R	163	6% 99%
2	S	163	99%
2	a	163	91% 98%
2	b	163	10% 99%
2	c	163	62% 99%
2	d	163	6% 99%
2	e	163	59% 98%
2	f	163	21% 99%
3	G	172	30% 100%
3	H	172	33% 100%
3	I	172	7% 100%
3	J	172	99%
3	K	172	100%
3	L	172	99%
3	T	172	34% 100%
3	U	172	34% 100%
3	V	172	6% 99%
3	W	172	100%
3	X	172	100%
3	Y	172	100%
3	g	172	92% 100%
3	h	172	73% 100%
3	i	172	65% 100%

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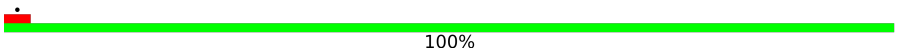
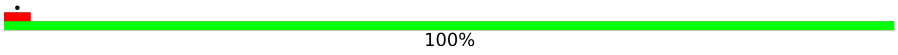
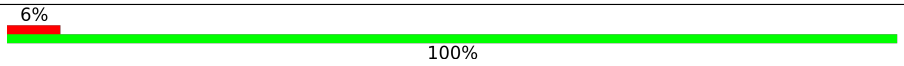
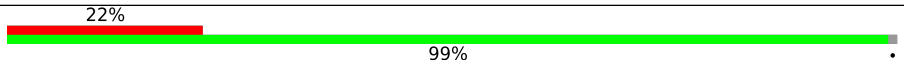
Mol	Chain	Length	Quality of chain
3	j	172	
3	k	172	
3	l	172	
4	M	78	
4	Z	78	
4	m	78	
5	4	252	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 55862 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 CpcJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	515	Total	C	N	O	S	0	0
			4129	2614	717	790	8		

- Molecule 2 is a protein called CpcA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	B	163	Total	C	N	O	S	0	0
			1262	804	217	239	2		
2	C	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	D	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	E	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	F	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	N	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	O	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	P	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	Q	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	R	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	S	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	a	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	b	163	Total	C	N	O	S	0	0
			1262	804	217	239	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	d	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	e	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	f	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		

- Molecule 3 is a protein called CpcB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	H	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	I	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	J	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	K	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	L	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	T	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	U	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	V	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	W	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	X	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	Y	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	g	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	h	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	i	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	j	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	k	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	l	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		

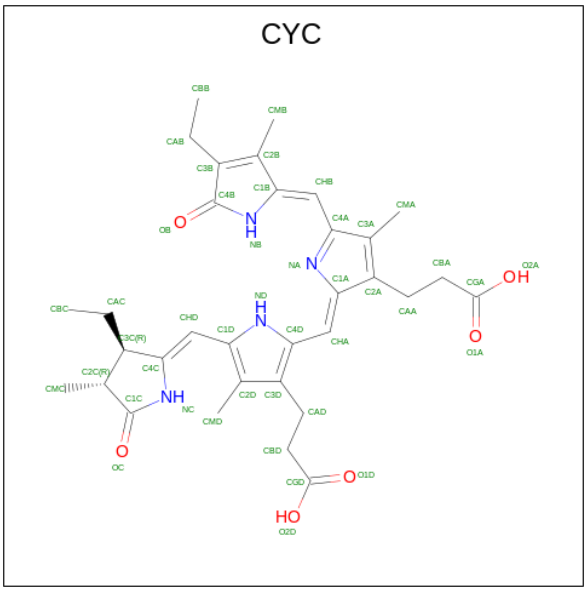
- Molecule 4 is a protein called CpcD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	60	Total	C	N	O	S	0	0
			483	306	90	86	1		
4	Z	60	Total	C	N	O	S	0	0
			483	306	90	86	1		
4	m	69	Total	C	N	O	S	0	0
			546	345	101	99	1		

- Molecule 5 is a protein called CpcG.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	250	Total	C	N	O	S	0	0
			2037	1312	349	373	3		

- Molecule 6 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	3	1	Total	C	N	O	0
			43	33	4	6	
6	A	1	Total	C	N	O	0
			43	33	4	6	
6	A	1	Total	C	N	O	0
			43	33	4	6	
6	B	1	Total	C	N	O	0
			43	33	4	6	
6	B	1	Total	C	N	O	0
			43	33	4	6	
6	C	1	Total	C	N	O	0
			43	33	4	6	
6	D	1	Total	C	N	O	0
			43	33	4	6	
6	E	1	Total	C	N	O	0
			43	33	4	6	
6	F	1	Total	C	N	O	0
			43	33	4	6	
6	G	1	Total	C	N	O	0
			43	33	4	6	
6	G	1	Total	C	N	O	0
			43	33	4	6	
6	H	1	Total	C	N	O	0
			43	33	4	6	
6	I	1	Total	C	N	O	0
			43	33	4	6	
6	I	1	Total	C	N	O	0
			43	33	4	6	
6	J	1	Total	C	N	O	0
			43	33	4	6	
6	K	1	Total	C	N	O	0
			43	33	4	6	
6	K	1	Total	C	N	O	0
			43	33	4	6	
6	L	1	Total	C	N	O	0
			43	33	4	6	
6	N	1	Total	C	N	O	0
			43	33	4	6	
6	O	1	Total	C	N	O	0
			43	33	4	6	
6	P	1	Total	C	N	O	0
			43	33	4	6	
6	Q	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
6	R	1	Total	C	N	O	0
			43	33	4	6	
6	S	1	Total	C	N	O	0
			43	33	4	6	
6	T	1	Total	C	N	O	0
			43	33	4	6	
6	T	1	Total	C	N	O	0
			43	33	4	6	
6	U	1	Total	C	N	O	0
			43	33	4	6	
6	V	1	Total	C	N	O	0
			43	33	4	6	
6	V	1	Total	C	N	O	0
			43	33	4	6	
6	W	1	Total	C	N	O	0
			43	33	4	6	
6	W	1	Total	C	N	O	0
			43	33	4	6	
6	X	1	Total	C	N	O	0
			43	33	4	6	
6	X	1	Total	C	N	O	0
			43	33	4	6	
6	Y	1	Total	C	N	O	0
			43	33	4	6	
6	Y	1	Total	C	N	O	0
			43	33	4	6	
6	Z	1	Total	C	N	O	0
			43	33	4	6	
6	4	1	Total	C	N	O	0
			43	33	4	6	
6	a	1	Total	C	N	O	0
			43	33	4	6	
6	b	1	Total	C	N	O	0
			43	33	4	6	
6	c	1	Total	C	N	O	0
			43	33	4	6	
6	d	1	Total	C	N	O	0
			43	33	4	6	
6	e	1	Total	C	N	O	0
			43	33	4	6	
6	f	1	Total	C	N	O	0
			43	33	4	6	

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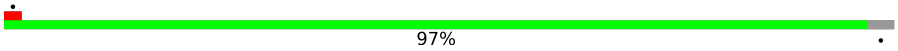
Mol	Chain	Residues	Atoms				AltConf
6	g	1	Total	C	N	O	0
			43	33	4	6	
6	g	1	Total	C	N	O	0
			43	33	4	6	
6	h	1	Total	C	N	O	0
			43	33	4	6	
6	h	1	Total	C	N	O	0
			43	33	4	6	
6	i	1	Total	C	N	O	0
			43	33	4	6	
6	j	1	Total	C	N	O	0
			43	33	4	6	
6	j	1	Total	C	N	O	0
			43	33	4	6	
6	k	1	Total	C	N	O	0
			43	33	4	6	
6	k	1	Total	C	N	O	0
			43	33	4	6	
6	l	1	Total	C	N	O	0
			43	33	4	6	
6	l	1	Total	C	N	O	0
			43	33	4	6	

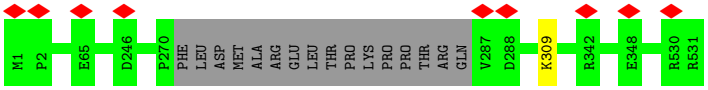
3 Residue-property plots (i)

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: CpcJ

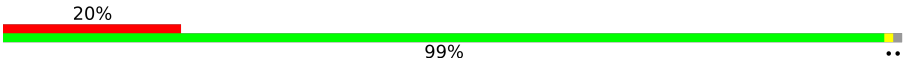
Chain 3:

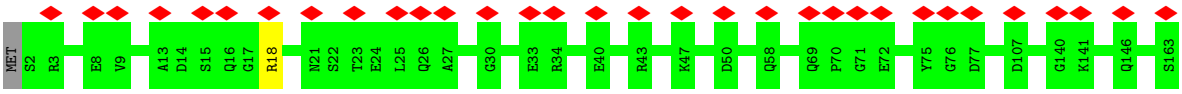




• Molecule 2: CpcA

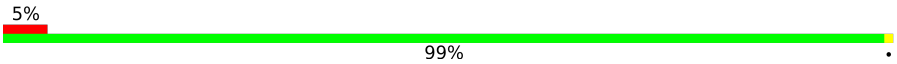
Chain A:

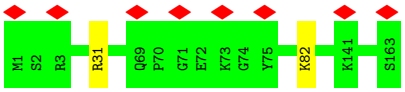




• Molecule 2: CpcA

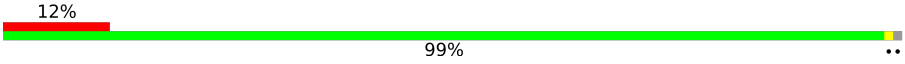
Chain B:

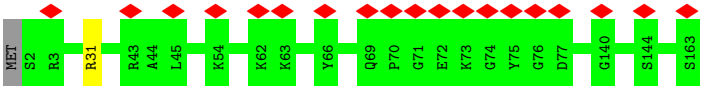




• Molecule 2: CpcA

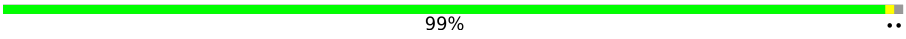
Chain C:





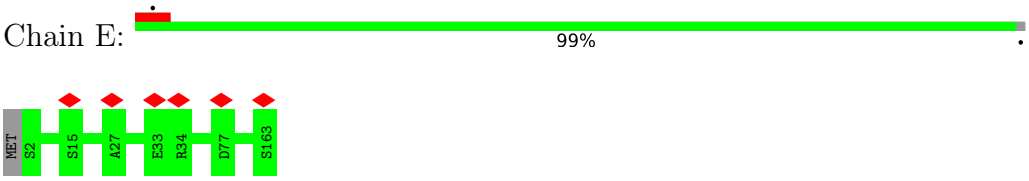
• Molecule 2: CpcA

Chain D:



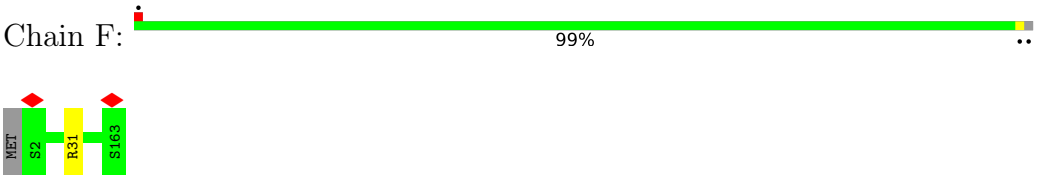
• Molecule 2: CpcA

Chain E:



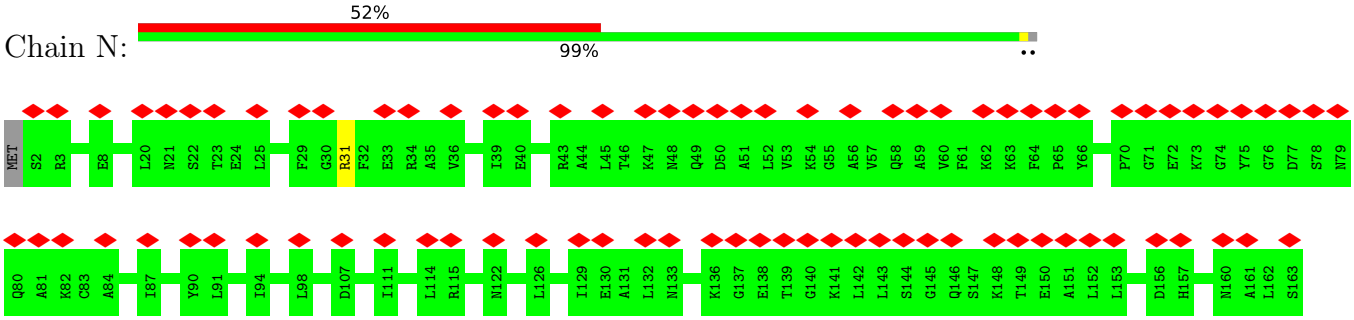
• Molecule 2: CpcA

Chain F:



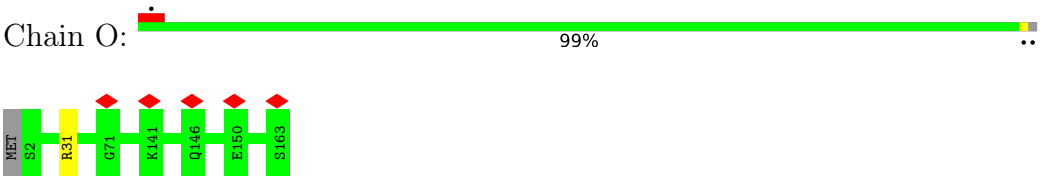
• Molecule 2: CpcA

Chain N:



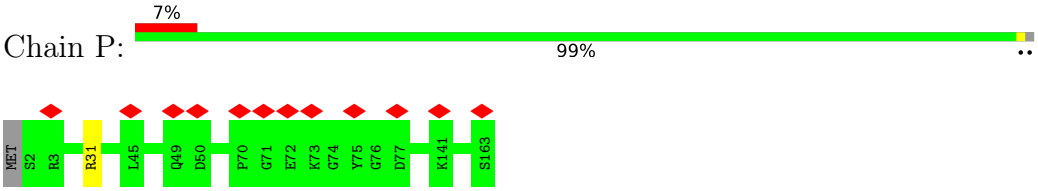
• Molecule 2: CpcA

Chain O:



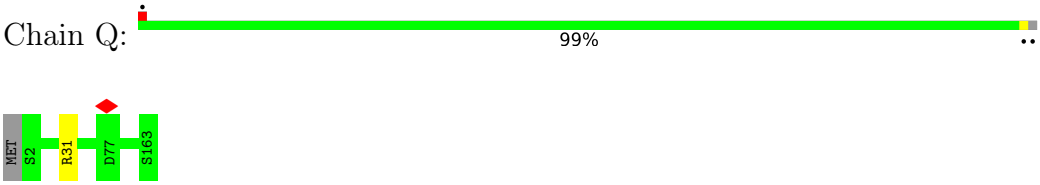
• Molecule 2: CpcA

Chain P:



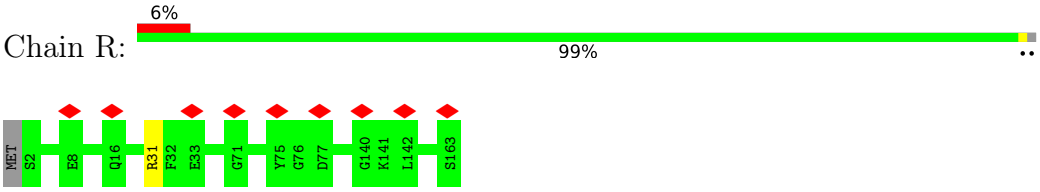
• Molecule 2: CpcA

Chain Q:



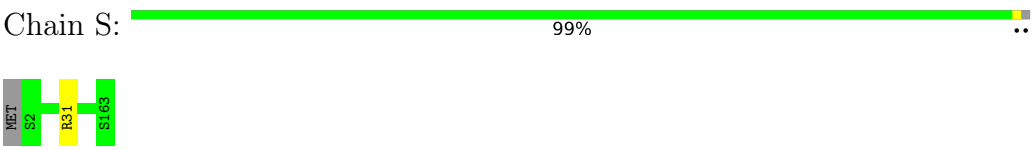
• Molecule 2: CpcA

Chain R:



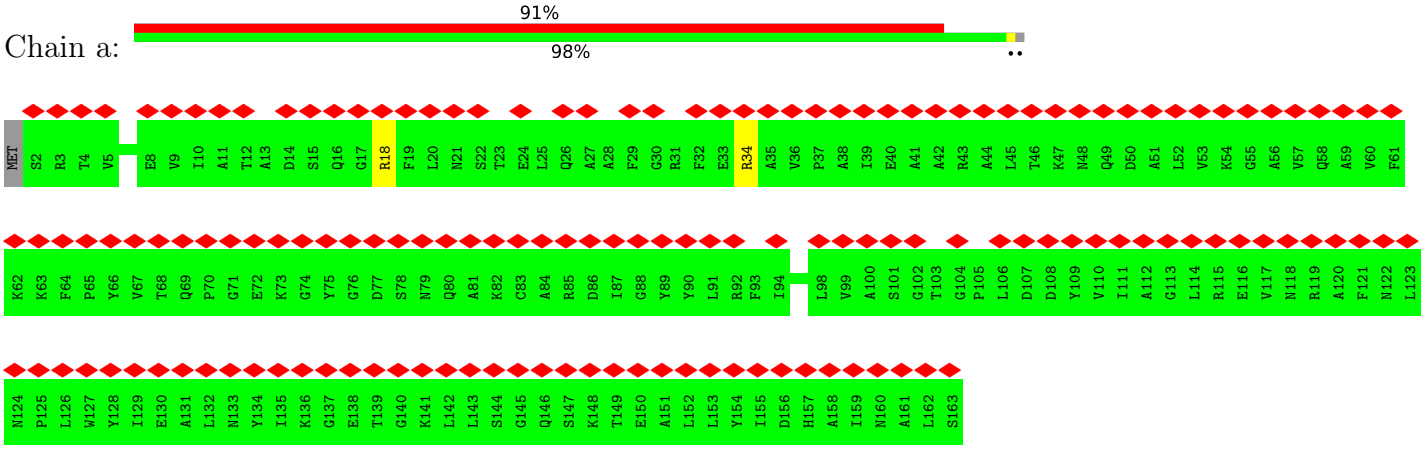
• Molecule 2: CpcA

Chain S:



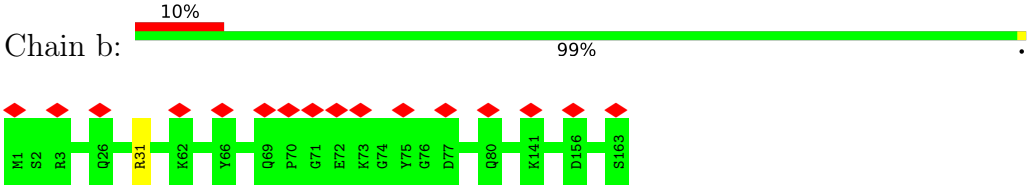
• Molecule 2: CpcA

Chain a:



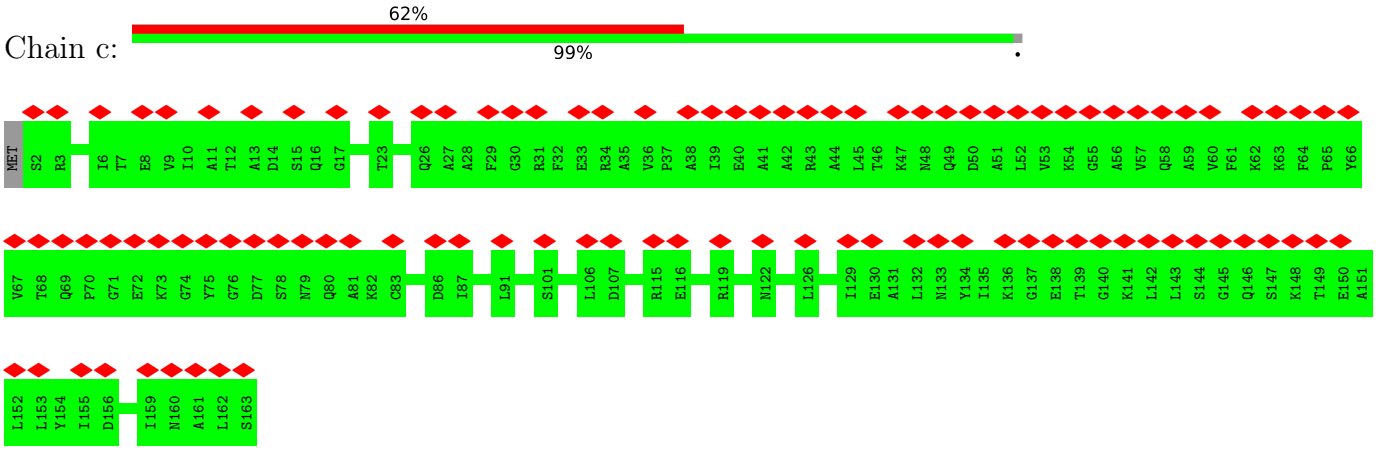
• Molecule 2: CpcA

Chain b:



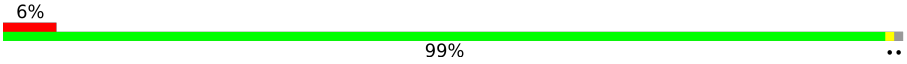
• Molecule 2: CpcA

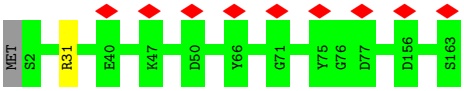
Chain c:



• Molecule 2: CpcA

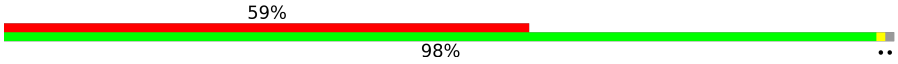
Chain d:

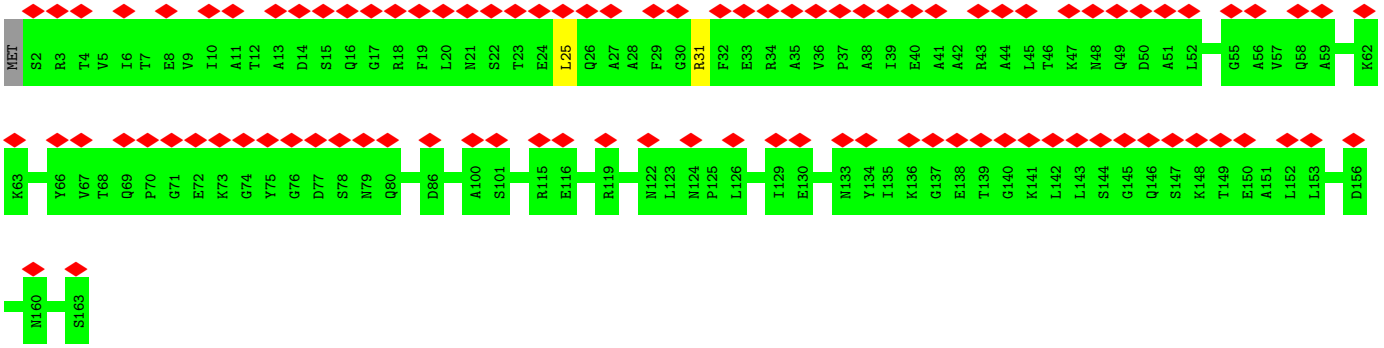




• Molecule 2: CpcA

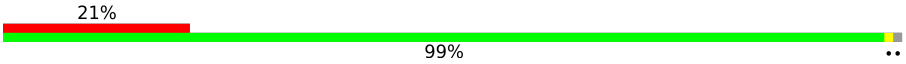
Chain e:

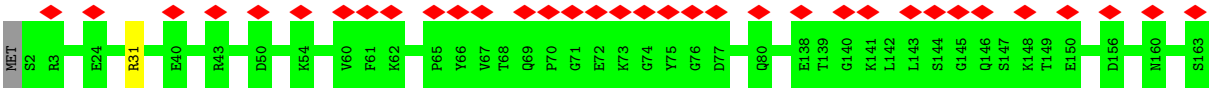




• Molecule 2: CpcA

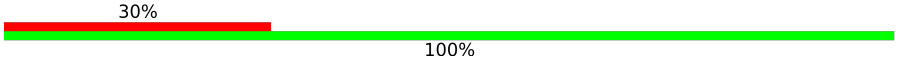
Chain f:





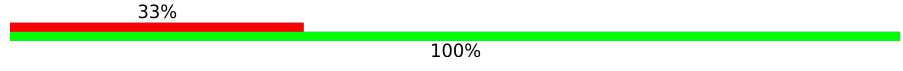
• Molecule 3: CpcB

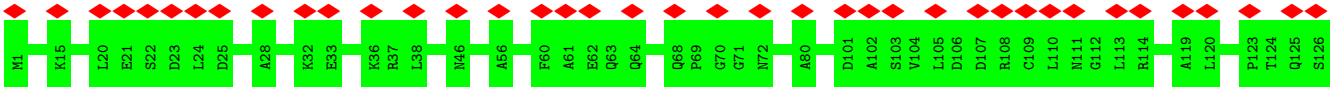
Chain G:

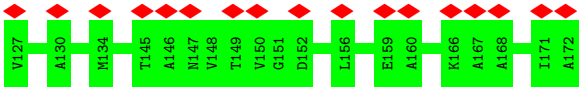


• Molecule 3: CpcB

Chain H:

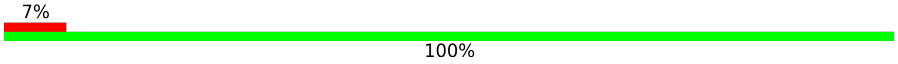


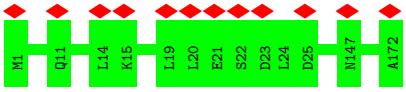




• Molecule 3: CpcB

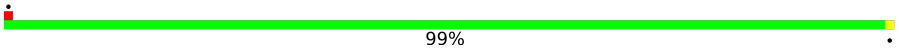
Chain I:





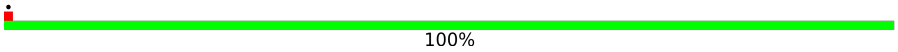
• Molecule 3: CpcB

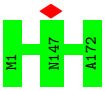
Chain J:



• Molecule 3: CpcB

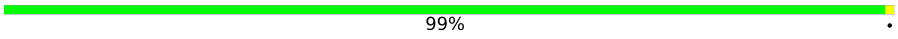
Chain K:





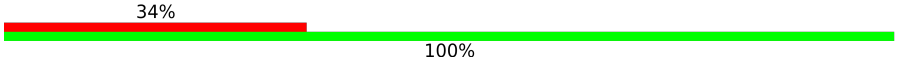
• Molecule 3: CpcB

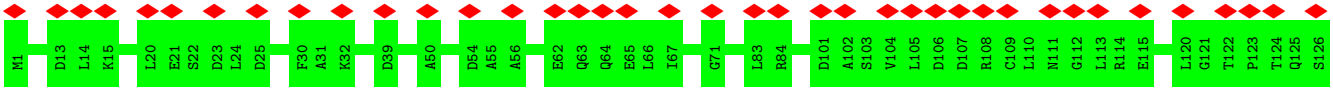
Chain L:

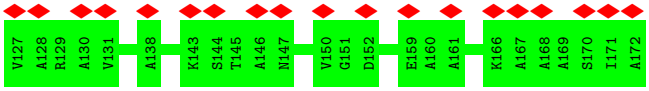


• Molecule 3: CpcB

Chain T:

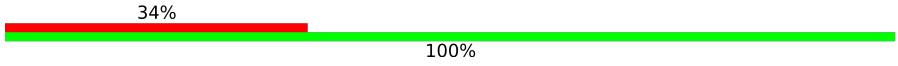


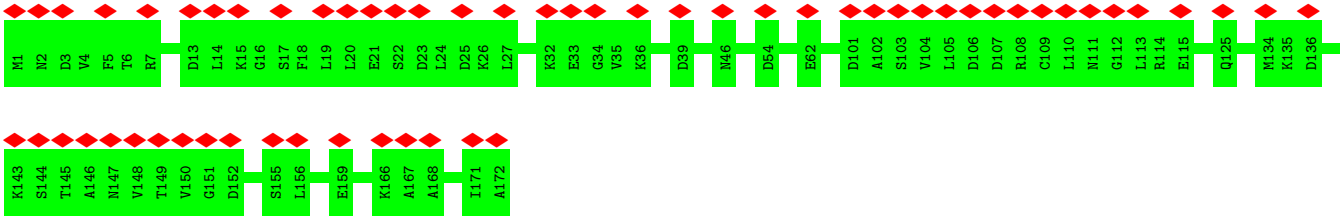




• Molecule 3: CpcB

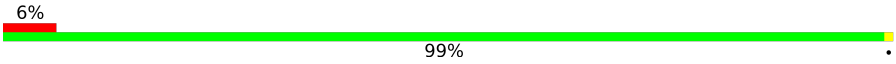
Chain U:

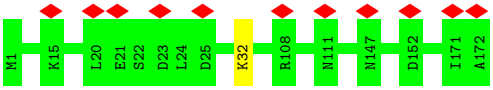




• Molecule 3: CpcB

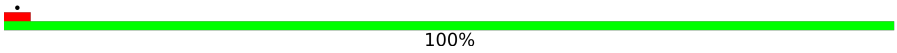
Chain V:

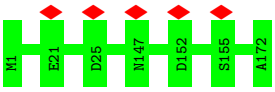




• Molecule 3: CpcB

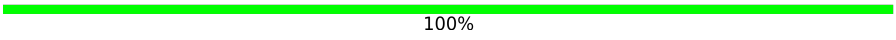
Chain W:





• Molecule 3: CpcB

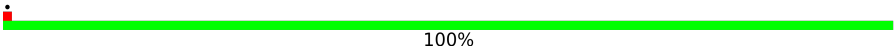
Chain X:

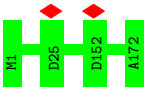


There are no outlier residues recorded for this chain.

• Molecule 3: CpcB

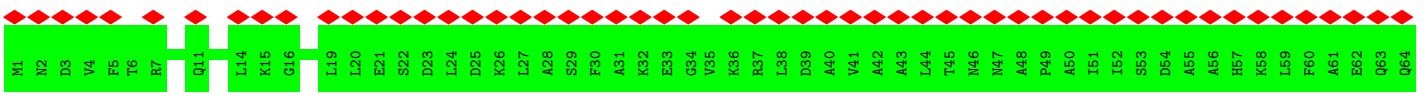
Chain Y:

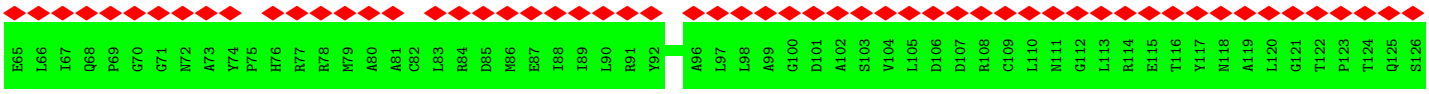


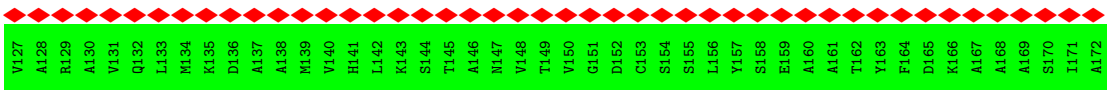


• Molecule 3: CpcB

Chain g:

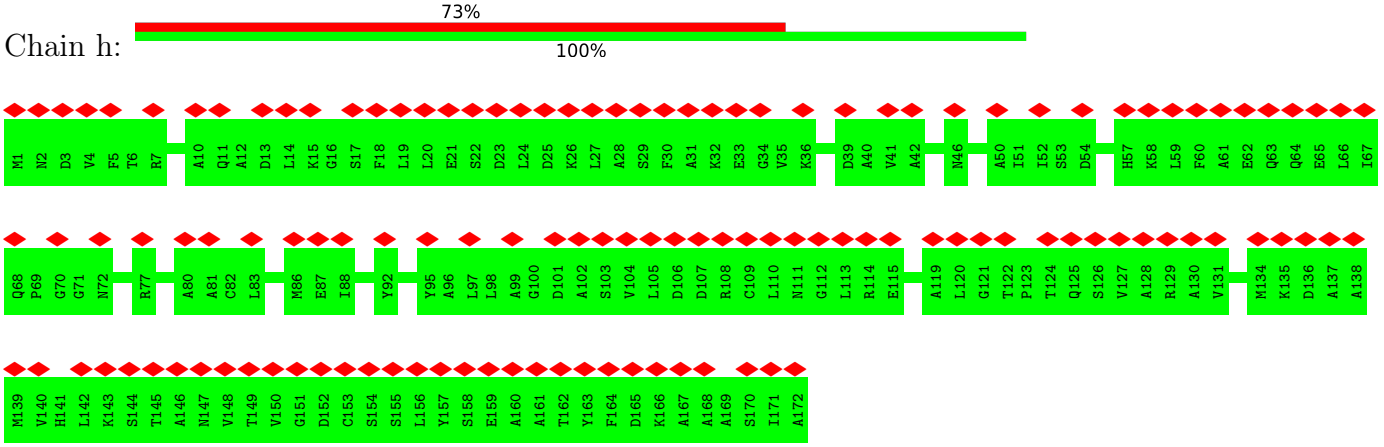






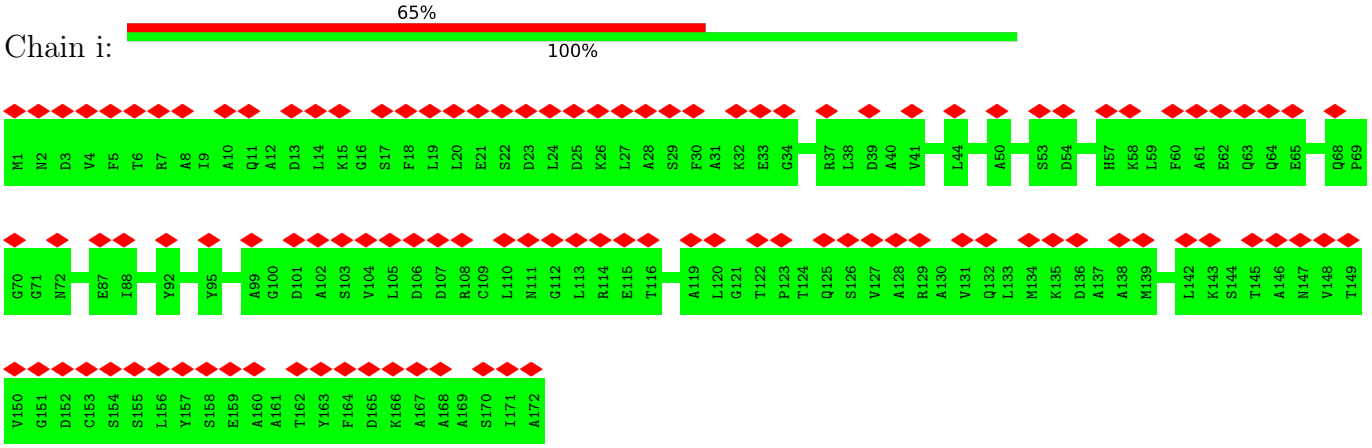
• Molecule 3: CpcB

Chain h:



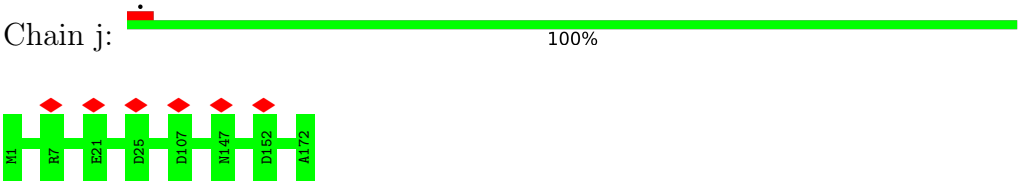
• Molecule 3: CpcB

Chain i:



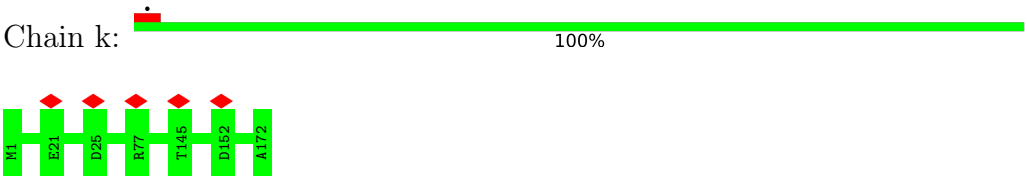
• Molecule 3: CpcB

Chain j:



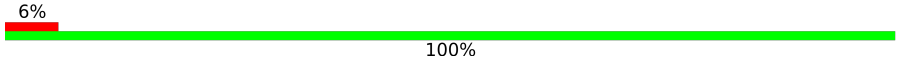
• Molecule 3: CpcB

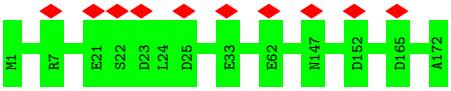
Chain k:



• Molecule 3: CpcB

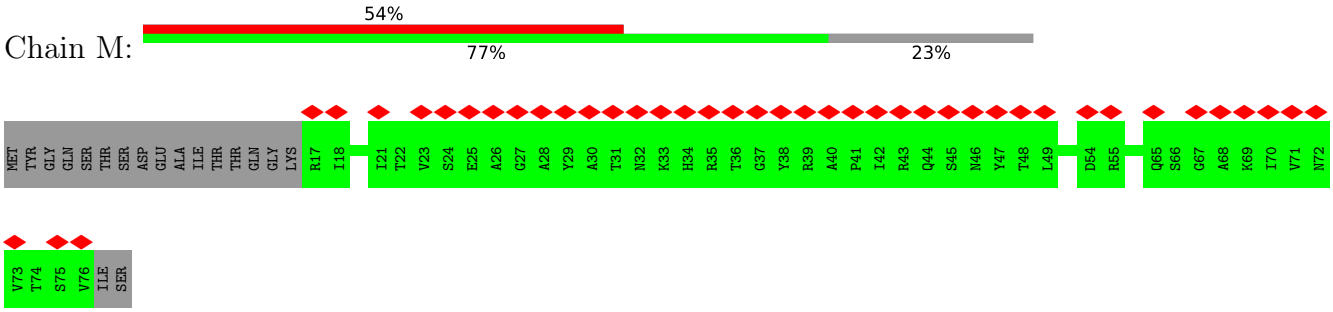
Chain l:





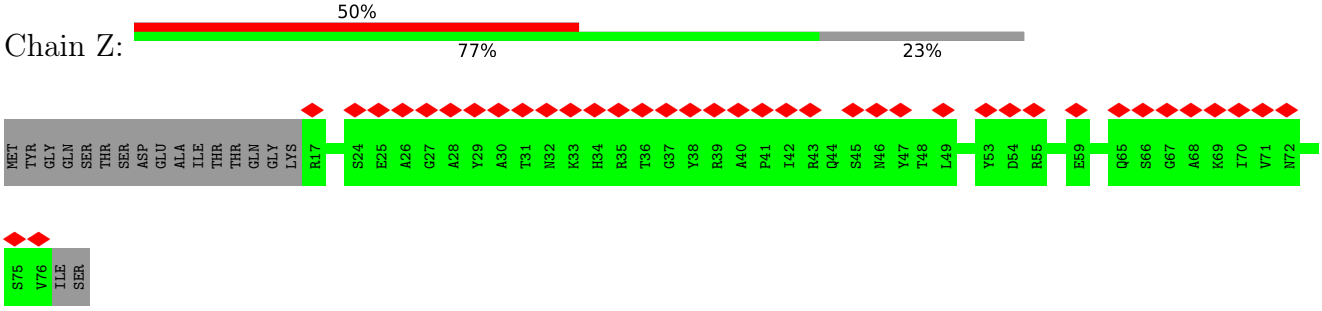
• Molecule 4: CpcD

Chain M:



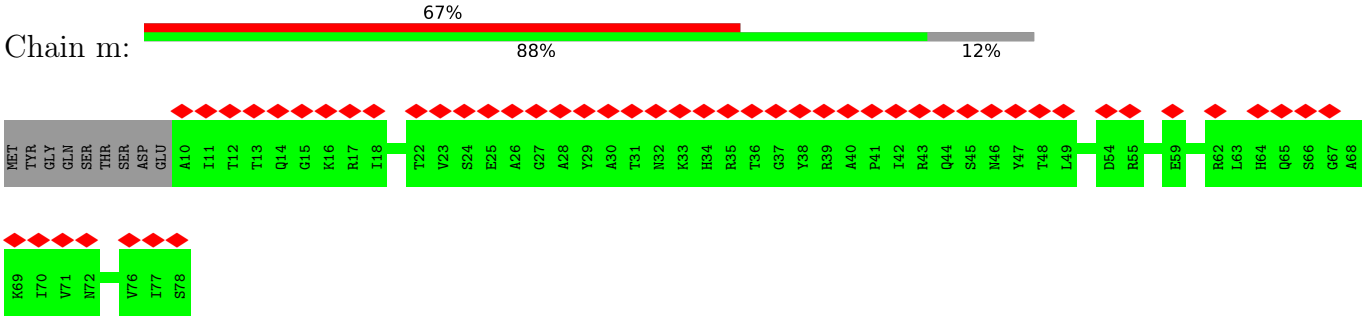
• Molecule 4: CpcD

Chain Z:



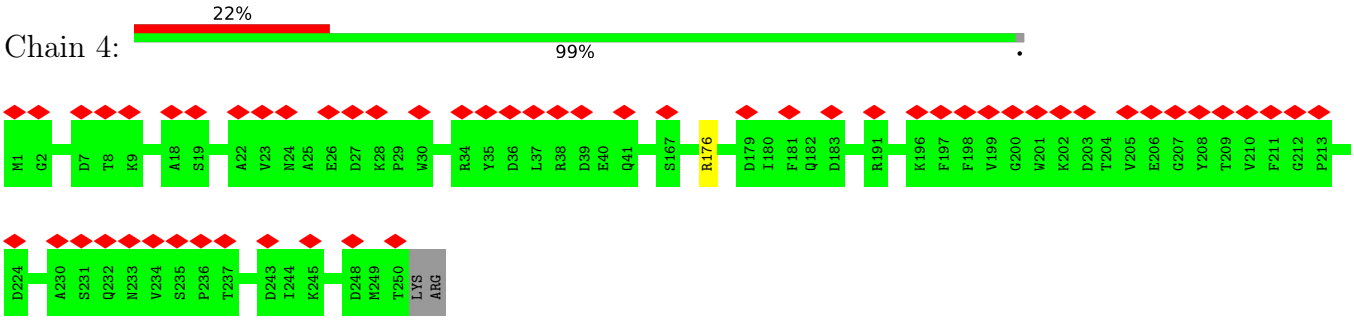
• Molecule 4: CpcD

Chain m:



• Molecule 5: CpcG

Chain 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1109579	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	8100	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.920	Depositor
Minimum map value	-0.235	Depositor
Average map value	0.065	Depositor
Map value standard deviation	0.123	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	721.48, 721.48, 721.48	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CYC

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	3	0.47	0/4224	0.51	0/5713
2	A	0.35	0/1277	0.46	0/1729
2	B	0.39	0/1285	0.49	0/1739
2	C	0.33	0/1277	0.43	0/1729
2	D	0.43	0/1277	0.47	0/1729
2	E	0.34	0/1277	0.45	0/1729
2	F	0.43	0/1277	0.46	0/1729
2	N	0.30	0/1277	0.44	0/1729
2	O	0.38	0/1277	0.45	0/1729
2	P	0.36	0/1277	0.45	0/1729
2	Q	0.41	0/1277	0.44	0/1729
2	R	0.34	0/1277	0.41	0/1729
2	S	0.42	0/1277	0.49	0/1729
2	a	0.32	0/1277	0.52	1/1729 (0.1%)
2	b	0.39	0/1285	0.47	0/1739
2	c	0.30	0/1277	0.46	0/1729
2	d	0.39	0/1277	0.43	0/1729
2	e	0.31	0/1277	0.46	1/1729 (0.1%)
2	f	0.35	0/1277	0.44	0/1729
3	G	0.28	0/1310	0.42	0/1772
3	H	0.29	0/1310	0.44	0/1772
3	I	0.32	0/1310	0.44	0/1772
3	J	0.44	0/1310	0.49	0/1772
3	K	0.41	0/1310	0.45	0/1772
3	L	0.40	0/1310	0.43	0/1772
3	T	0.28	0/1310	0.41	0/1772
3	U	0.29	0/1310	0.45	0/1772
3	V	0.32	0/1310	0.43	0/1772
3	W	0.39	0/1310	0.46	0/1772
3	X	0.44	0/1310	0.47	0/1772
3	Y	0.41	0/1310	0.43	0/1772
3	g	0.27	0/1310	0.45	0/1772

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	h	0.26	0/1310	0.45	0/1772
3	i	0.28	0/1310	0.45	0/1772
3	j	0.36	0/1310	0.45	0/1772
3	k	0.39	0/1310	0.44	0/1772
3	l	0.36	0/1310	0.42	0/1772
4	M	0.28	0/493	0.43	0/668
4	Z	0.28	0/493	0.47	0/668
4	m	0.27	0/556	0.48	0/753
5	4	0.39	0/2091	0.49	0/2836
All	All	0.37	0/54439	0.46	2/73676 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	34	ARG	NE-CZ-NH1	-8.68	115.96	120.30
2	e	25	LEU	CA-CB-CG	5.31	127.50	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	82	LYS	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	3	511/531 (96%)	499 (98%)	12 (2%)	0	100	100
2	A	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	B	161/163 (99%)	159 (99%)	2 (1%)	0	100	100
2	C	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	D	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
2	E	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	F	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	N	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
2	O	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	P	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	Q	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	R	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	S	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
2	a	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
2	b	161/163 (99%)	160 (99%)	1 (1%)	0	100	100
2	c	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	d	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	e	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	f	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
3	G	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
3	H	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	I	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
3	J	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
3	K	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	L	170/172 (99%)	166 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	T	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
3	U	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	V	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	W	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	X	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
3	Y	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
3	g	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
3	h	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
3	i	170/172 (99%)	170 (100%)	0	0	100	100
3	j	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
3	k	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
3	l	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
4	M	58/78 (74%)	57 (98%)	1 (2%)	0	100	100
4	Z	58/78 (74%)	56 (97%)	2 (3%)	0	100	100
4	m	67/78 (86%)	61 (91%)	6 (9%)	0	100	100
5	4	248/252 (98%)	228 (92%)	20 (8%)	0	100	100
All	All	6884/7047 (98%)	6730 (98%)	154 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	3	430/445 (97%)	429 (100%)	1 (0%)	93	96
2	A	128/129 (99%)	127 (99%)	1 (1%)	81	89
2	B	129/129 (100%)	128 (99%)	1 (1%)	81	89
2	C	128/129 (99%)	127 (99%)	1 (1%)	81	89
2	D	128/129 (99%)	127 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	128/129 (99%)	128 (100%)	0	100	100
2	F	128/129 (99%)	127 (99%)	1 (1%)	81	89
2	N	128/129 (99%)	127 (99%)	1 (1%)	81	89
2	O	128/129 (99%)	127 (99%)	1 (1%)	81	89
2	P	128/129 (99%)	127 (99%)	1 (1%)	81	89
2	Q	128/129 (99%)	127 (99%)	1 (1%)	81	89
2	R	128/129 (99%)	127 (99%)	1 (1%)	81	89
2	S	128/129 (99%)	127 (99%)	1 (1%)	81	89
2	a	128/129 (99%)	127 (99%)	1 (1%)	81	89
2	b	129/129 (100%)	128 (99%)	1 (1%)	81	89
2	c	128/129 (99%)	128 (100%)	0	100	100
2	d	128/129 (99%)	127 (99%)	1 (1%)	81	89
2	e	128/129 (99%)	127 (99%)	1 (1%)	81	89
2	f	128/129 (99%)	127 (99%)	1 (1%)	81	89
3	G	133/133 (100%)	133 (100%)	0	100	100
3	H	133/133 (100%)	133 (100%)	0	100	100
3	I	133/133 (100%)	133 (100%)	0	100	100
3	J	133/133 (100%)	132 (99%)	1 (1%)	81	89
3	K	133/133 (100%)	133 (100%)	0	100	100
3	L	133/133 (100%)	132 (99%)	1 (1%)	81	89
3	T	133/133 (100%)	133 (100%)	0	100	100
3	U	133/133 (100%)	133 (100%)	0	100	100
3	V	133/133 (100%)	132 (99%)	1 (1%)	81	89
3	W	133/133 (100%)	133 (100%)	0	100	100
3	X	133/133 (100%)	133 (100%)	0	100	100
3	Y	133/133 (100%)	133 (100%)	0	100	100
3	g	133/133 (100%)	133 (100%)	0	100	100
3	h	133/133 (100%)	133 (100%)	0	100	100
3	i	133/133 (100%)	133 (100%)	0	100	100
3	j	133/133 (100%)	133 (100%)	0	100	100
3	k	133/133 (100%)	133 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	l	133/133 (100%)	133 (100%)	0	100 100
4	M	52/67 (78%)	52 (100%)	0	100 100
4	Z	52/67 (78%)	52 (100%)	0	100 100
4	m	59/67 (88%)	59 (100%)	0	100 100
5	4	220/222 (99%)	219 (100%)	1 (0%)	88 92
All	All	5513/5584 (99%)	5492 (100%)	21 (0%)	91 94

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	309	LYS
2	A	18	ARG
2	B	31	ARG
2	C	31	ARG
2	D	31	ARG
2	F	31	ARG
3	J	15	LYS
3	L	32	LYS
2	N	31	ARG
2	O	31	ARG
2	P	31	ARG
2	Q	31	ARG
2	R	31	ARG
2	S	31	ARG
3	V	32	LYS
5	4	176	ARG
2	a	18	ARG
2	b	31	ARG
2	d	31	ARG
2	e	31	ARG
2	f	31	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	219	GLN
2	C	21	ASN
2	F	146	GLN
3	J	46	ASN

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Mol	Chain	Res	Type
3	J	72	ASN
3	K	72	ASN
2	P	79	ASN
2	Q	160	ASN
3	T	72	ASN
3	U	64	GLN
3	U	72	ASN
3	U	76	HIS
3	V	72	ASN
3	W	72	ASN
3	X	64	GLN
3	Y	72	ASN
5	4	138	HIS
5	4	185	GLN
2	a	133	ASN
2	e	58	GLN
3	k	72	ASN
3	l	72	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

54 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	CYC	S	200	-	42,46,46	6.36	24 (57%)	50,67,67	4.39	12 (24%)
6	CYC	I	201	-	42,46,46	6.47	25 (59%)	50,67,67	4.33	13 (26%)
6	CYC	X	200	-	42,46,46	6.30	23 (54%)	50,67,67	4.51	15 (30%)
6	CYC	W	201	-	42,46,46	6.50	25 (59%)	50,67,67	4.40	13 (26%)
6	CYC	G	200	-	42,46,46	6.48	25 (59%)	50,67,67	4.24	10 (20%)
6	CYC	I	200	-	42,46,46	6.46	23 (54%)	50,67,67	4.27	11 (22%)
6	CYC	P	200	-	42,46,46	6.38	23 (54%)	50,67,67	4.81	13 (26%)
6	CYC	N	200	-	42,46,46	6.51	24 (57%)	50,67,67	4.50	10 (20%)
6	CYC	B	201	-	42,46,46	6.52	23 (54%)	50,67,67	4.24	12 (24%)
6	CYC	R	200	-	42,46,46	6.40	23 (54%)	50,67,67	4.46	12 (24%)
6	CYC	J	200	-	42,46,46	6.32	24 (57%)	50,67,67	4.58	15 (30%)
6	CYC	Y	201	-	42,46,46	6.46	23 (54%)	50,67,67	4.80	14 (28%)
6	CYC	a	200	-	42,46,46	6.53	24 (57%)	50,67,67	4.28	12 (24%)
6	CYC	A	201	-	42,46,46	6.45	24 (57%)	50,67,67	4.53	13 (26%)
6	CYC	C	200	-	42,46,46	6.48	25 (59%)	50,67,67	4.34	12 (24%)
6	CYC	H	200	-	42,46,46	6.53	24 (57%)	50,67,67	4.44	13 (26%)
6	CYC	T	200	-	42,46,46	6.47	24 (57%)	50,67,67	4.38	13 (26%)
6	CYC	Z	200	-	42,46,46	6.49	24 (57%)	50,67,67	4.25	13 (26%)
6	CYC	E	200	-	42,46,46	6.36	23 (54%)	50,67,67	4.60	12 (24%)
6	CYC	Q	200	-	42,46,46	6.39	24 (57%)	50,67,67	4.52	14 (28%)
6	CYC	e	200	-	42,46,46	6.48	24 (57%)	50,67,67	4.19	11 (22%)
6	CYC	O	200	-	42,46,46	6.35	23 (54%)	50,67,67	4.48	14 (28%)
6	CYC	B	200	-	42,46,46	6.44	23 (54%)	50,67,67	4.39	12 (24%)
6	CYC	i	201	-	42,46,46	6.56	25 (59%)	50,67,67	4.62	13 (26%)
6	CYC	l	201	-	42,46,46	6.51	24 (57%)	50,67,67	4.36	12 (24%)
6	CYC	A	200	-	42,46,46	6.47	23 (54%)	50,67,67	4.40	10 (20%)
6	CYC	K	200	-	42,46,46	6.35	23 (54%)	50,67,67	4.54	15 (30%)
6	CYC	h	200	-	42,46,46	6.51	24 (57%)	50,67,67	4.32	11 (22%)
6	CYC	h	201	-	42,46,46	6.60	24 (57%)	50,67,67	4.46	10 (20%)
6	CYC	K	201	-	42,46,46	6.49	25 (59%)	50,67,67	4.46	12 (24%)
6	CYC	g	201	-	42,46,46	6.54	24 (57%)	50,67,67	4.64	11 (22%)
6	CYC	D	200	-	42,46,46	6.24	23 (54%)	50,67,67	4.52	14 (28%)
6	CYC	W	200	-	42,46,46	6.40	23 (54%)	50,67,67	4.45	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CYC	l	200	-	42,46,46	6.35	24 (57%)	50,67,67	4.59	12 (24%)
6	CYC	k	201	-	42,46,46	6.47	24 (57%)	50,67,67	4.49	12 (24%)
6	CYC	b	200	-	42,46,46	6.46	23 (54%)	50,67,67	4.40	11 (22%)
6	CYC	f	200	-	42,46,46	6.49	23 (54%)	50,67,67	4.45	11 (22%)
6	CYC	j	201	-	42,46,46	6.52	24 (57%)	50,67,67	4.71	15 (30%)
6	CYC	3	601	-	42,46,46	6.37	22 (52%)	50,67,67	4.47	12 (24%)
6	CYC	T	201	-	42,46,46	6.59	24 (57%)	50,67,67	4.39	14 (28%)
6	CYC	V	200	-	42,46,46	6.44	24 (57%)	50,67,67	4.31	12 (24%)
6	CYC	k	200	-	42,46,46	6.37	23 (54%)	50,67,67	4.57	17 (34%)
6	CYC	F	200	-	42,46,46	6.32	23 (54%)	50,67,67	4.45	13 (26%)
6	CYC	j	200	-	42,46,46	6.38	23 (54%)	50,67,67	4.46	15 (30%)
6	CYC	g	200	-	42,46,46	6.57	25 (59%)	50,67,67	4.48	12 (24%)
6	CYC	L	201	-	42,46,46	6.50	23 (54%)	50,67,67	4.34	13 (26%)
6	CYC	V	201	-	42,46,46	6.58	25 (59%)	50,67,67	4.36	12 (24%)
6	CYC	4	301	-	42,46,46	6.58	24 (57%)	50,67,67	4.40	14 (28%)
6	CYC	c	200	-	42,46,46	6.48	23 (54%)	50,67,67	4.37	11 (22%)
6	CYC	G	201	-	42,46,46	6.51	24 (57%)	50,67,67	4.63	12 (24%)
6	CYC	U	201	-	42,46,46	6.50	24 (57%)	50,67,67	4.73	12 (24%)
6	CYC	Y	200	-	42,46,46	6.32	23 (54%)	50,67,67	4.48	14 (28%)
6	CYC	X	201	-	42,46,46	6.44	23 (54%)	50,67,67	4.54	14 (28%)
6	CYC	d	200	-	42,46,46	6.40	23 (54%)	50,67,67	4.63	12 (24%)

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
6	CYC	S	200	-	-	15/25/74/74	0/4/4/4
6	CYC	I	201	-	-	13/25/74/74	0/4/4/4
6	CYC	X	200	-	-	10/25/74/74	0/4/4/4
6	CYC	W	201	-	-	16/25/74/74	0/4/4/4
6	CYC	G	200	-	-	8/25/74/74	0/4/4/4
6	CYC	I	200	-	-	8/25/74/74	0/4/4/4
6	CYC	P	200	-	-	16/25/74/74	0/4/4/4
6	CYC	N	200	-	-	15/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	B	201	-	-	13/25/74/74	0/4/4/4
6	CYC	R	200	-	-	15/25/74/74	0/4/4/4
6	CYC	J	200	-	-	9/25/74/74	0/4/4/4
6	CYC	Y	201	-	-	16/25/74/74	0/4/4/4
6	CYC	a	200	-	-	12/25/74/74	0/4/4/4
6	CYC	A	201	-	-	13/25/74/74	0/4/4/4
6	CYC	C	200	-	-	15/25/74/74	0/4/4/4
6	CYC	H	200	-	-	13/25/74/74	0/4/4/4
6	CYC	T	200	-	-	9/25/74/74	0/4/4/4
6	CYC	Z	200	-	-	9/25/74/74	0/4/4/4
6	CYC	E	200	-	-	13/25/74/74	0/4/4/4
6	CYC	Q	200	-	-	15/25/74/74	0/4/4/4
6	CYC	e	200	-	-	15/25/74/74	0/4/4/4
6	CYC	O	200	-	-	15/25/74/74	0/4/4/4
6	CYC	B	200	-	-	13/25/74/74	0/4/4/4
6	CYC	i	201	-	-	17/25/74/74	0/4/4/4
6	CYC	l	201	-	-	18/25/74/74	0/4/4/4
6	CYC	A	200	-	-	16/25/74/74	0/4/4/4
6	CYC	K	200	-	-	11/25/74/74	0/4/4/4
6	CYC	h	200	-	-	13/25/74/74	0/4/4/4
6	CYC	h	201	-	-	15/25/74/74	0/4/4/4
6	CYC	K	201	-	-	16/25/74/74	0/4/4/4
6	CYC	g	201	-	-	14/25/74/74	0/4/4/4
6	CYC	D	200	-	-	13/25/74/74	0/4/4/4
6	CYC	W	200	-	-	7/25/74/74	0/4/4/4
6	CYC	l	200	-	-	9/25/74/74	0/4/4/4
6	CYC	k	201	-	-	9/25/74/74	0/4/4/4
6	CYC	b	200	-	-	16/25/74/74	0/4/4/4
6	CYC	f	200	-	-	14/25/74/74	0/4/4/4
6	CYC	j	201	-	-	16/25/74/74	0/4/4/4
6	CYC	3	601	-	-	6/25/74/74	0/4/4/4
6	CYC	T	201	-	-	17/25/74/74	0/4/4/4
6	CYC	V	200	-	-	13/25/74/74	0/4/4/4
6	CYC	k	200	-	-	10/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	F	200	-	-	15/25/74/74	0/4/4/4
6	CYC	j	200	-	-	9/25/74/74	0/4/4/4
6	CYC	g	200	-	-	10/25/74/74	0/4/4/4
6	CYC	L	201	-	-	15/25/74/74	0/4/4/4
6	CYC	V	201	-	-	14/25/74/74	0/4/4/4
6	CYC	4	301	-	-	11/25/74/74	0/4/4/4
6	CYC	c	200	-	-	15/25/74/74	0/4/4/4
6	CYC	G	201	-	-	19/25/74/74	0/4/4/4
6	CYC	U	201	-	-	9/25/74/74	0/4/4/4
6	CYC	Y	200	-	-	5/25/74/74	0/4/4/4
6	CYC	X	201	-	-	13/25/74/74	0/4/4/4
6	CYC	d	200	-	-	13/25/74/74	0/4/4/4

All (1279) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	4	301	CYC	CHA-C1A	26.84	1.57	1.35
6	j	201	CYC	CHA-C1A	26.62	1.57	1.35
6	H	200	CYC	CHA-C1A	26.58	1.57	1.35
6	i	201	CYC	CHA-C1A	26.57	1.57	1.35
6	V	201	CYC	CHA-C1A	26.55	1.57	1.35
6	h	201	CYC	CHA-C1A	26.52	1.57	1.35
6	g	200	CYC	CHA-C1A	26.46	1.57	1.35
6	T	201	CYC	CHA-C1A	26.28	1.57	1.35
6	g	201	CYC	CHA-C1A	26.23	1.57	1.35
6	A	201	CYC	CHA-C1A	26.17	1.57	1.35
6	I	201	CYC	CHA-C1A	26.15	1.57	1.35
6	B	201	CYC	CHA-C1A	26.15	1.57	1.35
6	K	201	CYC	CHA-C1A	26.15	1.57	1.35
6	h	200	CYC	CHA-C1A	26.14	1.57	1.35
6	a	200	CYC	CHA-C1A	26.09	1.56	1.35
6	W	201	CYC	CHA-C1A	26.09	1.56	1.35
6	N	200	CYC	CHA-C1A	26.06	1.56	1.35
6	f	200	CYC	CHA-C1A	26.05	1.56	1.35
6	k	201	CYC	CHA-C1A	26.04	1.56	1.35
6	Y	201	CYC	CHA-C1A	26.01	1.56	1.35
6	Z	200	CYC	CHA-C1A	25.97	1.56	1.35
6	U	201	CYC	CHA-C1A	25.94	1.56	1.35
6	G	200	CYC	CHA-C1A	25.93	1.56	1.35
6	V	200	CYC	CHA-C1A	25.93	1.56	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	201	CYC	CHA-C1A	25.91	1.56	1.35
6	e	200	CYC	CHA-C1A	25.90	1.56	1.35
6	I	200	CYC	CHA-C1A	25.90	1.56	1.35
6	l	201	CYC	CHA-C1A	25.89	1.56	1.35
6	G	201	CYC	CHA-C1A	25.88	1.56	1.35
6	b	200	CYC	CHA-C1A	25.86	1.56	1.35
6	X	201	CYC	CHA-C1A	25.83	1.56	1.35
6	C	200	CYC	CHA-C1A	25.78	1.56	1.35
6	j	200	CYC	CHA-C1A	25.76	1.56	1.35
6	A	200	CYC	CHA-C1A	25.75	1.56	1.35
6	c	200	CYC	CHA-C1A	25.74	1.56	1.35
6	T	200	CYC	CHA-C1A	25.65	1.56	1.35
6	B	200	CYC	CHA-C1A	25.64	1.56	1.35
6	l	200	CYC	CHA-C1A	25.60	1.56	1.35
6	k	200	CYC	CHA-C1A	25.57	1.56	1.35
6	d	200	CYC	CHA-C1A	25.51	1.56	1.35
6	W	200	CYC	CHA-C1A	25.50	1.56	1.35
6	R	200	CYC	CHA-C1A	25.49	1.56	1.35
6	Q	200	CYC	CHA-C1A	25.37	1.56	1.35
6	3	601	CYC	CHA-C1A	25.34	1.56	1.35
6	Y	200	CYC	CHA-C1A	25.34	1.56	1.35
6	K	200	CYC	CHA-C1A	25.31	1.56	1.35
6	P	200	CYC	CHA-C1A	25.28	1.56	1.35
6	X	200	CYC	CHA-C1A	25.24	1.56	1.35
6	S	200	CYC	CHA-C1A	25.15	1.56	1.35
6	O	200	CYC	CHA-C1A	25.14	1.56	1.35
6	J	200	CYC	CHA-C1A	25.06	1.56	1.35
6	E	200	CYC	CHA-C1A	24.99	1.56	1.35
6	F	200	CYC	CHA-C1A	24.83	1.55	1.35
6	D	200	CYC	CHA-C1A	24.10	1.55	1.35
6	T	201	CYC	C2C-C1C	13.94	1.64	1.52
6	h	201	CYC	C2C-C1C	13.94	1.64	1.52
6	V	201	CYC	C2C-C1C	13.58	1.64	1.52
6	Z	200	CYC	C2C-C1C	13.57	1.64	1.52
6	C	200	CYC	C2C-C1C	13.53	1.64	1.52
6	N	200	CYC	C2C-C1C	13.51	1.64	1.52
6	B	201	CYC	C2C-C1C	13.51	1.64	1.52
6	g	200	CYC	C2C-C1C	13.27	1.63	1.52
6	G	200	CYC	C3C-C4C	13.26	1.70	1.50
6	A	200	CYC	C2C-C1C	13.25	1.63	1.52
6	a	200	CYC	C3C-C4C	13.24	1.70	1.50
6	R	200	CYC	C2C-C1C	13.24	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	200	CYC	C2C-C1C	13.21	1.63	1.52
6	b	200	CYC	C2C-C1C	13.18	1.63	1.52
6	W	201	CYC	C2C-C1C	13.17	1.63	1.52
6	B	200	CYC	C2C-C1C	13.16	1.63	1.52
6	U	201	CYC	C2C-C1C	13.16	1.63	1.52
6	g	201	CYC	C2C-C1C	13.14	1.63	1.52
6	H	200	CYC	C3C-C4C	13.14	1.70	1.50
6	L	201	CYC	C3C-C4C	13.10	1.69	1.50
6	E	200	CYC	C2C-C1C	13.10	1.63	1.52
6	l	201	CYC	C3C-C4C	13.08	1.69	1.50
6	i	201	CYC	C3C-C4C	13.06	1.69	1.50
6	j	201	CYC	C3C-C4C	13.05	1.69	1.50
6	S	200	CYC	C2C-C1C	13.04	1.63	1.52
6	W	200	CYC	C3C-C4C	13.04	1.69	1.50
6	l	200	CYC	C3C-C4C	13.03	1.69	1.50
6	g	200	CYC	C3C-C4C	13.02	1.69	1.50
6	I	201	CYC	C3C-C4C	13.02	1.69	1.50
6	c	200	CYC	C2C-C1C	13.01	1.63	1.52
6	T	200	CYC	C3C-C4C	12.99	1.69	1.50
6	F	200	CYC	C2C-C1C	12.98	1.63	1.52
6	P	200	CYC	C2C-C1C	12.96	1.63	1.52
6	U	201	CYC	C3C-C4C	12.95	1.69	1.50
6	K	201	CYC	C3C-C4C	12.93	1.69	1.50
6	V	200	CYC	C3C-C4C	12.93	1.69	1.50
6	k	201	CYC	C3C-C4C	12.92	1.69	1.50
6	c	200	CYC	C3C-C4C	12.91	1.69	1.50
6	O	200	CYC	C2C-C1C	12.91	1.63	1.52
6	Y	201	CYC	C3C-C4C	12.89	1.69	1.50
6	G	201	CYC	C3C-C4C	12.89	1.69	1.50
6	e	200	CYC	C2C-C1C	12.85	1.63	1.52
6	e	200	CYC	C3C-C4C	12.84	1.69	1.50
6	4	301	CYC	C3C-C4C	12.83	1.69	1.50
6	Y	200	CYC	C3C-C4C	12.82	1.69	1.50
6	g	201	CYC	C3C-C4C	12.82	1.69	1.50
6	d	200	CYC	C2C-C1C	12.81	1.63	1.52
6	K	200	CYC	C3C-C4C	12.81	1.69	1.50
6	I	200	CYC	C3C-C4C	12.80	1.69	1.50
6	I	200	CYC	C2C-C1C	12.79	1.63	1.52
6	3	601	CYC	C3C-C4C	12.78	1.69	1.50
6	G	201	CYC	C2C-C1C	12.76	1.63	1.52
6	X	200	CYC	C3C-C4C	12.76	1.69	1.50
6	D	200	CYC	C2C-C1C	12.76	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	l	201	CYC	C2C-C1C	12.76	1.63	1.52
6	A	201	CYC	C3C-C4C	12.76	1.69	1.50
6	i	201	CYC	C2C-C1C	12.74	1.63	1.52
6	N	200	CYC	C3C-C4C	12.74	1.69	1.50
6	X	201	CYC	C3C-C4C	12.73	1.69	1.50
6	k	201	CYC	C2C-C1C	12.72	1.63	1.52
6	W	201	CYC	C3C-C4C	12.72	1.69	1.50
6	j	200	CYC	C3C-C4C	12.70	1.69	1.50
6	4	301	CYC	C2C-C1C	12.70	1.63	1.52
6	h	200	CYC	C3C-C4C	12.70	1.69	1.50
6	J	200	CYC	C3C-C4C	12.69	1.69	1.50
6	K	201	CYC	C2C-C1C	12.66	1.63	1.52
6	a	200	CYC	C2C-C1C	12.65	1.63	1.52
6	T	200	CYC	C2C-C1C	12.61	1.63	1.52
6	B	200	CYC	C3C-C4C	12.58	1.69	1.50
6	Q	200	CYC	C3C-C4C	12.58	1.69	1.50
6	F	200	CYC	C3C-C4C	12.56	1.69	1.50
6	h	200	CYC	C2C-C1C	12.56	1.63	1.52
6	B	201	CYC	C3C-C4C	12.55	1.69	1.50
6	L	201	CYC	C2C-C1C	12.55	1.63	1.52
6	P	200	CYC	C3C-C4C	12.51	1.69	1.50
6	f	200	CYC	C3C-C4C	12.50	1.69	1.50
6	E	200	CYC	C3C-C4C	12.50	1.69	1.50
6	b	200	CYC	C3C-C4C	12.50	1.69	1.50
6	Q	200	CYC	C2C-C1C	12.49	1.63	1.52
6	A	201	CYC	C2C-C1C	12.48	1.63	1.52
6	H	200	CYC	C2C-C1C	12.48	1.63	1.52
6	A	200	CYC	C3C-C4C	12.48	1.69	1.50
6	h	201	CYC	C3C-C4C	12.47	1.69	1.50
6	h	201	CYC	C1C-NC	12.46	1.53	1.37
6	k	200	CYC	C3C-C4C	12.43	1.68	1.50
6	j	201	CYC	C2C-C1C	12.42	1.63	1.52
6	T	201	CYC	C3C-C4C	12.42	1.68	1.50
6	S	200	CYC	C3C-C4C	12.36	1.68	1.50
6	I	201	CYC	C2C-C1C	12.32	1.63	1.52
6	G	200	CYC	C2C-C1C	12.30	1.63	1.52
6	g	201	CYC	C1C-NC	12.29	1.53	1.37
6	Y	201	CYC	C2C-C1C	12.28	1.63	1.52
6	C	200	CYC	C3C-C4C	12.27	1.68	1.50
6	V	201	CYC	C3C-C4C	12.27	1.68	1.50
6	d	200	CYC	C3C-C4C	12.26	1.68	1.50
6	D	200	CYC	C3C-C4C	12.25	1.68	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	200	CYC	C3C-C4C	12.24	1.68	1.50
6	T	201	CYC	C1C-NC	12.23	1.53	1.37
6	h	200	CYC	C1C-NC	12.19	1.53	1.37
6	V	200	CYC	C2C-C1C	12.18	1.62	1.52
6	Z	200	CYC	C3C-C4C	12.12	1.68	1.50
6	c	200	CYC	C1C-NC	12.12	1.53	1.37
6	B	201	CYC	C1C-NC	12.11	1.53	1.37
6	W	200	CYC	C2C-C1C	12.08	1.62	1.52
6	V	201	CYC	C1C-NC	12.07	1.53	1.37
6	Z	200	CYC	C1C-NC	12.05	1.53	1.37
6	a	200	CYC	C1C-NC	12.05	1.53	1.37
6	g	200	CYC	C1C-NC	12.03	1.53	1.37
6	X	201	CYC	C2C-C1C	12.02	1.62	1.52
6	O	200	CYC	C3C-C4C	11.99	1.68	1.50
6	G	201	CYC	C1C-NC	11.98	1.53	1.37
6	k	200	CYC	C2C-C1C	11.98	1.62	1.52
6	e	200	CYC	C1C-NC	11.96	1.53	1.37
6	J	200	CYC	C2C-C1C	11.95	1.62	1.52
6	U	201	CYC	C1C-NC	11.90	1.53	1.37
6	B	200	CYC	C1C-NC	11.88	1.53	1.37
6	I	200	CYC	C1C-NC	11.86	1.53	1.37
6	T	200	CYC	C1C-NC	11.86	1.53	1.37
6	f	200	CYC	C1C-NC	11.85	1.53	1.37
6	Q	200	CYC	C1C-NC	11.84	1.52	1.37
6	O	200	CYC	C1C-NC	11.83	1.52	1.37
6	3	601	CYC	C2C-C1C	11.83	1.62	1.52
6	l	201	CYC	C1C-NC	11.81	1.52	1.37
6	K	200	CYC	C2C-C1C	11.81	1.62	1.52
6	H	200	CYC	C1C-NC	11.80	1.52	1.37
6	N	200	CYC	C1C-NC	11.78	1.52	1.37
6	i	201	CYC	C1C-NC	11.76	1.52	1.37
6	X	201	CYC	C1C-NC	11.75	1.52	1.37
6	G	200	CYC	C1C-NC	11.72	1.52	1.37
6	I	201	CYC	C1C-NC	11.70	1.52	1.37
6	C	200	CYC	C1C-NC	11.68	1.52	1.37
6	A	200	CYC	C1C-NC	11.68	1.52	1.37
6	4	301	CYC	C1C-NC	11.67	1.52	1.37
6	L	201	CYC	C1C-NC	11.65	1.52	1.37
6	Y	200	CYC	C2C-C1C	11.64	1.62	1.52
6	k	200	CYC	C1C-NC	11.60	1.52	1.37
6	k	201	CYC	C1C-NC	11.58	1.52	1.37
6	b	200	CYC	C1C-NC	11.58	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	200	CYC	C1C-NC	11.57	1.52	1.37
6	W	201	CYC	C1C-NC	11.57	1.52	1.37
6	3	601	CYC	C1C-NC	11.51	1.52	1.37
6	g	201	CYC	OB-C4B	11.47	1.45	1.23
6	E	200	CYC	C1C-NC	11.46	1.52	1.37
6	X	200	CYC	C2C-C1C	11.45	1.62	1.52
6	j	201	CYC	C1C-NC	11.44	1.52	1.37
6	j	200	CYC	C1C-NC	11.44	1.52	1.37
6	h	200	CYC	OB-C4B	11.42	1.45	1.23
6	R	200	CYC	C1C-NC	11.41	1.52	1.37
6	d	200	CYC	C1C-NC	11.41	1.52	1.37
6	V	201	CYC	OB-C4B	11.40	1.45	1.23
6	T	200	CYC	OB-C4B	11.39	1.45	1.23
6	g	200	CYC	OB-C4B	11.39	1.45	1.23
6	c	200	CYC	OB-C4B	11.39	1.45	1.23
6	j	200	CYC	C2C-C1C	11.36	1.62	1.52
6	l	201	CYC	OB-C4B	11.36	1.45	1.23
6	K	200	CYC	C1C-NC	11.35	1.52	1.37
6	G	200	CYC	OB-C4B	11.35	1.45	1.23
6	Y	201	CYC	C1C-NC	11.35	1.52	1.37
6	Y	201	CYC	OB-C4B	11.33	1.45	1.23
6	C	200	CYC	OB-C4B	11.33	1.45	1.23
6	W	201	CYC	OB-C4B	11.32	1.45	1.23
6	S	200	CYC	C1C-NC	11.32	1.52	1.37
6	P	200	CYC	OB-C4B	11.32	1.45	1.23
6	a	200	CYC	OB-C4B	11.31	1.45	1.23
6	i	201	CYC	OB-C4B	11.31	1.45	1.23
6	l	200	CYC	C2C-C1C	11.31	1.62	1.52
6	e	200	CYC	OB-C4B	11.30	1.45	1.23
6	K	201	CYC	C1C-NC	11.29	1.52	1.37
6	G	201	CYC	OB-C4B	11.28	1.45	1.23
6	4	301	CYC	OB-C4B	11.27	1.45	1.23
6	D	200	CYC	C1C-NC	11.27	1.52	1.37
6	Z	200	CYC	OB-C4B	11.27	1.45	1.23
6	X	201	CYC	OB-C4B	11.27	1.45	1.23
6	N	200	CYC	OB-C4B	11.26	1.45	1.23
6	T	201	CYC	OB-C4B	11.25	1.45	1.23
6	l	200	CYC	OB-C4B	11.24	1.45	1.23
6	W	200	CYC	C1C-NC	11.24	1.52	1.37
6	K	201	CYC	OB-C4B	11.24	1.45	1.23
6	A	201	CYC	C1C-NC	11.23	1.52	1.37
6	j	201	CYC	OB-C4B	11.23	1.45	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	h	201	CYC	OB-C4B	11.22	1.44	1.23
6	j	200	CYC	OB-C4B	11.22	1.44	1.23
6	f	200	CYC	OB-C4B	11.21	1.44	1.23
6	P	200	CYC	C1C-NC	11.21	1.52	1.37
6	L	201	CYC	OB-C4B	11.21	1.44	1.23
6	H	200	CYC	OB-C4B	11.21	1.44	1.23
6	A	200	CYC	OB-C4B	11.20	1.44	1.23
6	Y	200	CYC	OB-C4B	11.19	1.44	1.23
6	A	201	CYC	OB-C4B	11.17	1.44	1.23
6	k	200	CYC	OB-C4B	11.15	1.44	1.23
6	R	200	CYC	OB-C4B	11.15	1.44	1.23
6	V	200	CYC	OB-C4B	11.14	1.44	1.23
6	d	200	CYC	OB-C4B	11.14	1.44	1.23
6	3	601	CYC	OB-C4B	11.14	1.44	1.23
6	K	200	CYC	OB-C4B	11.13	1.44	1.23
6	U	201	CYC	OB-C4B	11.12	1.44	1.23
6	b	200	CYC	OB-C4B	11.12	1.44	1.23
6	I	200	CYC	OB-C4B	11.12	1.44	1.23
6	k	201	CYC	OB-C4B	11.11	1.44	1.23
6	F	200	CYC	C1C-NC	11.08	1.52	1.37
6	E	200	CYC	OB-C4B	11.08	1.44	1.23
6	W	200	CYC	OB-C4B	11.04	1.44	1.23
6	J	200	CYC	OB-C4B	11.02	1.44	1.23
6	B	200	CYC	OB-C4B	11.01	1.44	1.23
6	l	200	CYC	C1C-NC	10.98	1.51	1.37
6	J	200	CYC	C1C-NC	10.97	1.51	1.37
6	S	200	CYC	OB-C4B	10.90	1.44	1.23
6	B	201	CYC	OB-C4B	10.90	1.44	1.23
6	X	200	CYC	C1C-NC	10.86	1.51	1.37
6	O	200	CYC	OB-C4B	10.86	1.44	1.23
6	X	200	CYC	OB-C4B	10.86	1.44	1.23
6	I	201	CYC	OB-C4B	10.84	1.44	1.23
6	D	200	CYC	OB-C4B	10.78	1.44	1.23
6	Q	200	CYC	OB-C4B	10.74	1.44	1.23
6	Y	200	CYC	C1C-NC	10.70	1.51	1.37
6	F	200	CYC	OB-C4B	10.64	1.43	1.23
6	Q	200	CYC	C2C-C3C	-10.17	1.26	1.54
6	j	200	CYC	C2C-C3C	-10.17	1.26	1.54
6	h	200	CYC	C2C-C3C	-10.13	1.26	1.54
6	k	200	CYC	C2C-C3C	-10.01	1.26	1.54
6	a	200	CYC	C2C-C3C	-10.01	1.26	1.54
6	J	200	CYC	C2C-C3C	-9.98	1.26	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	4	301	CYC	CHB-C4A	9.96	1.63	1.40
6	V	201	CYC	C2C-C3C	-9.96	1.26	1.54
6	G	201	CYC	CHB-C4A	9.95	1.63	1.40
6	H	200	CYC	C2C-C3C	-9.95	1.26	1.54
6	O	200	CYC	C2C-C3C	-9.95	1.26	1.54
6	d	200	CYC	C2C-C3C	-9.92	1.26	1.54
6	l	201	CYC	C2C-C3C	-9.92	1.26	1.54
6	G	201	CYC	C2C-C3C	-9.91	1.26	1.54
6	h	201	CYC	C2C-C3C	-9.91	1.26	1.54
6	3	601	CYC	C2C-C3C	-9.91	1.26	1.54
6	i	201	CYC	CHB-C4A	9.91	1.63	1.40
6	V	200	CYC	C2C-C3C	-9.90	1.26	1.54
6	L	201	CYC	CHB-C4A	9.89	1.63	1.40
6	K	200	CYC	C2C-C3C	-9.89	1.26	1.54
6	Z	200	CYC	C2C-C3C	-9.89	1.26	1.54
6	B	201	CYC	C2C-C3C	-9.89	1.26	1.54
6	T	201	CYC	C2C-C3C	-9.89	1.26	1.54
6	g	201	CYC	C2C-C3C	-9.89	1.26	1.54
6	I	200	CYC	C2C-C3C	-9.88	1.26	1.54
6	l	201	CYC	CHB-C4A	9.87	1.63	1.40
6	l	200	CYC	C2C-C3C	-9.86	1.26	1.54
6	R	200	CYC	C2C-C3C	-9.86	1.26	1.54
6	f	200	CYC	C2C-C3C	-9.85	1.26	1.54
6	4	301	CYC	C2C-C3C	-9.85	1.26	1.54
6	Y	201	CYC	CHB-C4A	9.85	1.63	1.40
6	V	201	CYC	CHB-C4A	9.85	1.63	1.40
6	S	200	CYC	C2C-C3C	-9.85	1.27	1.54
6	I	201	CYC	C2C-C3C	-9.85	1.27	1.54
6	T	201	CYC	CHB-C4A	9.85	1.63	1.40
6	C	200	CYC	C2C-C3C	-9.84	1.27	1.54
6	X	201	CYC	C2C-C3C	-9.82	1.27	1.54
6	B	200	CYC	C2C-C3C	-9.82	1.27	1.54
6	D	200	CYC	C2C-C3C	-9.82	1.27	1.54
6	L	201	CYC	C2C-C3C	-9.82	1.27	1.54
6	A	200	CYC	C2C-C3C	-9.81	1.27	1.54
6	E	200	CYC	C2C-C3C	-9.81	1.27	1.54
6	i	201	CYC	C2C-C3C	-9.81	1.27	1.54
6	K	201	CYC	C2C-C3C	-9.80	1.27	1.54
6	W	200	CYC	C2C-C3C	-9.80	1.27	1.54
6	T	200	CYC	C2C-C3C	-9.80	1.27	1.54
6	g	200	CYC	C2C-C3C	-9.79	1.27	1.54
6	T	200	CYC	CHB-C4A	9.78	1.63	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	201	CYC	CHB-C4A	9.78	1.63	1.40
6	j	201	CYC	CHB-C4A	9.77	1.63	1.40
6	k	201	CYC	C2C-C3C	-9.77	1.27	1.54
6	c	200	CYC	C2C-C3C	-9.77	1.27	1.54
6	Y	201	CYC	C2C-C3C	-9.76	1.27	1.54
6	G	200	CYC	C2C-C3C	-9.75	1.27	1.54
6	Y	200	CYC	C2C-C3C	-9.74	1.27	1.54
6	W	200	CYC	CHB-C4A	9.72	1.63	1.40
6	b	200	CYC	C2C-C3C	-9.72	1.27	1.54
6	X	200	CYC	C2C-C3C	-9.71	1.27	1.54
6	V	200	CYC	CHB-C4A	9.70	1.63	1.40
6	P	200	CYC	C2C-C3C	-9.70	1.27	1.54
6	A	201	CYC	C2C-C3C	-9.70	1.27	1.54
6	N	200	CYC	C2C-C3C	-9.70	1.27	1.54
6	G	200	CYC	CHB-C4A	9.69	1.63	1.40
6	e	200	CYC	C2C-C3C	-9.69	1.27	1.54
6	X	201	CYC	CHB-C4A	9.69	1.63	1.40
6	F	200	CYC	C2C-C3C	-9.68	1.27	1.54
6	U	201	CYC	C2C-C3C	-9.67	1.27	1.54
6	W	201	CYC	C2C-C3C	-9.67	1.27	1.54
6	j	201	CYC	C2C-C3C	-9.66	1.27	1.54
6	W	201	CYC	CHB-C4A	9.65	1.63	1.40
6	k	200	CYC	CHB-C4A	9.65	1.63	1.40
6	j	200	CYC	CHB-C4A	9.60	1.62	1.40
6	C	200	CYC	CHB-C4A	9.59	1.62	1.40
6	h	200	CYC	CHB-C4A	9.58	1.62	1.40
6	A	200	CYC	CHB-C4A	9.58	1.62	1.40
6	e	200	CYC	CHB-C4A	9.58	1.62	1.40
6	J	200	CYC	CHB-C4A	9.58	1.62	1.40
6	g	200	CYC	CHB-C4A	9.55	1.62	1.40
6	F	200	CYC	CHB-C4A	9.54	1.62	1.40
6	c	200	CYC	CHB-C4A	9.52	1.62	1.40
6	S	200	CYC	CHB-C4A	9.52	1.62	1.40
6	I	200	CYC	CHB-C4A	9.51	1.62	1.40
6	k	201	CYC	CHB-C4A	9.49	1.62	1.40
6	Y	200	CYC	CHB-C4A	9.49	1.62	1.40
6	d	200	CYC	CHB-C4A	9.49	1.62	1.40
6	H	200	CYC	CHB-C4A	9.49	1.62	1.40
6	Q	200	CYC	CHB-C4A	9.48	1.62	1.40
6	a	200	CYC	CHB-C4A	9.48	1.62	1.40
6	3	601	CYC	CHB-C4A	9.48	1.62	1.40
6	B	201	CYC	CHB-C4A	9.47	1.62	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	200	CYC	CHB-C4A	9.47	1.62	1.40
6	h	201	CYC	CHB-C4A	9.47	1.62	1.40
6	O	200	CYC	CHB-C4A	9.46	1.62	1.40
6	E	200	CYC	CHB-C4A	9.43	1.62	1.40
6	I	201	CYC	CHB-C4A	9.40	1.62	1.40
6	N	200	CYC	CHB-C4A	9.40	1.62	1.40
6	X	200	CYC	CHB-C4A	9.39	1.62	1.40
6	U	201	CYC	CHB-C4A	9.38	1.62	1.40
6	K	200	CYC	CHB-C4A	9.37	1.62	1.40
6	b	200	CYC	CHB-C4A	9.36	1.62	1.40
6	f	200	CYC	CHB-C4A	9.35	1.62	1.40
6	P	200	CYC	CHB-C4A	9.35	1.62	1.40
6	B	200	CYC	CHB-C4A	9.33	1.62	1.40
6	D	200	CYC	CHB-C4A	9.33	1.62	1.40
6	A	201	CYC	CHB-C4A	9.33	1.62	1.40
6	l	200	CYC	CHB-C4A	9.32	1.62	1.40
6	g	201	CYC	CHB-C4A	9.25	1.62	1.40
6	Z	200	CYC	CHB-C4A	9.21	1.62	1.40
6	4	301	CYC	CHB-C1B	6.51	1.53	1.38
6	Y	200	CYC	C4B-C3B	-6.51	1.35	1.48
6	J	200	CYC	C4B-C3B	-6.33	1.36	1.48
6	I	201	CYC	C4B-C3B	-6.33	1.36	1.48
6	k	200	CYC	C4B-C3B	-6.29	1.36	1.48
6	3	601	CYC	C4B-C3B	-6.29	1.36	1.48
6	K	200	CYC	C4B-C3B	-6.28	1.36	1.48
6	L	201	CYC	C4B-C3B	-6.26	1.36	1.48
6	X	200	CYC	C4B-C3B	-6.25	1.36	1.48
6	j	200	CYC	C4B-C3B	-6.24	1.36	1.48
6	W	200	CYC	C4B-C3B	-6.19	1.36	1.48
6	l	201	CYC	CHB-C1B	6.18	1.52	1.38
6	Q	200	CYC	C4B-C3B	-6.18	1.36	1.48
6	4	301	CYC	C4B-C3B	-6.17	1.36	1.48
6	V	201	CYC	CHB-C1B	6.17	1.52	1.38
6	G	200	CYC	CHB-C1B	6.16	1.52	1.38
6	T	200	CYC	CHB-C1B	6.14	1.52	1.38
6	i	201	CYC	CHB-C1B	6.13	1.52	1.38
6	F	200	CYC	C4B-C3B	-6.13	1.36	1.48
6	A	201	CYC	C4B-C3B	-6.12	1.36	1.48
6	R	200	CYC	C4B-C3B	-6.12	1.36	1.48
6	k	201	CYC	C4B-C3B	-6.12	1.36	1.48
6	V	200	CYC	C4B-C3B	-6.12	1.36	1.48
6	I	200	CYC	C4B-C3B	-6.11	1.36	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	O	200	CYC	C4B-C3B	-6.09	1.36	1.48
6	G	201	CYC	CHB-C1B	6.09	1.52	1.38
6	Y	201	CYC	CHB-C1B	6.07	1.52	1.38
6	U	201	CYC	C4B-C3B	-6.07	1.36	1.48
6	K	201	CYC	C4B-C3B	-6.07	1.36	1.48
6	T	200	CYC	C4B-C3B	-6.07	1.36	1.48
6	T	201	CYC	C4B-C3B	-6.07	1.36	1.48
6	B	201	CYC	C4B-C3B	-6.06	1.36	1.48
6	V	201	CYC	C4B-C3B	-6.06	1.36	1.48
6	D	200	CYC	C4B-C3B	-6.05	1.36	1.48
6	L	201	CYC	CHB-C1B	6.05	1.52	1.38
6	d	200	CYC	C4B-C3B	-6.03	1.36	1.48
6	A	200	CYC	C4B-C3B	-6.03	1.36	1.48
6	a	200	CYC	CHB-C1B	6.02	1.52	1.38
6	X	201	CYC	C4B-C3B	-6.02	1.36	1.48
6	T	201	CYC	CHB-C1B	6.02	1.52	1.38
6	Z	200	CYC	C4B-C3B	-6.00	1.36	1.48
6	H	200	CYC	C4B-C3B	-6.00	1.36	1.48
6	l	200	CYC	C4B-C3B	-6.00	1.36	1.48
6	l	201	CYC	C4B-C3B	-5.99	1.36	1.48
6	G	201	CYC	C4B-C3B	-5.99	1.36	1.48
6	W	201	CYC	C4B-C3B	-5.98	1.36	1.48
6	A	200	CYC	CHB-C1B	5.98	1.52	1.38
6	j	201	CYC	C4B-C3B	-5.98	1.36	1.48
6	j	201	CYC	CHB-C1B	5.97	1.52	1.38
6	B	201	CYC	CHB-C1B	5.97	1.52	1.38
6	f	200	CYC	CHB-C1B	5.97	1.52	1.38
6	d	200	CYC	CHB-C1B	5.96	1.52	1.38
6	g	200	CYC	CHB-C1B	5.96	1.52	1.38
6	K	201	CYC	CHB-C1B	5.96	1.52	1.38
6	P	200	CYC	CHB-C1B	5.96	1.52	1.38
6	S	200	CYC	C4B-C3B	-5.95	1.36	1.48
6	W	201	CYC	CHB-C1B	5.95	1.52	1.38
6	E	200	CYC	C4B-C3B	-5.95	1.36	1.48
6	3	601	CYC	CHB-C1B	5.95	1.52	1.38
6	V	200	CYC	CHB-C1B	5.94	1.52	1.38
6	k	200	CYC	CHB-C1B	5.93	1.52	1.38
6	B	200	CYC	C4B-C3B	-5.93	1.36	1.48
6	U	201	CYC	CHB-C1B	5.93	1.52	1.38
6	I	200	CYC	CHB-C1B	5.92	1.52	1.38
6	a	200	CYC	C4B-C3B	-5.92	1.37	1.48
6	I	201	CYC	CHB-C1B	5.90	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	201	CYC	C4B-C3B	-5.90	1.37	1.48
6	C	200	CYC	CHB-C1B	5.90	1.52	1.38
6	e	200	CYC	CHB-C1B	5.90	1.52	1.38
6	h	200	CYC	CHB-C1B	5.89	1.52	1.38
6	h	201	CYC	CHB-C1B	5.89	1.52	1.38
6	i	201	CYC	C4B-C3B	-5.89	1.37	1.48
6	b	200	CYC	C4B-C3B	-5.89	1.37	1.48
6	k	201	CYC	CHB-C1B	5.88	1.52	1.38
6	c	200	CYC	CHB-C1B	5.88	1.52	1.38
6	C	200	CYC	C4B-C3B	-5.88	1.37	1.48
6	l	200	CYC	CHB-C1B	5.88	1.52	1.38
6	W	200	CYC	CHB-C1B	5.87	1.52	1.38
6	N	200	CYC	CHB-C1B	5.87	1.52	1.38
6	G	200	CYC	C4B-C3B	-5.87	1.37	1.48
6	g	201	CYC	CHB-C1B	5.86	1.52	1.38
6	R	200	CYC	CHB-C1B	5.86	1.52	1.38
6	e	200	CYC	C4B-C3B	-5.86	1.37	1.48
6	Z	200	CYC	CHB-C1B	5.85	1.52	1.38
6	Y	200	CYC	CHB-C1B	5.84	1.51	1.38
6	b	200	CYC	CHB-C1B	5.84	1.51	1.38
6	X	201	CYC	CHB-C1B	5.83	1.51	1.38
6	j	200	CYC	CHB-C1B	5.82	1.51	1.38
6	H	200	CYC	CHB-C1B	5.82	1.51	1.38
6	B	200	CYC	CHB-C1B	5.81	1.51	1.38
6	c	200	CYC	C4B-C3B	-5.78	1.37	1.48
6	P	200	CYC	C4B-C3B	-5.77	1.37	1.48
6	g	201	CYC	C4B-C3B	-5.77	1.37	1.48
6	h	201	CYC	C4B-C3B	-5.75	1.37	1.48
6	J	200	CYC	CHB-C1B	5.74	1.51	1.38
6	g	200	CYC	C4B-C3B	-5.74	1.37	1.48
6	f	200	CYC	C4B-C3B	-5.73	1.37	1.48
6	Q	200	CYC	CHB-C1B	5.72	1.51	1.38
6	S	200	CYC	CHB-C1B	5.72	1.51	1.38
6	A	201	CYC	CHB-C1B	5.70	1.51	1.38
6	F	200	CYC	CHB-C1B	5.64	1.51	1.38
6	N	200	CYC	C4B-C3B	-5.62	1.37	1.48
6	X	200	CYC	CHB-C1B	5.61	1.51	1.38
6	E	200	CYC	CHB-C1B	5.61	1.51	1.38
6	K	200	CYC	CHB-C1B	5.53	1.51	1.38
6	O	200	CYC	CHB-C1B	5.52	1.51	1.38
6	D	200	CYC	CHB-C1B	5.49	1.51	1.38
6	h	200	CYC	C4B-C3B	-5.48	1.37	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	200	CYC	CHD-C4C	5.42	1.51	1.38
6	B	201	CYC	CHD-C4C	5.37	1.51	1.38
6	a	200	CYC	C4D-CHA	5.32	1.61	1.41
6	l	200	CYC	CHD-C4C	5.31	1.51	1.38
6	G	200	CYC	CHD-C4C	5.31	1.51	1.38
6	U	201	CYC	CHD-C4C	5.30	1.51	1.38
6	e	200	CYC	CHD-C4C	5.23	1.51	1.38
6	D	200	CYC	C1A-C2A	-5.23	1.37	1.45
6	I	201	CYC	C4D-CHA	5.22	1.61	1.41
6	K	201	CYC	C4D-CHA	5.21	1.61	1.41
6	G	200	CYC	C4D-CHA	5.21	1.61	1.41
6	J	200	CYC	C1A-C2A	-5.21	1.37	1.45
6	A	201	CYC	CHD-C4C	5.21	1.51	1.38
6	h	200	CYC	C4D-CHA	5.20	1.61	1.41
6	4	301	CYC	C4D-CHA	5.20	1.61	1.41
6	i	201	CYC	CHD-C4C	5.19	1.51	1.38
6	N	200	CYC	C4D-CHA	5.19	1.61	1.41
6	g	200	CYC	C4D-CHA	5.19	1.61	1.41
6	g	201	CYC	C4D-CHA	5.19	1.61	1.41
6	L	201	CYC	CHD-C4C	5.19	1.51	1.38
6	h	201	CYC	C4D-CHA	5.19	1.61	1.41
6	j	201	CYC	C4D-CHA	5.18	1.61	1.41
6	b	200	CYC	C4D-CHA	5.18	1.61	1.41
6	g	200	CYC	CHD-C4C	5.18	1.51	1.38
6	N	200	CYC	CHD-C4C	5.18	1.51	1.38
6	T	201	CYC	CHD-C4C	5.18	1.51	1.38
6	W	201	CYC	C4D-CHA	5.16	1.61	1.41
6	i	201	CYC	C4D-CHA	5.16	1.61	1.41
6	X	201	CYC	CHD-C4C	5.16	1.51	1.38
6	Z	200	CYC	CHD-C4C	5.16	1.51	1.38
6	T	201	CYC	C4D-CHA	5.16	1.61	1.41
6	H	200	CYC	C4D-CHA	5.16	1.61	1.41
6	F	200	CYC	C1A-C2A	-5.16	1.37	1.45
6	I	201	CYC	CHD-C4C	5.16	1.51	1.38
6	c	200	CYC	CHD-C4C	5.15	1.51	1.38
6	j	201	CYC	CHD-C4C	5.15	1.51	1.38
6	h	200	CYC	CHD-C4C	5.15	1.51	1.38
6	W	201	CYC	CHD-C4C	5.15	1.51	1.38
6	U	201	CYC	C1D-CHD	5.15	1.61	1.41
6	f	200	CYC	C4D-CHA	5.15	1.61	1.41
6	h	201	CYC	CHD-C4C	5.14	1.51	1.38
6	B	201	CYC	C4D-CHA	5.14	1.61	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	201	CYC	C4D-CHA	5.13	1.61	1.41
6	k	201	CYC	CHD-C4C	5.13	1.51	1.38
6	4	301	CYC	CHD-C4C	5.13	1.51	1.38
6	l	200	CYC	C4D-CHA	5.13	1.61	1.41
6	k	201	CYC	C4D-CHA	5.13	1.61	1.41
6	L	201	CYC	C4D-CHA	5.12	1.61	1.41
6	b	200	CYC	CHD-C4C	5.12	1.51	1.38
6	T	200	CYC	CHD-C4C	5.12	1.51	1.38
6	e	200	CYC	C4D-CHA	5.11	1.61	1.41
6	I	200	CYC	C4D-CHA	5.11	1.61	1.41
6	Z	200	CYC	C4D-CHA	5.11	1.61	1.41
6	X	201	CYC	C4D-CHA	5.10	1.61	1.41
6	G	201	CYC	C4D-CHA	5.10	1.61	1.41
6	d	200	CYC	C4D-CHA	5.10	1.61	1.41
6	V	200	CYC	CHD-C4C	5.10	1.51	1.38
6	V	201	CYC	C4D-CHA	5.10	1.61	1.41
6	G	201	CYC	CHD-C4C	5.09	1.51	1.38
6	V	201	CYC	CHD-C4C	5.09	1.51	1.38
6	X	200	CYC	C1A-C2A	-5.09	1.37	1.45
6	Y	201	CYC	C4D-CHA	5.09	1.60	1.41
6	N	200	CYC	C1D-CHD	5.08	1.60	1.41
6	A	201	CYC	C4D-CHA	5.08	1.60	1.41
6	C	200	CYC	C4D-CHA	5.08	1.60	1.41
6	P	200	CYC	C1D-CHD	5.08	1.60	1.41
6	Z	200	CYC	C1D-CHD	5.08	1.60	1.41
6	K	201	CYC	CHD-C4C	5.08	1.51	1.38
6	c	200	CYC	C4D-CHA	5.08	1.60	1.41
6	T	200	CYC	C4D-CHA	5.08	1.60	1.41
6	X	200	CYC	CHD-C4C	5.08	1.51	1.38
6	P	200	CYC	C4D-CHA	5.08	1.60	1.41
6	A	200	CYC	C4D-CHA	5.08	1.60	1.41
6	H	200	CYC	CHD-C4C	5.08	1.51	1.38
6	j	200	CYC	CHD-C4C	5.07	1.51	1.38
6	l	201	CYC	CHD-C4C	5.07	1.51	1.38
6	l	201	CYC	C4D-CHA	5.06	1.60	1.41
6	j	200	CYC	C4D-CHA	5.06	1.60	1.41
6	I	200	CYC	CHD-C4C	5.05	1.50	1.38
6	B	200	CYC	C4D-CHA	5.05	1.60	1.41
6	Q	200	CYC	C4D-CHA	5.05	1.60	1.41
6	C	200	CYC	CHD-C4C	5.05	1.50	1.38
6	W	200	CYC	C4D-CHA	5.04	1.60	1.41
6	d	200	CYC	CHD-C4C	5.04	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	l	200	CYC	C1D-CHD	5.03	1.60	1.41
6	P	200	CYC	CHD-C4C	5.03	1.50	1.38
6	3	601	CYC	C1A-C2A	-5.03	1.37	1.45
6	b	200	CYC	C1D-CHD	5.03	1.60	1.41
6	h	201	CYC	C1D-CHD	5.03	1.60	1.41
6	O	200	CYC	C1A-C2A	-5.02	1.37	1.45
6	g	201	CYC	CHD-C4C	5.02	1.50	1.38
6	K	200	CYC	C1B-C2B	-5.01	1.36	1.45
6	Y	201	CYC	CHD-C4C	5.01	1.50	1.38
6	A	200	CYC	C1D-CHD	5.01	1.60	1.41
6	F	200	CYC	CHD-C4C	5.00	1.50	1.38
6	C	200	CYC	C1D-CHD	5.00	1.60	1.41
6	4	301	CYC	C1D-CHD	5.00	1.60	1.41
6	e	200	CYC	C1D-CHD	5.00	1.60	1.41
6	S	200	CYC	CHD-C4C	5.00	1.50	1.38
6	V	200	CYC	C4D-CHA	4.99	1.60	1.41
6	D	200	CYC	CHD-C4C	4.98	1.50	1.38
6	X	200	CYC	C4D-CHA	4.98	1.60	1.41
6	S	200	CYC	C4D-CHA	4.98	1.60	1.41
6	G	200	CYC	C1D-CHD	4.97	1.60	1.41
6	f	200	CYC	CHD-C4C	4.97	1.50	1.38
6	T	201	CYC	C1D-CHD	4.96	1.60	1.41
6	E	200	CYC	CHD-C4C	4.96	1.50	1.38
6	d	200	CYC	C1D-CHD	4.96	1.60	1.41
6	E	200	CYC	C1D-CHD	4.96	1.60	1.41
6	a	200	CYC	C1D-CHD	4.95	1.60	1.41
6	E	200	CYC	C4D-CHA	4.95	1.60	1.41
6	V	201	CYC	C1D-CHD	4.94	1.60	1.41
6	O	200	CYC	C4D-CHA	4.94	1.60	1.41
6	3	601	CYC	C1B-C2B	-4.94	1.36	1.45
6	g	201	CYC	C1D-CHD	4.94	1.60	1.41
6	K	200	CYC	C1A-C2A	-4.93	1.37	1.45
6	A	200	CYC	CHD-C4C	4.93	1.50	1.38
6	c	200	CYC	C1D-CHD	4.93	1.60	1.41
6	W	200	CYC	CHD-C4C	4.92	1.50	1.38
6	Y	200	CYC	CHD-C4C	4.92	1.50	1.38
6	B	201	CYC	C1D-CHD	4.92	1.60	1.41
6	K	200	CYC	CHD-C4C	4.92	1.50	1.38
6	S	200	CYC	C1D-CHD	4.91	1.60	1.41
6	k	200	CYC	C4D-CHA	4.91	1.60	1.41
6	X	200	CYC	C1D-CHD	4.91	1.60	1.41
6	R	200	CYC	C4D-CHA	4.90	1.60	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	200	CYC	C1D-CHD	4.89	1.60	1.41
6	I	201	CYC	C1D-CHD	4.89	1.60	1.41
6	Y	200	CYC	C4D-CHA	4.89	1.60	1.41
6	3	601	CYC	C4D-CHA	4.89	1.60	1.41
6	F	200	CYC	C4D-CHA	4.88	1.60	1.41
6	3	601	CYC	CHD-C4C	4.87	1.50	1.38
6	K	200	CYC	C4D-CHA	4.87	1.60	1.41
6	K	201	CYC	C1D-CHD	4.87	1.60	1.41
6	W	200	CYC	C1D-CHD	4.87	1.60	1.41
6	k	201	CYC	C1D-CHD	4.86	1.60	1.41
6	B	200	CYC	C1B-C2B	-4.86	1.36	1.45
6	D	200	CYC	C1D-CHD	4.86	1.60	1.41
6	F	200	CYC	C1D-CHD	4.86	1.60	1.41
6	F	200	CYC	C1B-C2B	-4.86	1.36	1.45
6	h	200	CYC	C1D-CHD	4.85	1.60	1.41
6	D	200	CYC	C1B-C2B	-4.85	1.36	1.45
6	D	200	CYC	C4D-CHA	4.85	1.60	1.41
6	R	200	CYC	CHD-C4C	4.85	1.50	1.38
6	Q	200	CYC	CHD-C4C	4.85	1.50	1.38
6	Y	200	CYC	C1A-C2A	-4.84	1.38	1.45
6	W	201	CYC	C1D-CHD	4.84	1.60	1.41
6	B	200	CYC	CHD-C4C	4.84	1.50	1.38
6	H	200	CYC	C1D-CHD	4.83	1.59	1.41
6	W	200	CYC	C1A-C2A	-4.82	1.38	1.45
6	j	200	CYC	C1D-CHD	4.82	1.59	1.41
6	i	201	CYC	C1D-CHD	4.82	1.59	1.41
6	A	200	CYC	C1A-C2A	-4.81	1.38	1.45
6	k	200	CYC	CHD-C4C	4.81	1.50	1.38
6	R	200	CYC	C1D-CHD	4.81	1.59	1.41
6	J	200	CYC	C4D-CHA	4.81	1.59	1.41
6	A	201	CYC	C1D-CHD	4.80	1.59	1.41
6	V	200	CYC	C1D-CHD	4.80	1.59	1.41
6	B	200	CYC	C1A-C2A	-4.79	1.38	1.45
6	X	200	CYC	C1B-C2B	-4.79	1.36	1.45
6	3	601	CYC	C1D-CHD	4.79	1.59	1.41
6	g	200	CYC	C1D-CHD	4.78	1.59	1.41
6	l	201	CYC	C1D-CHD	4.77	1.59	1.41
6	j	201	CYC	C1D-CHD	4.77	1.59	1.41
6	S	200	CYC	C1A-C2A	-4.77	1.38	1.45
6	O	200	CYC	CHD-C4C	4.76	1.50	1.38
6	L	201	CYC	C1D-CHD	4.76	1.59	1.41
6	J	200	CYC	CHD-C4C	4.75	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	200	CYC	C1B-C2B	-4.74	1.36	1.45
6	I	200	CYC	C1D-CHD	4.74	1.59	1.41
6	G	201	CYC	C1D-CHD	4.74	1.59	1.41
6	J	200	CYC	C1D-CHD	4.73	1.59	1.41
6	P	200	CYC	C1A-C2A	-4.73	1.38	1.45
6	E	200	CYC	C1A-C2A	-4.73	1.38	1.45
6	W	200	CYC	C1B-NB	-4.72	1.29	1.37
6	Y	201	CYC	C1D-CHD	4.71	1.59	1.41
6	Q	200	CYC	C1D-CHD	4.70	1.59	1.41
6	Y	200	CYC	C1B-C2B	-4.70	1.36	1.45
6	b	200	CYC	C1B-C2B	-4.68	1.36	1.45
6	K	200	CYC	C1D-CHD	4.68	1.59	1.41
6	J	200	CYC	C1B-C2B	-4.67	1.36	1.45
6	X	201	CYC	C1D-CHD	4.67	1.59	1.41
6	Y	200	CYC	C1D-CHD	4.66	1.59	1.41
6	d	200	CYC	C1A-C2A	-4.66	1.38	1.45
6	O	200	CYC	C1B-NB	-4.66	1.30	1.37
6	X	200	CYC	C1B-NB	-4.65	1.30	1.37
6	j	200	CYC	C1A-C2A	-4.65	1.38	1.45
6	R	200	CYC	C1A-C2A	-4.65	1.38	1.45
6	A	201	CYC	C1B-C2B	-4.65	1.36	1.45
6	D	200	CYC	C1B-NB	-4.64	1.30	1.37
6	f	200	CYC	C1D-CHD	4.63	1.59	1.41
6	e	200	CYC	C1A-C2A	-4.62	1.38	1.45
6	k	200	CYC	C1D-CHD	4.62	1.59	1.41
6	K	201	CYC	C1A-C2A	-4.60	1.38	1.45
6	c	200	CYC	C1A-C2A	-4.60	1.38	1.45
6	Q	200	CYC	C1B-C2B	-4.60	1.36	1.45
6	Q	200	CYC	C1A-C2A	-4.59	1.38	1.45
6	J	200	CYC	C1B-NB	-4.59	1.30	1.37
6	d	200	CYC	C1B-C2B	-4.58	1.36	1.45
6	C	200	CYC	C1A-C2A	-4.58	1.38	1.45
6	B	200	CYC	C1D-CHD	4.57	1.58	1.41
6	X	201	CYC	C1A-C2A	-4.56	1.38	1.45
6	E	200	CYC	C1B-C2B	-4.56	1.36	1.45
6	l	201	CYC	C1A-C2A	-4.56	1.38	1.45
6	H	200	CYC	C1B-C2B	-4.55	1.36	1.45
6	P	200	CYC	C1B-C2B	-4.55	1.36	1.45
6	S	200	CYC	C1B-C2B	-4.55	1.36	1.45
6	I	200	CYC	C1B-C2B	-4.54	1.36	1.45
6	T	200	CYC	C1A-C2A	-4.54	1.38	1.45
6	Q	200	CYC	C1B-NB	-4.53	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	200	CYC	C1B-C2B	-4.53	1.37	1.45
6	l	200	CYC	C1B-C2B	-4.53	1.37	1.45
6	O	200	CYC	C1D-CHD	4.53	1.58	1.41
6	O	200	CYC	C1B-C2B	-4.52	1.37	1.45
6	L	201	CYC	C1A-C2A	-4.51	1.38	1.45
6	G	201	CYC	C1A-C2A	-4.51	1.38	1.45
6	b	200	CYC	C1A-C2A	-4.51	1.38	1.45
6	F	200	CYC	C1B-NB	-4.50	1.30	1.37
6	R	200	CYC	C1B-C2B	-4.50	1.37	1.45
6	W	201	CYC	C1B-C2B	-4.50	1.37	1.45
6	W	200	CYC	C1B-C2B	-4.49	1.37	1.45
6	k	200	CYC	C1B-C2B	-4.49	1.37	1.45
6	A	200	CYC	C1B-C2B	-4.48	1.37	1.45
6	G	200	CYC	C1A-C2A	-4.48	1.38	1.45
6	N	200	CYC	C1B-C2B	-4.47	1.37	1.45
6	j	200	CYC	C1B-C2B	-4.47	1.37	1.45
6	Y	200	CYC	C1B-NB	-4.46	1.30	1.37
6	K	200	CYC	C1B-NB	-4.45	1.30	1.37
6	E	200	CYC	C1B-NB	-4.45	1.30	1.37
6	I	200	CYC	C1A-C2A	-4.45	1.38	1.45
6	c	200	CYC	C1B-C2B	-4.45	1.37	1.45
6	Z	200	CYC	C1A-C2A	-4.44	1.38	1.45
6	a	200	CYC	C1B-C2B	-4.44	1.37	1.45
6	V	200	CYC	C1A-C2A	-4.44	1.38	1.45
6	A	201	CYC	C1B-NB	-4.44	1.30	1.37
6	S	200	CYC	C1B-NB	-4.44	1.30	1.37
6	l	200	CYC	C1A-C2A	-4.44	1.38	1.45
6	h	200	CYC	C1B-C2B	-4.43	1.37	1.45
6	W	201	CYC	C1A-C2A	-4.43	1.38	1.45
6	Y	201	CYC	C1A-C2A	-4.41	1.38	1.45
6	e	200	CYC	C1B-C2B	-4.40	1.37	1.45
6	g	201	CYC	C1B-C2B	-4.40	1.37	1.45
6	C	200	CYC	C1B-C2B	-4.40	1.37	1.45
6	C	200	CYC	C1B-NB	-4.39	1.30	1.37
6	k	200	CYC	C1B-NB	-4.39	1.30	1.37
6	L	201	CYC	C1B-C2B	-4.38	1.37	1.45
6	X	201	CYC	C1B-C2B	-4.37	1.37	1.45
6	4	301	CYC	C1A-C2A	-4.37	1.38	1.45
6	Y	201	CYC	C1B-C2B	-4.35	1.37	1.45
6	B	201	CYC	C1A-C2A	-4.34	1.38	1.45
6	i	201	CYC	C1A-C2A	-4.33	1.38	1.45
6	k	201	CYC	C1B-C2B	-4.32	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	201	CYC	C1A-C2A	-4.32	1.38	1.45
6	K	201	CYC	C1B-C2B	-4.31	1.37	1.45
6	f	200	CYC	C1A-C2A	-4.30	1.38	1.45
6	X	201	CYC	C1B-NB	-4.30	1.30	1.37
6	3	601	CYC	C1B-NB	-4.29	1.30	1.37
6	V	201	CYC	C1A-C2A	-4.29	1.38	1.45
6	I	201	CYC	C1B-NB	-4.29	1.30	1.37
6	B	200	CYC	C1B-NB	-4.28	1.30	1.37
6	j	200	CYC	C1B-NB	-4.27	1.30	1.37
6	l	201	CYC	C1B-C2B	-4.27	1.37	1.45
6	h	200	CYC	C1A-C2A	-4.26	1.38	1.45
6	Z	200	CYC	C1B-C2B	-4.26	1.37	1.45
6	G	201	CYC	C1B-NB	-4.26	1.30	1.37
6	I	201	CYC	C1B-C2B	-4.25	1.37	1.45
6	i	201	CYC	C1B-C2B	-4.23	1.37	1.45
6	b	200	CYC	C1B-NB	-4.23	1.30	1.37
6	N	200	CYC	C1A-C2A	-4.23	1.39	1.45
6	T	201	CYC	C1B-C2B	-4.22	1.37	1.45
6	G	201	CYC	C1B-C2B	-4.21	1.37	1.45
6	V	201	CYC	C1B-C2B	-4.21	1.37	1.45
6	L	201	CYC	C1B-NB	-4.21	1.30	1.37
6	a	200	CYC	C1A-C2A	-4.20	1.39	1.45
6	j	201	CYC	C1B-C2B	-4.20	1.37	1.45
6	d	200	CYC	C1B-NB	-4.19	1.30	1.37
6	A	201	CYC	C1A-C2A	-4.19	1.39	1.45
6	T	200	CYC	C1B-C2B	-4.18	1.37	1.45
6	R	200	CYC	C1B-NB	-4.18	1.30	1.37
6	f	200	CYC	C1B-NB	-4.16	1.30	1.37
6	K	201	CYC	C1B-NB	-4.16	1.30	1.37
6	T	200	CYC	C1B-NB	-4.16	1.30	1.37
6	Y	201	CYC	C1B-NB	-4.16	1.30	1.37
6	G	200	CYC	C1B-C2B	-4.15	1.37	1.45
6	g	200	CYC	C1B-C2B	-4.15	1.37	1.45
6	I	201	CYC	C1A-C2A	-4.14	1.39	1.45
6	k	200	CYC	C1A-C2A	-4.12	1.39	1.45
6	h	200	CYC	C1B-NB	-4.12	1.30	1.37
6	A	200	CYC	C1B-NB	-4.11	1.30	1.37
6	l	201	CYC	C1B-NB	-4.11	1.30	1.37
6	U	201	CYC	C1B-C2B	-4.10	1.37	1.45
6	H	200	CYC	C1A-C2A	-4.10	1.39	1.45
6	V	200	CYC	C1B-NB	-4.10	1.31	1.37
6	g	200	CYC	C1A-C2A	-4.09	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	l	200	CYC	C1B-NB	-4.08	1.31	1.37
6	U	201	CYC	C1A-C2A	-4.08	1.39	1.45
6	k	201	CYC	C1A-C2A	-4.08	1.39	1.45
6	U	201	CYC	C1B-NB	-4.06	1.31	1.37
6	I	200	CYC	C1B-NB	-4.05	1.31	1.37
6	g	201	CYC	C1A-C2A	-4.05	1.39	1.45
6	h	201	CYC	C1B-NB	-4.05	1.31	1.37
6	N	200	CYC	C1B-NB	-4.05	1.31	1.37
6	T	201	CYC	C1B-NB	-4.04	1.31	1.37
6	P	200	CYC	C1B-NB	-4.04	1.31	1.37
6	B	201	CYC	C1B-C2B	-4.04	1.37	1.45
6	B	201	CYC	C1B-NB	-4.04	1.31	1.37
6	i	201	CYC	C1B-NB	-4.03	1.31	1.37
6	Z	200	CYC	C1B-NB	-4.03	1.31	1.37
6	G	200	CYC	C1B-NB	-4.03	1.31	1.37
6	k	201	CYC	C1B-NB	-4.00	1.31	1.37
6	j	201	CYC	C1A-C2A	-4.00	1.39	1.45
6	e	200	CYC	C1B-NB	-3.99	1.31	1.37
6	h	201	CYC	C1A-C2A	-3.98	1.39	1.45
6	T	200	CYC	CBA-CGA	3.98	1.59	1.50
6	4	301	CYC	CBA-CGA	3.98	1.59	1.50
6	h	201	CYC	C1B-C2B	-3.97	1.38	1.45
6	4	301	CYC	C1B-C2B	-3.96	1.38	1.45
6	j	201	CYC	C1B-NB	-3.96	1.31	1.37
6	V	201	CYC	C1B-NB	-3.95	1.31	1.37
6	T	201	CYC	CBA-CGA	3.94	1.59	1.50
6	g	200	CYC	CBA-CGA	3.93	1.59	1.50
6	X	201	CYC	CBA-CGA	3.93	1.59	1.50
6	P	200	CYC	CBA-CGA	3.92	1.59	1.50
6	W	201	CYC	CBA-CGA	3.91	1.59	1.50
6	G	201	CYC	CBA-CGA	3.91	1.59	1.50
6	U	201	CYC	CBA-CGA	3.91	1.59	1.50
6	K	201	CYC	CBA-CGA	3.90	1.59	1.50
6	A	200	CYC	CBA-CGA	3.90	1.59	1.50
6	h	201	CYC	CBA-CGA	3.90	1.59	1.50
6	c	200	CYC	C1B-NB	-3.89	1.31	1.37
6	H	200	CYC	C1B-NB	-3.89	1.31	1.37
6	L	201	CYC	CBA-CGA	3.89	1.59	1.50
6	g	201	CYC	CBA-CGA	3.88	1.59	1.50
6	C	200	CYC	CBA-CGA	3.88	1.59	1.50
6	W	201	CYC	C1B-NB	-3.87	1.31	1.37
6	G	200	CYC	CBA-CGA	3.87	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	k	201	CYC	CBA-CGA	3.87	1.59	1.50
6	j	201	CYC	CBA-CGA	3.86	1.59	1.50
6	l	201	CYC	CBA-CGA	3.86	1.59	1.50
6	i	201	CYC	CBA-CGA	3.86	1.59	1.50
6	V	201	CYC	CBA-CGA	3.86	1.59	1.50
6	I	201	CYC	CBA-CGA	3.85	1.59	1.50
6	c	200	CYC	CBA-CGA	3.85	1.59	1.50
6	Y	201	CYC	CBA-CGA	3.85	1.59	1.50
6	a	200	CYC	CBA-CGA	3.83	1.59	1.50
6	H	200	CYC	CBA-CGA	3.82	1.59	1.50
6	e	200	CYC	CBA-CGA	3.82	1.59	1.50
6	B	201	CYC	CBA-CGA	3.81	1.59	1.50
6	g	200	CYC	C1B-NB	-3.81	1.31	1.37
6	f	200	CYC	CBA-CGA	3.79	1.59	1.50
6	3	601	CYC	CBA-CGA	3.78	1.59	1.50
6	h	200	CYC	CBA-CGA	3.78	1.59	1.50
6	N	200	CYC	CBA-CGA	3.76	1.59	1.50
6	g	201	CYC	C1B-NB	-3.76	1.31	1.37
6	G	200	CYC	CMC-C2C	3.75	1.61	1.53
6	j	200	CYC	CBA-CGA	3.75	1.59	1.50
6	g	200	CYC	CMC-C2C	3.75	1.61	1.53
6	N	200	CYC	CMC-C2C	3.74	1.61	1.53
6	i	201	CYC	CMC-C2C	3.74	1.61	1.53
6	U	201	CYC	CMC-C2C	3.74	1.61	1.53
6	T	201	CYC	CMC-C2C	3.73	1.61	1.53
6	h	201	CYC	CMC-C2C	3.73	1.61	1.53
6	b	200	CYC	CBA-CGA	3.70	1.59	1.50
6	a	200	CYC	C1B-NB	-3.69	1.31	1.37
6	H	200	CYC	CMC-C2C	3.69	1.61	1.53
6	l	201	CYC	CMC-C2C	3.68	1.61	1.53
6	B	200	CYC	CMC-C2C	3.68	1.61	1.53
6	A	201	CYC	CBA-CGA	3.68	1.59	1.50
6	V	200	CYC	CBA-CGA	3.68	1.59	1.50
6	g	201	CYC	CMC-C2C	3.67	1.61	1.53
6	d	200	CYC	CBA-CGA	3.67	1.59	1.50
6	4	301	CYC	C1B-NB	-3.67	1.31	1.37
6	J	200	CYC	CBA-CGA	3.67	1.59	1.50
6	k	201	CYC	CMC-C2C	3.66	1.61	1.53
6	B	201	CYC	CMC-C2C	3.65	1.61	1.53
6	h	200	CYC	CMC-C2C	3.65	1.61	1.53
6	f	200	CYC	CMC-C2C	3.64	1.61	1.53
6	A	200	CYC	CMC-C2C	3.63	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	j	201	CYC	CMC-C2C	3.63	1.61	1.53
6	G	201	CYC	CMC-C2C	3.62	1.61	1.53
6	I	200	CYC	CBA-CGA	3.62	1.59	1.50
6	E	200	CYC	CBA-CGA	3.61	1.59	1.50
6	Z	200	CYC	CBA-CGA	3.60	1.59	1.50
6	e	200	CYC	CMC-C2C	3.60	1.60	1.53
6	b	200	CYC	CMC-C2C	3.60	1.60	1.53
6	a	200	CYC	CMC-C2C	3.60	1.60	1.53
6	K	201	CYC	CMC-C2C	3.60	1.60	1.53
6	E	200	CYC	CMC-C2C	3.59	1.60	1.53
6	R	200	CYC	CBA-CGA	3.59	1.58	1.50
6	3	601	CYC	CMC-C2C	3.58	1.60	1.53
6	K	200	CYC	CBA-CGA	3.58	1.58	1.50
6	Y	201	CYC	CMC-C2C	3.58	1.60	1.53
6	T	200	CYC	CMC-C2C	3.58	1.60	1.53
6	Z	200	CYC	CMC-C2C	3.58	1.60	1.53
6	I	200	CYC	CMC-C2C	3.58	1.60	1.53
6	W	200	CYC	CMC-C2C	3.58	1.60	1.53
6	W	201	CYC	CMC-C2C	3.58	1.60	1.53
6	d	200	CYC	CMC-C2C	3.58	1.60	1.53
6	X	201	CYC	CMC-C2C	3.57	1.60	1.53
6	R	200	CYC	CMC-C2C	3.57	1.60	1.53
6	l	200	CYC	CMC-C2C	3.56	1.60	1.53
6	V	201	CYC	CMC-C2C	3.56	1.60	1.53
6	4	301	CYC	CMC-C2C	3.55	1.60	1.53
6	A	201	CYC	CMC-C2C	3.55	1.60	1.53
6	K	200	CYC	C1A-NA	-3.55	1.31	1.38
6	Q	200	CYC	CBA-CGA	3.55	1.58	1.50
6	O	200	CYC	CMC-C2C	3.53	1.60	1.53
6	j	200	CYC	CMC-C2C	3.53	1.60	1.53
6	P	200	CYC	CMC-C2C	3.53	1.60	1.53
6	l	200	CYC	CBA-CGA	3.51	1.58	1.50
6	k	200	CYC	CMC-C2C	3.51	1.60	1.53
6	D	200	CYC	CMC-C2C	3.51	1.60	1.53
6	C	200	CYC	CMC-C2C	3.49	1.60	1.53
6	F	200	CYC	CBA-CGA	3.49	1.58	1.50
6	S	200	CYC	CBA-CGA	3.49	1.58	1.50
6	I	201	CYC	CMC-C2C	3.48	1.60	1.53
6	c	200	CYC	CMC-C2C	3.48	1.60	1.53
6	F	200	CYC	CMC-C2C	3.47	1.60	1.53
6	S	200	CYC	CMC-C2C	3.47	1.60	1.53
6	L	201	CYC	CMC-C2C	3.46	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	200	CYC	CBA-CGA	3.46	1.58	1.50
6	X	200	CYC	CBA-CGA	3.46	1.58	1.50
6	Y	200	CYC	CMC-C2C	3.45	1.60	1.53
6	W	200	CYC	CBA-CGA	3.45	1.58	1.50
6	D	200	CYC	CBA-CGA	3.44	1.58	1.50
6	X	200	CYC	C1A-NA	-3.44	1.31	1.38
6	V	200	CYC	CMC-C2C	3.43	1.60	1.53
6	k	200	CYC	CBA-CGA	3.41	1.58	1.50
6	Q	200	CYC	CMC-C2C	3.38	1.60	1.53
6	X	200	CYC	C4B-NB	-3.38	1.30	1.38
6	K	200	CYC	CMC-C2C	3.38	1.60	1.53
6	J	200	CYC	CMC-C2C	3.36	1.60	1.53
6	O	200	CYC	CBA-CGA	3.33	1.58	1.50
6	W	200	CYC	C1A-NA	-3.31	1.31	1.38
6	O	200	CYC	C1A-NA	-3.31	1.31	1.38
6	D	200	CYC	C1A-NA	-3.31	1.31	1.38
6	X	200	CYC	CMC-C2C	3.31	1.60	1.53
6	F	200	CYC	C1A-NA	-3.30	1.31	1.38
6	Y	200	CYC	CBA-CGA	3.29	1.58	1.50
6	h	200	CYC	CAB-C3B	3.24	1.59	1.51
6	J	200	CYC	C1A-NA	-3.24	1.31	1.38
6	W	200	CYC	C4B-NB	-3.21	1.31	1.38
6	3	601	CYC	C1A-NA	-3.20	1.31	1.38
6	O	200	CYC	C4B-NB	-3.16	1.31	1.38
6	L	201	CYC	C1A-NA	-3.16	1.31	1.38
6	B	201	CYC	CAB-C3B	3.14	1.59	1.51
6	Q	200	CYC	C1A-NA	-3.13	1.31	1.38
6	N	200	CYC	CAB-C3B	3.12	1.59	1.51
6	X	201	CYC	C1A-NA	-3.11	1.31	1.38
6	J	200	CYC	C4B-NB	-3.11	1.31	1.38
6	K	201	CYC	C1A-NA	-3.10	1.31	1.38
6	Y	201	CYC	C1A-NA	-3.10	1.31	1.38
6	Y	200	CYC	C1A-NA	-3.09	1.31	1.38
6	F	200	CYC	C4B-NB	-3.07	1.31	1.38
6	K	200	CYC	C4B-NB	-3.07	1.31	1.38
6	f	200	CYC	CAB-C3B	3.06	1.59	1.51
6	A	201	CYC	C1A-NA	-3.05	1.32	1.38
6	S	200	CYC	C1A-NA	-3.05	1.32	1.38
6	k	200	CYC	C1A-NA	-3.05	1.32	1.38
6	h	201	CYC	CAB-C3B	3.05	1.58	1.51
6	E	200	CYC	C1A-NA	-3.05	1.32	1.38
6	B	201	CYC	C4A-C3A	-3.04	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	200	CYC	C4B-NB	-3.03	1.31	1.38
6	g	200	CYC	CAB-C3B	3.03	1.58	1.51
6	R	200	CYC	C1A-NA	-3.02	1.32	1.38
6	D	200	CYC	C4B-NB	-3.01	1.31	1.38
6	V	200	CYC	C1A-NA	-3.00	1.32	1.38
6	4	301	CYC	CAB-C3B	3.00	1.58	1.51
6	Y	201	CYC	CAB-C3B	3.00	1.58	1.51
6	Y	200	CYC	C4B-NB	-3.00	1.31	1.38
6	P	200	CYC	C1A-NA	-3.00	1.32	1.38
6	h	201	CYC	C4A-C3A	-3.00	1.39	1.45
6	G	200	CYC	CAB-C3B	2.99	1.58	1.51
6	a	200	CYC	CAB-C3B	2.99	1.58	1.51
6	T	201	CYC	C1A-NA	-2.98	1.32	1.38
6	C	200	CYC	CAB-C3B	2.97	1.58	1.51
6	U	201	CYC	CAB-C3B	2.97	1.58	1.51
6	V	201	CYC	CAB-C3B	2.97	1.58	1.51
6	I	200	CYC	C1A-NA	-2.96	1.32	1.38
6	i	201	CYC	CAB-C3B	2.96	1.58	1.51
6	G	201	CYC	CAB-C3B	2.96	1.58	1.51
6	b	200	CYC	CAB-C3B	2.96	1.58	1.51
6	B	200	CYC	C1A-NA	-2.96	1.32	1.38
6	f	200	CYC	C4A-C3A	-2.95	1.39	1.45
6	e	200	CYC	CAB-C3B	2.95	1.58	1.51
6	l	201	CYC	CAB-C3B	2.95	1.58	1.51
6	K	201	CYC	CAB-C3B	2.94	1.58	1.51
6	W	201	CYC	C1A-NA	-2.94	1.32	1.38
6	T	201	CYC	CAB-C3B	2.94	1.58	1.51
6	Q	200	CYC	CAB-C3B	2.94	1.58	1.51
6	I	201	CYC	CAB-C3B	2.94	1.58	1.51
6	T	200	CYC	C4B-NB	-2.94	1.31	1.38
6	Q	200	CYC	C4B-NB	-2.93	1.31	1.38
6	j	200	CYC	C1A-NA	-2.93	1.32	1.38
6	l	200	CYC	C1A-NA	-2.93	1.32	1.38
6	D	200	CYC	CAB-C3B	2.93	1.58	1.51
6	B	200	CYC	CAB-C3B	2.92	1.58	1.51
6	I	201	CYC	C1A-NA	-2.92	1.32	1.38
6	S	200	CYC	CAB-C3B	2.92	1.58	1.51
6	A	200	CYC	CAB-C3B	2.92	1.58	1.51
6	Z	200	CYC	C4A-C3A	-2.92	1.39	1.45
6	E	200	CYC	C4B-NB	-2.91	1.31	1.38
6	b	200	CYC	C1A-NA	-2.91	1.32	1.38
6	Z	200	CYC	CAB-C3B	2.91	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	d	200	CYC	CAB-C3B	2.90	1.58	1.51
6	W	201	CYC	CAB-C3B	2.90	1.58	1.51
6	U	201	CYC	C4A-C3A	-2.90	1.39	1.45
6	j	200	CYC	C4B-NB	-2.90	1.31	1.38
6	P	200	CYC	CAB-C3B	2.89	1.58	1.51
6	c	200	CYC	CAB-C3B	2.89	1.58	1.51
6	V	200	CYC	CAB-C3B	2.88	1.58	1.51
6	j	201	CYC	CAB-C3B	2.88	1.58	1.51
6	C	200	CYC	C4B-NB	-2.88	1.31	1.38
6	W	200	CYC	CAB-C3B	2.88	1.58	1.51
6	R	200	CYC	CAB-C3B	2.88	1.58	1.51
6	T	200	CYC	CAB-C3B	2.88	1.58	1.51
6	T	200	CYC	C1A-NA	-2.87	1.32	1.38
6	X	201	CYC	C4B-NB	-2.87	1.31	1.38
6	V	201	CYC	C1A-NA	-2.87	1.32	1.38
6	A	201	CYC	CAC-C3C	2.87	1.59	1.54
6	N	200	CYC	C1A-NA	-2.86	1.32	1.38
6	g	201	CYC	C4A-C3A	-2.86	1.39	1.45
6	H	200	CYC	C1A-NA	-2.86	1.32	1.38
6	d	200	CYC	C1A-NA	-2.86	1.32	1.38
6	k	201	CYC	C1A-NA	-2.86	1.32	1.38
6	l	200	CYC	C4B-NB	-2.85	1.31	1.38
6	Y	200	CYC	CAC-C3C	2.85	1.59	1.54
6	B	200	CYC	C4B-NB	-2.85	1.31	1.38
6	k	200	CYC	C4B-NB	-2.85	1.31	1.38
6	L	201	CYC	CAB-C3B	2.85	1.58	1.51
6	3	601	CYC	CAB-C3B	2.84	1.58	1.51
6	I	200	CYC	CAB-C3B	2.84	1.58	1.51
6	c	200	CYC	C4A-C3A	-2.83	1.39	1.45
6	G	201	CYC	C1A-NA	-2.83	1.32	1.38
6	k	201	CYC	CAB-C3B	2.82	1.58	1.51
6	C	200	CYC	C1A-NA	-2.82	1.32	1.38
6	l	201	CYC	C1A-NA	-2.82	1.32	1.38
6	g	201	CYC	CAB-C3B	2.82	1.58	1.51
6	E	200	CYC	CAB-C3B	2.82	1.58	1.51
6	B	200	CYC	C4A-C3A	-2.82	1.39	1.45
6	A	201	CYC	C4B-NB	-2.81	1.32	1.38
6	F	200	CYC	CAB-C3B	2.81	1.58	1.51
6	3	601	CYC	C4A-C3A	-2.81	1.39	1.45
6	e	200	CYC	C1A-NA	-2.81	1.32	1.38
6	3	601	CYC	C4B-NB	-2.80	1.32	1.38
6	K	200	CYC	CAB-C3B	2.80	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	b	200	CYC	CMD-C2D	2.80	1.57	1.51
6	A	200	CYC	C1A-NA	-2.79	1.32	1.38
6	J	200	CYC	CAB-C3B	2.79	1.58	1.51
6	A	201	CYC	CAB-C3B	2.79	1.58	1.51
6	X	201	CYC	CAB-C3B	2.79	1.58	1.51
6	h	200	CYC	C1A-NA	-2.79	1.32	1.38
6	O	200	CYC	CAB-C3B	2.79	1.58	1.51
6	Y	200	CYC	C4A-C3A	-2.79	1.39	1.45
6	I	200	CYC	C4B-NB	-2.79	1.32	1.38
6	G	201	CYC	C4B-NB	-2.78	1.32	1.38
6	b	200	CYC	C4B-NB	-2.78	1.32	1.38
6	V	200	CYC	C4B-NB	-2.78	1.32	1.38
6	l	200	CYC	CAB-C3B	2.78	1.58	1.51
6	j	201	CYC	C1A-NA	-2.78	1.32	1.38
6	R	200	CYC	C4B-NB	-2.78	1.32	1.38
6	Q	200	CYC	C4A-C3A	-2.77	1.39	1.45
6	Y	201	CYC	CAC-C3C	2.77	1.59	1.54
6	K	200	CYC	C4A-C3A	-2.77	1.39	1.45
6	h	201	CYC	CAC-C3C	2.77	1.59	1.54
6	b	200	CYC	C4A-C3A	-2.77	1.39	1.45
6	k	200	CYC	CAB-C3B	2.77	1.58	1.51
6	h	201	CYC	C4B-NB	-2.76	1.32	1.38
6	i	201	CYC	C1A-NA	-2.76	1.32	1.38
6	l	201	CYC	C4B-NB	-2.76	1.32	1.38
6	k	201	CYC	CAC-C3C	2.75	1.59	1.54
6	K	201	CYC	C4B-NB	-2.75	1.32	1.38
6	d	200	CYC	C4B-NB	-2.75	1.32	1.38
6	P	200	CYC	C4B-NB	-2.75	1.32	1.38
6	H	200	CYC	CAB-C3B	2.75	1.58	1.51
6	W	201	CYC	CAC-C3C	2.75	1.59	1.54
6	L	201	CYC	CAC-C3C	2.74	1.59	1.54
6	A	200	CYC	C4A-C3A	-2.74	1.39	1.45
6	X	200	CYC	CAB-C3B	2.74	1.58	1.51
6	g	201	CYC	C1A-NA	-2.73	1.32	1.38
6	I	201	CYC	C4B-NB	-2.73	1.32	1.38
6	G	200	CYC	C4B-NB	-2.72	1.32	1.38
6	j	201	CYC	CAC-C3C	2.72	1.59	1.54
6	N	200	CYC	C4B-NB	-2.72	1.32	1.38
6	Y	200	CYC	CAB-C3B	2.72	1.58	1.51
6	N	200	CYC	C4A-C3A	-2.71	1.40	1.45
6	k	201	CYC	C4A-C3A	-2.71	1.40	1.45
6	Z	200	CYC	C1A-NA	-2.71	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	4	301	CYC	C4A-C3A	-2.71	1.40	1.45
6	a	200	CYC	C1A-NA	-2.70	1.32	1.38
6	a	200	CYC	C4B-NB	-2.70	1.32	1.38
6	T	201	CYC	C4B-NB	-2.69	1.32	1.38
6	f	200	CYC	C1A-NA	-2.69	1.32	1.38
6	A	200	CYC	C4B-NB	-2.69	1.32	1.38
6	I	200	CYC	C4A-C3A	-2.69	1.40	1.45
6	O	200	CYC	C4A-C3A	-2.68	1.40	1.45
6	k	201	CYC	C4B-NB	-2.68	1.32	1.38
6	d	200	CYC	C4A-C3A	-2.68	1.40	1.45
6	h	200	CYC	C4B-NB	-2.67	1.32	1.38
6	G	200	CYC	CAC-C3C	2.67	1.59	1.54
6	h	201	CYC	CMD-C2D	2.67	1.57	1.51
6	R	200	CYC	CMD-C2D	2.67	1.57	1.51
6	i	201	CYC	CAC-C3C	2.66	1.59	1.54
6	j	200	CYC	CAB-C3B	2.66	1.57	1.51
6	G	200	CYC	C1A-NA	-2.66	1.32	1.38
6	l	200	CYC	C4A-C3A	-2.66	1.40	1.45
6	e	200	CYC	C4B-NB	-2.66	1.32	1.38
6	B	200	CYC	CAC-C3C	2.66	1.59	1.54
6	U	201	CYC	C4B-NB	-2.66	1.32	1.38
6	L	201	CYC	C4B-NB	-2.65	1.32	1.38
6	W	201	CYC	C4B-NB	-2.65	1.32	1.38
6	R	200	CYC	C4A-C3A	-2.65	1.40	1.45
6	F	200	CYC	C4A-C3A	-2.64	1.40	1.45
6	I	201	CYC	CAC-C3C	2.64	1.59	1.54
6	C	200	CYC	CMD-C2D	2.64	1.57	1.51
6	P	200	CYC	CMD-C2D	2.63	1.57	1.51
6	U	201	CYC	C1A-NA	-2.63	1.32	1.38
6	c	200	CYC	C4B-NB	-2.63	1.32	1.38
6	S	200	CYC	CMD-C2D	2.62	1.57	1.51
6	i	201	CYC	C4B-NB	-2.62	1.32	1.38
6	g	200	CYC	C1A-NA	-2.62	1.33	1.38
6	Y	201	CYC	C4B-NB	-2.61	1.32	1.38
6	F	200	CYC	CMD-C2D	2.61	1.57	1.51
6	A	201	CYC	C4A-C3A	-2.61	1.40	1.45
6	E	200	CYC	C4A-C3A	-2.61	1.40	1.45
6	K	201	CYC	CAC-C3C	2.61	1.59	1.54
6	B	201	CYC	C4B-NB	-2.61	1.32	1.38
6	f	200	CYC	C4B-NB	-2.60	1.32	1.38
6	d	200	CYC	CMD-C2D	2.60	1.57	1.51
6	G	201	CYC	CAC-C3C	2.60	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	201	CYC	C4B-NB	-2.60	1.32	1.38
6	g	200	CYC	CAC-C3C	2.59	1.59	1.54
6	E	200	CYC	CMD-C2D	2.59	1.57	1.51
6	V	200	CYC	C4A-C3A	-2.58	1.40	1.45
6	a	200	CYC	C4A-C3A	-2.58	1.40	1.45
6	D	200	CYC	C4A-C3A	-2.58	1.40	1.45
6	Z	200	CYC	C4B-NB	-2.57	1.32	1.38
6	N	200	CYC	CMD-C2D	2.56	1.57	1.51
6	A	200	CYC	CMD-C2D	2.56	1.57	1.51
6	V	201	CYC	CMD-C2D	2.56	1.57	1.51
6	Q	200	CYC	CAC-C3C	2.55	1.59	1.54
6	X	201	CYC	CAC-C3C	2.55	1.59	1.54
6	K	200	CYC	CAC-C3C	2.54	1.59	1.54
6	H	200	CYC	C4B-NB	-2.54	1.32	1.38
6	k	200	CYC	C4A-C3A	-2.54	1.40	1.45
6	j	201	CYC	C4B-NB	-2.54	1.32	1.38
6	g	201	CYC	CAC-C3C	2.54	1.59	1.54
6	D	200	CYC	CAC-C3C	2.54	1.59	1.54
6	c	200	CYC	C1A-NA	-2.53	1.33	1.38
6	4	301	CYC	CAC-C3C	2.53	1.59	1.54
6	H	200	CYC	CAC-C3C	2.53	1.58	1.54
6	g	200	CYC	C4A-C3A	-2.52	1.40	1.45
6	B	201	CYC	C1A-NA	-2.52	1.33	1.38
6	g	200	CYC	C4B-NB	-2.52	1.32	1.38
6	X	200	CYC	C4A-C3A	-2.52	1.40	1.45
6	l	200	CYC	CAC-C3C	2.52	1.58	1.54
6	I	201	CYC	C4A-C3A	-2.51	1.40	1.45
6	e	200	CYC	C4A-C3A	-2.50	1.40	1.45
6	4	301	CYC	C1A-NA	-2.50	1.33	1.38
6	B	201	CYC	CAC-C3C	2.50	1.58	1.54
6	4	301	CYC	C4B-NB	-2.49	1.32	1.38
6	f	200	CYC	CMD-C2D	2.49	1.56	1.51
6	X	200	CYC	CAC-C3C	2.49	1.58	1.54
6	3	601	CYC	CAC-C3C	2.49	1.58	1.54
6	Z	200	CYC	CMD-C2D	2.48	1.56	1.51
6	R	200	CYC	CAC-C3C	2.48	1.58	1.54
6	f	200	CYC	CAC-C3C	2.48	1.58	1.54
6	P	200	CYC	C4A-C3A	-2.48	1.40	1.45
6	B	200	CYC	CMD-C2D	2.47	1.56	1.51
6	U	201	CYC	CAC-C3C	2.47	1.58	1.54
6	Z	200	CYC	CAC-C3C	2.47	1.58	1.54
6	D	200	CYC	CMD-C2D	2.47	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	200	CYC	C4A-C3A	-2.47	1.40	1.45
6	A	200	CYC	CAC-C3C	2.46	1.58	1.54
6	h	200	CYC	C4A-C3A	-2.45	1.40	1.45
6	O	200	CYC	CAC-C3C	2.45	1.58	1.54
6	T	201	CYC	CAC-C3C	2.45	1.58	1.54
6	k	200	CYC	CAC-C3C	2.45	1.58	1.54
6	4	301	CYC	CMD-C2D	2.45	1.56	1.51
6	a	200	CYC	CMD-C2D	2.45	1.56	1.51
6	G	201	CYC	CMD-C2D	2.45	1.56	1.51
6	g	201	CYC	CMD-C2D	2.45	1.56	1.51
6	h	201	CYC	C1A-NA	-2.44	1.33	1.38
6	V	201	CYC	CAC-C3C	2.44	1.58	1.54
6	L	201	CYC	C4A-C3A	-2.44	1.40	1.45
6	b	200	CYC	CAC-C3C	2.44	1.58	1.54
6	e	200	CYC	CAC-C3C	2.44	1.58	1.54
6	N	200	CYC	CAC-C3C	2.44	1.58	1.54
6	j	201	CYC	CMD-C2D	2.43	1.56	1.51
6	g	201	CYC	C4B-NB	-2.43	1.32	1.38
6	W	201	CYC	C4A-C3A	-2.43	1.40	1.45
6	W	200	CYC	C4A-C3A	-2.43	1.40	1.45
6	I	200	CYC	CAC-C3C	2.43	1.58	1.54
6	j	201	CYC	C4A-C3A	-2.43	1.40	1.45
6	h	200	CYC	CAC-C3C	2.43	1.58	1.54
6	C	200	CYC	C4A-C3A	-2.42	1.40	1.45
6	a	200	CYC	CAC-C3C	2.42	1.58	1.54
6	c	200	CYC	CMD-C2D	2.42	1.56	1.51
6	W	201	CYC	CMD-C2D	2.42	1.56	1.51
6	j	200	CYC	CAC-C3C	2.42	1.58	1.54
6	c	200	CYC	CAC-C3C	2.41	1.58	1.54
6	J	200	CYC	C4A-C3A	-2.41	1.40	1.45
6	H	200	CYC	CMD-C2D	2.41	1.56	1.51
6	l	201	CYC	CMD-C2D	2.40	1.56	1.51
6	S	200	CYC	CAC-C3C	2.40	1.58	1.54
6	T	200	CYC	CAC-C3C	2.40	1.58	1.54
6	k	201	CYC	CMD-C2D	2.39	1.56	1.51
6	Y	201	CYC	CMD-C2D	2.39	1.56	1.51
6	A	201	CYC	CMD-C2D	2.38	1.56	1.51
6	j	200	CYC	C4A-C3A	-2.38	1.40	1.45
6	X	201	CYC	CMD-C2D	2.38	1.56	1.51
6	F	200	CYC	CAC-C3C	2.38	1.58	1.54
6	T	200	CYC	CMD-C2D	2.38	1.56	1.51
6	P	200	CYC	CAC-C3C	2.37	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	201	CYC	CMD-C2D	2.37	1.56	1.51
6	V	200	CYC	CAC-C3C	2.37	1.58	1.54
6	G	200	CYC	C4A-C3A	-2.37	1.40	1.45
6	L	201	CYC	CMD-C2D	2.37	1.56	1.51
6	E	200	CYC	CAC-C3C	2.37	1.58	1.54
6	e	200	CYC	CMD-C2D	2.36	1.56	1.51
6	C	200	CYC	CAC-C3C	2.36	1.58	1.54
6	Y	201	CYC	C4A-C3A	-2.36	1.40	1.45
6	Q	200	CYC	CMD-C2D	2.36	1.56	1.51
6	h	200	CYC	CMD-C2D	2.35	1.56	1.51
6	X	201	CYC	C4A-C3A	-2.35	1.40	1.45
6	O	200	CYC	CMD-C2D	2.34	1.56	1.51
6	K	201	CYC	C4A-C3A	-2.34	1.40	1.45
6	a	200	CYC	CMA-C3A	2.34	1.55	1.50
6	W	200	CYC	CAC-C3C	2.33	1.58	1.54
6	i	201	CYC	CMD-C2D	2.31	1.56	1.51
6	l	201	CYC	CAC-C3C	2.31	1.58	1.54
6	B	201	CYC	CMD-C2D	2.29	1.56	1.51
6	K	201	CYC	CMD-C2D	2.28	1.56	1.51
6	S	200	CYC	C4A-C3A	-2.28	1.40	1.45
6	I	201	CYC	CMD-C2D	2.27	1.56	1.51
6	W	200	CYC	CMD-C2D	2.26	1.56	1.51
6	l	201	CYC	C4A-C3A	-2.26	1.40	1.45
6	J	200	CYC	CAC-C3C	2.26	1.58	1.54
6	g	200	CYC	CMD-C2D	2.25	1.56	1.51
6	J	200	CYC	CMD-C2D	2.25	1.56	1.51
6	g	200	CYC	CMA-C3A	2.23	1.55	1.50
6	X	200	CYC	C4C-NC	-2.23	1.32	1.37
6	V	201	CYC	C4A-C3A	-2.22	1.41	1.45
6	G	201	CYC	C4A-C3A	-2.21	1.41	1.45
6	H	200	CYC	CMA-C3A	2.20	1.55	1.50
6	G	200	CYC	CMD-C2D	2.19	1.56	1.51
6	V	200	CYC	CMD-C2D	2.18	1.56	1.51
6	V	201	CYC	CMA-C3A	2.18	1.55	1.50
6	C	200	CYC	CMA-C3A	2.18	1.55	1.50
6	T	200	CYC	C4A-C3A	-2.16	1.41	1.45
6	d	200	CYC	CAC-C3C	2.16	1.58	1.54
6	e	200	CYC	CMA-C3A	2.16	1.55	1.50
6	i	201	CYC	CMA-C3A	2.15	1.55	1.50
6	4	301	CYC	CBA-CAA	2.15	1.58	1.52
6	l	200	CYC	C4C-NC	-2.14	1.32	1.37
6	h	200	CYC	CMA-C3A	2.14	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	201	CYC	CMD-C2D	2.14	1.56	1.51
6	j	200	CYC	CMD-C2D	2.13	1.56	1.51
6	T	201	CYC	CMA-C3A	2.13	1.55	1.50
6	A	201	CYC	CMA-C3A	2.13	1.55	1.50
6	T	201	CYC	C4A-C3A	-2.13	1.41	1.45
6	I	201	CYC	CMA-C3A	2.12	1.55	1.50
6	G	200	CYC	CMA-C3A	2.12	1.55	1.50
6	W	201	CYC	CMA-C3A	2.11	1.55	1.50
6	i	201	CYC	C4A-C3A	-2.10	1.41	1.45
6	l	200	CYC	CMA-C3A	2.09	1.55	1.50
6	U	201	CYC	CMA-C3A	2.09	1.55	1.50
6	N	200	CYC	CMA-C3A	2.08	1.55	1.50
6	k	200	CYC	CMD-C2D	2.08	1.56	1.51
6	K	200	CYC	CMD-C2D	2.07	1.55	1.51
6	Z	200	CYC	CMA-C3A	2.07	1.55	1.50
6	G	201	CYC	CBA-CAA	2.05	1.58	1.52
6	k	201	CYC	CMA-C3A	2.05	1.55	1.50
6	G	200	CYC	CBA-CAA	2.04	1.58	1.52
6	l	201	CYC	CMA-C3A	2.04	1.55	1.50
6	g	200	CYC	CBA-CAA	2.04	1.58	1.52
6	h	201	CYC	CBA-CAA	2.04	1.58	1.52
6	J	200	CYC	C4C-NC	-2.04	1.33	1.37
6	V	200	CYC	CMA-C3A	2.04	1.55	1.50
6	T	200	CYC	CBA-CAA	2.03	1.58	1.52
6	S	200	CYC	CMA-C3A	2.03	1.55	1.50
6	I	201	CYC	CBA-CAA	2.03	1.58	1.52
6	g	201	CYC	CBA-CAA	2.02	1.58	1.52
6	Y	200	CYC	CMA-C3A	2.02	1.55	1.50
6	I	200	CYC	CMA-C3A	2.02	1.55	1.50
6	Q	200	CYC	C4A-NA	-2.01	1.32	1.36
6	j	201	CYC	CBA-CAA	2.01	1.58	1.52
6	K	201	CYC	CBA-CAA	2.01	1.58	1.52
6	V	201	CYC	CBA-CAA	2.01	1.58	1.52
6	i	201	CYC	CBA-CAA	2.01	1.58	1.52
6	W	201	CYC	CBA-CAA	2.01	1.58	1.52
6	C	200	CYC	CBA-CAA	2.00	1.58	1.52
6	K	201	CYC	C4C-NC	-2.00	1.33	1.37

All (681) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	3	601	CYC	OC-C1C-C2C	-22.68	108.14	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	l	200	CYC	OC-C1C-C2C	-22.62	108.19	126.17
6	K	200	CYC	OC-C1C-C2C	-22.57	108.23	126.17
6	X	201	CYC	OC-C1C-C2C	-22.43	108.34	126.17
6	k	200	CYC	OC-C1C-C2C	-22.43	108.34	126.17
6	X	200	CYC	OC-C1C-C2C	-22.34	108.41	126.17
6	J	200	CYC	OC-C1C-C2C	-22.08	108.62	126.17
6	j	200	CYC	OC-C1C-C2C	-22.03	108.66	126.17
6	Y	201	CYC	OC-C1C-C2C	-21.71	108.91	126.17
6	j	201	CYC	OC-C1C-C2C	-21.62	108.99	126.17
6	P	200	CYC	OC-C1C-C2C	-21.28	109.25	126.17
6	d	200	CYC	OC-C1C-C2C	-21.17	109.34	126.17
6	W	200	CYC	OC-C1C-C2C	-21.15	109.36	126.17
6	A	201	CYC	OC-C1C-C2C	-21.10	109.39	126.17
6	Q	200	CYC	OC-C1C-C2C	-20.88	109.57	126.17
6	V	200	CYC	OC-C1C-C2C	-20.79	109.64	126.17
6	L	201	CYC	OC-C1C-C2C	-20.77	109.66	126.17
6	G	201	CYC	OC-C1C-C2C	-20.75	109.67	126.17
6	i	201	CYC	OC-C1C-C2C	-20.70	109.72	126.17
6	K	201	CYC	OC-C1C-C2C	-20.69	109.72	126.17
6	T	200	CYC	OC-C1C-C2C	-20.64	109.76	126.17
6	4	301	CYC	OC-C1C-C2C	-20.56	109.82	126.17
6	U	201	CYC	OC-C1C-C2C	-20.54	109.84	126.17
6	I	200	CYC	OC-C1C-C2C	-20.52	109.86	126.17
6	k	201	CYC	OC-C1C-C2C	-20.50	109.88	126.17
6	Z	200	CYC	OC-C1C-C2C	-20.42	109.94	126.17
6	G	200	CYC	OC-C1C-C2C	-20.41	109.94	126.17
6	g	201	CYC	OC-C1C-C2C	-20.40	109.95	126.17
6	H	200	CYC	OC-C1C-C2C	-20.39	109.96	126.17
6	Y	200	CYC	OC-C1C-C2C	-20.38	109.97	126.17
6	g	200	CYC	OC-C1C-C2C	-20.38	109.97	126.17
6	a	200	CYC	OC-C1C-C2C	-20.30	110.03	126.17
6	D	200	CYC	OC-C1C-C2C	-20.27	110.06	126.17
6	V	201	CYC	OC-C1C-C2C	-20.22	110.09	126.17
6	h	200	CYC	OC-C1C-C2C	-20.18	110.13	126.17
6	W	201	CYC	OC-C1C-C2C	-20.05	110.23	126.17
6	O	200	CYC	OC-C1C-C2C	-20.01	110.26	126.17
6	B	201	CYC	OC-C1C-C2C	-19.99	110.28	126.17
6	h	201	CYC	OC-C1C-C2C	-19.85	110.39	126.17
6	I	201	CYC	OC-C1C-C2C	-19.70	110.51	126.17
6	B	200	CYC	OC-C1C-C2C	-19.70	110.51	126.17
6	l	201	CYC	OC-C1C-C2C	-19.67	110.54	126.17
6	c	200	CYC	OC-C1C-C2C	-19.58	110.61	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	200	CYC	OC-C1C-C2C	-19.58	110.61	126.17
6	R	200	CYC	OC-C1C-C2C	-19.47	110.70	126.17
6	E	200	CYC	OC-C1C-C2C	-19.38	110.77	126.17
6	f	200	CYC	OC-C1C-C2C	-19.36	110.78	126.17
6	b	200	CYC	OC-C1C-C2C	-19.23	110.89	126.17
6	T	201	CYC	OC-C1C-C2C	-19.19	110.92	126.17
6	S	200	CYC	OC-C1C-C2C	-19.15	110.94	126.17
6	C	200	CYC	OC-C1C-C2C	-19.13	110.96	126.17
6	e	200	CYC	OC-C1C-C2C	-18.88	111.16	126.17
6	N	200	CYC	OC-C1C-C2C	-18.86	111.17	126.17
6	F	200	CYC	OC-C1C-C2C	-18.50	111.46	126.17
6	E	200	CYC	C4D-CHA-C1A	-14.82	111.11	128.81
6	g	201	CYC	C4D-CHA-C1A	-14.80	111.12	128.81
6	U	201	CYC	C4D-CHA-C1A	-14.78	111.16	128.81
6	N	200	CYC	C4D-CHA-C1A	-14.61	111.36	128.81
6	O	200	CYC	C4D-CHA-C1A	-14.47	111.52	128.81
6	Y	201	CYC	C4D-CHA-C1A	-14.38	111.63	128.81
6	T	201	CYC	C4D-CHA-C1A	-14.28	111.75	128.81
6	i	201	CYC	C4D-CHA-C1A	-13.48	112.70	128.81
6	G	201	CYC	C4D-CHA-C1A	-13.47	112.71	128.81
6	J	200	CYC	OC-C1C-NC	-13.39	108.73	124.94
6	P	200	CYC	C4D-CHA-C1A	-13.32	112.90	128.81
6	W	200	CYC	OC-C1C-NC	-13.31	108.82	124.94
6	P	200	CYC	CHD-C4C-NC	-13.23	109.47	125.20
6	F	200	CYC	CHD-C4C-NC	-13.15	109.57	125.20
6	h	201	CYC	C4D-CHA-C1A	-13.10	113.16	128.81
6	D	200	CYC	CHD-C4C-NC	-13.09	109.64	125.20
6	k	200	CYC	OC-C1C-NC	-13.03	109.16	124.94
6	E	200	CYC	CHD-C4C-NC	-13.00	109.75	125.20
6	3	601	CYC	OC-C1C-NC	-13.00	109.20	124.94
6	P	200	CYC	OC-C1C-NC	-12.97	109.23	124.94
6	g	201	CYC	CHD-C4C-NC	-12.94	109.82	125.20
6	C	200	CYC	C4D-CHA-C1A	-12.91	113.38	128.81
6	j	201	CYC	CHD-C4C-NC	-12.90	109.87	125.20
6	j	201	CYC	OC-C1C-NC	-12.86	109.37	124.94
6	G	201	CYC	CHD-C4C-NC	-12.86	109.92	125.20
6	d	200	CYC	CHD-C4C-NC	-12.81	109.97	125.20
6	K	201	CYC	OC-C1C-NC	-12.79	109.45	124.94
6	S	200	CYC	CHD-C4C-NC	-12.79	110.00	125.20
6	R	200	CYC	CHD-C4C-NC	-12.78	110.00	125.20
6	j	200	CYC	OC-C1C-NC	-12.75	109.50	124.94
6	Y	201	CYC	CHD-C4C-NC	-12.74	110.06	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	U	201	CYC	CHD-C4C-NC	-12.72	110.08	125.20
6	A	201	CYC	OC-C1C-NC	-12.67	109.60	124.94
6	g	200	CYC	C4D-CHA-C1A	-12.65	113.70	128.81
6	4	301	CYC	CHD-C4C-NC	-12.65	110.16	125.20
6	V	201	CYC	OC-C1C-NC	-12.59	109.70	124.94
6	A	200	CYC	CHD-C4C-NC	-12.58	110.25	125.20
6	d	200	CYC	OC-C1C-NC	-12.55	109.75	124.94
6	f	200	CYC	CHD-C4C-NC	-12.54	110.30	125.20
6	Y	201	CYC	OC-C1C-NC	-12.53	109.76	124.94
6	c	200	CYC	CHD-C4C-NC	-12.51	110.33	125.20
6	d	200	CYC	C4D-CHA-C1A	-12.49	113.89	128.81
6	Y	200	CYC	CHD-C4C-NC	-12.48	110.37	125.20
6	Z	200	CYC	OC-C1C-NC	-12.47	109.84	124.94
6	i	201	CYC	CHD-C4C-NC	-12.46	110.39	125.20
6	Q	200	CYC	OC-C1C-NC	-12.46	109.86	124.94
6	j	201	CYC	C4D-CHA-C1A	-12.43	113.96	128.81
6	O	200	CYC	OC-C1C-NC	-12.43	109.89	124.94
6	b	200	CYC	C4D-CHA-C1A	-12.39	114.01	128.81
6	c	200	CYC	C4D-CHA-C1A	-12.39	114.01	128.81
6	K	200	CYC	OC-C1C-NC	-12.39	109.94	124.94
6	K	201	CYC	CHD-C4C-NC	-12.38	110.48	125.20
6	R	200	CYC	C4D-CHA-C1A	-12.38	114.02	128.81
6	A	200	CYC	C4D-CHA-C1A	-12.37	114.03	128.81
6	a	200	CYC	CHD-C4C-NC	-12.35	110.53	125.20
6	i	201	CYC	OC-C1C-NC	-12.34	110.00	124.94
6	f	200	CYC	C4D-CHA-C1A	-12.33	114.08	128.81
6	I	201	CYC	CHD-C4C-NC	-12.32	110.56	125.20
6	I	200	CYC	OC-C1C-NC	-12.29	110.05	124.94
6	D	200	CYC	OC-C1C-NC	-12.26	110.09	124.94
6	I	201	CYC	OC-C1C-NC	-12.25	110.10	124.94
6	N	200	CYC	CHD-C4C-NC	-12.23	110.66	125.20
6	k	200	CYC	CHD-C4C-NC	-12.23	110.66	125.20
6	h	201	CYC	OC-C1C-NC	-12.23	110.13	124.94
6	W	201	CYC	OC-C1C-NC	-12.22	110.14	124.94
6	k	201	CYC	OC-C1C-NC	-12.20	110.17	124.94
6	g	200	CYC	CHD-C4C-NC	-12.17	110.74	125.20
6	B	200	CYC	OC-C1C-NC	-12.17	110.21	124.94
6	J	200	CYC	CHD-C4C-NC	-12.15	110.76	125.20
6	Q	200	CYC	C4D-CHA-C1A	-12.14	114.30	128.81
6	b	200	CYC	CHD-C4C-NC	-12.14	110.78	125.20
6	f	200	CYC	OC-C1C-NC	-12.13	110.25	124.94
6	R	200	CYC	OC-C1C-NC	-12.12	110.26	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	l	201	CYC	CHD-C4C-NC	-12.11	110.81	125.20
6	Q	200	CYC	CHD-C4C-NC	-12.09	110.83	125.20
6	B	200	CYC	C4D-CHA-C1A	-12.06	114.41	128.81
6	F	200	CYC	C4D-CHA-C1A	-12.04	114.42	128.81
6	V	200	CYC	OC-C1C-NC	-12.04	110.37	124.94
6	X	200	CYC	OC-C1C-NC	-12.03	110.38	124.94
6	l	200	CYC	OC-C1C-NC	-12.02	110.38	124.94
6	F	200	CYC	OC-C1C-NC	-12.00	110.42	124.94
6	H	200	CYC	OC-C1C-NC	-11.99	110.42	124.94
6	a	200	CYC	OC-C1C-NC	-11.98	110.43	124.94
6	U	201	CYC	OC-C1C-NC	-11.97	110.44	124.94
6	S	200	CYC	OC-C1C-NC	-11.97	110.44	124.94
6	G	201	CYC	OC-C1C-NC	-11.97	110.44	124.94
6	g	200	CYC	OC-C1C-NC	-11.96	110.46	124.94
6	L	201	CYC	OC-C1C-NC	-11.93	110.50	124.94
6	g	201	CYC	OC-C1C-NC	-11.92	110.51	124.94
6	Y	200	CYC	OC-C1C-NC	-11.90	110.53	124.94
6	h	201	CYC	CHD-C4C-NC	-11.90	111.06	125.20
6	W	201	CYC	CHD-C4C-NC	-11.90	111.06	125.20
6	X	201	CYC	OC-C1C-NC	-11.89	110.55	124.94
6	T	200	CYC	OC-C1C-NC	-11.88	110.55	124.94
6	e	200	CYC	CHD-C4C-NC	-11.88	111.08	125.20
6	k	201	CYC	CHD-C4C-NC	-11.82	111.15	125.20
6	X	200	CYC	CHD-C4C-NC	-11.82	111.15	125.20
6	B	200	CYC	CHD-C4C-NC	-11.81	111.16	125.20
6	T	201	CYC	OC-C1C-NC	-11.80	110.65	124.94
6	B	201	CYC	OC-C1C-NC	-11.80	110.66	124.94
6	X	201	CYC	CHD-C4C-NC	-11.79	111.18	125.20
6	H	200	CYC	CHD-C4C-NC	-11.79	111.18	125.20
6	4	301	CYC	OC-C1C-NC	-11.79	110.66	124.94
6	C	200	CYC	CHD-C4C-NC	-11.78	111.19	125.20
6	E	200	CYC	OC-C1C-NC	-11.75	110.71	124.94
6	G	200	CYC	OC-C1C-NC	-11.72	110.75	124.94
6	h	200	CYC	OC-C1C-NC	-11.71	110.76	124.94
6	b	200	CYC	OC-C1C-NC	-11.71	110.77	124.94
6	G	200	CYC	CHD-C4C-NC	-11.70	111.29	125.20
6	k	201	CYC	C4D-CHA-C1A	-11.69	114.85	128.81
6	W	200	CYC	CHD-C4C-NC	-11.60	111.41	125.20
6	N	200	CYC	OC-C1C-NC	-11.59	110.91	124.94
6	T	200	CYC	CHD-C4C-NC	-11.57	111.45	125.20
6	D	200	CYC	C4D-CHA-C1A	-11.48	115.10	128.81
6	V	201	CYC	C4D-CHA-C1A	-11.47	115.10	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	V	200	CYC	CHD-C4C-NC	-11.47	111.57	125.20
6	K	200	CYC	CHD-C4C-NC	-11.47	111.57	125.20
6	l	201	CYC	OC-C1C-NC	-11.47	111.06	124.94
6	W	201	CYC	C4D-CHA-C1A	-11.46	115.11	128.81
6	A	201	CYC	C4D-CHA-C1A	-11.40	115.19	128.81
6	H	200	CYC	C4D-CHA-C1A	-11.37	115.22	128.81
6	A	200	CYC	OC-C1C-NC	-11.37	111.17	124.94
6	C	200	CYC	OC-C1C-NC	-11.36	111.18	124.94
6	h	200	CYC	CHD-C4C-NC	-11.34	111.72	125.20
6	T	201	CYC	CHD-C4C-NC	-11.22	111.87	125.20
6	h	200	CYC	C4D-CHA-C1A	-11.15	115.49	128.81
6	V	201	CYC	CHD-C4C-NC	-11.12	111.98	125.20
6	j	200	CYC	CHD-C4C-NC	-11.05	112.07	125.20
6	L	201	CYC	CHD-C4C-NC	-11.04	112.08	125.20
6	S	200	CYC	C4D-CHA-C1A	-11.02	115.64	128.81
6	l	201	CYC	C4D-CHA-C1A	-10.99	115.68	128.81
6	3	601	CYC	CHD-C4C-NC	-10.99	112.14	125.20
6	A	201	CYC	CHD-C4C-NC	-10.96	112.17	125.20
6	I	200	CYC	CHD-C4C-NC	-10.94	112.20	125.20
6	e	200	CYC	OC-C1C-NC	-10.89	111.75	124.94
6	Z	200	CYC	CHD-C4C-NC	-10.88	112.27	125.20
6	l	200	CYC	CHD-C4C-NC	-10.74	112.43	125.20
6	e	200	CYC	C4D-CHA-C1A	-10.54	116.22	128.81
6	T	200	CYC	C4D-CHA-C1A	-10.53	116.23	128.81
6	B	201	CYC	C4D-CHA-C1A	-10.44	116.33	128.81
6	c	200	CYC	OC-C1C-NC	-10.34	112.41	124.94
6	X	201	CYC	C4D-CHA-C1A	-10.27	116.54	128.81
6	I	201	CYC	C4D-CHA-C1A	-9.99	116.87	128.81
6	L	201	CYC	C4D-CHA-C1A	-9.97	116.89	128.81
6	4	301	CYC	C4D-CHA-C1A	-9.94	116.93	128.81
6	B	201	CYC	CHD-C4C-NC	-9.91	113.42	125.20
6	l	200	CYC	C4D-CHA-C1A	-9.74	117.18	128.81
6	O	200	CYC	CHD-C4C-NC	-9.66	113.71	125.20
6	J	200	CYC	C4D-CHA-C1A	-9.49	117.47	128.81
6	Z	200	CYC	C4D-CHA-C1A	-9.47	117.49	128.81
6	K	201	CYC	C4D-CHA-C1A	-9.37	117.61	128.81
6	I	200	CYC	C4D-CHA-C1A	-9.16	117.87	128.81
6	Y	200	CYC	C2C-C1C-NC	-9.12	100.41	108.27
6	Y	200	CYC	C4D-CHA-C1A	-9.08	117.96	128.81
6	3	601	CYC	C4D-CHA-C1A	-8.57	118.57	128.81
6	K	200	CYC	C4D-CHA-C1A	-8.54	118.61	128.81
6	V	200	CYC	C4D-CHA-C1A	-8.54	118.61	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	W	200	CYC	C4D-CHA-C1A	-8.44	118.73	128.81
6	G	200	CYC	C4D-CHA-C1A	-8.41	118.77	128.81
6	j	200	CYC	C4D-CHA-C1A	-8.40	118.77	128.81
6	l	200	CYC	C2C-C1C-NC	-8.06	101.33	108.27
6	h	201	CYC	C1B-CHB-C4A	-8.05	108.41	128.08
6	k	200	CYC	C4D-CHA-C1A	-7.99	119.26	128.81
6	a	200	CYC	C4D-CHA-C1A	-7.95	119.31	128.81
6	X	200	CYC	C4D-CHA-C1A	-7.85	119.43	128.81
6	P	200	CYC	C2C-C1C-NC	-7.63	101.69	108.27
6	U	201	CYC	C1B-CHB-C4A	-7.48	109.80	128.08
6	F	200	CYC	C2C-C1C-NC	-7.33	101.95	108.27
6	B	201	CYC	C1B-CHB-C4A	-7.26	110.35	128.08
6	a	200	CYC	C1B-CHB-C4A	-7.24	110.40	128.08
6	l	201	CYC	C2C-C1C-NC	-7.22	102.05	108.27
6	c	200	CYC	C1B-CHB-C4A	-7.14	110.64	128.08
6	A	201	CYC	C2C-C1C-NC	-7.14	102.12	108.27
6	H	200	CYC	C2C-C1C-NC	-6.71	102.49	108.27
6	S	200	CYC	C2C-C1C-NC	-6.51	102.66	108.27
6	k	201	CYC	C2C-C1C-NC	-6.48	102.69	108.27
6	E	200	CYC	C2C-C1C-NC	-6.34	102.81	108.27
6	g	201	CYC	C1B-CHB-C4A	-6.24	112.84	128.08
6	N	200	CYC	C2C-C1C-NC	-6.22	102.92	108.27
6	b	200	CYC	C2C-C1C-NC	-6.11	103.01	108.27
6	D	200	CYC	C2C-C1C-NC	-6.07	103.04	108.27
6	U	201	CYC	C2C-C1C-NC	-6.06	103.05	108.27
6	W	201	CYC	C2C-C1C-NC	-6.02	103.08	108.27
6	A	200	CYC	C2C-C1C-NC	-6.02	103.09	108.27
6	g	200	CYC	C1B-CHB-C4A	-5.98	113.46	128.08
6	f	200	CYC	C1B-CHB-C4A	-5.93	113.61	128.08
6	4	301	CYC	C2C-C1C-NC	-5.91	103.18	108.27
6	K	201	CYC	C2C-C1C-NC	-5.88	103.21	108.27
6	X	200	CYC	C2C-C1C-NC	-5.85	103.23	108.27
6	G	200	CYC	C2C-C1C-NC	-5.80	103.27	108.27
6	C	200	CYC	C2C-C1C-NC	-5.77	103.30	108.27
6	j	201	CYC	C2C-C1C-NC	-5.70	103.36	108.27
6	R	200	CYC	C2C-C1C-NC	-5.70	103.36	108.27
6	N	200	CYC	C1B-CHB-C4A	-5.54	114.56	128.08
6	e	200	CYC	C1B-CHB-C4A	-5.44	114.79	128.08
6	I	201	CYC	C2C-C1C-NC	-5.42	103.60	108.27
6	h	200	CYC	C2C-C1C-NC	-5.41	103.61	108.27
6	k	201	CYC	C1B-CHB-C4A	-5.36	114.99	128.08
6	Z	200	CYC	C1B-CHB-C4A	-5.35	115.01	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	200	CYC	CAB-C3B-C4B	5.32	129.78	121.38
6	l	200	CYC	C1B-CHB-C4A	-5.25	115.26	128.08
6	X	201	CYC	C2C-C3C-C4C	5.17	109.08	101.34
6	b	200	CYC	C1B-CHB-C4A	-5.13	115.55	128.08
6	h	200	CYC	CAB-C3B-C4B	5.11	129.45	121.38
6	O	200	CYC	C1B-CHB-C4A	-5.09	115.64	128.08
6	B	200	CYC	C1B-CHB-C4A	-5.08	115.67	128.08
6	B	200	CYC	CAB-C3B-C4B	5.07	129.39	121.38
6	L	201	CYC	C2C-C1C-NC	-5.07	103.91	108.27
6	T	200	CYC	C2C-C3C-C4C	5.03	108.88	101.34
6	F	200	CYC	CAB-C3B-C4B	5.03	129.32	121.38
6	E	200	CYC	C1B-CHB-C4A	-5.02	115.81	128.08
6	I	200	CYC	C2C-C3C-C4C	5.01	108.84	101.34
6	X	200	CYC	CMA-C3A-C4A	4.99	132.75	125.06
6	W	200	CYC	C2C-C3C-C4C	4.98	108.80	101.34
6	c	200	CYC	C2C-C1C-NC	-4.93	104.02	108.27
6	J	200	CYC	C2C-C3C-C4C	4.90	108.68	101.34
6	e	200	CYC	C2C-C1C-NC	-4.90	104.05	108.27
6	g	200	CYC	C2C-C3C-C4C	4.90	108.67	101.34
6	d	200	CYC	CAB-C3B-C4B	4.85	129.05	121.38
6	3	601	CYC	C2C-C3C-C4C	4.84	108.59	101.34
6	d	200	CYC	C2C-C1C-NC	-4.84	104.10	108.27
6	R	200	CYC	C1B-CHB-C4A	-4.84	116.27	128.08
6	K	200	CYC	C2C-C1C-NC	-4.81	104.13	108.27
6	j	200	CYC	C2C-C1C-NC	-4.80	104.14	108.27
6	k	200	CYC	C2C-C3C-C4C	4.76	108.47	101.34
6	j	200	CYC	CMA-C3A-C4A	4.76	132.39	125.06
6	V	200	CYC	C2C-C1C-NC	-4.72	104.20	108.27
6	Z	200	CYC	C2C-C1C-NC	-4.72	104.21	108.27
6	H	200	CYC	C1B-CHB-C4A	-4.71	116.57	128.08
6	l	200	CYC	C2C-C3C-C4C	4.71	108.40	101.34
6	A	200	CYC	C1B-CHB-C4A	-4.71	116.58	128.08
6	W	200	CYC	C2C-C1C-NC	-4.70	104.22	108.27
6	V	200	CYC	C2C-C3C-C4C	4.67	108.33	101.34
6	K	200	CYC	C2C-C3C-C4C	4.67	108.33	101.34
6	T	200	CYC	C2C-C1C-NC	-4.64	104.27	108.27
6	i	201	CYC	C2C-C3C-C4C	4.63	108.27	101.34
6	X	200	CYC	C2C-C3C-C4C	4.62	108.26	101.34
6	e	200	CYC	C2C-C3C-C4C	4.59	108.22	101.34
6	4	301	CYC	C1B-CHB-C4A	-4.59	116.87	128.08
6	b	200	CYC	CAB-C3B-C4B	4.58	128.61	121.38
6	S	200	CYC	C1B-CHB-C4A	-4.57	116.91	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	200	CYC	C1B-CHB-C4A	-4.57	116.93	128.08
6	4	301	CYC	C2C-C3C-C4C	4.56	108.17	101.34
6	S	200	CYC	CAB-C3B-C4B	4.52	128.53	121.38
6	B	200	CYC	C2C-C3C-C4C	4.50	108.08	101.34
6	G	201	CYC	C2C-C3C-C4C	4.49	108.06	101.34
6	Y	201	CYC	C2C-C1C-NC	-4.46	104.42	108.27
6	G	201	CYC	C2C-C1C-NC	-4.46	104.43	108.27
6	N	200	CYC	CAB-C3B-C4B	4.45	128.41	121.38
6	f	200	CYC	C2C-C3C-C4C	4.44	107.99	101.34
6	L	201	CYC	C2C-C3C-C4C	4.44	107.98	101.34
6	K	200	CYC	CMA-C3A-C4A	4.42	131.86	125.06
6	f	200	CYC	C2C-C1C-NC	-4.38	104.50	108.27
6	X	201	CYC	CMA-C3A-C4A	4.37	131.80	125.06
6	a	200	CYC	C2C-C1C-NC	-4.37	104.51	108.27
6	P	200	CYC	CAB-C3B-C4B	4.37	128.27	121.38
6	Y	201	CYC	C2C-C3C-C4C	4.33	107.83	101.34
6	D	200	CYC	CAB-C3B-C4B	4.33	128.22	121.38
6	k	201	CYC	C2C-C3C-C4C	4.33	107.82	101.34
6	J	200	CYC	CMA-C3A-C4A	4.33	131.73	125.06
6	k	200	CYC	CMA-C3A-C4A	4.32	131.72	125.06
6	W	200	CYC	CMA-C3A-C4A	4.30	131.69	125.06
6	T	200	CYC	CMA-C3A-C4A	4.28	131.66	125.06
6	G	200	CYC	C2C-C3C-C4C	4.27	107.73	101.34
6	I	201	CYC	C2C-C3C-C4C	4.24	107.69	101.34
6	P	200	CYC	C1B-CHB-C4A	-4.24	117.73	128.08
6	O	200	CYC	CAB-C3B-C4B	4.23	128.06	121.38
6	G	201	CYC	CMA-C3A-C4A	4.21	131.55	125.06
6	h	200	CYC	C1B-CHB-C4A	-4.21	117.80	128.08
6	I	200	CYC	C1B-CHB-C4A	-4.20	117.82	128.08
6	c	200	CYC	C2C-C3C-C4C	4.18	107.59	101.34
6	K	201	CYC	C2C-C3C-C4C	4.17	107.58	101.34
6	Q	200	CYC	CAB-C3B-C4B	4.16	127.95	121.38
6	j	201	CYC	C2C-C3C-C4C	4.15	107.56	101.34
6	Q	200	CYC	C2C-C3C-C4C	4.14	107.54	101.34
6	Y	200	CYC	CMA-C3A-C4A	4.14	131.44	125.06
6	Q	200	CYC	C1B-CHB-C4A	-4.12	118.00	128.08
6	g	201	CYC	CAB-C3B-C4B	4.09	127.84	121.38
6	i	201	CYC	C2C-C1C-NC	-4.06	104.77	108.27
6	A	201	CYC	C2C-C3C-C4C	4.05	107.40	101.34
6	F	200	CYC	C1B-CHB-C4A	-4.04	118.20	128.08
6	i	201	CYC	CMA-C3A-C4A	4.04	131.29	125.06
6	A	200	CYC	CAB-C3B-C4B	4.03	127.74	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	200	CYC	CAB-C3B-C4B	4.01	127.71	121.38
6	e	200	CYC	CAB-C3B-C4B	3.99	127.68	121.38
6	K	201	CYC	CMA-C3A-C4A	3.95	131.14	125.06
6	d	200	CYC	C1B-CHB-C4A	-3.91	118.52	128.08
6	Y	201	CYC	CAB-C3B-C4B	3.88	127.50	121.38
6	B	201	CYC	C2C-C1C-NC	-3.87	104.93	108.27
6	g	201	CYC	C2C-C3C-C4C	3.87	107.13	101.34
6	l	201	CYC	C2C-C3C-C4C	3.87	107.13	101.34
6	Y	201	CYC	CMA-C3A-C4A	3.86	131.01	125.06
6	l	201	CYC	CMA-C3A-C4A	3.86	131.01	125.06
6	T	201	CYC	C2C-C1C-NC	-3.86	104.95	108.27
6	d	200	CYC	C2C-C3C-C4C	3.85	107.11	101.34
6	G	201	CYC	CAB-C3B-C4B	3.84	127.45	121.38
6	A	201	CYC	CAB-C3B-C4B	3.84	127.44	121.38
6	N	200	CYC	C2C-C3C-C4C	3.83	107.08	101.34
6	H	200	CYC	C2C-C3C-C4C	3.82	107.06	101.34
6	O	200	CYC	C2C-C3C-C4C	3.80	107.03	101.34
6	c	200	CYC	CAB-C3B-C4B	3.79	127.37	121.38
6	j	201	CYC	CAB-C3B-C4B	3.79	127.37	121.38
6	V	201	CYC	CMA-C3A-C4A	3.79	130.91	125.06
6	g	200	CYC	C2C-C1C-NC	-3.78	105.02	108.27
6	Y	200	CYC	C2C-C3C-C4C	3.78	107.00	101.34
6	V	200	CYC	C1B-CHB-C4A	-3.78	118.85	128.08
6	A	200	CYC	C2C-C3C-C4C	3.77	106.99	101.34
6	i	201	CYC	CAB-C3B-C4B	3.77	127.33	121.38
6	G	200	CYC	C1B-CHB-C4A	-3.77	118.88	128.08
6	W	200	CYC	CAB-C3B-C4B	3.76	127.32	121.38
6	U	201	CYC	C2C-C3C-C4C	3.75	106.96	101.34
6	R	200	CYC	CAB-C3B-C4B	3.73	127.28	121.38
6	D	200	CYC	C1B-CHB-C4A	-3.72	119.00	128.08
6	W	201	CYC	C2C-C3C-C4C	3.72	106.91	101.34
6	T	201	CYC	CMA-C3A-C4A	3.72	130.79	125.06
6	l	201	CYC	CAB-C3B-C4B	3.68	127.19	121.38
6	Y	200	CYC	C1B-CHB-C4A	-3.66	119.13	128.08
6	C	200	CYC	CAB-C3B-C4B	3.65	127.14	121.38
6	F	200	CYC	CMA-C3A-C4A	3.64	130.67	125.06
6	W	201	CYC	CAB-C3B-C4B	3.63	127.11	121.38
6	B	201	CYC	CAB-C3B-C4B	3.62	127.10	121.38
6	K	201	CYC	CHB-C4A-C3A	3.62	134.21	124.90
6	g	200	CYC	CAB-C3B-C4B	3.62	127.09	121.38
6	K	201	CYC	CAB-C3B-C4B	3.62	127.09	121.38
6	E	200	CYC	C2C-C3C-C4C	3.62	106.75	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	V	201	CYC	CAB-C3B-C4B	3.61	127.08	121.38
6	L	201	CYC	CMA-C3A-C4A	3.61	130.62	125.06
6	S	200	CYC	C2C-C3C-C4C	3.61	106.74	101.34
6	C	200	CYC	CMA-C3A-C4A	3.61	130.62	125.06
6	V	201	CYC	C2C-C1C-NC	-3.60	105.17	108.27
6	V	200	CYC	CAB-C3B-C4B	3.60	127.06	121.38
6	D	200	CYC	C2C-C3C-C4C	3.59	106.72	101.34
6	R	200	CYC	C2C-C3C-C4C	3.57	106.69	101.34
6	I	201	CYC	C1B-CHB-C4A	-3.57	119.36	128.08
6	S	200	CYC	CMA-C3A-C4A	3.57	130.56	125.06
6	B	201	CYC	C2C-C3C-C4C	3.54	106.65	101.34
6	D	200	CYC	CMA-C3A-C4A	3.51	130.47	125.06
6	P	200	CYC	CMA-C3A-C4A	3.50	130.45	125.06
6	G	200	CYC	CAB-C3B-C4B	3.48	126.88	121.38
6	G	201	CYC	CHB-C4A-C3A	3.48	133.85	124.90
6	h	201	CYC	CAB-C3B-C4B	3.47	126.87	121.38
6	b	200	CYC	C2C-C3C-C4C	3.47	106.54	101.34
6	j	200	CYC	C2C-C3C-C4C	3.47	106.54	101.34
6	W	200	CYC	CHB-C4A-C3A	3.47	133.82	124.90
6	J	200	CYC	CAB-C3B-C4B	3.45	126.83	121.38
6	O	200	CYC	CMA-C3A-C4A	3.45	130.38	125.06
6	3	601	CYC	C1B-CHB-C4A	-3.45	119.65	128.08
6	U	201	CYC	CAB-C3B-C4B	3.45	126.83	121.38
6	X	201	CYC	CAB-C3B-C4B	3.43	126.80	121.38
6	X	201	CYC	CHB-C4A-C3A	3.43	133.72	124.90
6	L	201	CYC	CHB-C4A-C3A	3.42	133.70	124.90
6	F	200	CYC	C2C-C3C-C4C	3.42	106.46	101.34
6	I	200	CYC	CAB-C3B-C4B	3.42	126.78	121.38
6	a	200	CYC	CAB-C3B-C4B	3.42	126.78	121.38
6	K	200	CYC	CAB-C3B-C4B	3.41	126.77	121.38
6	V	201	CYC	CHB-C4A-C3A	3.40	133.63	124.90
6	L	201	CYC	CAB-C3B-C4B	3.38	126.72	121.38
6	k	201	CYC	CAB-C3B-C4B	3.38	126.71	121.38
6	I	200	CYC	CMA-C3A-C4A	3.38	130.26	125.06
6	T	201	CYC	CHB-C4A-C3A	3.37	133.56	124.90
6	i	201	CYC	CHB-C4A-C3A	3.36	133.55	124.90
6	Y	201	CYC	CHB-C4A-C3A	3.36	133.54	124.90
6	A	201	CYC	C1B-CHB-C4A	-3.36	119.88	128.08
6	J	200	CYC	CHB-C4A-C3A	3.36	133.53	124.90
6	T	201	CYC	CAB-C3B-C4B	3.34	126.66	121.38
6	X	200	CYC	CHB-C4A-C3A	3.34	133.48	124.90
6	W	201	CYC	CMA-C3A-C4A	3.33	130.19	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	k	200	CYC	CAB-C3B-C4B	3.32	126.62	121.38
6	l	200	CYC	CAB-C3B-C4B	3.31	126.61	121.38
6	3	601	CYC	CAB-C3B-C4B	3.30	126.60	121.38
6	K	201	CYC	C1A-NA-C4A	3.30	112.73	106.51
6	h	201	CYC	C2C-C1C-NC	-3.30	105.43	108.27
6	Z	200	CYC	CAB-C3B-C4B	3.30	126.58	121.38
6	V	200	CYC	CMA-C3A-C4A	3.29	130.13	125.06
6	O	200	CYC	CAC-C3C-C4C	-3.28	104.26	112.67
6	I	201	CYC	CAB-C3B-C4B	3.26	126.53	121.38
6	A	201	CYC	CMA-C3A-C4A	3.25	130.08	125.06
6	I	201	CYC	OB-C4B-C3B	-3.23	124.53	128.04
6	J	200	CYC	C2C-C1C-NC	-3.22	105.50	108.27
6	I	200	CYC	C2C-C1C-NC	-3.22	105.50	108.27
6	j	201	CYC	CMA-C3A-C4A	3.22	130.02	125.06
6	a	200	CYC	C2C-C3C-C4C	3.19	106.12	101.34
6	K	200	CYC	CHB-C4A-C3A	3.18	133.08	124.90
6	H	200	CYC	CAB-C3B-C4B	3.18	126.40	121.38
6	j	200	CYC	CAB-C3B-C4B	3.15	126.35	121.38
6	B	201	CYC	CMB-C2B-C1B	3.14	128.09	124.17
6	O	200	CYC	CMB-C2B-C1B	3.11	128.05	124.17
6	C	200	CYC	C2C-C3C-C4C	3.09	105.97	101.34
6	H	200	CYC	CMA-C3A-C4A	3.08	129.80	125.06
6	T	201	CYC	C1A-NA-C4A	3.07	112.30	106.51
6	k	200	CYC	C2C-C1C-NC	-3.07	105.62	108.27
6	G	200	CYC	CMA-C3A-C4A	3.07	129.79	125.06
6	V	201	CYC	C1A-NA-C4A	3.06	112.28	106.51
6	i	201	CYC	C1A-NA-C4A	3.06	112.27	106.51
6	L	201	CYC	C1A-NA-C4A	3.05	112.26	106.51
6	4	301	CYC	CAB-C3B-C4B	3.05	126.20	121.38
6	k	200	CYC	CHB-C4A-C3A	3.02	132.67	124.90
6	P	200	CYC	C2C-C3C-C4C	3.02	105.86	101.34
6	j	200	CYC	CHB-C4A-C3A	3.01	132.63	124.90
6	T	200	CYC	CAB-C3B-C4B	3.01	126.13	121.38
6	X	201	CYC	C1A-NA-C4A	2.99	112.15	106.51
6	W	201	CYC	C1B-CHB-C4A	-2.99	120.78	128.08
6	R	200	CYC	CMA-C3A-C4A	2.99	129.66	125.06
6	Y	200	CYC	CAB-C3B-C4B	2.98	126.08	121.38
6	T	200	CYC	C1B-CHB-C4A	-2.98	120.81	128.08
6	Y	201	CYC	C1A-NA-C4A	2.97	112.11	106.51
6	G	201	CYC	C1A-NA-C4A	2.97	112.11	106.51
6	j	201	CYC	CHB-C4A-C3A	2.97	132.54	124.90
6	e	200	CYC	CMA-C3A-C4A	2.97	129.63	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	j	201	CYC	C1A-NA-C4A	2.94	112.05	106.51
6	W	200	CYC	C1A-NA-C4A	2.93	112.04	106.51
6	h	200	CYC	CMA-C3A-C4A	2.92	129.56	125.06
6	Q	200	CYC	C2C-C1C-NC	-2.92	105.76	108.27
6	g	201	CYC	C2C-C1C-NC	-2.91	105.76	108.27
6	3	601	CYC	CMA-C3A-C4A	2.91	129.54	125.06
6	B	200	CYC	CMA-C3A-C4A	2.91	129.54	125.06
6	l	201	CYC	CHB-C4A-C3A	2.90	132.35	124.90
6	I	201	CYC	CMA-C3A-C4A	2.89	129.52	125.06
6	K	200	CYC	CBD-CAD-C3D	-2.89	107.69	112.62
6	b	200	CYC	CMA-C3A-C4A	2.88	129.50	125.06
6	E	200	CYC	CMA-C3A-C4A	2.87	129.48	125.06
6	l	201	CYC	C1A-NA-C4A	2.85	111.88	106.51
6	T	200	CYC	CHB-C4A-C3A	2.83	132.18	124.90
6	A	200	CYC	CMA-C3A-C4A	2.80	129.37	125.06
6	I	201	CYC	C3B-C4B-NB	2.79	109.03	106.78
6	W	201	CYC	CHB-C4A-C3A	2.77	132.01	124.90
6	W	201	CYC	C1A-NA-C4A	2.76	111.70	106.51
6	k	200	CYC	C1A-NA-C4A	2.75	111.69	106.51
6	F	200	CYC	CMD-C2D-C3D	-2.75	119.76	124.94
6	4	301	CYC	OB-C4B-C3B	-2.73	125.07	128.04
6	X	200	CYC	CHB-C4A-NA	-2.73	119.22	124.93
6	B	201	CYC	OB-C4B-C3B	-2.73	125.08	128.04
6	J	200	CYC	CHB-C4A-NA	-2.72	119.24	124.93
6	d	200	CYC	CMA-C3A-C4A	2.72	129.25	125.06
6	k	200	CYC	CAA-C2A-C1A	2.71	129.80	125.01
6	A	201	CYC	C1A-NA-C4A	2.71	111.61	106.51
6	l	201	CYC	C1B-CHB-C4A	-2.71	121.47	128.08
6	X	200	CYC	C1B-CHB-C4A	-2.69	121.50	128.08
6	K	200	CYC	CHB-C4A-NA	-2.68	119.33	124.93
6	V	200	CYC	C1A-NA-C4A	2.67	111.55	106.51
6	W	200	CYC	CHB-C4A-NA	-2.67	119.34	124.93
6	X	200	CYC	CAB-C3B-C4B	2.67	125.59	121.38
6	4	301	CYC	C1A-NA-C4A	2.66	111.52	106.51
6	Y	200	CYC	CMC-C2C-C1C	-2.65	106.69	112.40
6	U	201	CYC	CMB-C2B-C1B	2.64	127.47	124.17
6	k	201	CYC	OB-C4B-C3B	-2.63	125.18	128.04
6	j	200	CYC	C1A-NA-C4A	2.62	111.44	106.51
6	Y	201	CYC	CMC-C2C-C1C	-2.62	106.76	112.40
6	l	200	CYC	CMA-C3A-C4A	2.61	129.09	125.06
6	O	200	CYC	C1A-NA-C4A	2.61	111.42	106.51
6	Z	200	CYC	OB-C4B-C3B	-2.61	125.21	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Q	200	CYC	C1A-NA-C4A	2.60	111.42	106.51
6	H	200	CYC	OB-C4B-C3B	-2.60	125.22	128.04
6	f	200	CYC	CAC-C3C-C4C	-2.60	106.01	112.67
6	I	201	CYC	C1A-NA-C4A	2.57	111.35	106.51
6	h	200	CYC	C1A-NA-C4A	2.56	111.34	106.51
6	K	201	CYC	CHB-C4A-NA	-2.56	119.59	124.93
6	Q	200	CYC	CMA-C3A-C4A	2.54	128.98	125.06
6	J	200	CYC	C1A-NA-C4A	2.54	111.30	106.51
6	T	200	CYC	C1A-NA-C4A	2.54	111.30	106.51
6	X	200	CYC	C1A-NA-C4A	2.54	111.30	106.51
6	H	200	CYC	C1A-NA-C4A	2.54	111.30	106.51
6	K	200	CYC	C1A-NA-C4A	2.53	111.28	106.51
6	I	200	CYC	C1A-NA-C4A	2.52	111.27	106.51
6	T	201	CYC	C1B-CHB-C4A	-2.52	121.93	128.08
6	A	201	CYC	CHB-C4A-C3A	2.52	131.37	124.90
6	X	200	CYC	CMD-C2D-C3D	-2.51	120.21	124.94
6	g	201	CYC	C1A-NA-C4A	2.51	111.24	106.51
6	X	201	CYC	CHB-C4A-NA	-2.50	119.70	124.93
6	T	201	CYC	C2C-C3C-C4C	2.50	105.08	101.34
6	S	200	CYC	C1A-NA-C4A	2.50	111.21	106.51
6	R	200	CYC	C1A-NA-C4A	2.49	111.20	106.51
6	j	200	CYC	C1B-CHB-C4A	-2.48	122.01	128.08
6	L	201	CYC	CHB-C4A-NA	-2.48	119.75	124.93
6	b	200	CYC	C1A-NA-C4A	2.48	111.18	106.51
6	V	201	CYC	OB-C4B-C3B	-2.47	125.36	128.04
6	F	200	CYC	CHB-C4A-C3A	2.47	131.25	124.90
6	k	201	CYC	C1A-NA-C4A	2.46	111.15	106.51
6	B	200	CYC	C1A-NA-C4A	2.46	111.14	106.51
6	K	200	CYC	CHB-C1B-C2B	-2.45	122.08	126.95
6	k	201	CYC	CMA-C3A-C4A	2.45	128.84	125.06
6	V	201	CYC	CHB-C4A-NA	-2.45	119.81	124.93
6	G	201	CYC	CHB-C4A-NA	-2.45	119.82	124.93
6	E	200	CYC	C1A-NA-C4A	2.43	111.09	106.51
6	C	200	CYC	C1A-NA-C4A	2.42	111.08	106.51
6	N	200	CYC	C1A-NA-C4A	2.42	111.07	106.51
6	Y	200	CYC	C1A-NA-C4A	2.41	111.06	106.51
6	e	200	CYC	CMC-C2C-C1C	-2.41	107.21	112.40
6	O	200	CYC	CHB-C4A-C3A	2.41	131.09	124.90
6	h	200	CYC	C2C-C3C-C4C	2.40	104.94	101.34
6	P	200	CYC	CMD-C2D-C3D	-2.40	120.42	124.94
6	K	200	CYC	CMC-C2C-C1C	-2.39	107.24	112.40
6	e	200	CYC	C1A-NA-C4A	2.39	111.02	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	200	CYC	CMC-C2C-C1C	-2.39	107.25	112.40
6	j	201	CYC	CMC-C2C-C1C	-2.39	107.25	112.40
6	l	201	CYC	CMB-C2B-C1B	2.39	127.15	124.17
6	V	201	CYC	CMB-C2B-C1B	2.38	127.14	124.17
6	B	201	CYC	C3B-C4B-NB	2.38	108.70	106.78
6	h	201	CYC	CMB-C2B-C1B	2.38	127.14	124.17
6	T	201	CYC	CHB-C4A-NA	-2.38	119.96	124.93
6	F	200	CYC	C1A-NA-C4A	2.37	110.98	106.51
6	P	200	CYC	CHB-C4A-C3A	2.37	131.00	124.90
6	D	200	CYC	CHB-C4A-C3A	2.37	131.00	124.90
6	d	200	CYC	C1A-NA-C4A	2.37	110.97	106.51
6	Y	201	CYC	CHB-C4A-NA	-2.37	119.98	124.93
6	i	201	CYC	CHB-C4A-NA	-2.37	119.98	124.93
6	g	200	CYC	CMB-C2B-C1B	2.36	127.11	124.17
6	U	201	CYC	OB-C4B-C3B	-2.36	125.48	128.04
6	c	200	CYC	CMC-C2C-C1C	-2.36	107.32	112.40
6	P	200	CYC	C1A-NA-C4A	2.36	110.96	106.51
6	Q	200	CYC	CHB-C4A-C3A	2.36	130.97	124.90
6	L	201	CYC	OB-C4B-C3B	-2.36	125.48	128.04
6	Q	200	CYC	CAC-C3C-C2C	-2.35	108.38	114.26
6	K	200	CYC	C1B-CHB-C4A	-2.35	122.33	128.08
6	V	200	CYC	CHB-C4A-C3A	2.35	130.95	124.90
6	B	200	CYC	CMC-C2C-C1C	-2.35	107.34	112.40
6	A	200	CYC	C1A-NA-C4A	2.35	110.93	106.51
6	g	200	CYC	C1A-NA-C4A	2.34	110.93	106.51
6	O	200	CYC	C2C-C1C-NC	-2.34	106.25	108.27
6	O	200	CYC	CMC-C2C-C1C	-2.33	107.38	112.40
6	G	200	CYC	C1A-NA-C4A	2.33	110.89	106.51
6	k	200	CYC	CMC-C2C-C1C	-2.32	107.40	112.40
6	Q	200	CYC	C3B-C4B-NB	2.32	108.65	106.78
6	i	201	CYC	C1B-CHB-C4A	-2.32	122.42	128.08
6	4	301	CYC	CAC-C3C-C2C	-2.31	108.48	114.26
6	X	200	CYC	CMC-C2C-C1C	-2.31	107.43	112.40
6	4	301	CYC	CMB-C2B-C1B	2.30	127.04	124.17
6	S	200	CYC	CHB-C4A-C3A	2.30	130.82	124.90
6	3	601	CYC	CMC-C2C-C1C	-2.30	107.44	112.40
6	l	200	CYC	CMC-C2C-C1C	-2.29	107.47	112.40
6	D	200	CYC	CMD-C2D-C3D	-2.29	120.63	124.94
6	I	200	CYC	OB-C4B-C3B	-2.29	125.56	128.04
6	Y	200	CYC	CAA-CBA-CGA	-2.29	108.69	113.60
6	3	601	CYC	C1A-NA-C4A	2.28	110.80	106.51
6	a	200	CYC	CBD-CAD-C3D	2.28	116.51	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	200	CYC	C1B-CHB-C4A	-2.28	122.52	128.08
6	E	200	CYC	CHB-C4A-C3A	2.27	130.73	124.90
6	D	200	CYC	C1A-NA-C4A	2.26	110.78	106.51
6	Y	201	CYC	CHB-C1B-C2B	-2.26	122.46	126.95
6	P	200	CYC	CBD-CAD-C3D	-2.26	108.76	112.62
6	k	200	CYC	CHB-C1B-C2B	-2.26	122.47	126.95
6	f	200	CYC	C1A-NA-C4A	2.26	110.76	106.51
6	A	201	CYC	CHB-C1B-C2B	-2.25	122.48	126.95
6	Z	200	CYC	CMD-C2D-C3D	-2.25	120.70	124.94
6	X	201	CYC	CMC-C2C-C1C	-2.25	107.55	112.40
6	k	201	CYC	C3B-C4B-NB	2.25	108.59	106.78
6	l	200	CYC	C1A-NA-C4A	2.25	110.74	106.51
6	3	601	CYC	O2A-CGA-CBA	2.24	121.22	114.03
6	S	200	CYC	CMD-C2D-C3D	-2.23	120.73	124.94
6	a	200	CYC	CAC-C3C-C2C	-2.23	108.68	114.26
6	f	200	CYC	CMC-C2C-C1C	-2.22	107.61	112.40
6	a	200	CYC	C1A-NA-C4A	2.22	110.69	106.51
6	B	200	CYC	C2C-C1C-NC	-2.22	106.36	108.27
6	B	201	CYC	C1A-NA-C4A	2.20	110.66	106.51
6	h	201	CYC	C1A-NA-C4A	2.20	110.66	106.51
6	W	200	CYC	C1B-CHB-C4A	-2.19	122.73	128.08
6	j	200	CYC	CAD-CBD-CGD	-2.19	107.62	113.76
6	j	200	CYC	CHB-C4A-NA	-2.19	120.36	124.93
6	h	201	CYC	C3B-C4B-NB	2.19	108.54	106.78
6	3	601	CYC	CHB-C1B-C2B	-2.18	122.62	126.95
6	R	200	CYC	CMD-C2D-C3D	-2.18	120.83	124.94
6	X	201	CYC	C1B-CHB-C4A	-2.18	122.76	128.08
6	W	201	CYC	CMB-C2B-C1B	2.18	126.89	124.17
6	L	201	CYC	CHB-C1B-C2B	-2.18	122.63	126.95
6	B	200	CYC	CAC-C3C-C4C	-2.17	107.09	112.67
6	k	200	CYC	CHB-C4A-NA	-2.17	120.40	124.93
6	h	200	CYC	CHB-C4A-C3A	2.16	130.45	124.90
6	j	201	CYC	OB-C4B-C3B	-2.16	125.70	128.04
6	j	201	CYC	CMB-C2B-C1B	2.16	126.86	124.17
6	d	200	CYC	CBD-CAD-C3D	-2.15	108.94	112.62
6	F	200	CYC	CMC-C2C-C1C	-2.15	107.78	112.40
6	b	200	CYC	CMD-C2D-C3D	-2.14	120.90	124.94
6	I	201	CYC	CHB-C4A-C3A	2.14	130.41	124.90
6	W	200	CYC	CMC-C2C-C1C	-2.14	107.79	112.40
6	X	201	CYC	C2C-C1C-NC	-2.14	106.43	108.27
6	C	200	CYC	CHB-C4A-C3A	2.14	130.40	124.90
6	k	200	CYC	CAA-C2A-C3A	-2.14	123.90	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	200	CYC	CHB-C4A-C3A	2.13	130.39	124.90
6	U	201	CYC	C1A-NA-C4A	2.13	110.53	106.51
6	W	201	CYC	OB-C4B-C3B	-2.13	125.73	128.04
6	j	201	CYC	C1B-CHB-C4A	-2.13	122.88	128.08
6	4	301	CYC	CMA-C3A-C4A	2.13	128.34	125.06
6	X	201	CYC	CMB-C2B-C1B	2.13	126.82	124.17
6	G	201	CYC	CMB-C2B-C1B	2.12	126.82	124.17
6	V	200	CYC	OB-C4B-C3B	-2.12	125.73	128.04
6	W	200	CYC	O2D-CGD-CBD	2.12	120.85	114.03
6	k	200	CYC	C1B-CHB-C4A	-2.12	122.90	128.08
6	Z	200	CYC	CMB-C2B-C1B	2.12	126.81	124.17
6	g	201	CYC	CAC-C3C-C2C	-2.12	108.97	114.26
6	J	200	CYC	O2D-CGD-CBD	2.11	120.81	114.03
6	Y	200	CYC	O2A-CGA-CBA	2.11	120.81	114.03
6	Y	200	CYC	OB-C4B-C3B	-2.11	125.75	128.04
6	g	200	CYC	OB-C4B-C3B	-2.09	125.77	128.04
6	i	201	CYC	CMB-C2B-C1B	2.09	126.78	124.17
6	Z	200	CYC	C1A-NA-C4A	2.09	110.44	106.51
6	T	200	CYC	CMB-C2B-C1B	2.09	126.77	124.17
6	c	200	CYC	CMB-C2B-C1B	2.09	126.77	124.17
6	g	200	CYC	CMA-C3A-C4A	2.08	128.27	125.06
6	T	201	CYC	CHA-C1A-NA	-2.08	125.94	128.83
6	N	200	CYC	CMA-C3A-C4A	2.08	128.26	125.06
6	Z	200	CYC	O2A-CGA-CBA	2.08	120.70	114.03
6	j	200	CYC	O2D-CGD-CBD	2.07	120.67	114.03
6	k	200	CYC	OB-C4B-C3B	-2.07	125.80	128.04
6	D	200	CYC	C3B-C4B-NB	2.06	108.44	106.78
6	U	201	CYC	CAC-C3C-C2C	-2.06	109.11	114.26
6	T	200	CYC	CAC-C3C-C2C	-2.05	109.13	114.26
6	E	200	CYC	CMD-C2D-C3D	-2.05	121.08	124.94
6	c	200	CYC	C1A-NA-C4A	2.05	110.37	106.51
6	T	201	CYC	OB-C4B-C3B	-2.05	125.82	128.04
6	Q	200	CYC	CHA-C1A-NA	-2.04	125.99	128.83
6	g	201	CYC	CMB-C2B-C1B	2.04	126.72	124.17
6	j	201	CYC	CHB-C4A-NA	-2.04	120.67	124.93
6	D	200	CYC	CHB-C1B-C2B	-2.04	122.91	126.95
6	R	200	CYC	CHB-C4A-C3A	2.04	130.14	124.90
6	d	200	CYC	CMB-C2B-C1B	2.04	126.71	124.17
6	Z	200	CYC	CMA-C3A-C4A	2.03	128.19	125.06
6	Y	201	CYC	CHA-C1A-NA	-2.03	126.02	128.83
6	K	201	CYC	C3A-C4A-NA	-2.02	106.21	110.53
6	H	200	CYC	CAC-C3C-C2C	-2.02	109.21	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	4	301	CYC	O2A-CGA-CBA	2.02	120.51	114.03
6	j	200	CYC	CMC-C2C-C1C	-2.01	108.07	112.40
6	X	200	CYC	CHB-C1B-C2B	-2.01	122.96	126.95
6	a	200	CYC	CMA-C3A-C4A	2.01	128.16	125.06
6	C	200	CYC	O2A-CGA-CBA	2.01	120.48	114.03
6	l	200	CYC	O2D-CGD-CBD	2.01	120.48	114.03
6	J	200	CYC	O2A-CGA-CBA	2.00	120.47	114.03
6	A	201	CYC	CMC-C2C-C1C	-2.00	108.09	112.40

There are no chirality outliers.

All (694) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	3	601	CYC	NA-C4A-CHB-C1B
6	3	601	CYC	C3A-C4A-CHB-C1B
6	3	601	CYC	NC-C4C-CHD-C1D
6	3	601	CYC	ND-C1D-CHD-C4C
6	3	601	CYC	C2D-C1D-CHD-C4C
6	A	200	CYC	NA-C1A-CHA-C4D
6	A	200	CYC	C2A-C1A-CHA-C4D
6	A	200	CYC	ND-C4D-CHA-C1A
6	A	200	CYC	C3D-C4D-CHA-C1A
6	A	200	CYC	NA-C4A-CHB-C1B
6	A	200	CYC	C3A-C4A-CHB-C1B
6	A	200	CYC	NC-C4C-CHD-C1D
6	A	200	CYC	ND-C1D-CHD-C4C
6	A	200	CYC	C2D-C1D-CHD-C4C
6	A	201	CYC	NA-C4A-CHB-C1B
6	A	201	CYC	C3A-C4A-CHB-C1B
6	A	201	CYC	C2C-C3C-CAC-CBC
6	A	201	CYC	C4C-C3C-CAC-CBC
6	A	201	CYC	NC-C4C-CHD-C1D
6	A	201	CYC	ND-C1D-CHD-C4C
6	A	201	CYC	C2D-C1D-CHD-C4C
6	B	200	CYC	NA-C1A-CHA-C4D
6	B	200	CYC	C2A-C1A-CHA-C4D
6	B	200	CYC	ND-C4D-CHA-C1A
6	B	200	CYC	C3D-C4D-CHA-C1A
6	B	200	CYC	NA-C4A-CHB-C1B
6	B	200	CYC	C3A-C4A-CHB-C1B
6	B	200	CYC	C4B-C3B-CAB-CBB
6	B	200	CYC	NC-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
6	B	200	CYC	ND-C1D-CHD-C4C
6	B	200	CYC	C2D-C1D-CHD-C4C
6	B	201	CYC	NA-C4A-CHB-C1B
6	B	201	CYC	C3A-C4A-CHB-C1B
6	B	201	CYC	C2C-C3C-CAC-CBC
6	B	201	CYC	C4C-C3C-CAC-CBC
6	B	201	CYC	NC-C4C-CHD-C1D
6	B	201	CYC	ND-C1D-CHD-C4C
6	B	201	CYC	C2D-C1D-CHD-C4C
6	B	201	CYC	C3D-CAD-CBD-CGD
6	C	200	CYC	NA-C1A-CHA-C4D
6	C	200	CYC	ND-C4D-CHA-C1A
6	C	200	CYC	C3D-C4D-CHA-C1A
6	C	200	CYC	NA-C4A-CHB-C1B
6	C	200	CYC	C3A-C4A-CHB-C1B
6	C	200	CYC	C4B-C3B-CAB-CBB
6	C	200	CYC	NC-C4C-CHD-C1D
6	C	200	CYC	ND-C1D-CHD-C4C
6	C	200	CYC	C2D-C1D-CHD-C4C
6	D	200	CYC	NA-C1A-CHA-C4D
6	D	200	CYC	C2A-C1A-CHA-C4D
6	D	200	CYC	ND-C4D-CHA-C1A
6	D	200	CYC	C3D-C4D-CHA-C1A
6	D	200	CYC	NA-C4A-CHB-C1B
6	D	200	CYC	C3A-C4A-CHB-C1B
6	D	200	CYC	C4B-C3B-CAB-CBB
6	D	200	CYC	NC-C4C-CHD-C1D
6	D	200	CYC	ND-C1D-CHD-C4C
6	D	200	CYC	C2D-C1D-CHD-C4C
6	E	200	CYC	NA-C1A-CHA-C4D
6	E	200	CYC	C2A-C1A-CHA-C4D
6	E	200	CYC	ND-C4D-CHA-C1A
6	E	200	CYC	C3D-C4D-CHA-C1A
6	E	200	CYC	NA-C4A-CHB-C1B
6	E	200	CYC	C3A-C4A-CHB-C1B
6	E	200	CYC	C4B-C3B-CAB-CBB
6	E	200	CYC	NC-C4C-CHD-C1D
6	E	200	CYC	ND-C1D-CHD-C4C
6	E	200	CYC	C2D-C1D-CHD-C4C
6	F	200	CYC	NA-C1A-CHA-C4D
6	F	200	CYC	ND-C4D-CHA-C1A
6	F	200	CYC	C3D-C4D-CHA-C1A

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Mol	Chain	Res	Type	Atoms
6	F	200	CYC	NA-C4A-CHB-C1B
6	F	200	CYC	C3A-C4A-CHB-C1B
6	F	200	CYC	C2B-C3B-CAB-CBB
6	F	200	CYC	NC-C4C-CHD-C1D
6	F	200	CYC	ND-C1D-CHD-C4C
6	F	200	CYC	C2D-C1D-CHD-C4C
6	G	200	CYC	NA-C4A-CHB-C1B
6	G	200	CYC	C3A-C4A-CHB-C1B
6	G	200	CYC	NC-C4C-CHD-C1D
6	G	200	CYC	ND-C1D-CHD-C4C
6	G	200	CYC	C2D-C1D-CHD-C4C
6	G	201	CYC	NA-C1A-CHA-C4D
6	G	201	CYC	C2A-C1A-CHA-C4D
6	G	201	CYC	ND-C4D-CHA-C1A
6	G	201	CYC	C3D-C4D-CHA-C1A
6	G	201	CYC	C2C-C3C-CAC-CBC
6	G	201	CYC	C4C-C3C-CAC-CBC
6	G	201	CYC	NC-C4C-CHD-C1D
6	G	201	CYC	ND-C1D-CHD-C4C
6	G	201	CYC	C2D-C1D-CHD-C4C
6	G	201	CYC	C3D-CAD-CBD-CGD
6	H	200	CYC	NA-C4A-CHB-C1B
6	H	200	CYC	C2C-C3C-CAC-CBC
6	H	200	CYC	C4C-C3C-CAC-CBC
6	H	200	CYC	NC-C4C-CHD-C1D
6	H	200	CYC	ND-C1D-CHD-C4C
6	H	200	CYC	C2D-C1D-CHD-C4C
6	I	200	CYC	NA-C4A-CHB-C1B
6	I	200	CYC	C3A-C4A-CHB-C1B
6	I	200	CYC	NC-C4C-CHD-C1D
6	I	200	CYC	ND-C1D-CHD-C4C
6	I	200	CYC	C2D-C1D-CHD-C4C
6	I	201	CYC	NA-C4A-CHB-C1B
6	I	201	CYC	C3A-C4A-CHB-C1B
6	I	201	CYC	C4C-C3C-CAC-CBC
6	I	201	CYC	NC-C4C-CHD-C1D
6	I	201	CYC	ND-C1D-CHD-C4C
6	I	201	CYC	C2D-C1D-CHD-C4C
6	J	200	CYC	NC-C4C-CHD-C1D
6	J	200	CYC	ND-C1D-CHD-C4C
6	J	200	CYC	C2D-C1D-CHD-C4C
6	K	200	CYC	NC-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
6	K	200	CYC	ND-C1D-CHD-C4C
6	K	200	CYC	C2D-C1D-CHD-C4C
6	K	201	CYC	NA-C1A-CHA-C4D
6	K	201	CYC	ND-C4D-CHA-C1A
6	K	201	CYC	C3D-C4D-CHA-C1A
6	K	201	CYC	C3A-C4A-CHB-C1B
6	K	201	CYC	C4C-C3C-CAC-CBC
6	K	201	CYC	NC-C4C-CHD-C1D
6	K	201	CYC	ND-C1D-CHD-C4C
6	K	201	CYC	C2D-C1D-CHD-C4C
6	L	201	CYC	NA-C1A-CHA-C4D
6	L	201	CYC	ND-C4D-CHA-C1A
6	L	201	CYC	C3D-C4D-CHA-C1A
6	L	201	CYC	NA-C4A-CHB-C1B
6	L	201	CYC	C3A-C4A-CHB-C1B
6	L	201	CYC	C2C-C3C-CAC-CBC
6	L	201	CYC	C4C-C3C-CAC-CBC
6	L	201	CYC	NC-C4C-CHD-C1D
6	L	201	CYC	ND-C1D-CHD-C4C
6	L	201	CYC	C2D-C1D-CHD-C4C
6	N	200	CYC	NA-C1A-CHA-C4D
6	N	200	CYC	C2A-C1A-CHA-C4D
6	N	200	CYC	ND-C4D-CHA-C1A
6	N	200	CYC	C3D-C4D-CHA-C1A
6	N	200	CYC	NA-C4A-CHB-C1B
6	N	200	CYC	C3A-C4A-CHB-C1B
6	N	200	CYC	C4B-C3B-CAB-CBB
6	N	200	CYC	NC-C4C-CHD-C1D
6	N	200	CYC	ND-C1D-CHD-C4C
6	N	200	CYC	C2D-C1D-CHD-C4C
6	O	200	CYC	NA-C1A-CHA-C4D
6	O	200	CYC	C2A-C1A-CHA-C4D
6	O	200	CYC	ND-C4D-CHA-C1A
6	O	200	CYC	C3D-C4D-CHA-C1A
6	O	200	CYC	NA-C4A-CHB-C1B
6	O	200	CYC	C3A-C4A-CHB-C1B
6	O	200	CYC	C4B-C3B-CAB-CBB
6	O	200	CYC	NC-C4C-CHD-C1D
6	O	200	CYC	ND-C1D-CHD-C4C
6	O	200	CYC	C2D-C1D-CHD-C4C
6	P	200	CYC	NA-C1A-CHA-C4D
6	P	200	CYC	C2A-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
6	P	200	CYC	ND-C4D-CHA-C1A
6	P	200	CYC	C3D-C4D-CHA-C1A
6	P	200	CYC	NA-C4A-CHB-C1B
6	P	200	CYC	C3A-C4A-CHB-C1B
6	P	200	CYC	C4B-C3B-CAB-CBB
6	P	200	CYC	C4C-C3C-CAC-CBC
6	P	200	CYC	NC-C4C-CHD-C1D
6	P	200	CYC	ND-C1D-CHD-C4C
6	P	200	CYC	C2D-C1D-CHD-C4C
6	Q	200	CYC	NA-C1A-CHA-C4D
6	Q	200	CYC	C2A-C1A-CHA-C4D
6	Q	200	CYC	ND-C4D-CHA-C1A
6	Q	200	CYC	C3D-C4D-CHA-C1A
6	Q	200	CYC	NA-C4A-CHB-C1B
6	Q	200	CYC	C3A-C4A-CHB-C1B
6	Q	200	CYC	NC-C4C-CHD-C1D
6	Q	200	CYC	ND-C1D-CHD-C4C
6	Q	200	CYC	C2D-C1D-CHD-C4C
6	R	200	CYC	NA-C1A-CHA-C4D
6	R	200	CYC	C2A-C1A-CHA-C4D
6	R	200	CYC	ND-C4D-CHA-C1A
6	R	200	CYC	C3D-C4D-CHA-C1A
6	R	200	CYC	NA-C4A-CHB-C1B
6	R	200	CYC	C3A-C4A-CHB-C1B
6	R	200	CYC	NC-C4C-CHD-C1D
6	R	200	CYC	ND-C1D-CHD-C4C
6	R	200	CYC	C2D-C1D-CHD-C4C
6	S	200	CYC	NA-C1A-CHA-C4D
6	S	200	CYC	ND-C4D-CHA-C1A
6	S	200	CYC	C3D-C4D-CHA-C1A
6	S	200	CYC	NA-C4A-CHB-C1B
6	S	200	CYC	C3A-C4A-CHB-C1B
6	S	200	CYC	C4B-C3B-CAB-CBB
6	S	200	CYC	NC-C4C-CHD-C1D
6	S	200	CYC	ND-C1D-CHD-C4C
6	S	200	CYC	C2D-C1D-CHD-C4C
6	T	200	CYC	NA-C4A-CHB-C1B
6	T	200	CYC	C3A-C4A-CHB-C1B
6	T	200	CYC	NC-C4C-CHD-C1D
6	T	200	CYC	ND-C1D-CHD-C4C
6	T	200	CYC	C2D-C1D-CHD-C4C
6	T	201	CYC	NA-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
6	T	201	CYC	C2A-C1A-CHA-C4D
6	T	201	CYC	ND-C4D-CHA-C1A
6	T	201	CYC	C3D-C4D-CHA-C1A
6	T	201	CYC	C2C-C3C-CAC-CBC
6	T	201	CYC	C4C-C3C-CAC-CBC
6	T	201	CYC	NC-C4C-CHD-C1D
6	U	201	CYC	ND-C4D-CHA-C1A
6	U	201	CYC	C3D-C4D-CHA-C1A
6	U	201	CYC	NA-C4A-CHB-C1B
6	U	201	CYC	C3A-C4A-CHB-C1B
6	U	201	CYC	NC-C4C-CHD-C1D
6	V	200	CYC	NA-C4A-CHB-C1B
6	V	200	CYC	C2C-C3C-CAC-CBC
6	V	200	CYC	C4C-C3C-CAC-CBC
6	V	200	CYC	NC-C4C-CHD-C1D
6	V	200	CYC	ND-C1D-CHD-C4C
6	V	200	CYC	C2D-C1D-CHD-C4C
6	V	201	CYC	ND-C4D-CHA-C1A
6	V	201	CYC	C3D-C4D-CHA-C1A
6	V	201	CYC	C4C-C3C-CAC-CBC
6	V	201	CYC	NC-C4C-CHD-C1D
6	V	201	CYC	ND-C1D-CHD-C4C
6	V	201	CYC	C2D-C1D-CHD-C4C
6	W	200	CYC	NC-C4C-CHD-C1D
6	W	200	CYC	ND-C1D-CHD-C4C
6	W	200	CYC	C2D-C1D-CHD-C4C
6	W	201	CYC	ND-C4D-CHA-C1A
6	W	201	CYC	C3D-C4D-CHA-C1A
6	W	201	CYC	NA-C4A-CHB-C1B
6	W	201	CYC	C3A-C4A-CHB-C1B
6	W	201	CYC	C2A-CAA-CBA-CGA
6	W	201	CYC	C2B-C1B-CHB-C4A
6	W	201	CYC	C2C-C3C-CAC-CBC
6	W	201	CYC	C4C-C3C-CAC-CBC
6	W	201	CYC	NC-C4C-CHD-C1D
6	W	201	CYC	ND-C1D-CHD-C4C
6	W	201	CYC	C2D-C1D-CHD-C4C
6	X	200	CYC	C2C-C3C-CAC-CBC
6	X	200	CYC	NC-C4C-CHD-C1D
6	X	200	CYC	C3D-CAD-CBD-CGD
6	X	201	CYC	NA-C1A-CHA-C4D
6	X	201	CYC	ND-C4D-CHA-C1A

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Mol	Chain	Res	Type	Atoms
6	X	201	CYC	C3D-C4D-CHA-C1A
6	X	201	CYC	NC-C4C-CHD-C1D
6	X	201	CYC	ND-C1D-CHD-C4C
6	X	201	CYC	C2D-C1D-CHD-C4C
6	Y	200	CYC	NA-C4A-CHB-C1B
6	Y	200	CYC	C3A-C4A-CHB-C1B
6	Y	200	CYC	NC-C4C-CHD-C1D
6	Y	200	CYC	C2D-C1D-CHD-C4C
6	Y	201	CYC	NA-C1A-CHA-C4D
6	Y	201	CYC	C2A-C1A-CHA-C4D
6	Y	201	CYC	ND-C4D-CHA-C1A
6	Y	201	CYC	C3D-C4D-CHA-C1A
6	Y	201	CYC	NC-C4C-CHD-C1D
6	Y	201	CYC	ND-C1D-CHD-C4C
6	Y	201	CYC	C2D-C1D-CHD-C4C
6	Z	200	CYC	NA-C4A-CHB-C1B
6	Z	200	CYC	C3A-C4A-CHB-C1B
6	Z	200	CYC	NB-C1B-CHB-C4A
6	Z	200	CYC	C2B-C1B-CHB-C4A
6	Z	200	CYC	C2C-C3C-CAC-CBC
6	Z	200	CYC	C4C-C3C-CAC-CBC
6	Z	200	CYC	NC-C4C-CHD-C1D
6	Z	200	CYC	ND-C1D-CHD-C4C
6	Z	200	CYC	C2D-C1D-CHD-C4C
6	4	301	CYC	NA-C1A-CHA-C4D
6	4	301	CYC	NA-C4A-CHB-C1B
6	4	301	CYC	C3A-C4A-CHB-C1B
6	4	301	CYC	C4C-C3C-CAC-CBC
6	4	301	CYC	NC-C4C-CHD-C1D
6	4	301	CYC	ND-C1D-CHD-C4C
6	4	301	CYC	C2D-C1D-CHD-C4C
6	a	200	CYC	NA-C4A-CHB-C1B
6	a	200	CYC	C3A-C4A-CHB-C1B
6	a	200	CYC	C2C-C3C-CAC-CBC
6	a	200	CYC	C4C-C3C-CAC-CBC
6	a	200	CYC	NC-C4C-CHD-C1D
6	a	200	CYC	ND-C1D-CHD-C4C
6	a	200	CYC	C2D-C1D-CHD-C4C
6	b	200	CYC	NA-C1A-CHA-C4D
6	b	200	CYC	ND-C4D-CHA-C1A
6	b	200	CYC	C3D-C4D-CHA-C1A
6	b	200	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
6	b	200	CYC	C3A-C4A-CHB-C1B
6	b	200	CYC	C4B-C3B-CAB-CBB
6	b	200	CYC	NC-C4C-CHD-C1D
6	b	200	CYC	ND-C1D-CHD-C4C
6	b	200	CYC	C2D-C1D-CHD-C4C
6	c	200	CYC	NA-C1A-CHA-C4D
6	c	200	CYC	C2A-C1A-CHA-C4D
6	c	200	CYC	ND-C4D-CHA-C1A
6	c	200	CYC	C3D-C4D-CHA-C1A
6	c	200	CYC	NA-C4A-CHB-C1B
6	c	200	CYC	C3A-C4A-CHB-C1B
6	c	200	CYC	C4C-C3C-CAC-CBC
6	c	200	CYC	NC-C4C-CHD-C1D
6	c	200	CYC	ND-C1D-CHD-C4C
6	c	200	CYC	C2D-C1D-CHD-C4C
6	d	200	CYC	NA-C1A-CHA-C4D
6	d	200	CYC	ND-C4D-CHA-C1A
6	d	200	CYC	C3D-C4D-CHA-C1A
6	d	200	CYC	NA-C4A-CHB-C1B
6	d	200	CYC	C3A-C4A-CHB-C1B
6	d	200	CYC	C4B-C3B-CAB-CBB
6	d	200	CYC	NC-C4C-CHD-C1D
6	d	200	CYC	ND-C1D-CHD-C4C
6	d	200	CYC	C2D-C1D-CHD-C4C
6	e	200	CYC	NA-C1A-CHA-C4D
6	e	200	CYC	ND-C4D-CHA-C1A
6	e	200	CYC	C3D-C4D-CHA-C1A
6	e	200	CYC	NA-C4A-CHB-C1B
6	e	200	CYC	C3A-C4A-CHB-C1B
6	e	200	CYC	C4B-C3B-CAB-CBB
6	e	200	CYC	NC-C4C-CHD-C1D
6	e	200	CYC	C2D-C1D-CHD-C4C
6	f	200	CYC	NA-C1A-CHA-C4D
6	f	200	CYC	C2A-C1A-CHA-C4D
6	f	200	CYC	ND-C4D-CHA-C1A
6	f	200	CYC	C3D-C4D-CHA-C1A
6	f	200	CYC	NA-C4A-CHB-C1B
6	f	200	CYC	C3A-C4A-CHB-C1B
6	f	200	CYC	C2B-C3B-CAB-CBB
6	f	200	CYC	NC-C4C-CHD-C1D
6	f	200	CYC	ND-C1D-CHD-C4C
6	f	200	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
6	g	200	CYC	ND-C4D-CHA-C1A
6	g	200	CYC	C3D-C4D-CHA-C1A
6	g	200	CYC	NA-C4A-CHB-C1B
6	g	200	CYC	C3A-C4A-CHB-C1B
6	g	200	CYC	NC-C4C-CHD-C1D
6	g	200	CYC	ND-C1D-CHD-C4C
6	g	200	CYC	C2D-C1D-CHD-C4C
6	g	201	CYC	NA-C1A-CHA-C4D
6	g	201	CYC	ND-C4D-CHA-C1A
6	g	201	CYC	C3D-C4D-CHA-C1A
6	g	201	CYC	NA-C4A-CHB-C1B
6	g	201	CYC	C3A-C4A-CHB-C1B
6	g	201	CYC	NC-C4C-CHD-C1D
6	g	201	CYC	ND-C1D-CHD-C4C
6	g	201	CYC	C2D-C1D-CHD-C4C
6	h	200	CYC	NA-C4A-CHB-C1B
6	h	200	CYC	NB-C1B-CHB-C4A
6	h	200	CYC	C2B-C1B-CHB-C4A
6	h	200	CYC	C2B-C3B-CAB-CBB
6	h	200	CYC	C4B-C3B-CAB-CBB
6	h	200	CYC	C2C-C3C-CAC-CBC
6	h	200	CYC	C4C-C3C-CAC-CBC
6	h	200	CYC	NC-C4C-CHD-C1D
6	h	200	CYC	ND-C1D-CHD-C4C
6	h	200	CYC	C2D-C1D-CHD-C4C
6	h	201	CYC	NA-C1A-CHA-C4D
6	h	201	CYC	ND-C4D-CHA-C1A
6	h	201	CYC	C3D-C4D-CHA-C1A
6	h	201	CYC	NA-C4A-CHB-C1B
6	h	201	CYC	C3A-C4A-CHB-C1B
6	h	201	CYC	C2C-C3C-CAC-CBC
6	h	201	CYC	NC-C4C-CHD-C1D
6	h	201	CYC	ND-C1D-CHD-C4C
6	h	201	CYC	C2D-C1D-CHD-C4C
6	i	201	CYC	ND-C4D-CHA-C1A
6	i	201	CYC	C3D-C4D-CHA-C1A
6	i	201	CYC	NA-C4A-CHB-C1B
6	i	201	CYC	C3A-C4A-CHB-C1B
6	i	201	CYC	NC-C4C-CHD-C1D
6	i	201	CYC	ND-C1D-CHD-C4C
6	i	201	CYC	C2D-C1D-CHD-C4C
6	i	201	CYC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
6	j	200	CYC	C2C-C3C-CAC-CBC
6	j	200	CYC	C4C-C3C-CAC-CBC
6	j	200	CYC	NC-C4C-CHD-C1D
6	j	200	CYC	ND-C1D-CHD-C4C
6	j	200	CYC	C2D-C1D-CHD-C4C
6	j	201	CYC	ND-C4D-CHA-C1A
6	j	201	CYC	C3D-C4D-CHA-C1A
6	j	201	CYC	C3A-C4A-CHB-C1B
6	j	201	CYC	C2C-C3C-CAC-CBC
6	j	201	CYC	C4C-C3C-CAC-CBC
6	j	201	CYC	NC-C4C-CHD-C1D
6	j	201	CYC	ND-C1D-CHD-C4C
6	j	201	CYC	C2D-C1D-CHD-C4C
6	k	200	CYC	NC-C4C-CHD-C1D
6	k	200	CYC	ND-C1D-CHD-C4C
6	k	200	CYC	C2D-C1D-CHD-C4C
6	k	201	CYC	NA-C4A-CHB-C1B
6	k	201	CYC	C3A-C4A-CHB-C1B
6	k	201	CYC	C2C-C3C-CAC-CBC
6	k	201	CYC	C4C-C3C-CAC-CBC
6	k	201	CYC	NC-C4C-CHD-C1D
6	k	201	CYC	ND-C1D-CHD-C4C
6	k	201	CYC	C2D-C1D-CHD-C4C
6	l	200	CYC	NA-C4A-CHB-C1B
6	l	200	CYC	C3A-C4A-CHB-C1B
6	l	200	CYC	NC-C4C-CHD-C1D
6	l	201	CYC	ND-C4D-CHA-C1A
6	l	201	CYC	C3D-C4D-CHA-C1A
6	l	201	CYC	C4C-C3C-CAC-CBC
6	l	201	CYC	NC-C4C-CHD-C1D
6	l	201	CYC	ND-C1D-CHD-C4C
6	l	201	CYC	C2D-C1D-CHD-C4C
6	d	200	CYC	C2B-C3B-CAB-CBB
6	B	200	CYC	C2B-C3B-CAB-CBB
6	D	200	CYC	C2B-C3B-CAB-CBB
6	N	200	CYC	C2B-C3B-CAB-CBB
6	P	200	CYC	C2B-C3B-CAB-CBB
6	S	200	CYC	C2B-C3B-CAB-CBB
6	b	200	CYC	C2B-C3B-CAB-CBB
6	E	200	CYC	C2B-C3B-CAB-CBB
6	C	200	CYC	C2B-C3B-CAB-CBB
6	O	200	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
6	e	200	CYC	C2B-C3B-CAB-CBB
6	Q	200	CYC	C2B-C3B-CAB-CBB
6	l	201	CYC	C2B-C1B-CHB-C4A
6	G	201	CYC	C2B-C3B-CAB-CBB
6	l	201	CYC	C2B-C3B-CAB-CBB
6	W	200	CYC	C2B-C3B-CAB-CBB
6	i	201	CYC	C2B-C3B-CAB-CBB
6	J	200	CYC	C2B-C3B-CAB-CBB
6	B	201	CYC	C2A-CAA-CBA-CGA
6	Y	201	CYC	C2A-CAA-CBA-CGA
6	e	200	CYC	C2A-CAA-CBA-CGA
6	H	200	CYC	C3A-C4A-CHB-C1B
6	h	200	CYC	C3A-C4A-CHB-C1B
6	R	200	CYC	C2B-C3B-CAB-CBB
6	k	200	CYC	C1A-C2A-CAA-CBA
6	A	200	CYC	C2B-C3B-CAB-CBB
6	T	201	CYC	NB-C1B-CHB-C4A
6	W	201	CYC	NB-C1B-CHB-C4A
6	l	201	CYC	NB-C1B-CHB-C4A
6	G	200	CYC	C2B-C3B-CAB-CBB
6	Y	201	CYC	C2B-C3B-CAB-CBB
6	K	201	CYC	C2B-C3B-CAB-CBB
6	C	200	CYC	C3D-CAD-CBD-CGD
6	L	201	CYC	C3D-CAD-CBD-CGD
6	X	201	CYC	C3D-CAD-CBD-CGD
6	Y	201	CYC	C3D-CAD-CBD-CGD
6	c	200	CYC	C3D-CAD-CBD-CGD
6	A	201	CYC	NA-C1A-CHA-C4D
6	V	201	CYC	NA-C1A-CHA-C4D
6	i	201	CYC	NA-C1A-CHA-C4D
6	l	200	CYC	NA-C1A-CHA-C4D
6	l	201	CYC	NA-C1A-CHA-C4D
6	F	200	CYC	C4B-C3B-CAB-CBB
6	Q	200	CYC	C4B-C3B-CAB-CBB
6	f	200	CYC	C4B-C3B-CAB-CBB
6	l	200	CYC	C2B-C3B-CAB-CBB
6	H	200	CYC	NB-C1B-CHB-C4A
6	K	200	CYC	NB-C1B-CHB-C4A
6	g	200	CYC	NB-C1B-CHB-C4A
6	j	201	CYC	NB-C1B-CHB-C4A
6	T	201	CYC	C2B-C1B-CHB-C4A
6	g	200	CYC	C2B-C1B-CHB-C4A

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Mol	Chain	Res	Type	Atoms
6	V	200	CYC	C2A-CAA-CBA-CGA
6	g	201	CYC	C2A-CAA-CBA-CGA
6	j	201	CYC	C2A-CAA-CBA-CGA
6	k	201	CYC	C2A-CAA-CBA-CGA
6	V	201	CYC	C3A-C4A-CHB-C1B
6	X	201	CYC	C3A-C4A-CHB-C1B
6	T	200	CYC	C2B-C3B-CAB-CBB
6	C	200	CYC	C2A-C1A-CHA-C4D
6	b	200	CYC	C2A-C1A-CHA-C4D
6	e	200	CYC	C2A-C1A-CHA-C4D
6	h	201	CYC	C2A-C1A-CHA-C4D
6	k	200	CYC	C3A-C2A-CAA-CBA
6	G	201	CYC	NA-C4A-CHB-C1B
6	G	201	CYC	C2A-CAA-CBA-CGA
6	J	200	CYC	NA-C4A-CHB-C1B
6	K	200	CYC	NA-C4A-CHB-C1B
6	K	201	CYC	NA-C4A-CHB-C1B
6	T	201	CYC	NA-C4A-CHB-C1B
6	U	201	CYC	C2A-CAA-CBA-CGA
6	V	201	CYC	NA-C4A-CHB-C1B
6	W	200	CYC	NA-C4A-CHB-C1B
6	X	200	CYC	NA-C4A-CHB-C1B
6	X	201	CYC	NA-C4A-CHB-C1B
6	Y	200	CYC	C2A-CAA-CBA-CGA
6	Y	201	CYC	NA-C4A-CHB-C1B
6	j	200	CYC	NA-C4A-CHB-C1B
6	j	201	CYC	NA-C4A-CHB-C1B
6	k	200	CYC	NA-C4A-CHB-C1B
6	l	201	CYC	NA-C4A-CHB-C1B
6	l	201	CYC	C2A-CAA-CBA-CGA
6	G	201	CYC	C3A-C4A-CHB-C1B
6	J	200	CYC	C3A-C4A-CHB-C1B
6	K	200	CYC	C3A-C4A-CHB-C1B
6	T	201	CYC	C3A-C4A-CHB-C1B
6	V	200	CYC	C3A-C4A-CHB-C1B
6	W	200	CYC	C3A-C4A-CHB-C1B
6	X	200	CYC	C3A-C4A-CHB-C1B
6	Y	201	CYC	C3A-C4A-CHB-C1B
6	j	200	CYC	C3A-C4A-CHB-C1B
6	k	200	CYC	C3A-C4A-CHB-C1B
6	l	201	CYC	C3A-C4A-CHB-C1B
6	j	201	CYC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
6	G	201	CYC	C4B-C3B-CAB-CBB
6	W	200	CYC	C4B-C3B-CAB-CBB
6	l	201	CYC	C4B-C3B-CAB-CBB
6	j	201	CYC	C2B-C1B-CHB-C4A
6	c	200	CYC	C2B-C3B-CAB-CBB
6	3	601	CYC	C2A-CAA-CBA-CGA
6	A	200	CYC	C2A-CAA-CBA-CGA
6	F	200	CYC	C2A-C1A-CHA-C4D
6	K	201	CYC	C2A-C1A-CHA-C4D
6	L	201	CYC	C2A-C1A-CHA-C4D
6	S	200	CYC	C2A-C1A-CHA-C4D
6	X	201	CYC	C2A-C1A-CHA-C4D
6	4	301	CYC	C2A-C1A-CHA-C4D
6	d	200	CYC	C2A-C1A-CHA-C4D
6	g	201	CYC	C2A-C1A-CHA-C4D
6	l	201	CYC	C2A-C1A-CHA-C4D
6	b	200	CYC	C2A-CAA-CBA-CGA
6	I	201	CYC	C2C-C3C-CAC-CBC
6	K	201	CYC	C2C-C3C-CAC-CBC
6	V	201	CYC	C2C-C3C-CAC-CBC
6	l	201	CYC	C2C-C3C-CAC-CBC
6	H	200	CYC	C2B-C1B-CHB-C4A
6	J	200	CYC	C4B-C3B-CAB-CBB
6	i	201	CYC	C4B-C3B-CAB-CBB
6	h	201	CYC	C2A-CAA-CBA-CGA
6	l	200	CYC	C2A-CAA-CBA-CGA
6	A	201	CYC	C2A-C1A-CHA-C4D
6	V	201	CYC	C2A-C1A-CHA-C4D
6	l	200	CYC	C2A-C1A-CHA-C4D
6	T	200	CYC	NB-C1B-CHB-C4A
6	G	200	CYC	C2A-CAA-CBA-CGA
6	K	200	CYC	C2A-CAA-CBA-CGA
6	g	200	CYC	C2A-CAA-CBA-CGA
6	h	200	CYC	C2A-CAA-CBA-CGA
6	k	200	CYC	C2A-CAA-CBA-CGA
6	I	201	CYC	NA-C1A-CHA-C4D
6	j	201	CYC	NA-C1A-CHA-C4D
6	A	200	CYC	C4B-C3B-CAB-CBB
6	R	200	CYC	C4B-C3B-CAB-CBB
6	K	200	CYC	C2B-C1B-CHB-C4A
6	I	200	CYC	C4C-C3C-CAC-CBC
6	h	201	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
6	H	200	CYC	C2A-CAA-CBA-CGA
6	P	200	CYC	C2A-CAA-CBA-CGA
6	X	200	CYC	NB-C1B-CHB-C4A
6	X	201	CYC	NB-C1B-CHB-C4A
6	I	201	CYC	C3D-CAD-CBD-CGD
6	G	200	CYC	C4B-C3B-CAB-CBB
6	K	201	CYC	C4B-C3B-CAB-CBB
6	Y	201	CYC	C4B-C3B-CAB-CBB
6	l	200	CYC	C4B-C3B-CAB-CBB
6	P	200	CYC	C2C-C3C-CAC-CBC
6	T	201	CYC	C3D-CAD-CBD-CGD
6	4	301	CYC	C2C-C3C-CAC-CBC
6	h	200	CYC	C3D-CAD-CBD-CGD
6	i	201	CYC	NB-C1B-CHB-C4A
6	V	200	CYC	C3A-C2A-CAA-CBA
6	V	200	CYC	C1A-C2A-CAA-CBA
6	T	201	CYC	C2B-C3B-CAB-CBB
6	i	201	CYC	C2A-C1A-CHA-C4D
6	K	201	CYC	C3D-CAD-CBD-CGD
6	K	200	CYC	C2B-C3B-CAB-CBB
6	H	200	CYC	C2B-C3B-CAB-CBB
6	A	201	CYC	CAD-CBD-CGD-O1D
6	B	200	CYC	CAA-CBA-CGA-O2A
6	L	201	CYC	C2B-C3B-CAB-CBB
6	C	200	CYC	CAA-CBA-CGA-O2A
6	O	200	CYC	CAD-CBD-CGD-O2D
6	Y	201	CYC	CAA-CBA-CGA-O2A
6	a	200	CYC	CAA-CBA-CGA-O2A
6	c	200	CYC	CAA-CBA-CGA-O2A
6	k	200	CYC	CAA-CBA-CGA-O1A
6	A	200	CYC	CAA-CBA-CGA-O1A
6	d	200	CYC	CAA-CBA-CGA-O2A
6	i	201	CYC	CAA-CBA-CGA-O1A
6	j	200	CYC	CAA-CBA-CGA-O2A
6	B	201	CYC	CAD-CBD-CGD-O1D
6	T	201	CYC	CAA-CBA-CGA-O1A
6	f	200	CYC	CAA-CBA-CGA-O1A
6	V	200	CYC	CAA-CBA-CGA-O1A
6	X	200	CYC	CAD-CBD-CGD-O1D
6	a	200	CYC	CAA-CBA-CGA-O1A
6	b	200	CYC	CAD-CBD-CGD-O1D
6	k	201	CYC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
6	G	201	CYC	CAA-CBA-CGA-O1A
6	I	201	CYC	CAD-CBD-CGD-O1D
6	O	200	CYC	CAD-CBD-CGD-O1D
6	S	200	CYC	CAD-CBD-CGD-O1D
6	X	201	CYC	CAA-CBA-CGA-O1A
6	T	201	CYC	CAD-CBD-CGD-O1D
6	C	200	CYC	C2A-CAA-CBA-CGA
6	f	200	CYC	C2A-CAA-CBA-CGA
6	N	200	CYC	CAD-CBD-CGD-O1D
6	W	201	CYC	CAA-CBA-CGA-O1A
6	Y	201	CYC	CAA-CBA-CGA-O1A
6	U	201	CYC	CAD-CBD-CGD-O2D
6	V	200	CYC	CAA-CBA-CGA-O2A
6	V	201	CYC	CAA-CBA-CGA-O1A
6	T	200	CYC	C4B-C3B-CAB-CBB
6	V	200	CYC	NB-C1B-CHB-C4A
6	A	200	CYC	CAA-CBA-CGA-O2A
6	P	200	CYC	CAD-CBD-CGD-O1D
6	X	200	CYC	CAD-CBD-CGD-O2D
6	i	201	CYC	CAA-CBA-CGA-O2A
6	A	200	CYC	CAD-CBD-CGD-O1D
6	R	200	CYC	CAA-CBA-CGA-O1A
6	a	200	CYC	CAD-CBD-CGD-O1D
6	i	201	CYC	CAD-CBD-CGD-O1D
6	l	201	CYC	CAA-CBA-CGA-O2A
6	I	200	CYC	CAA-CBA-CGA-O1A
6	R	200	CYC	CAA-CBA-CGA-O2A
6	S	200	CYC	CAA-CBA-CGA-O1A
6	T	201	CYC	CAA-CBA-CGA-O2A
6	U	201	CYC	CAD-CBD-CGD-O1D
6	k	200	CYC	CAA-CBA-CGA-O2A
6	R	200	CYC	CAD-CBD-CGD-O1D
6	S	200	CYC	CAA-CBA-CGA-O2A
6	T	201	CYC	CAD-CBD-CGD-O2D
6	c	200	CYC	CAA-CBA-CGA-O1A
6	d	200	CYC	CAA-CBA-CGA-O1A
6	h	201	CYC	CAA-CBA-CGA-O1A
6	D	200	CYC	CAA-CBA-CGA-O1A
6	I	201	CYC	CAA-CBA-CGA-O1A
6	I	201	CYC	CAD-CBD-CGD-O2D
6	S	200	CYC	CAD-CBD-CGD-O2D
6	j	200	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
6	l	201	CYC	CAA-CBA-CGA-O1A
6	D	200	CYC	CAA-CBA-CGA-O2A
6	G	201	CYC	CAA-CBA-CGA-O2A
6	a	200	CYC	CAD-CBD-CGD-O2D
6	B	201	CYC	CAD-CBD-CGD-O2D
6	b	200	CYC	CAD-CBD-CGD-O2D
6	f	200	CYC	CAA-CBA-CGA-O2A
6	A	201	CYC	CAD-CBD-CGD-O2D
6	V	201	CYC	CAA-CBA-CGA-O2A
6	F	200	CYC	CAA-CBA-CGA-O1A
6	N	200	CYC	CAD-CBD-CGD-O2D
6	C	200	CYC	CAA-CBA-CGA-O1A
6	I	200	CYC	CAA-CBA-CGA-O2A
6	h	201	CYC	CAA-CBA-CGA-O2A
6	c	200	CYC	C2C-C3C-CAC-CBC
6	B	200	CYC	CAA-CBA-CGA-O1A
6	Q	200	CYC	CAA-CBA-CGA-O2A
6	R	200	CYC	CAD-CBD-CGD-O2D
6	F	200	CYC	CAA-CBA-CGA-O2A
6	F	200	CYC	CAD-CBD-CGD-O2D
6	I	201	CYC	CAA-CBA-CGA-O2A
6	i	201	CYC	CAD-CBD-CGD-O2D
6	A	200	CYC	CAD-CBD-CGD-O2D
6	e	200	CYC	CAD-CBD-CGD-O1D
6	X	200	CYC	CAA-CBA-CGA-O2A
6	G	201	CYC	CAD-CBD-CGD-O1D
6	X	201	CYC	CAA-CBA-CGA-O2A
6	b	200	CYC	CAA-CBA-CGA-O2A
6	g	201	CYC	CAD-CBD-CGD-O2D
6	J	200	CYC	CAA-CBA-CGA-O2A
6	G	201	CYC	CAD-CBD-CGD-O2D
6	A	201	CYC	CAA-CBA-CGA-O2A
6	e	200	CYC	CAA-CBA-CGA-O2A
6	Q	200	CYC	CAA-CBA-CGA-O1A
6	B	201	CYC	CAA-CBA-CGA-O1A
6	P	200	CYC	CAD-CBD-CGD-O2D
6	F	200	CYC	CAD-CBD-CGD-O1D
6	W	201	CYC	CAA-CBA-CGA-O2A
6	g	201	CYC	CAA-CBA-CGA-O2A
6	T	200	CYC	C2B-C1B-CHB-C4A
6	E	200	CYC	CAA-CBA-CGA-O2A
6	N	200	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
6	A	201	CYC	CAA-CBA-CGA-O1A
6	J	200	CYC	CAA-CBA-CGA-O1A
6	B	201	CYC	CAA-CBA-CGA-O2A
6	L	201	CYC	CAA-CBA-CGA-O1A
6	Q	200	CYC	CAD-CBD-CGD-O1D
6	X	200	CYC	CAA-CBA-CGA-O1A
6	g	201	CYC	CAA-CBA-CGA-O1A
6	E	200	CYC	CAA-CBA-CGA-O1A
6	K	201	CYC	CAA-CBA-CGA-O1A
6	K	201	CYC	CAA-CBA-CGA-O2A
6	N	200	CYC	CAA-CBA-CGA-O1A
6	g	201	CYC	CAD-CBD-CGD-O1D
6	j	201	CYC	CAD-CBD-CGD-O2D
6	O	200	CYC	CAA-CBA-CGA-O2A
6	j	201	CYC	CAD-CBD-CGD-O1D
6	Q	200	CYC	CAD-CBD-CGD-O2D
6	K	200	CYC	CAA-CBA-CGA-O2A
6	L	201	CYC	CAA-CBA-CGA-O2A
6	O	200	CYC	CAA-CBA-CGA-O1A
6	b	200	CYC	CAA-CBA-CGA-O1A
6	e	200	CYC	CAA-CBA-CGA-O1A
6	e	200	CYC	CAD-CBD-CGD-O2D
6	H	200	CYC	CAA-CBA-CGA-O2A
6	V	201	CYC	CAD-CBD-CGD-O1D
6	W	201	CYC	CAD-CBD-CGD-O2D
6	4	301	CYC	CAA-CBA-CGA-O2A
6	U	201	CYC	CAA-CBA-CGA-O2A
6	K	200	CYC	CAA-CBA-CGA-O1A
6	W	201	CYC	CAD-CBD-CGD-O1D
6	h	201	CYC	NB-C1B-CHB-C4A
6	a	200	CYC	C3A-C2A-CAA-CBA
6	H	200	CYC	CAA-CBA-CGA-O1A
6	Y	201	CYC	C1A-C2A-CAA-CBA
6	l	200	CYC	C3A-C2A-CAA-CBA
6	4	301	CYC	CAA-CBA-CGA-O1A

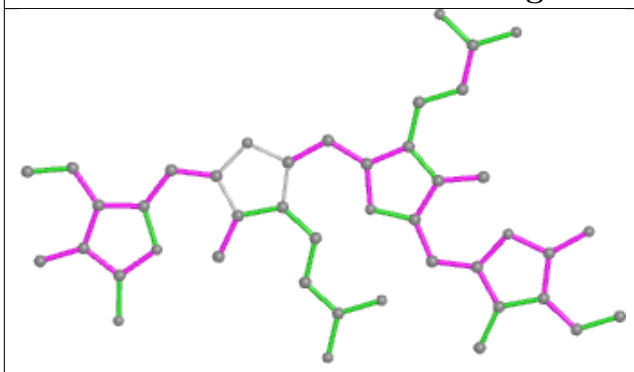
There are no ring outliers.

No monomer is involved in short contacts.

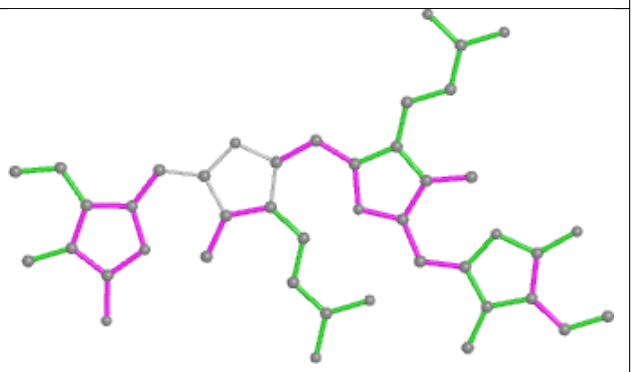
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

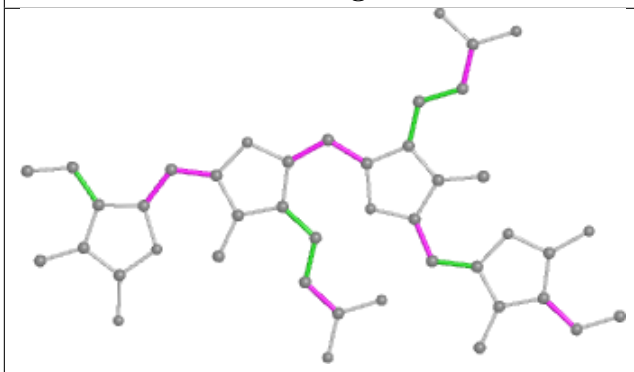
Ligand CYC S 200



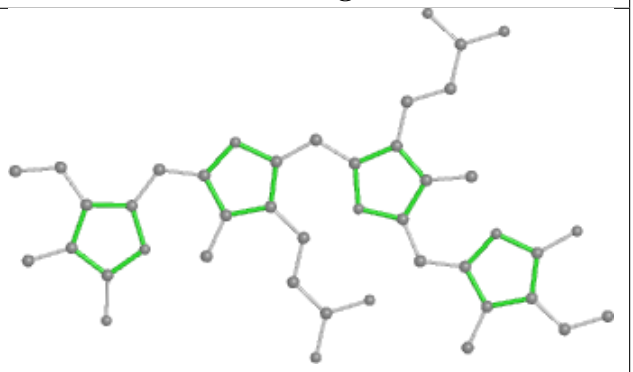
Bond lengths



Bond angles

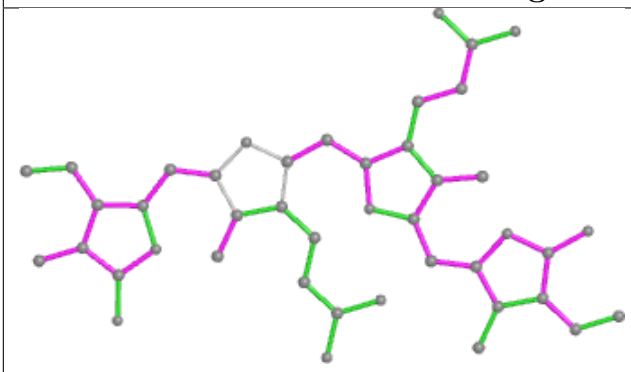


Torsions

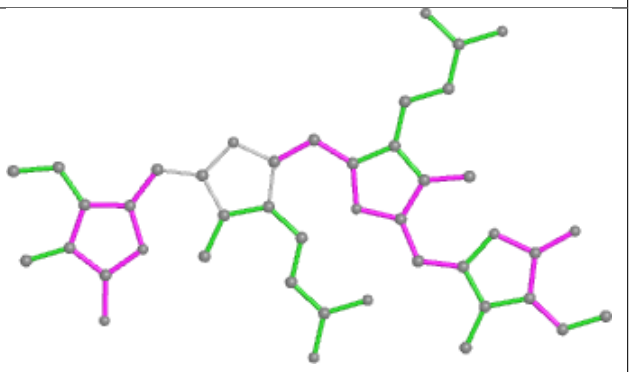


Rings

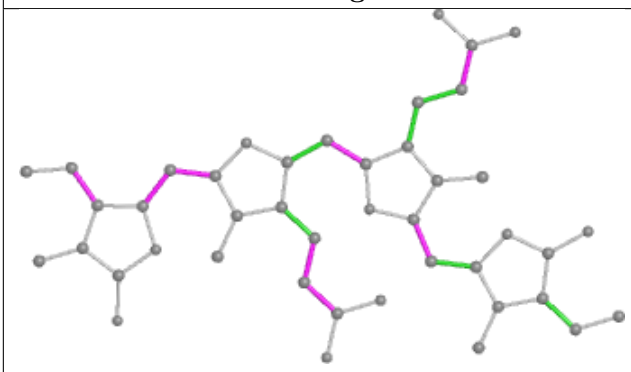
Ligand CYC I 201



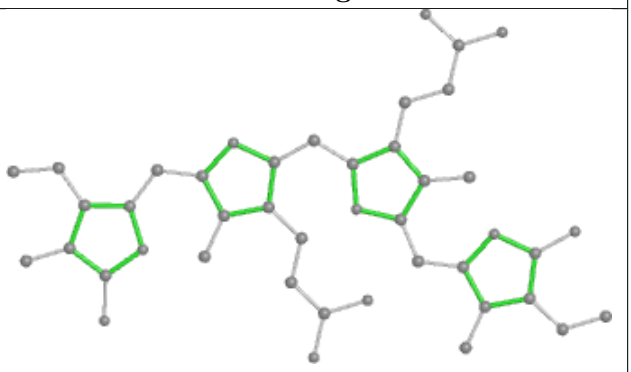
Bond lengths



Bond angles

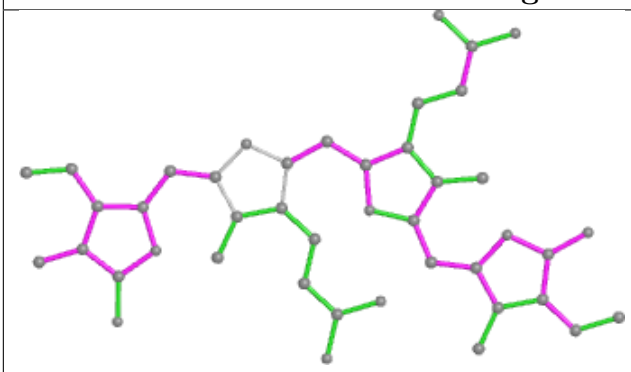


Torsions

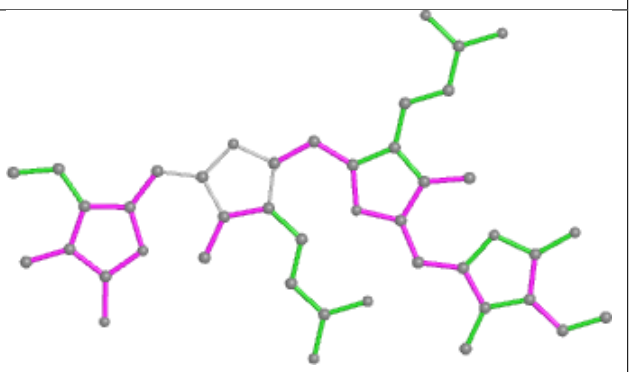


Rings

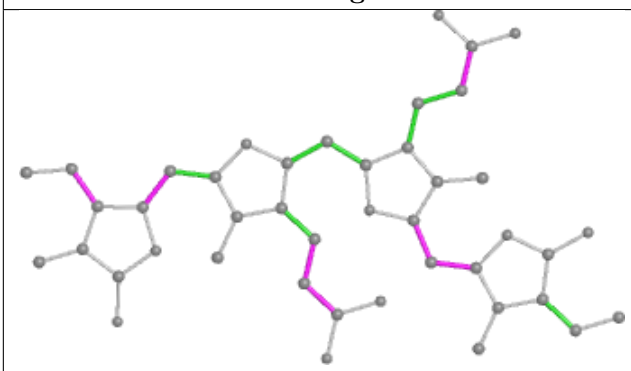
Ligand CYC X 200



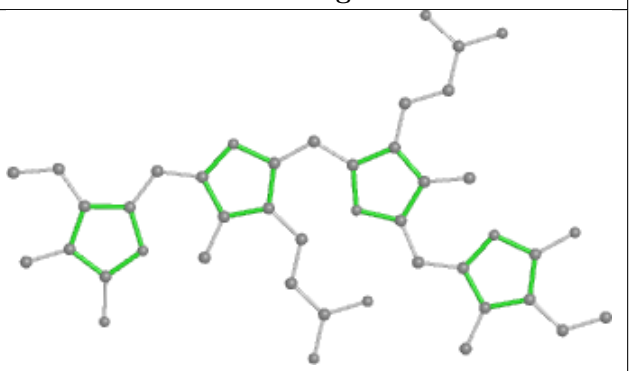
Bond lengths



Bond angles

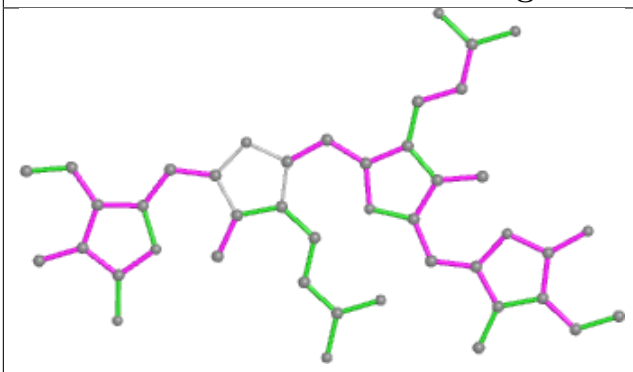


Torsions

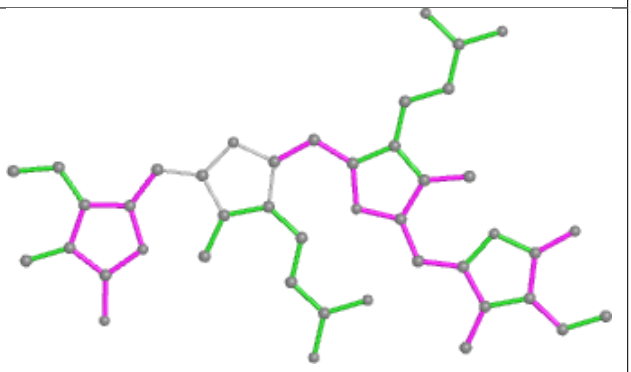


Rings

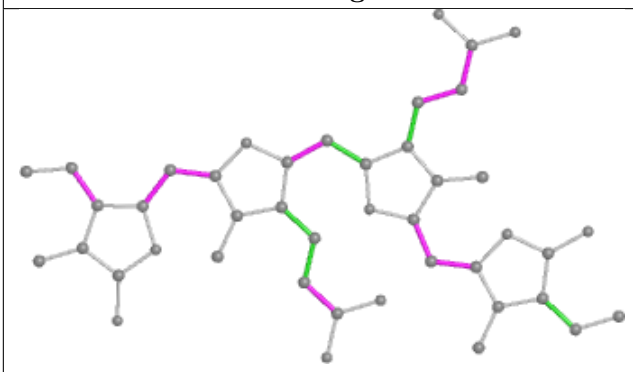
Ligand CYC W 201



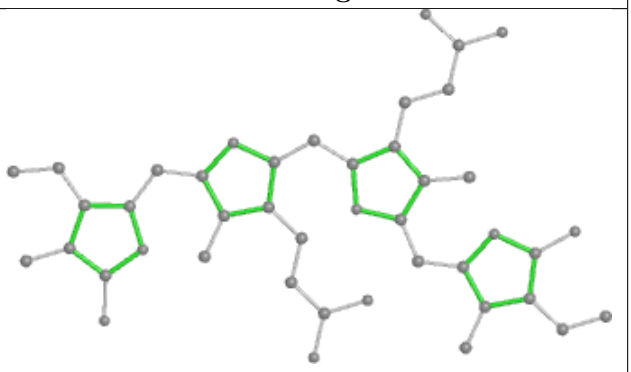
Bond lengths



Bond angles

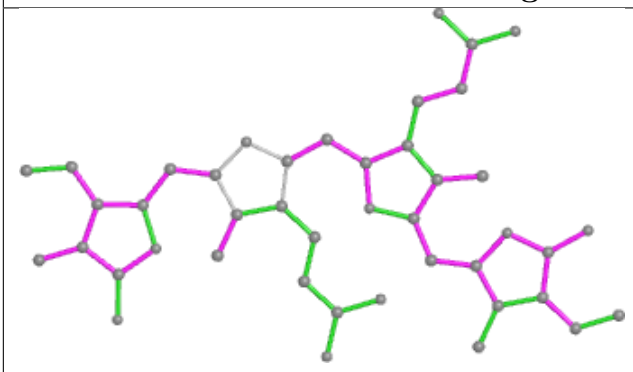


Torsions

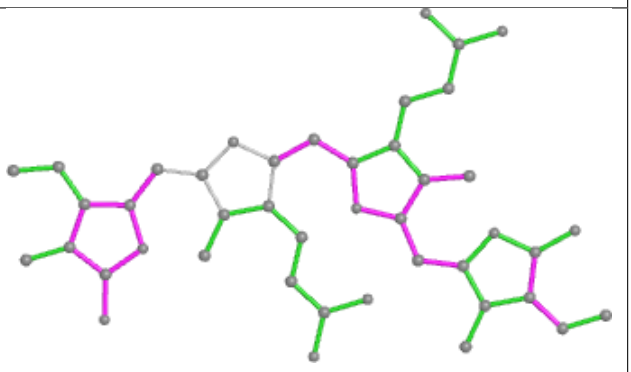


Rings

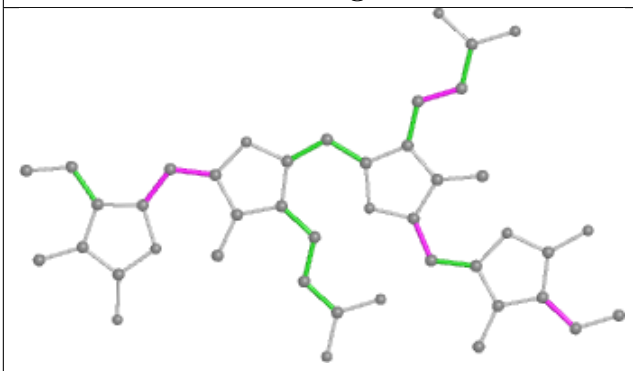
Ligand CYC G 200



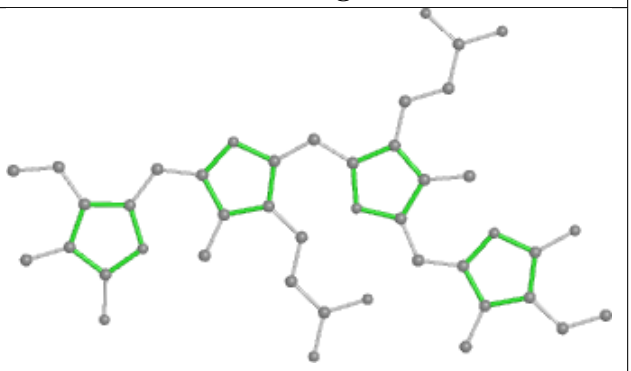
Bond lengths



Bond angles

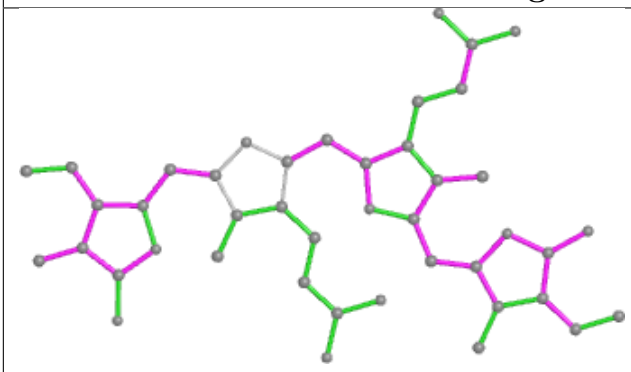


Torsions

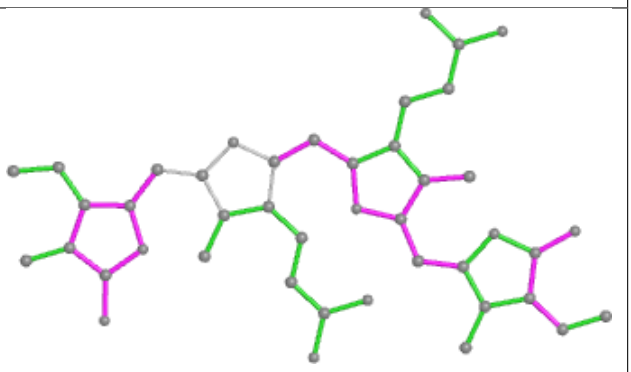


Rings

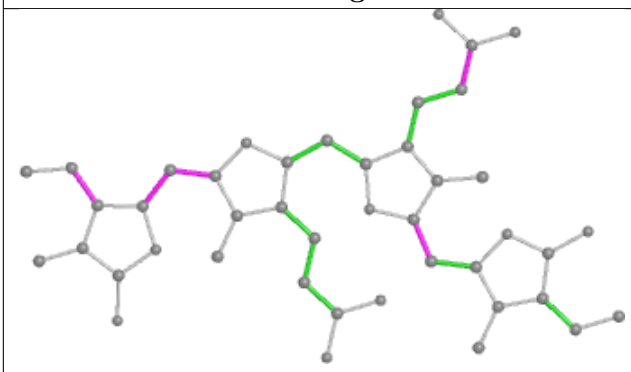
Ligand CYC I 200



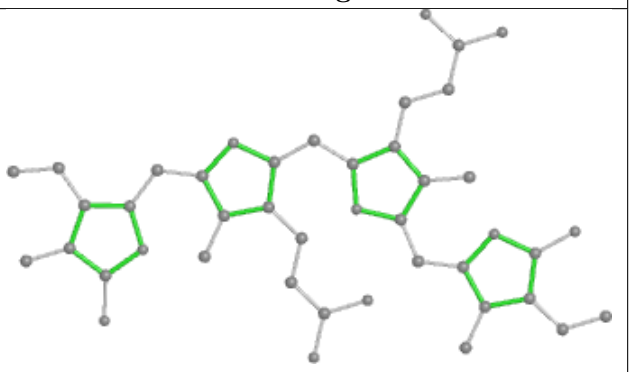
Bond lengths



Bond angles

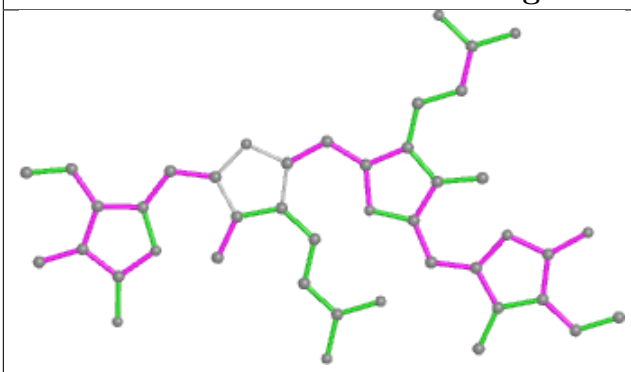


Torsions



Rings

Ligand CYC P 200



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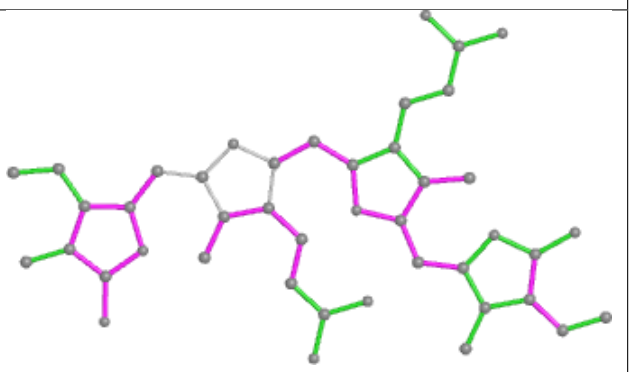

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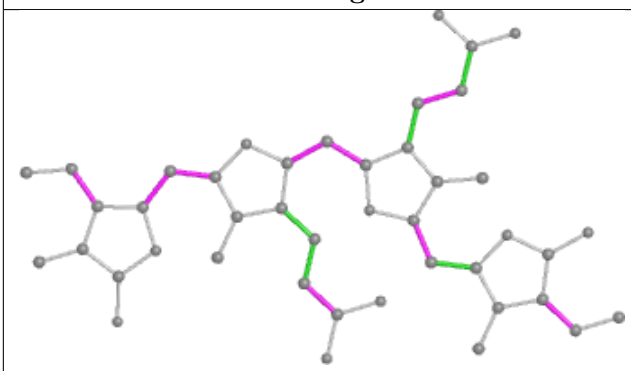

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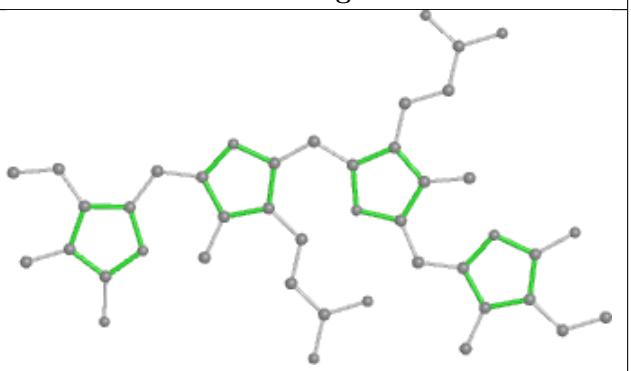

Rings

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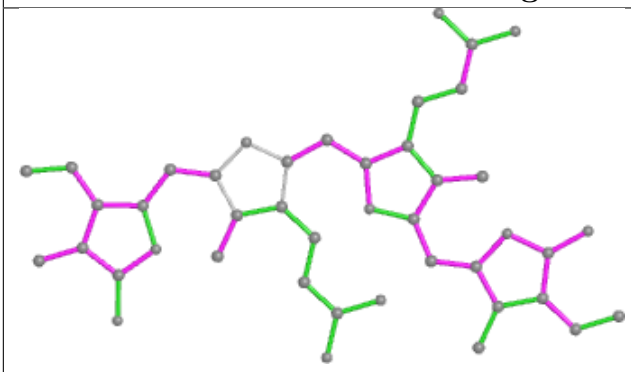

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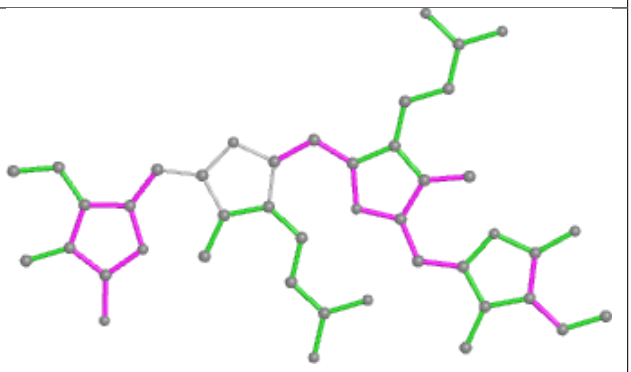

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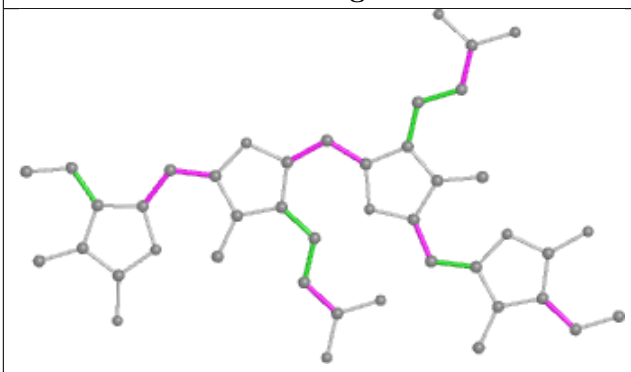

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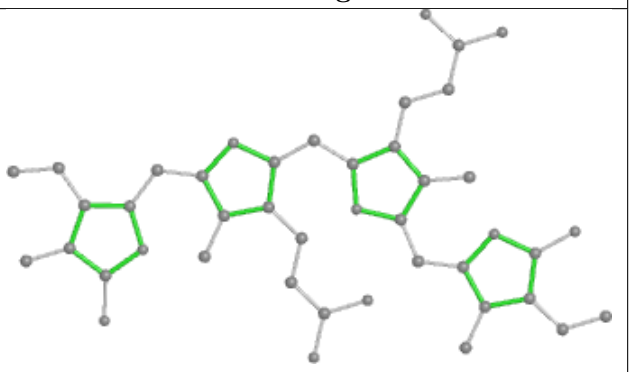

Rings

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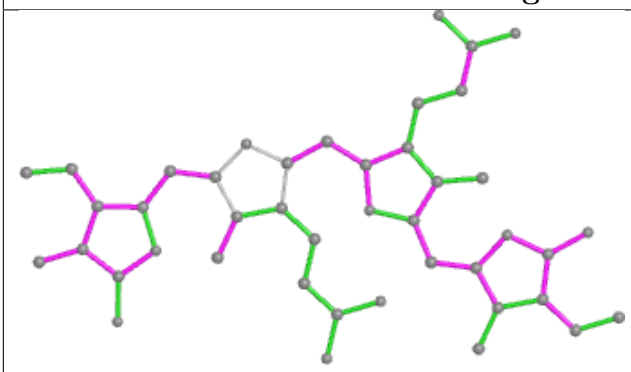

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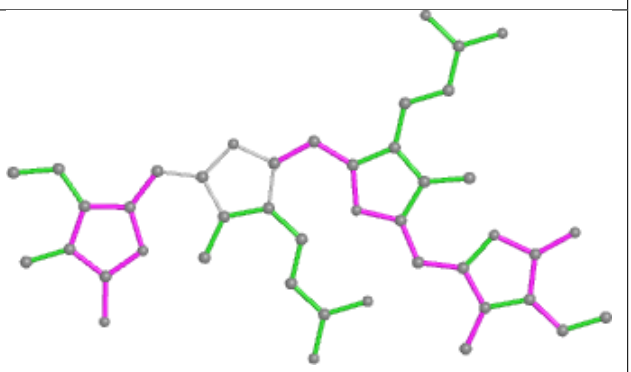

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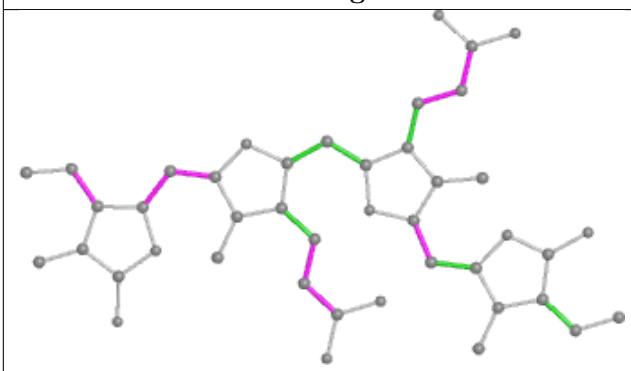

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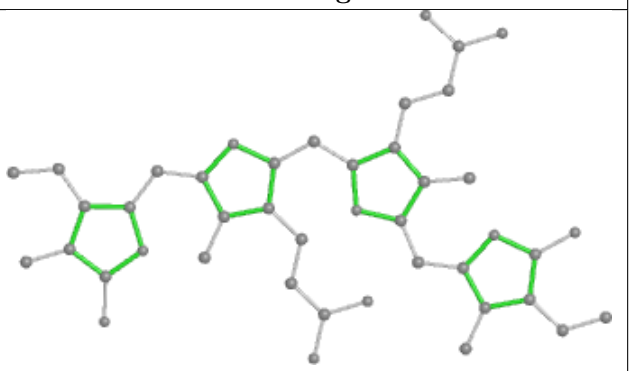

Rings

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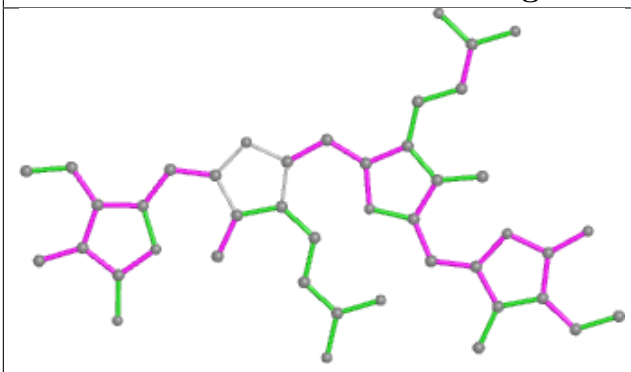

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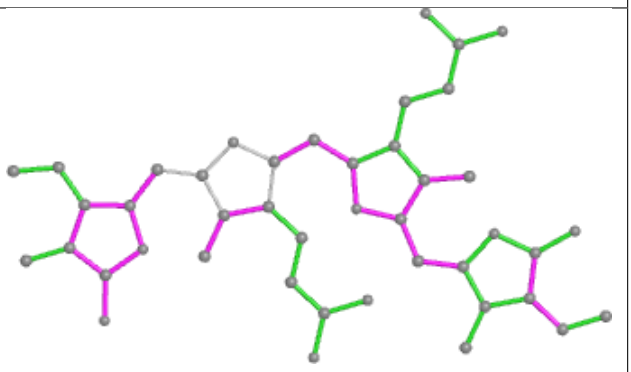

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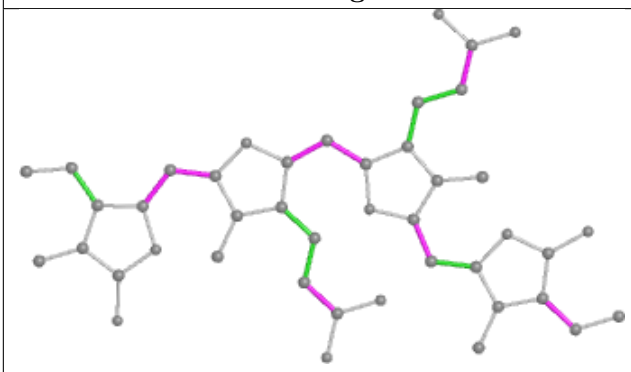

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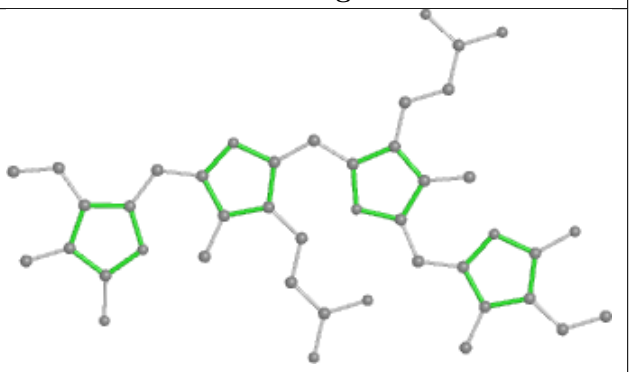

Rings

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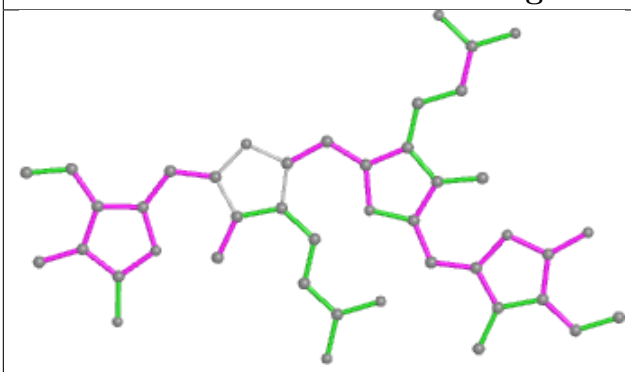

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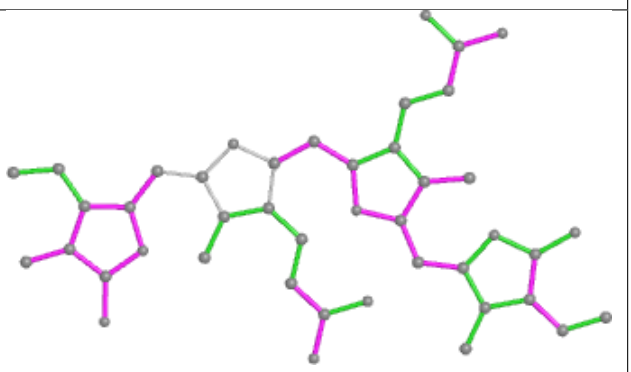

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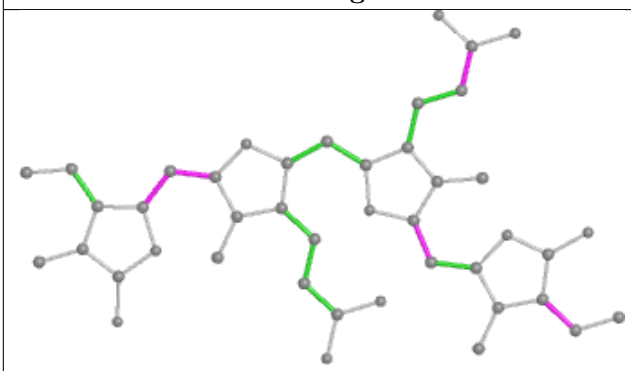

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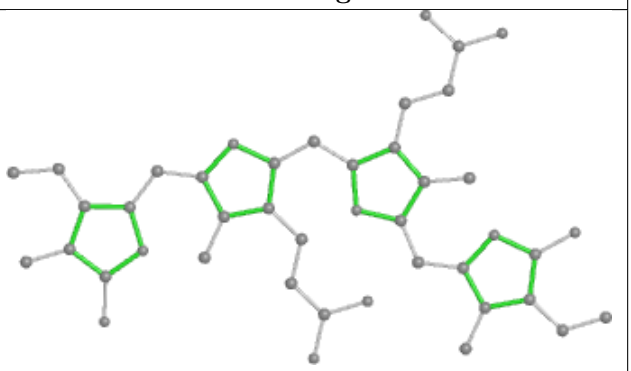

Rings

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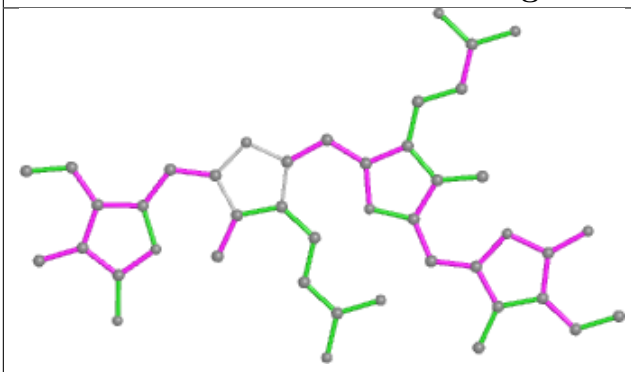

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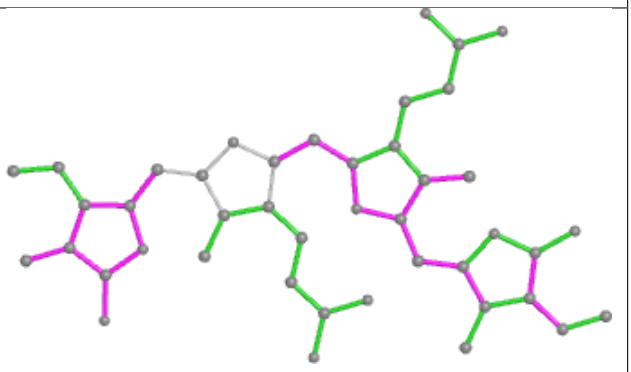

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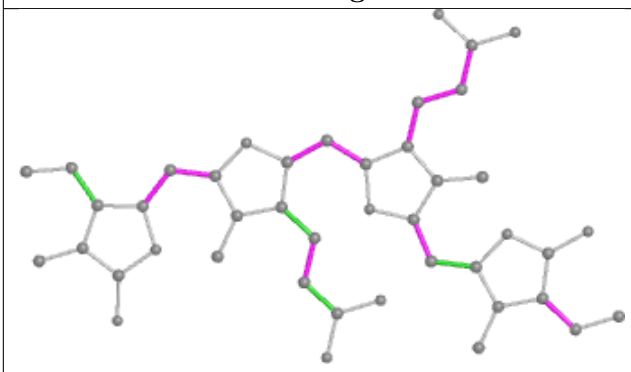

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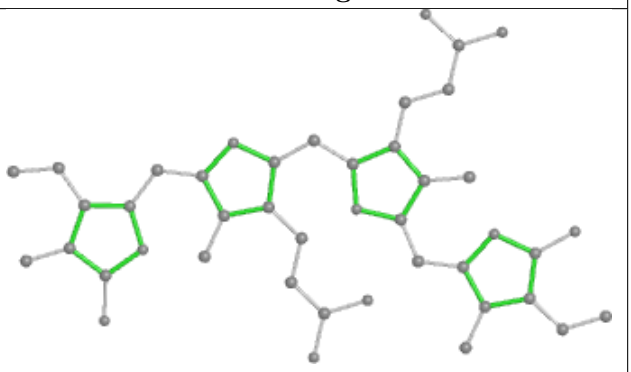

Rings

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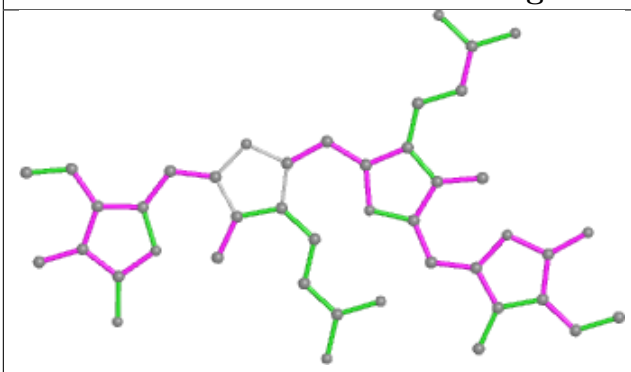

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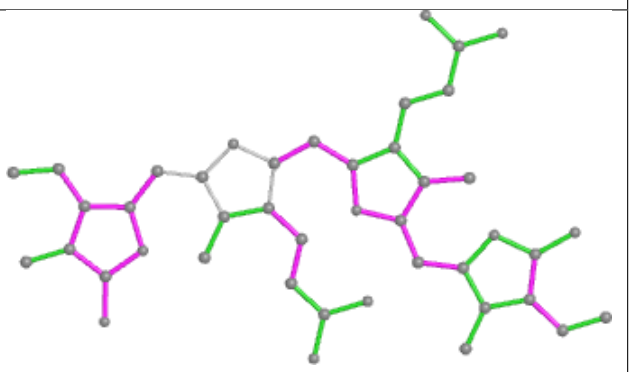

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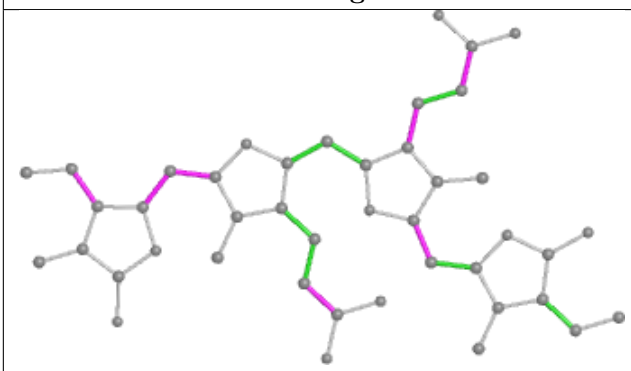

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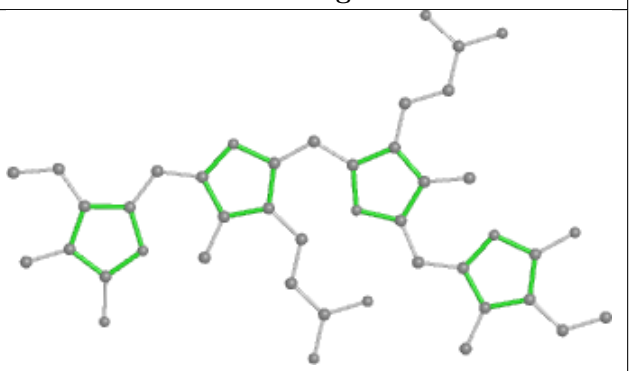

Rings

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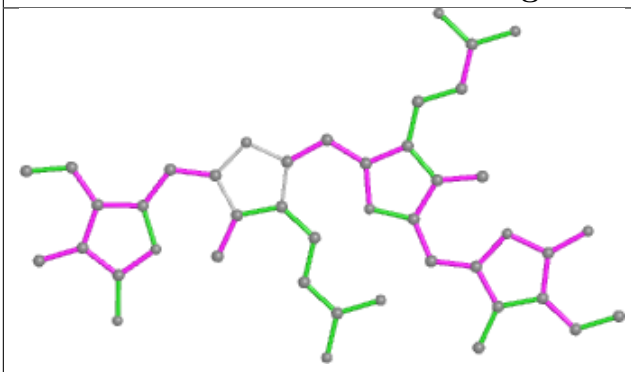

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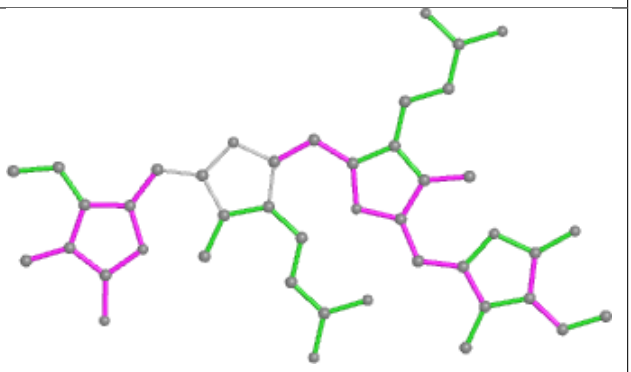

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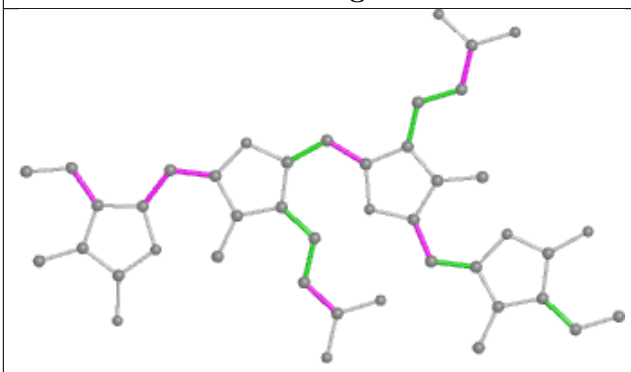

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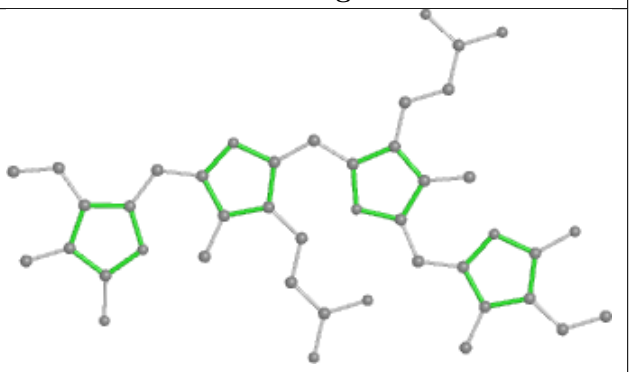
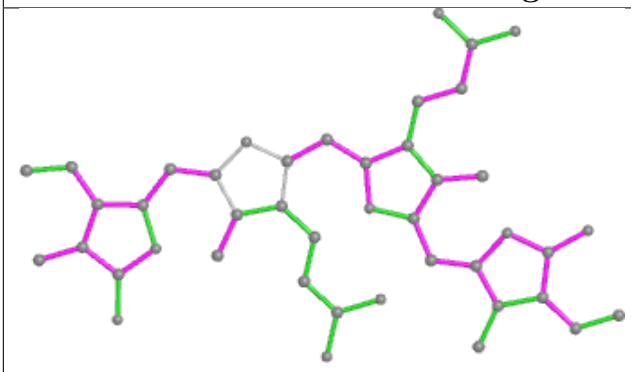


Rings

Ligand CYC C 200



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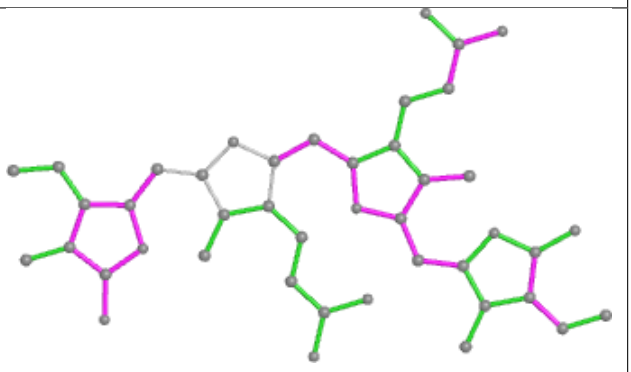

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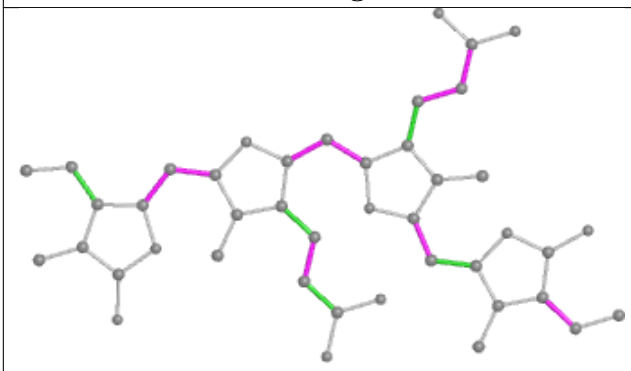

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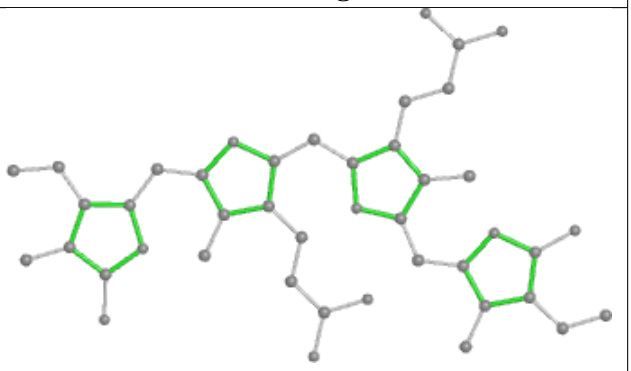

Rings

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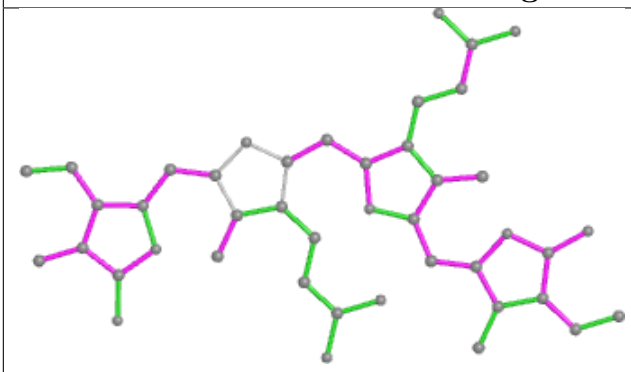

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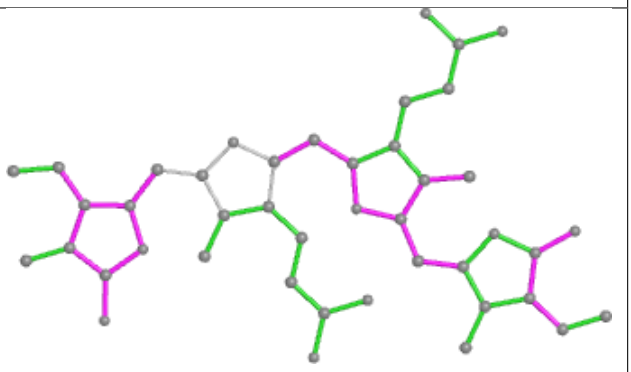

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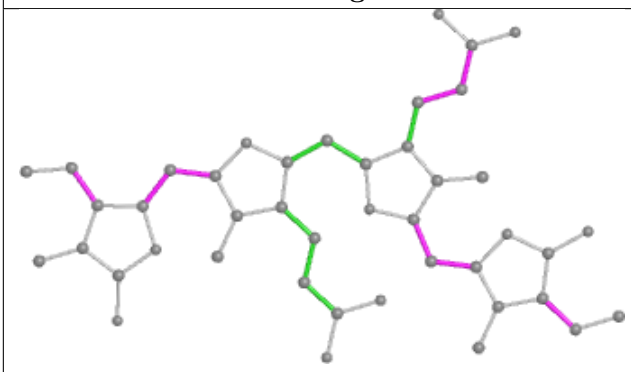

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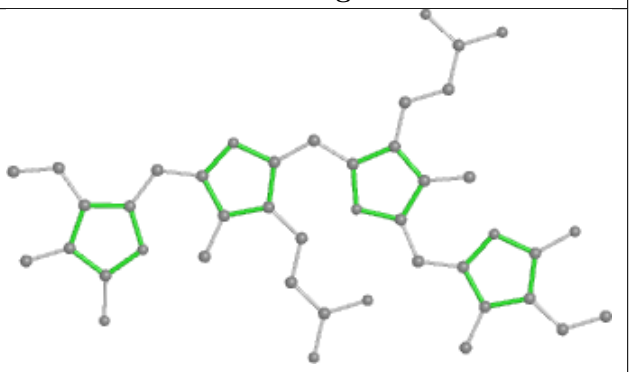
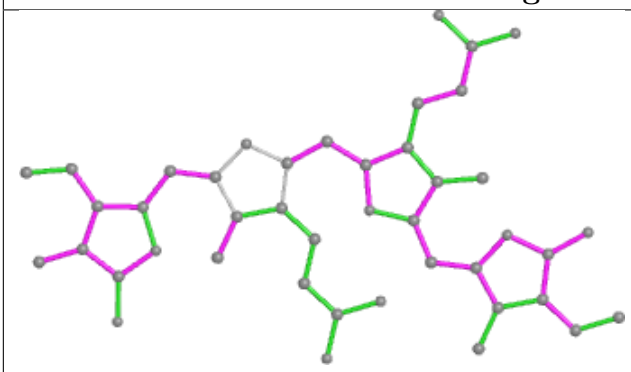


Rings

Ligand CYC T 200



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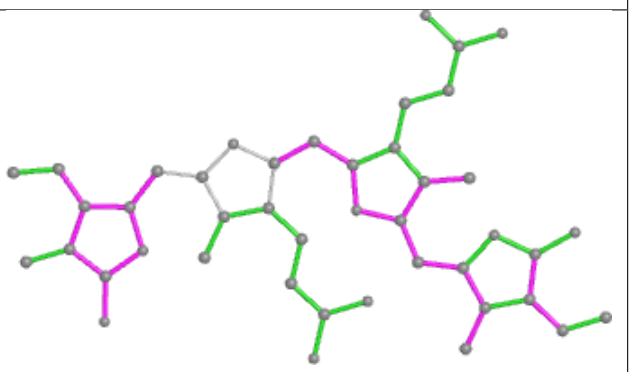

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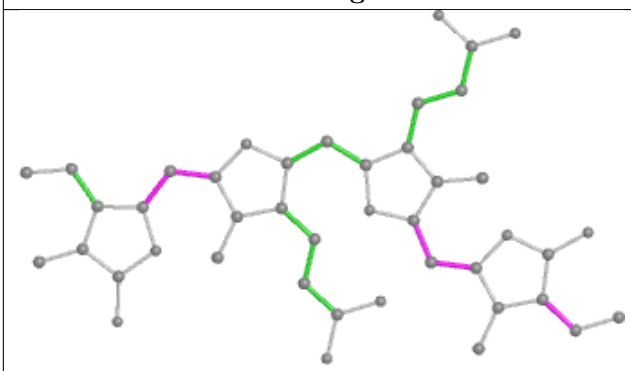

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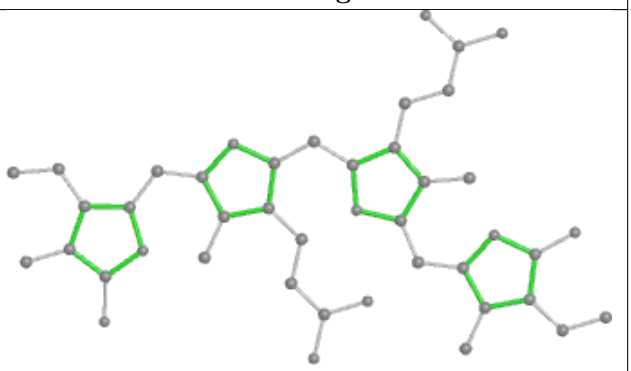
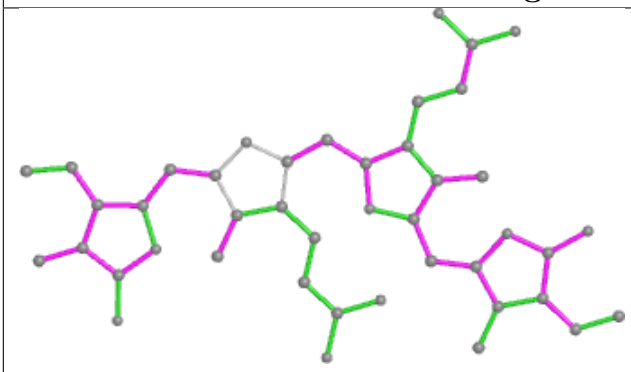


Rings

Ligand CYC Z 200



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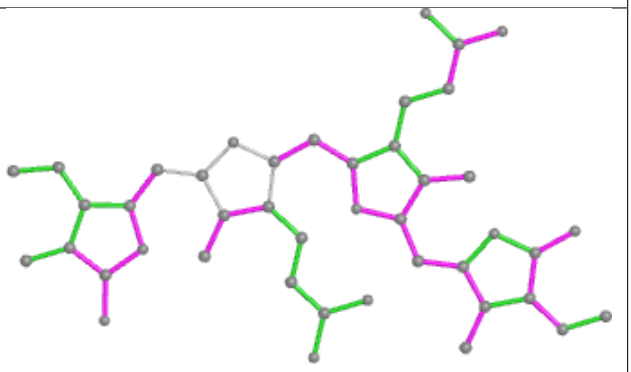

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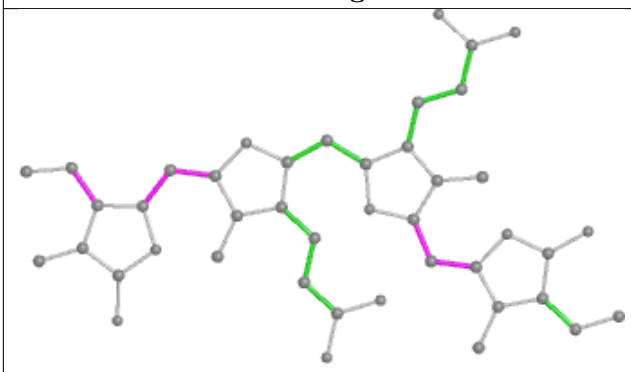

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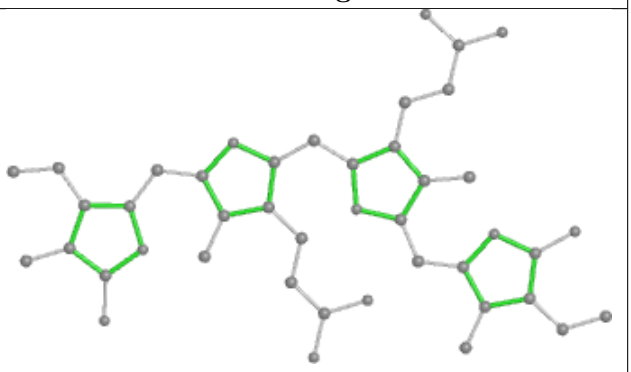
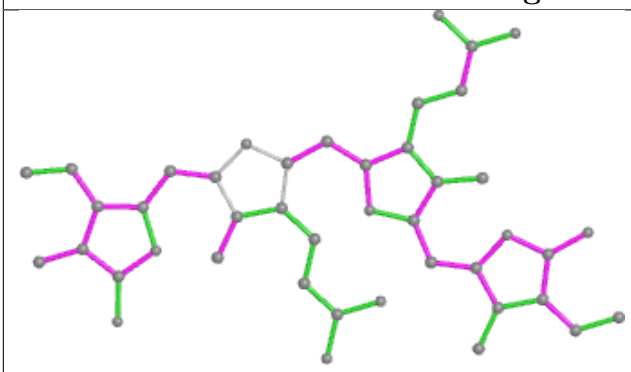


Rings

Ligand CYC E 200



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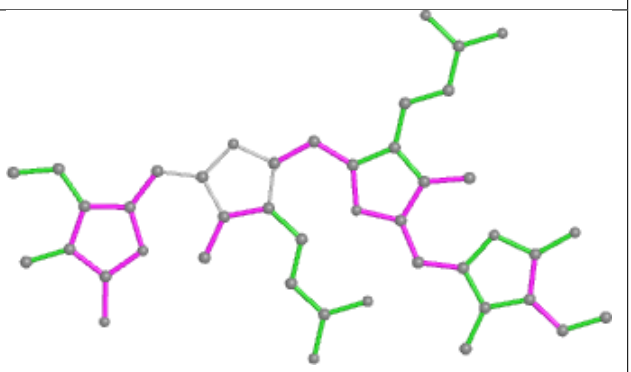

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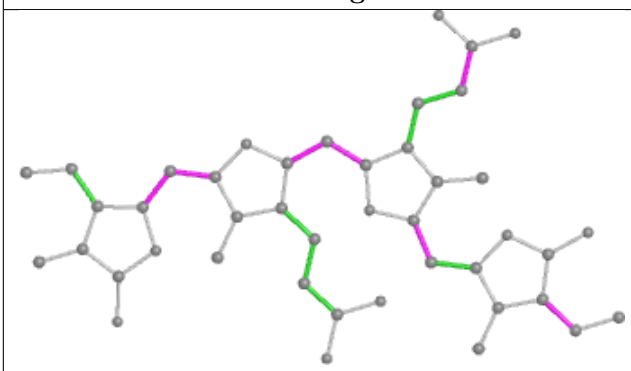

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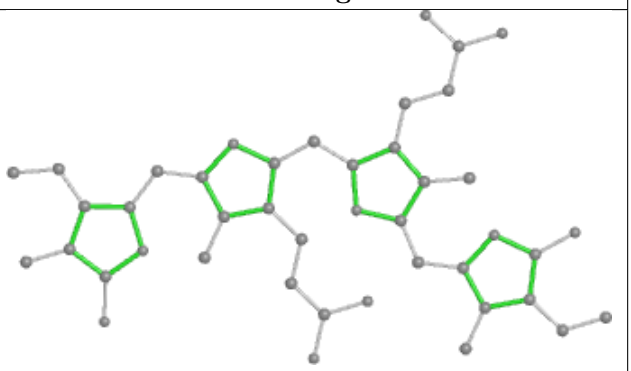
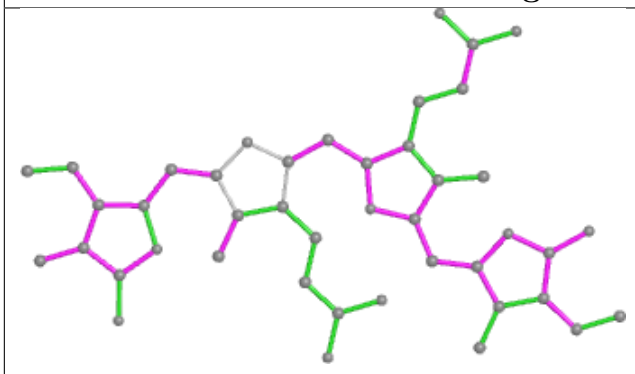


Rings

Ligand CYC Q 200



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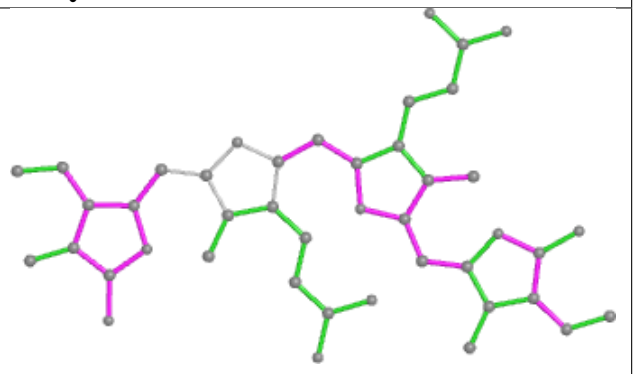

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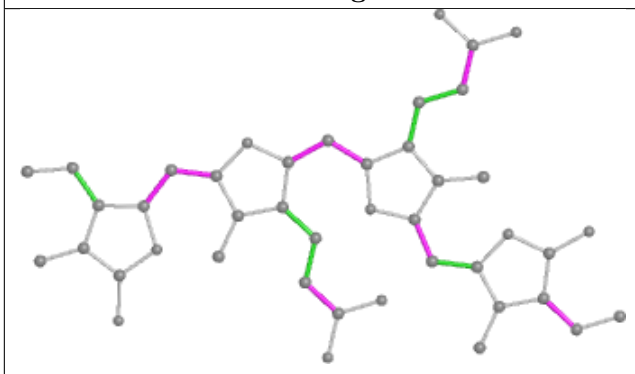

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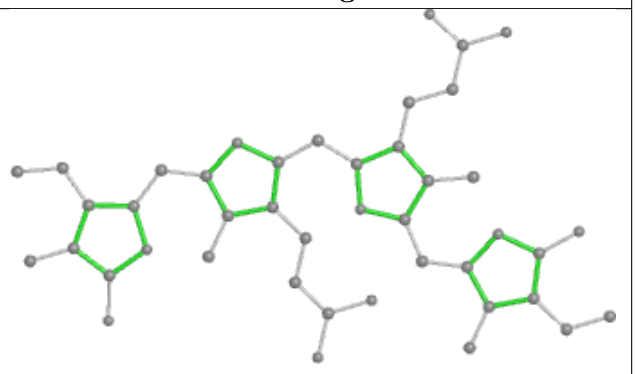
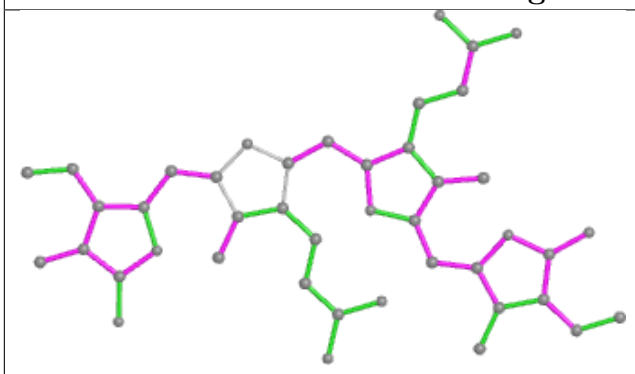
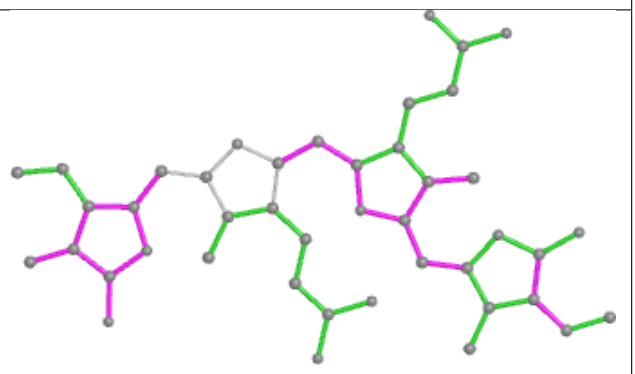


Rings

Ligand CYC e 200



Bond lengths



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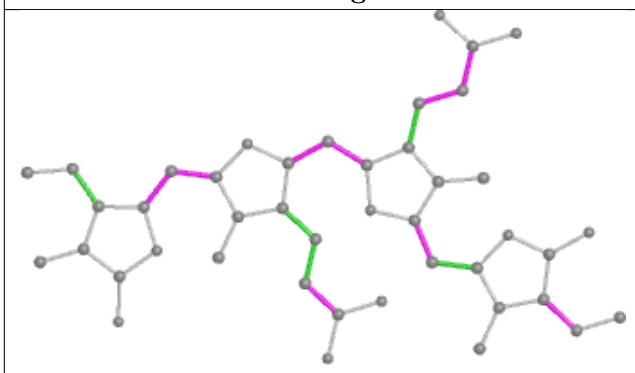

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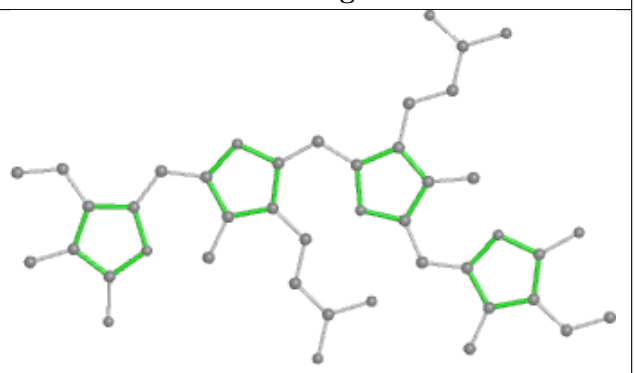

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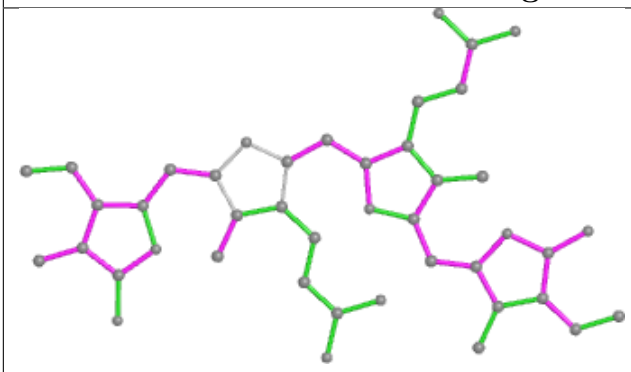

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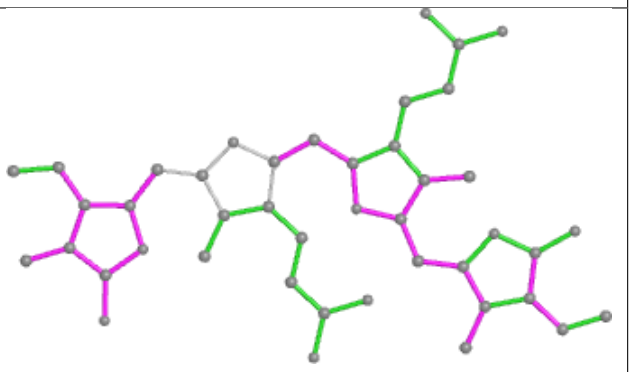

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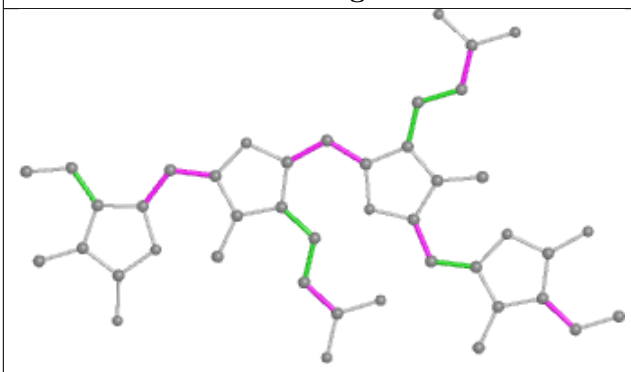

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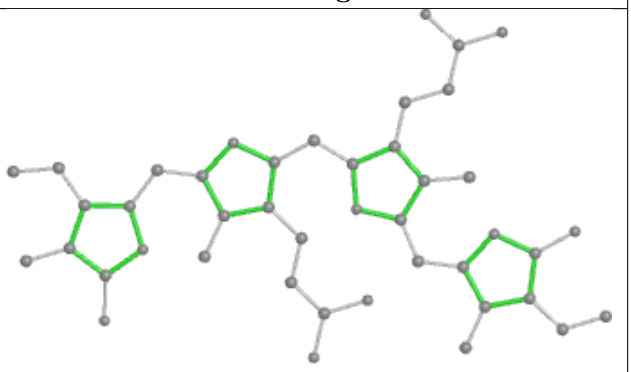

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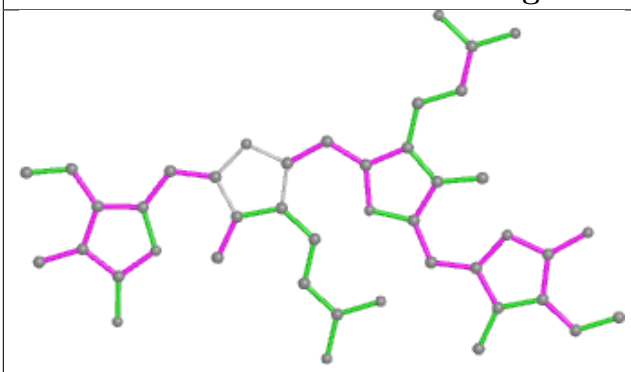

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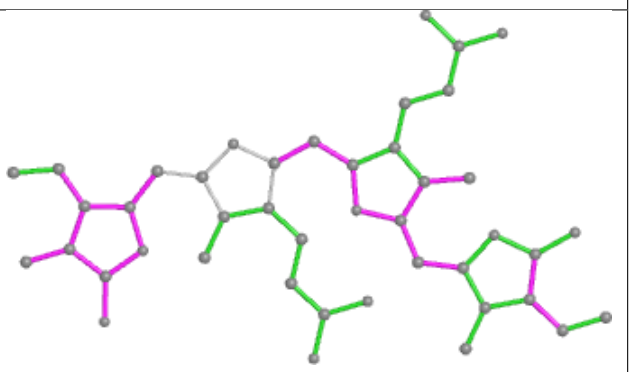

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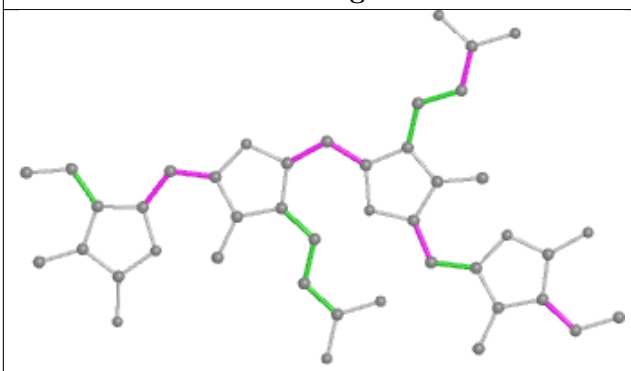

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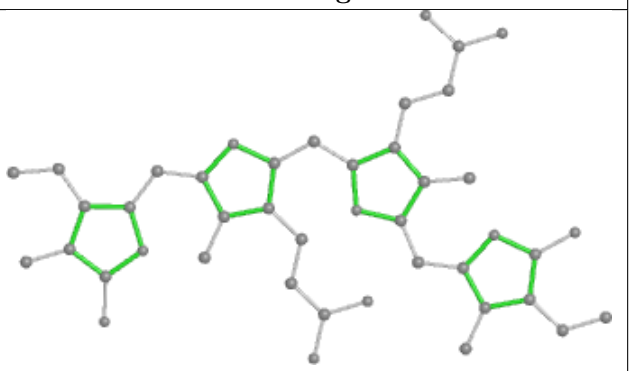

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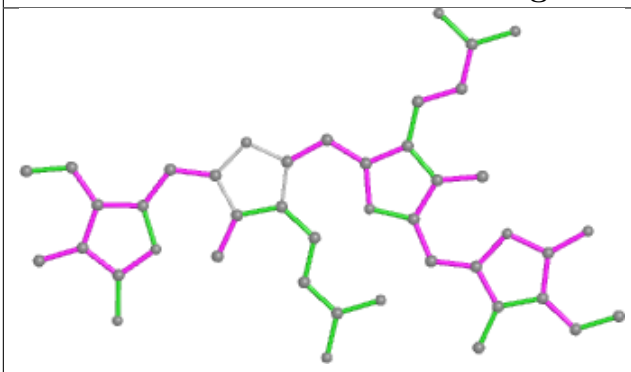

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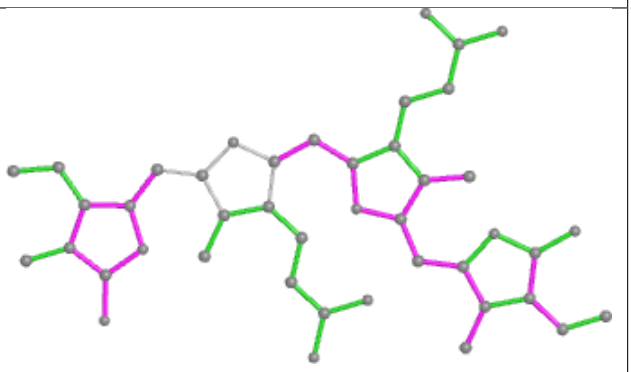

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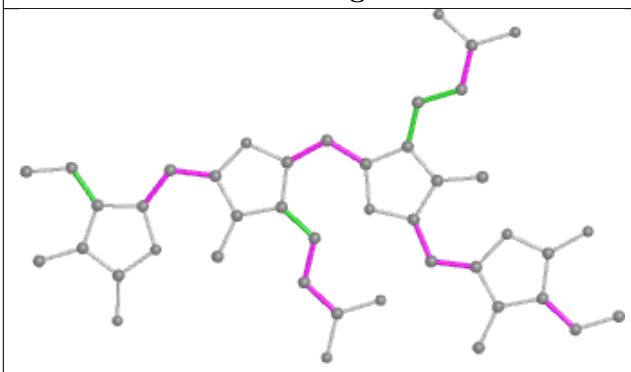

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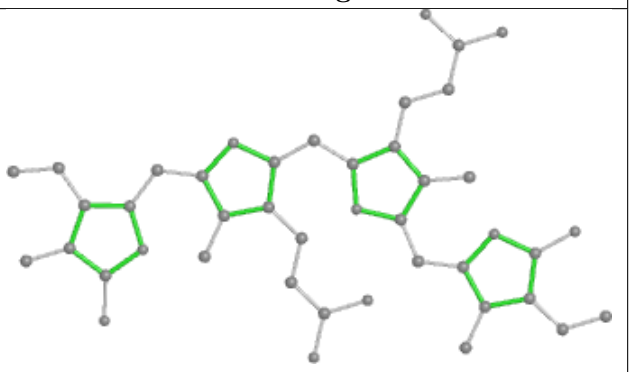

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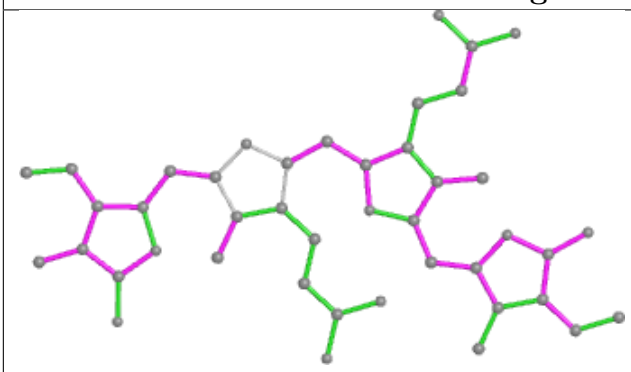

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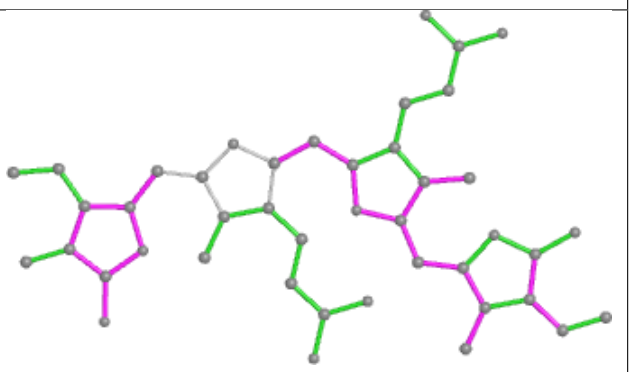

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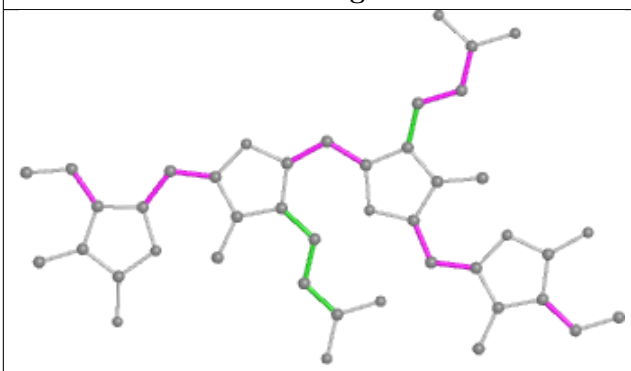

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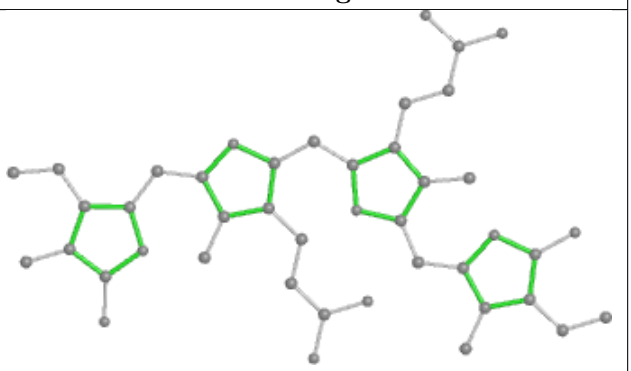

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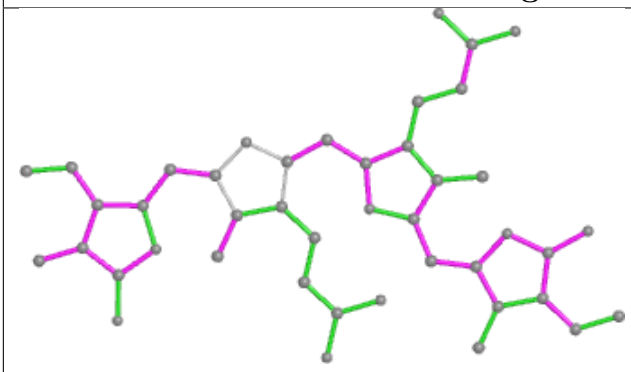

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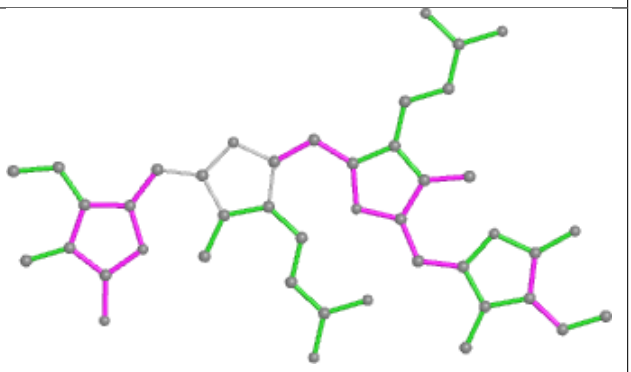

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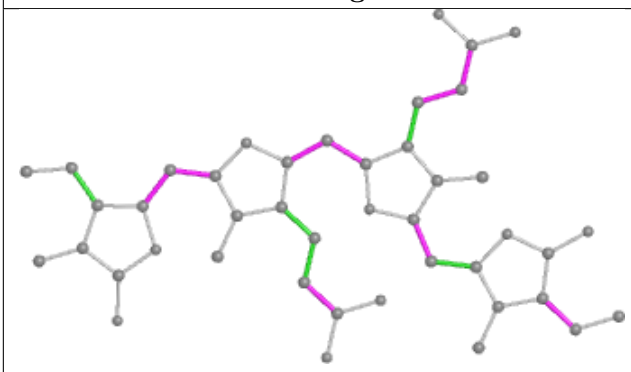

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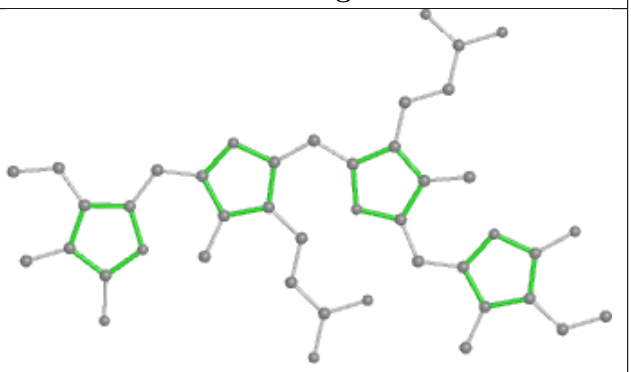

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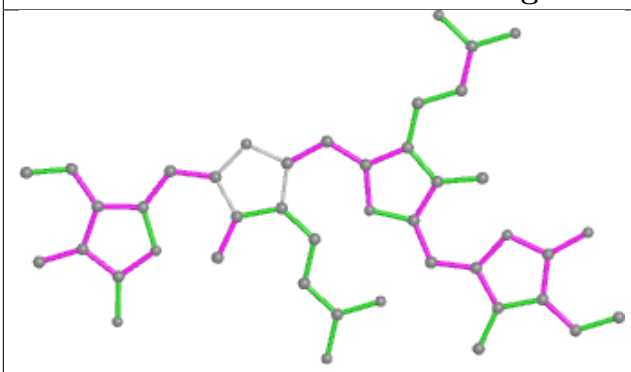

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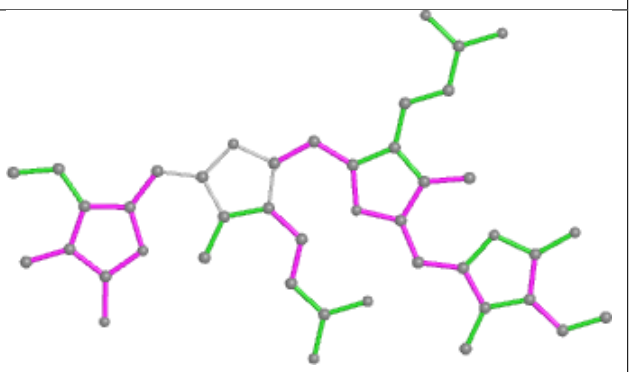

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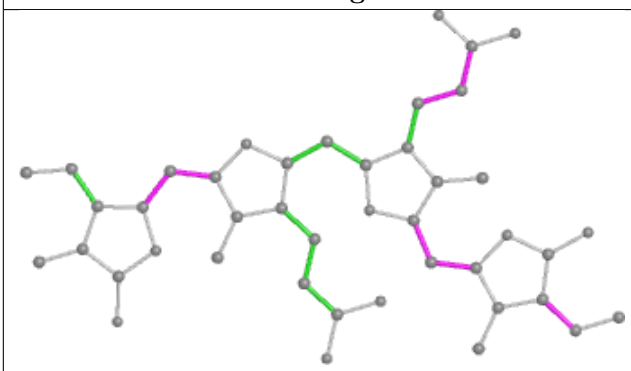

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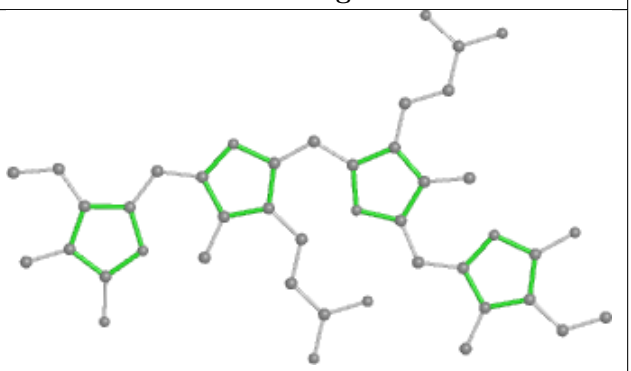

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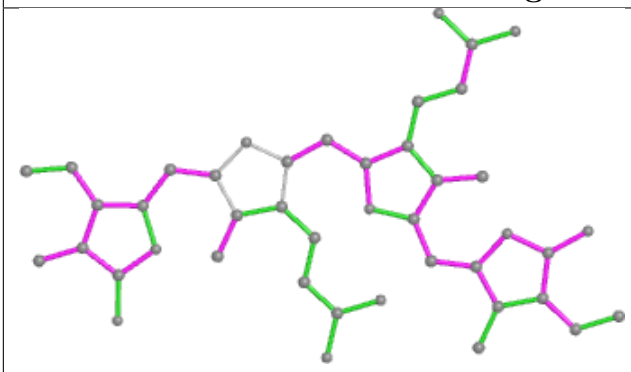

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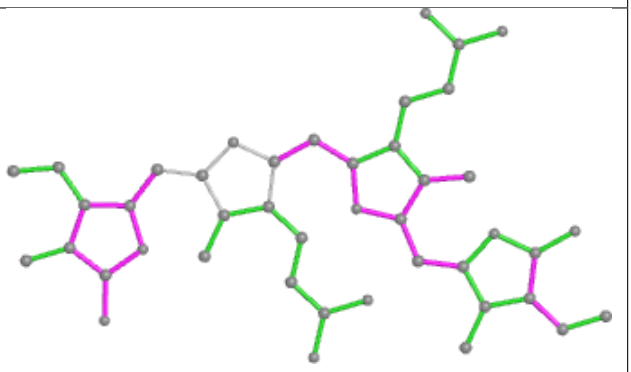

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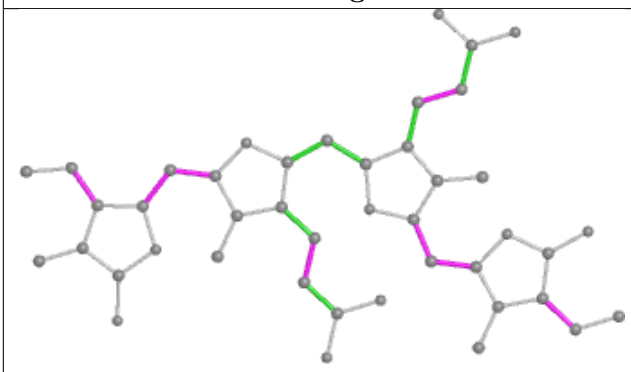

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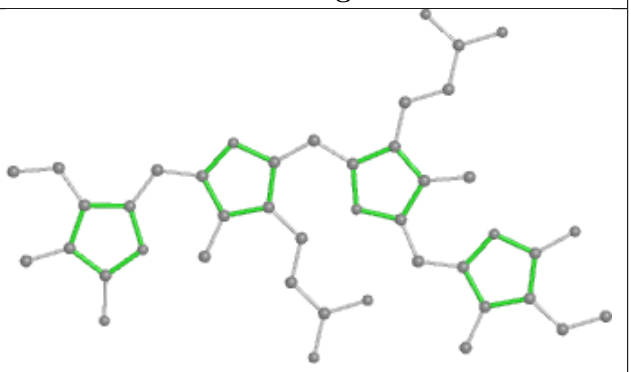

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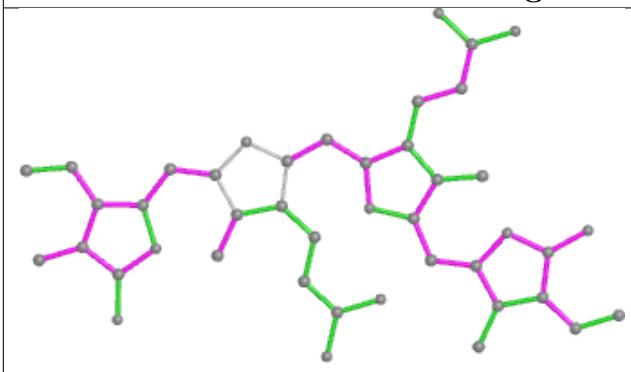

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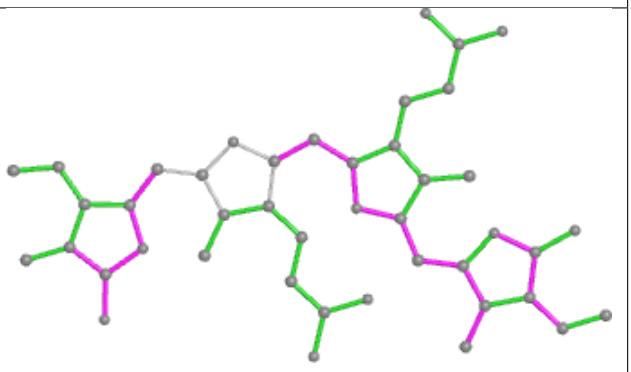

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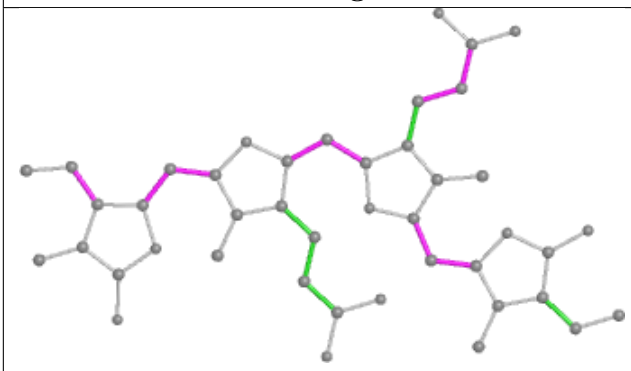

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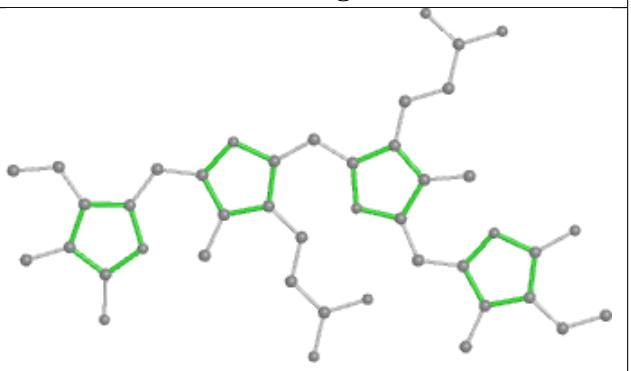

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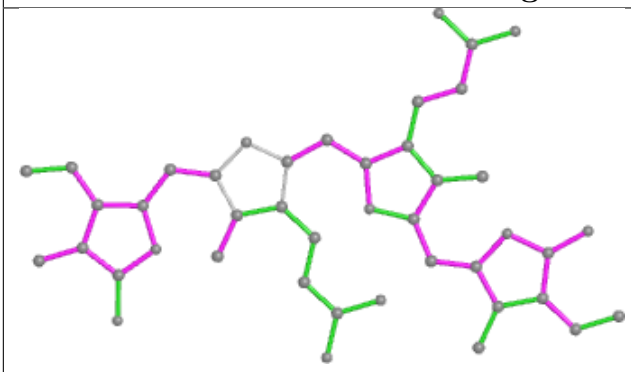

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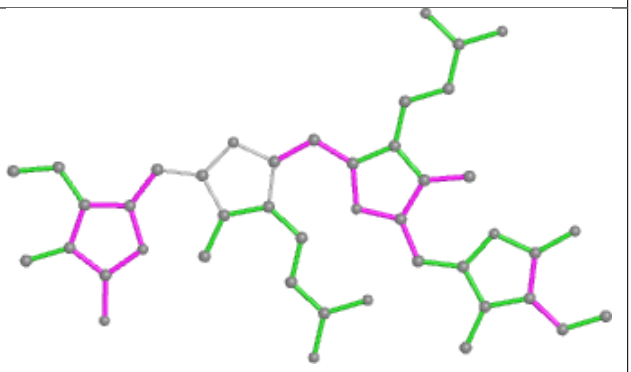

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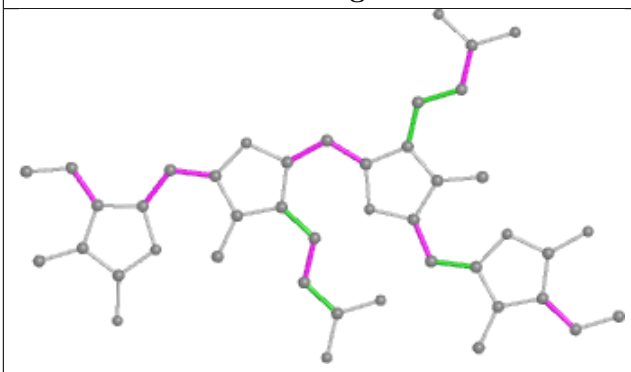

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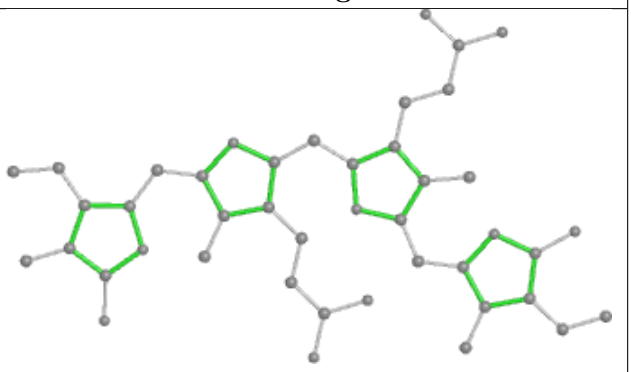

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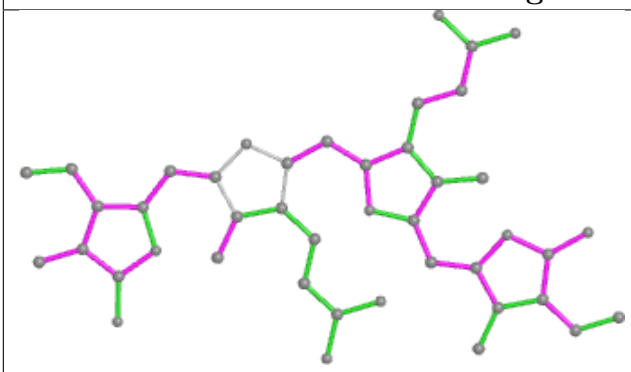

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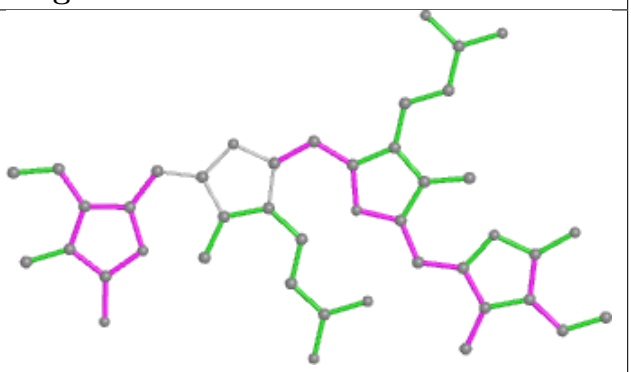

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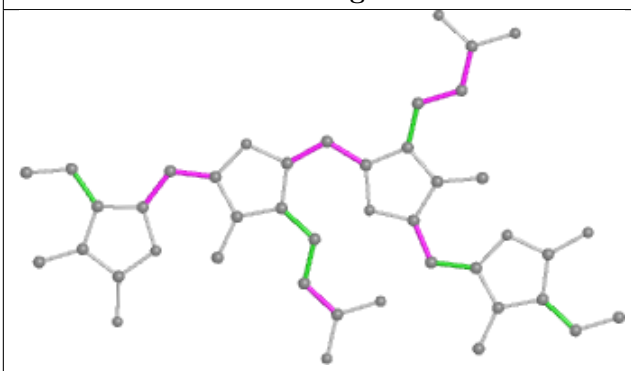

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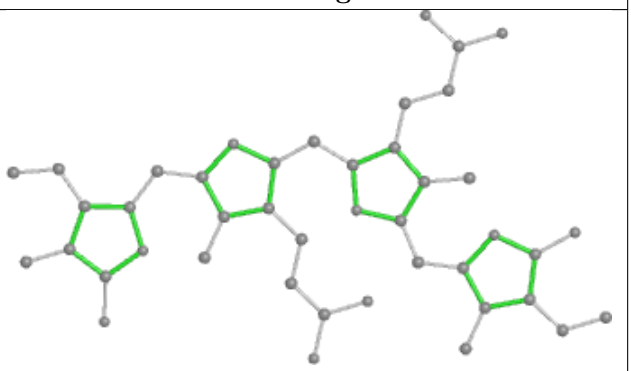

Rings

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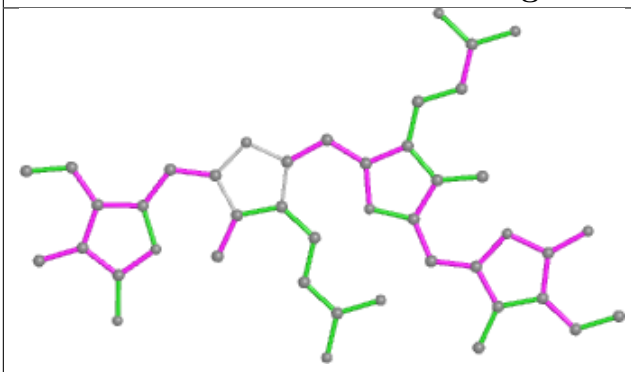

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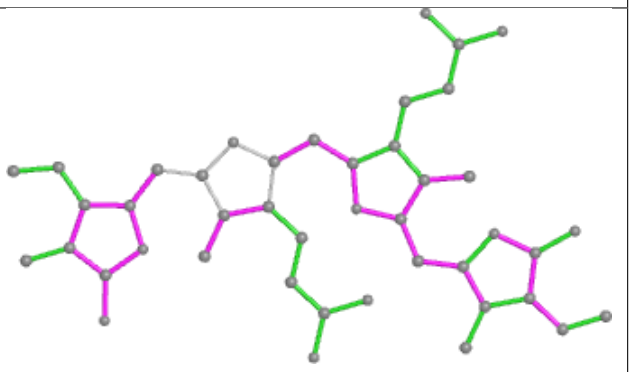

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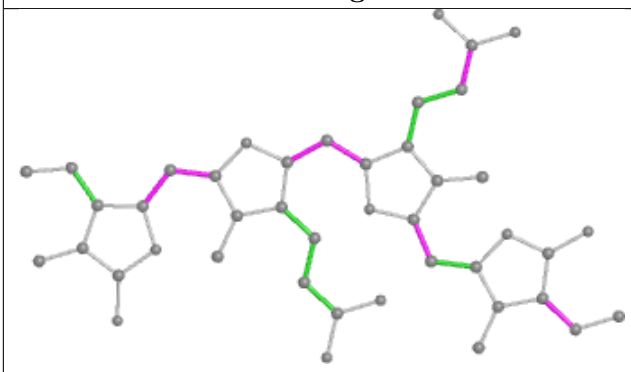

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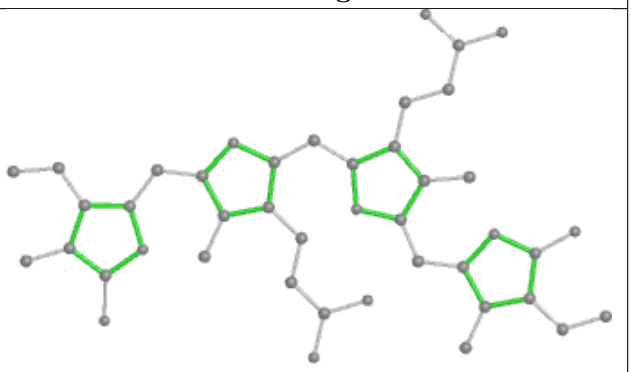

Rings

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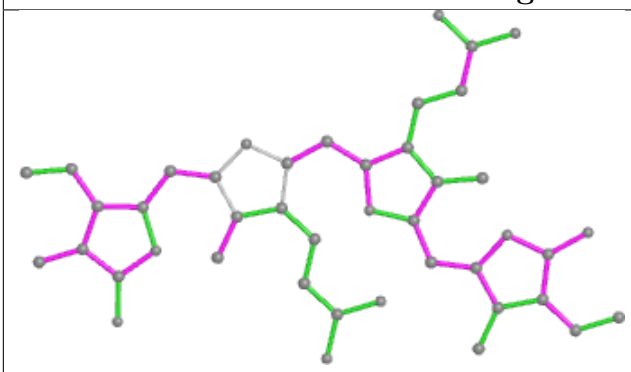

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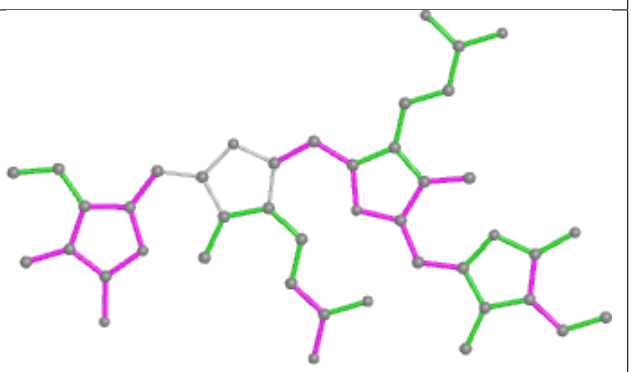

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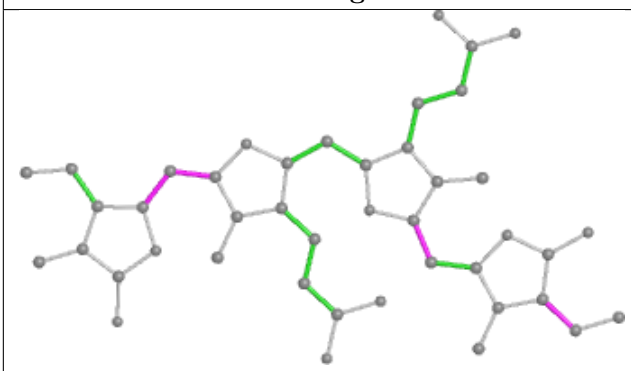

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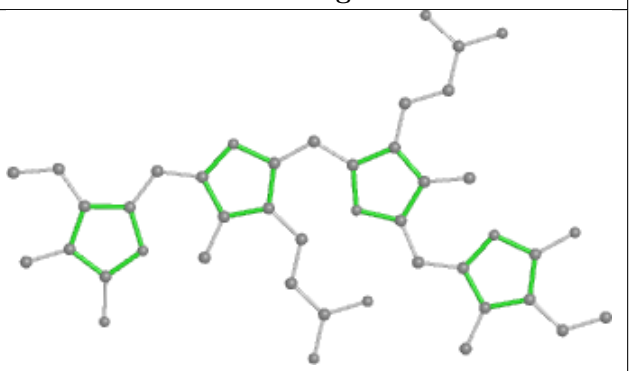

Rings

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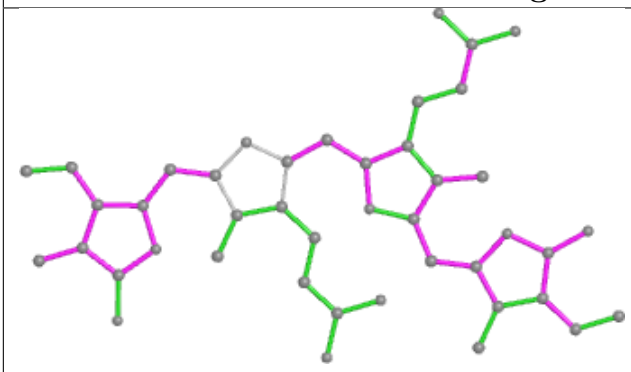

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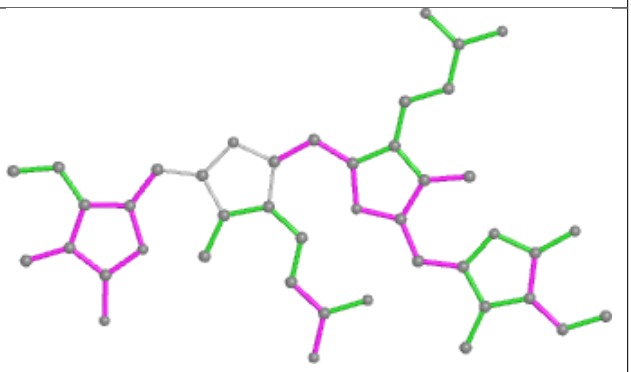

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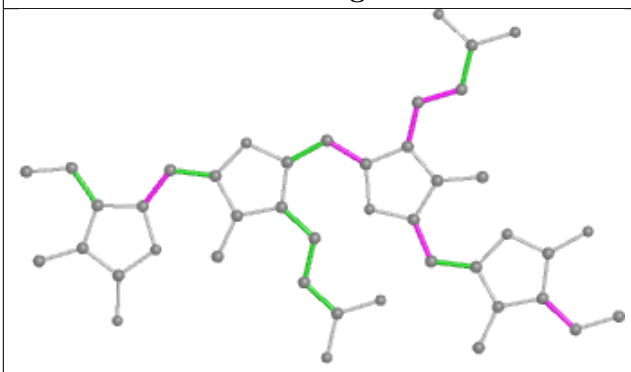

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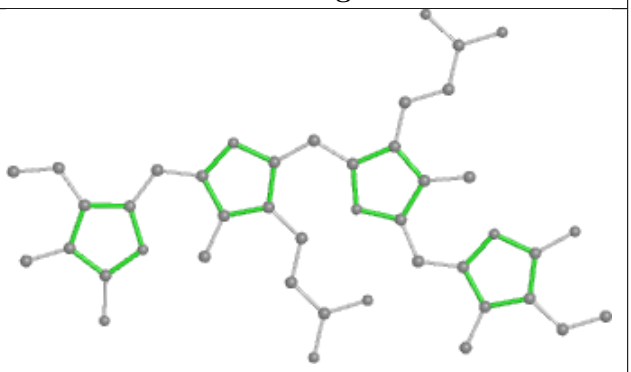

Rings

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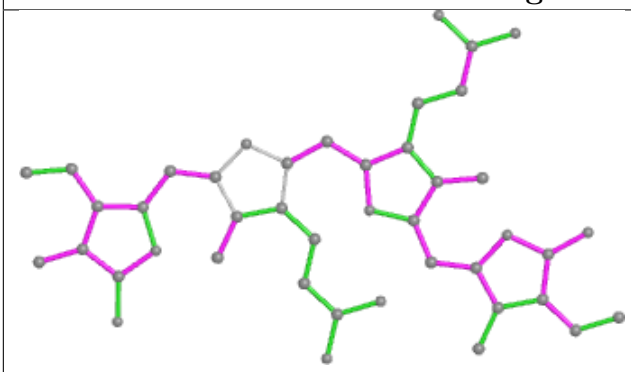

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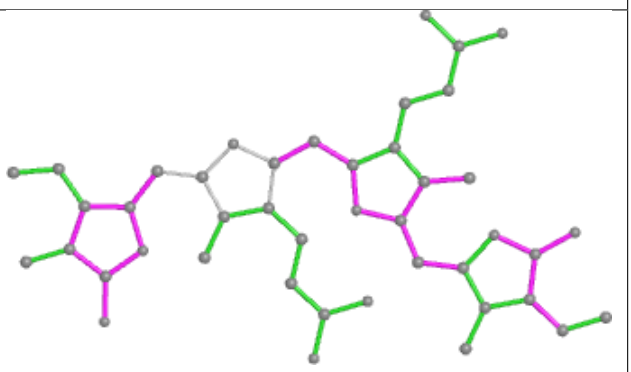

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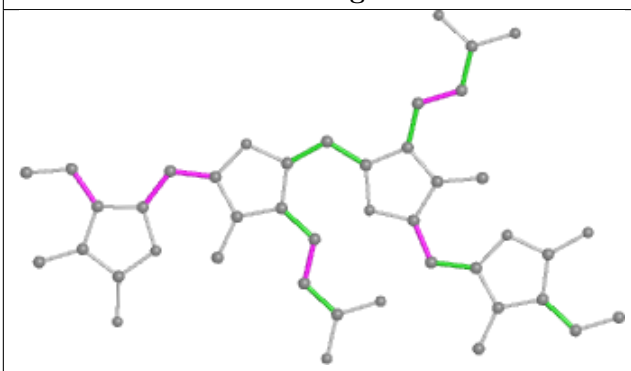
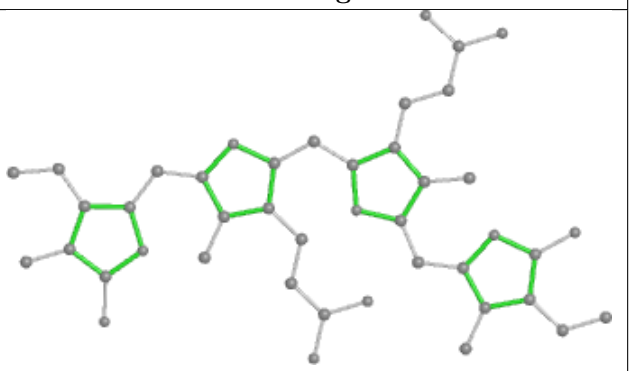
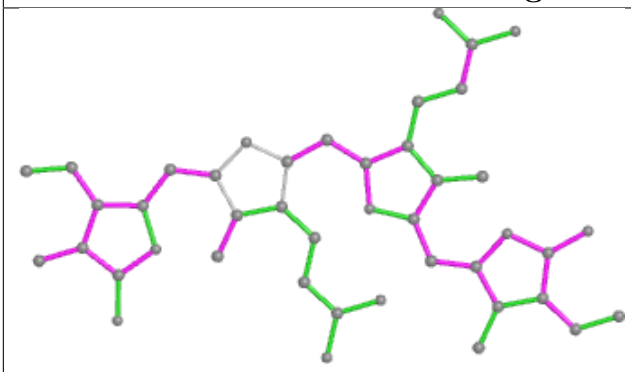


Torsions

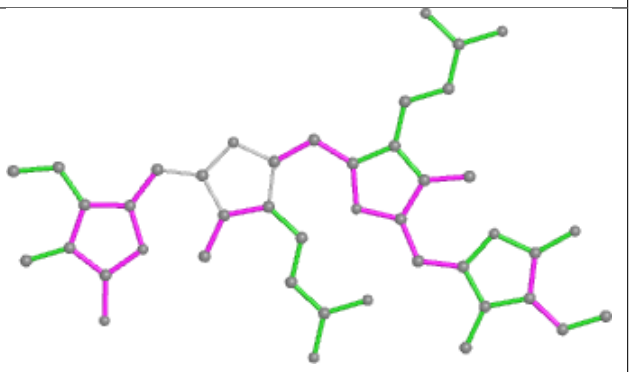


Rings

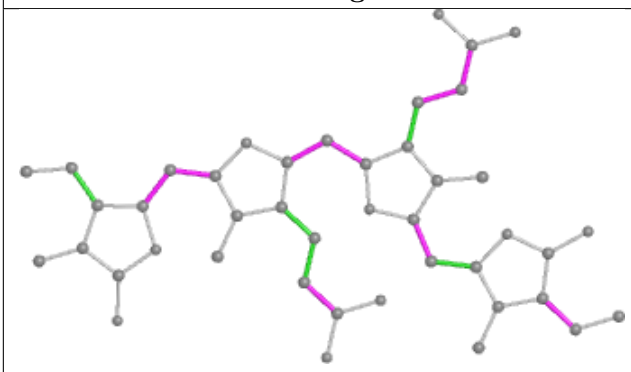
Ligand CYC b 200



Bond lengths



Bond angles



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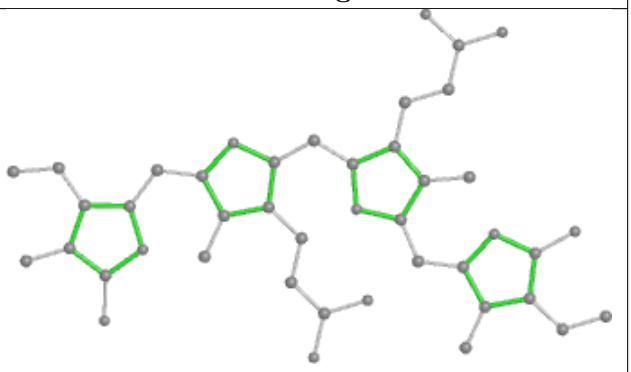
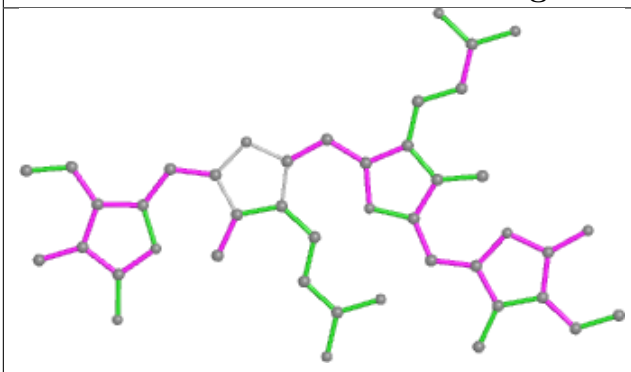


Rings

Ligand CYC f 200



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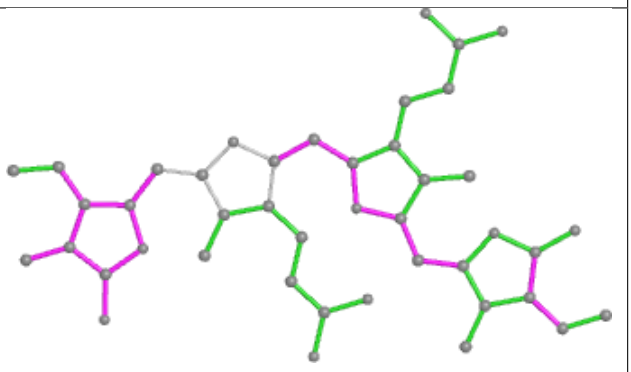
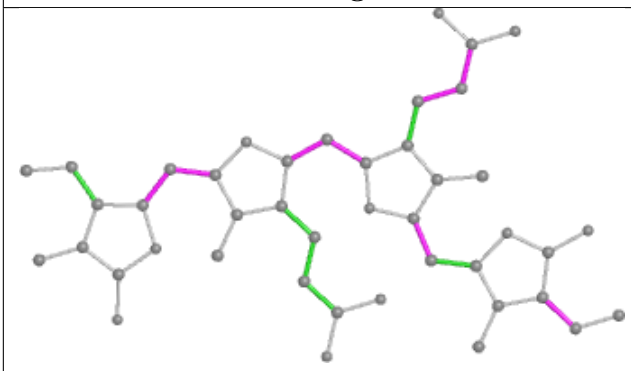


Bond angles



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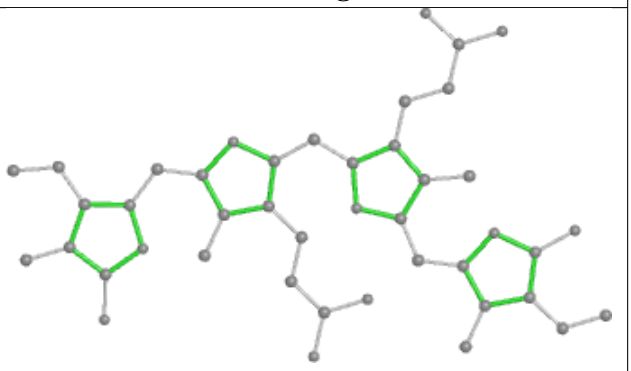
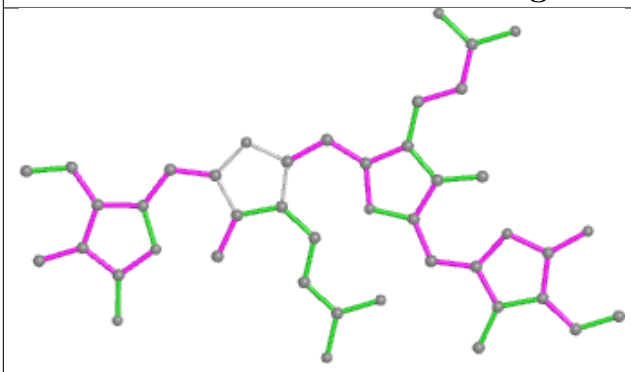


Rings

Ligand CYC j 201



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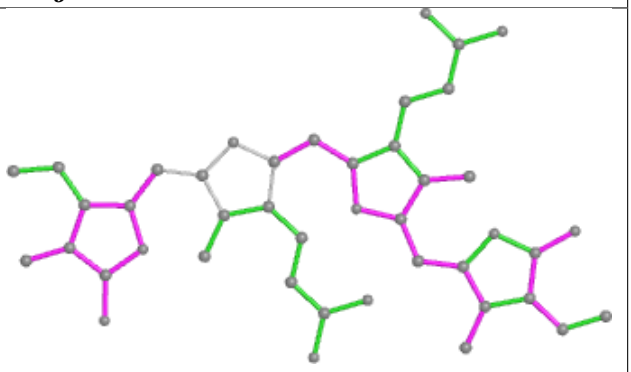
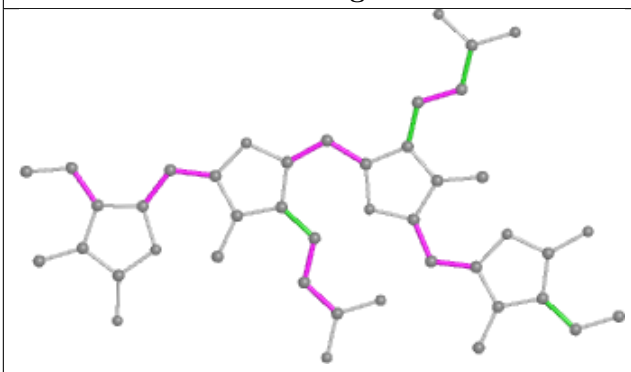


Bond angles



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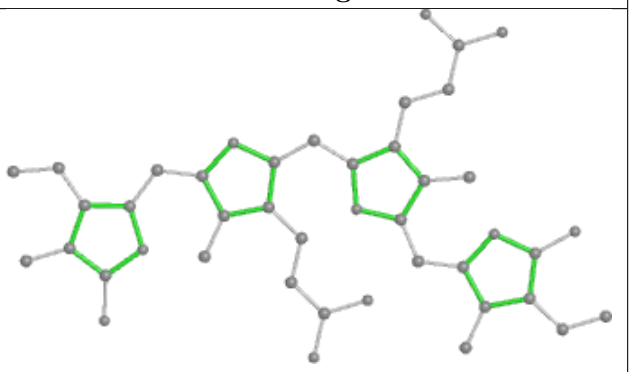
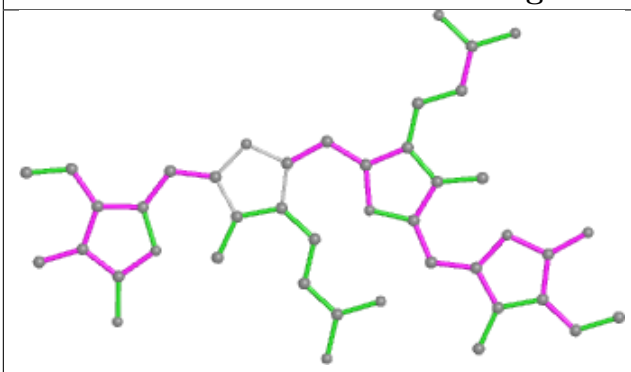


Rings

Ligand CYC 3 601



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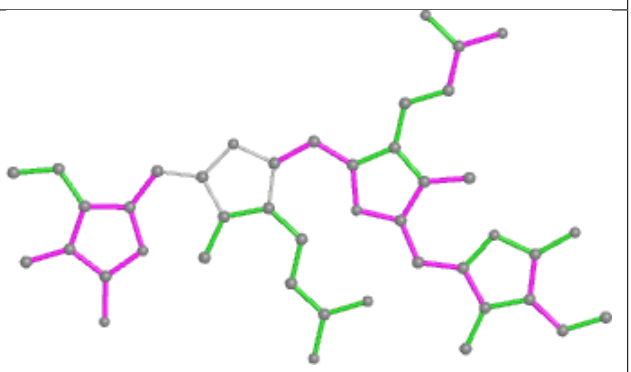

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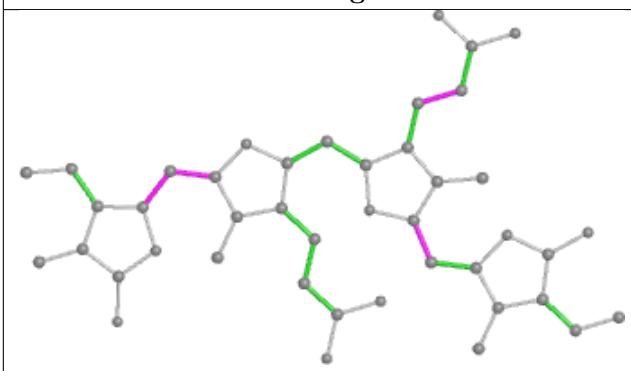

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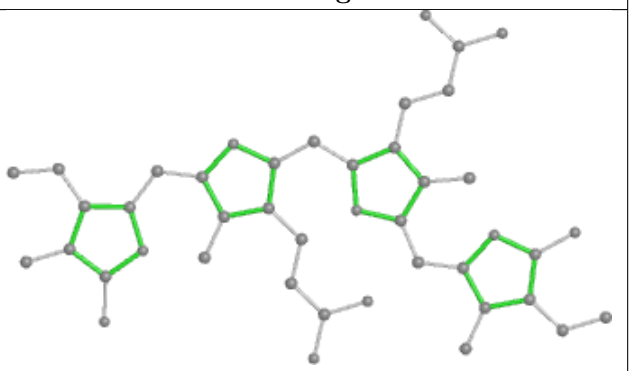
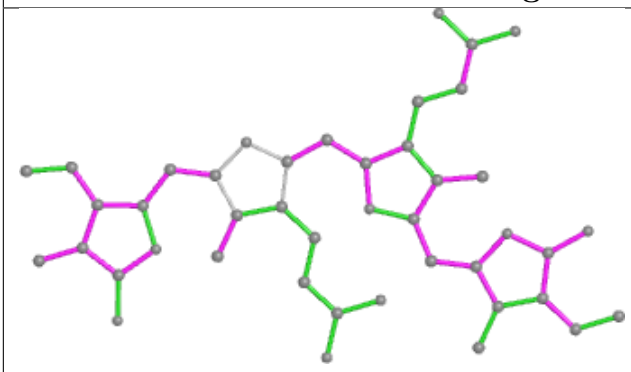


Rings

Ligand CYC T 201



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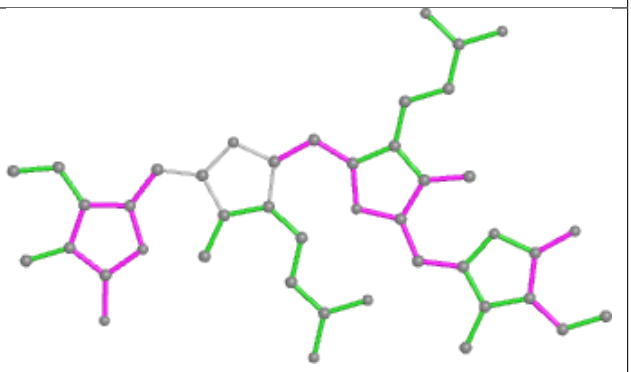

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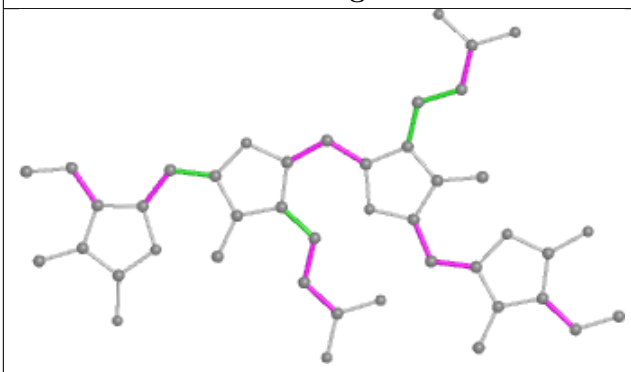

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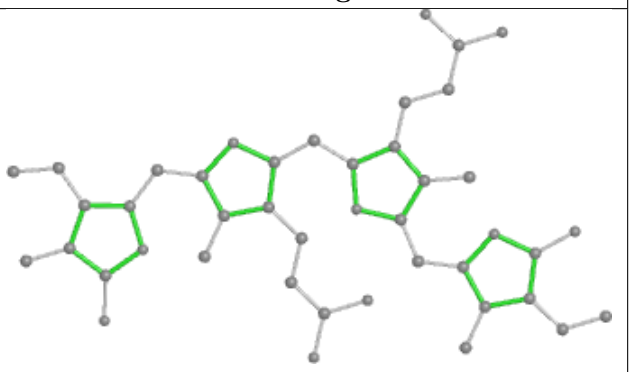
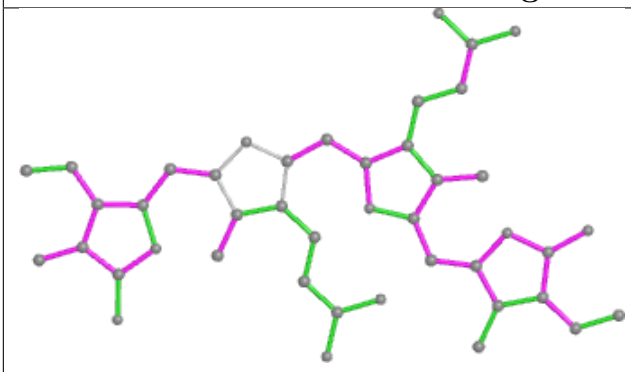


Rings

Ligand CYC V 200



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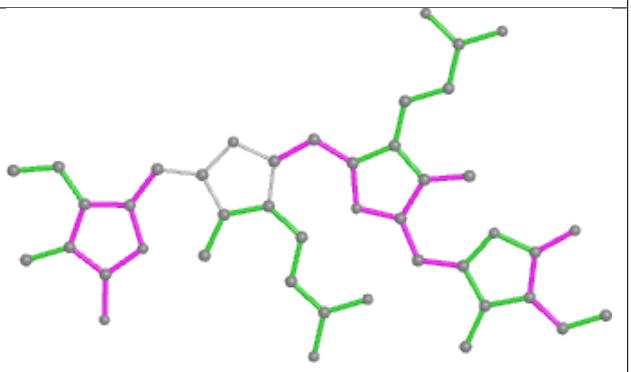

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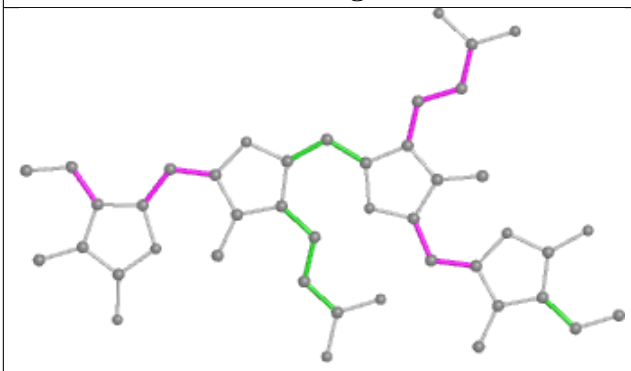

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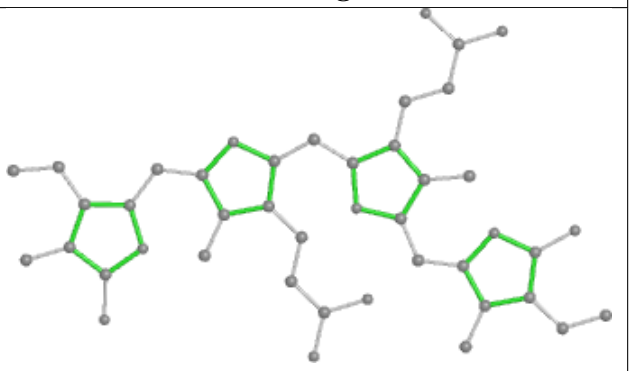

Rings

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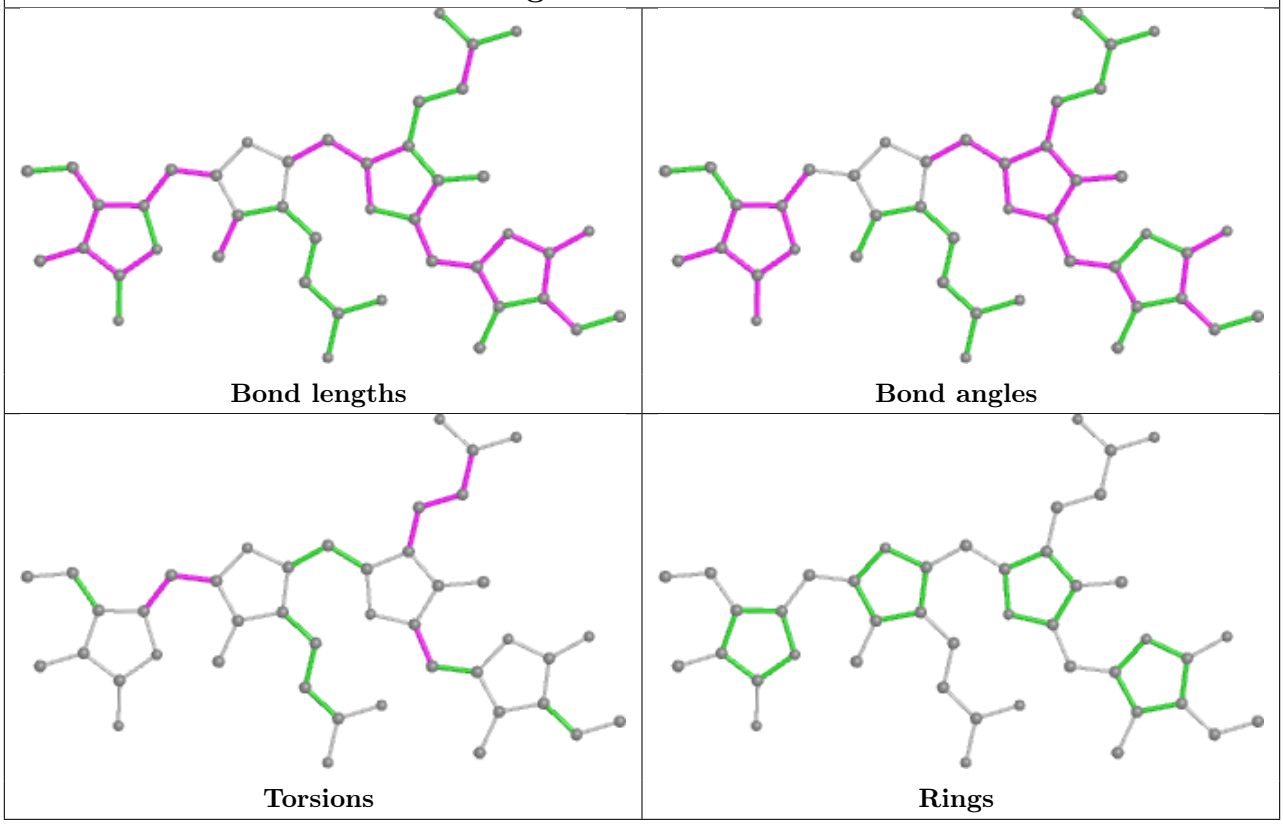

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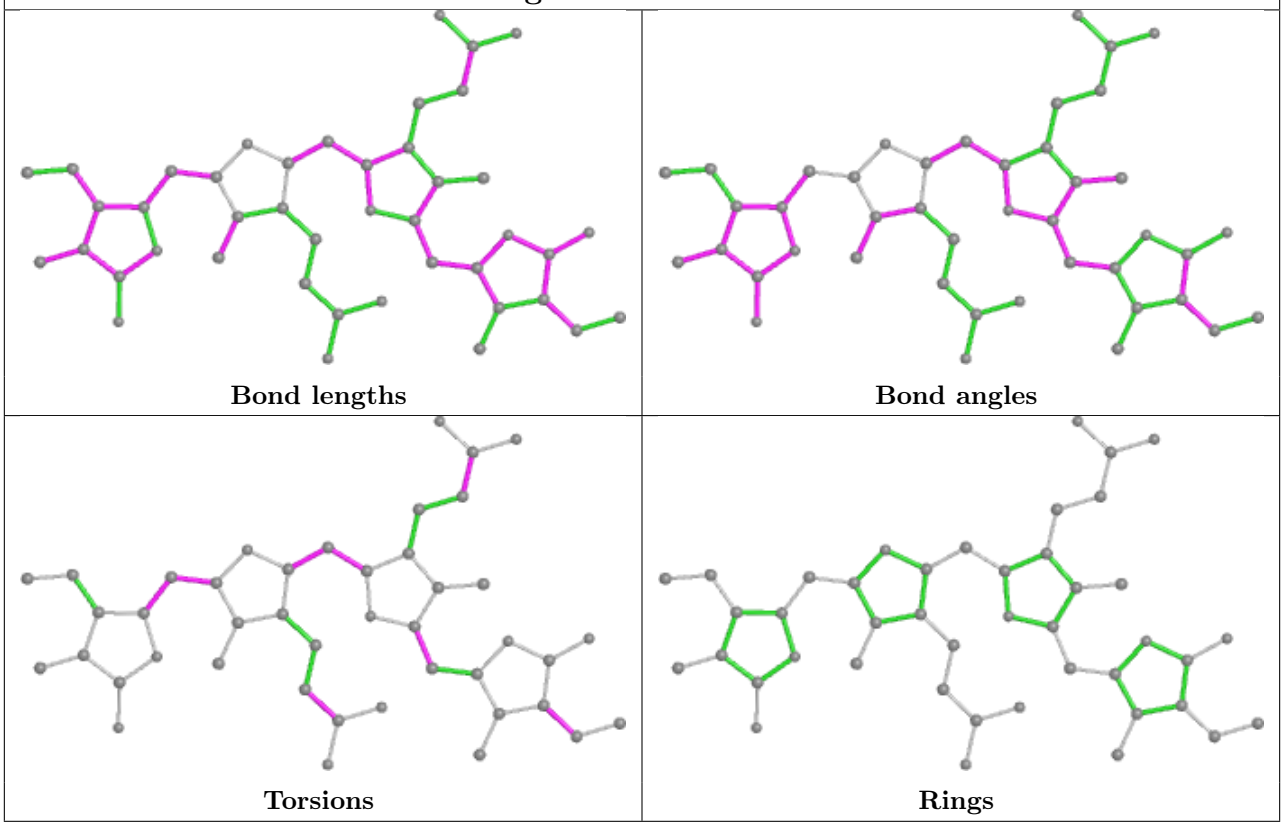

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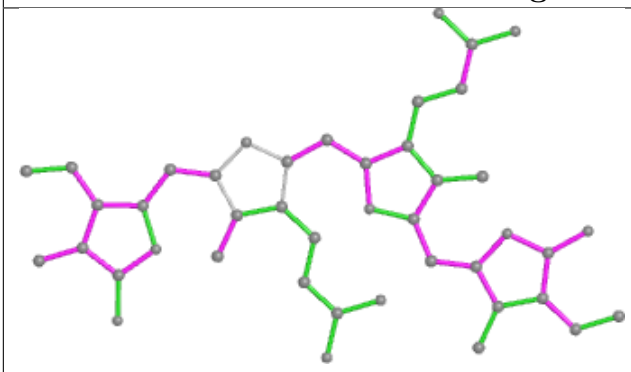

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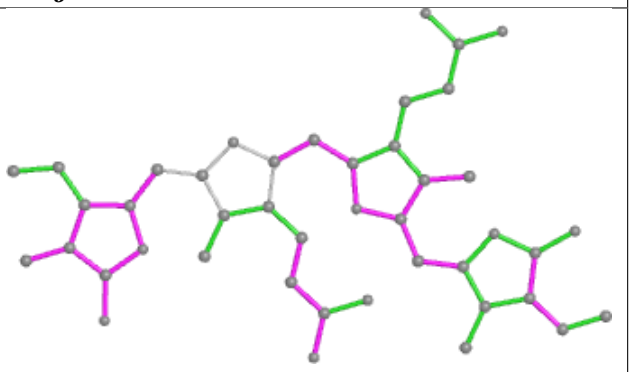
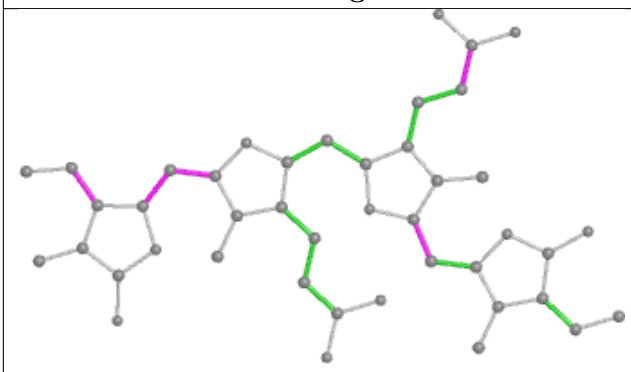


Bond angles



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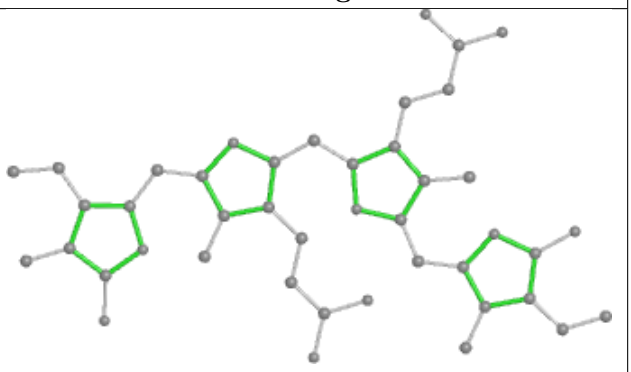

Rings

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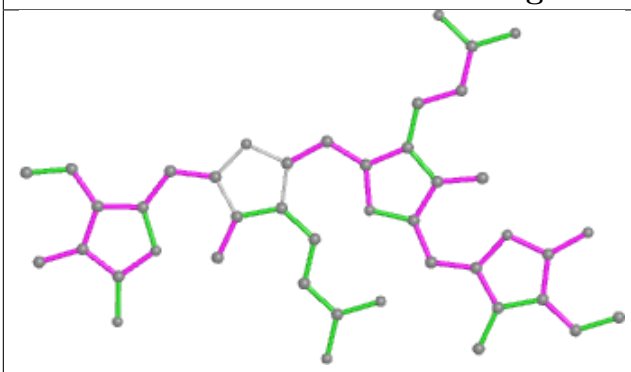

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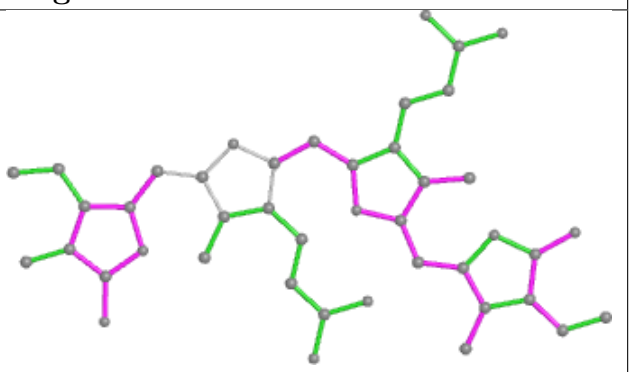
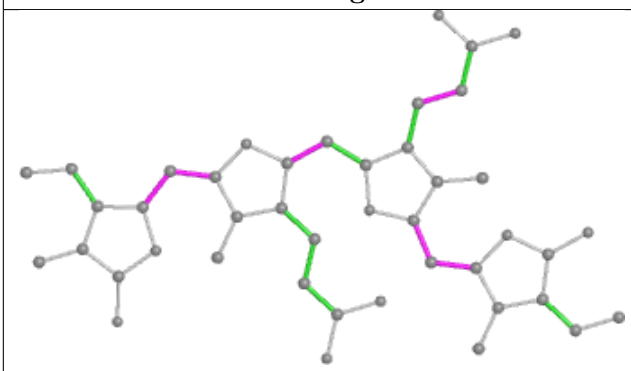


Bond angles



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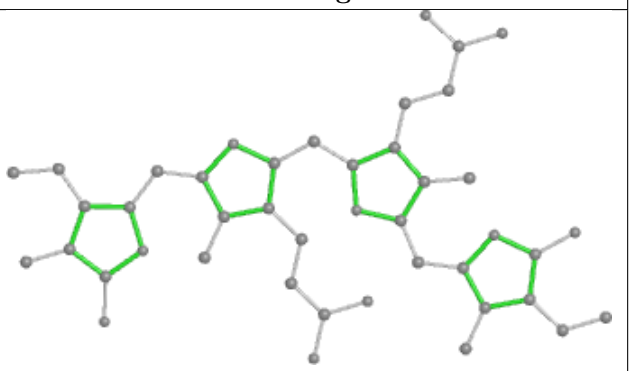
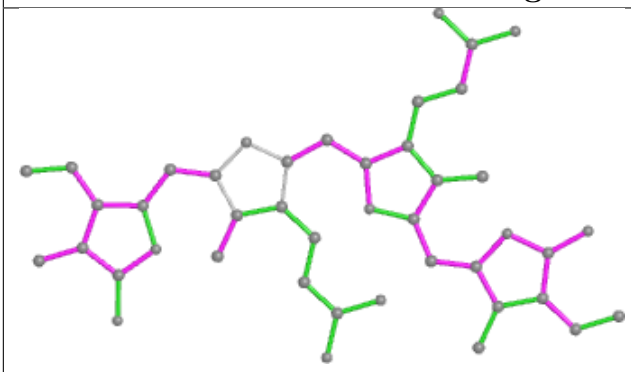


Rings

Ligand CYC L 201



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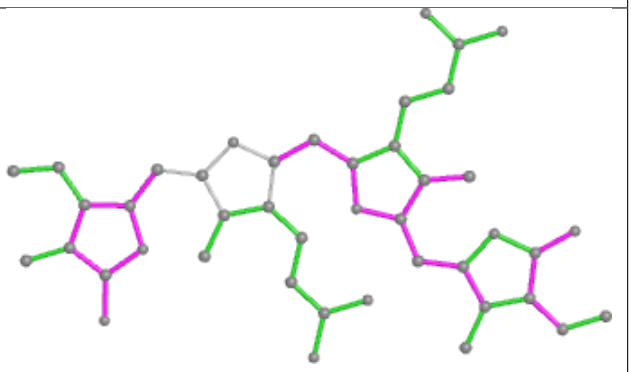
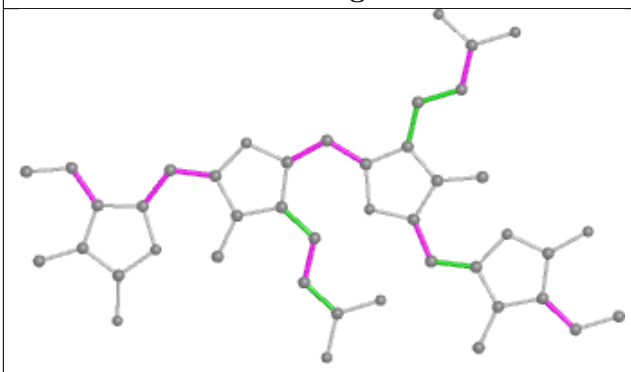


Bond angles



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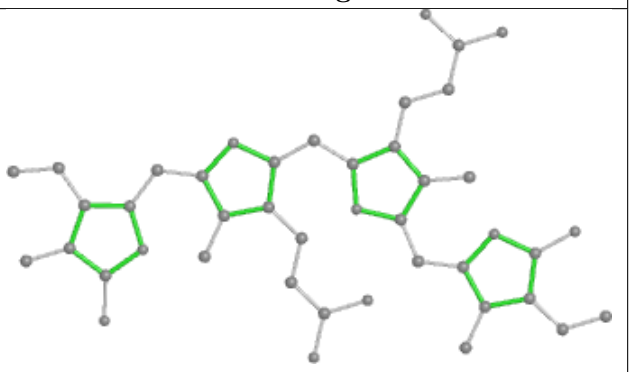
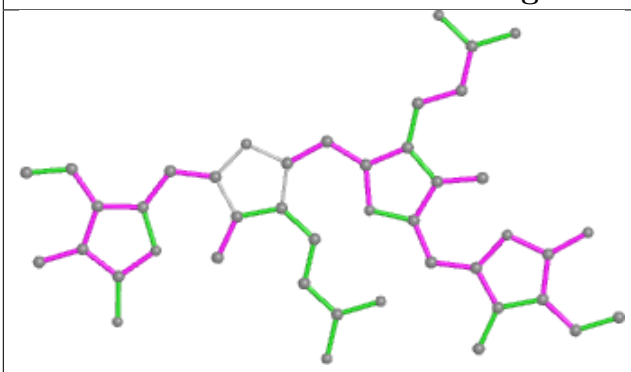


Rings

Ligand CYC V 201



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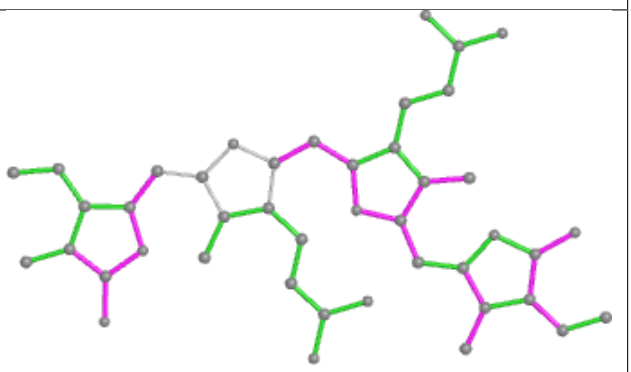
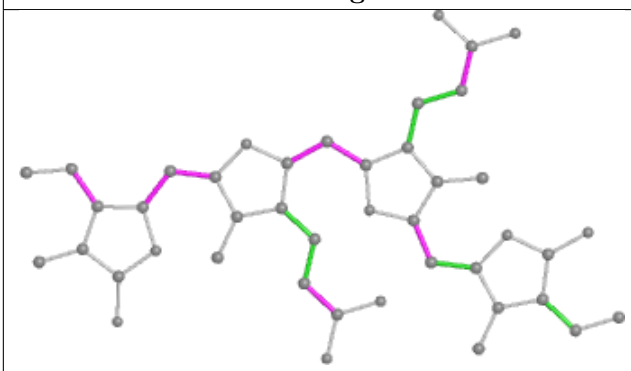


Bond angles



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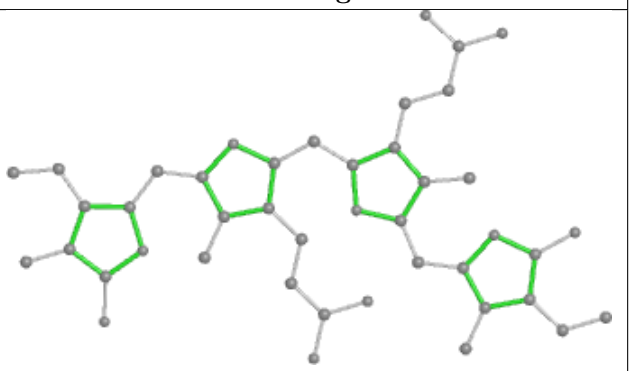
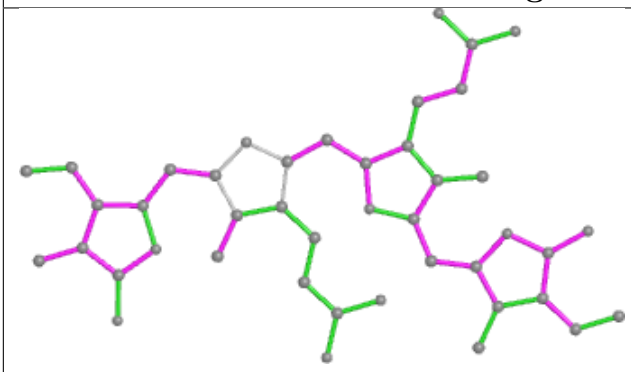


Rings

Ligand CYC 4 301



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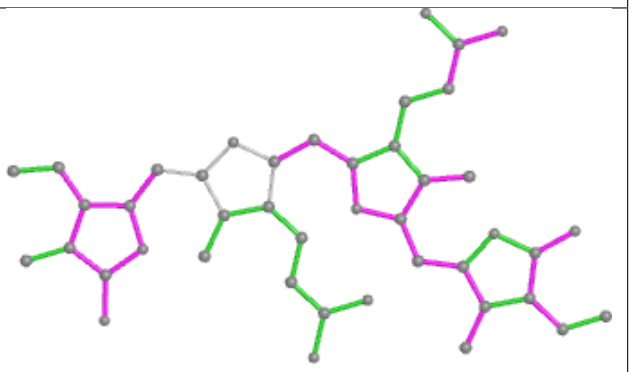

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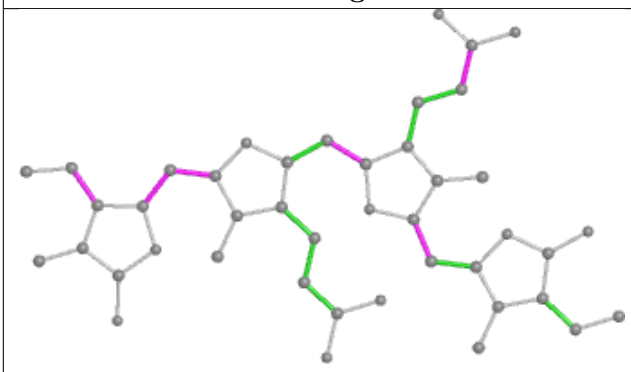

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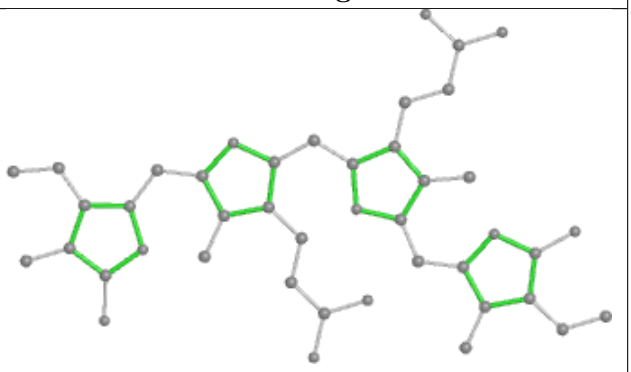
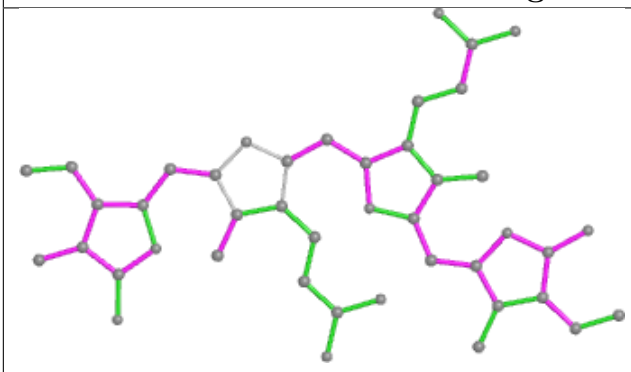


Rings

Ligand CYC c 200



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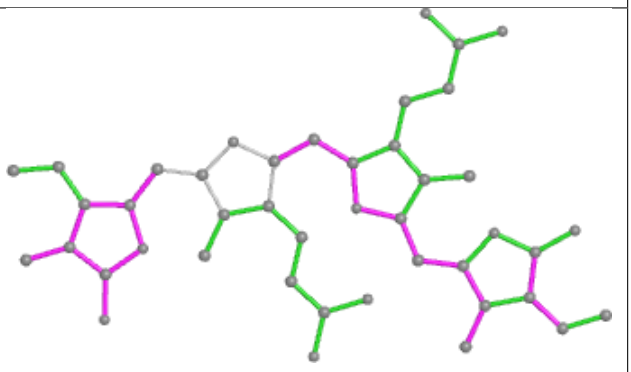
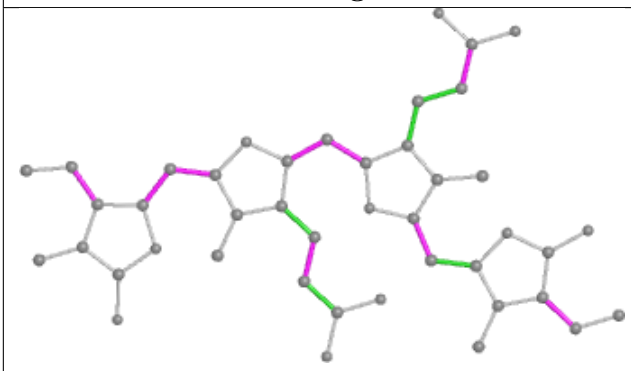


Bond angles



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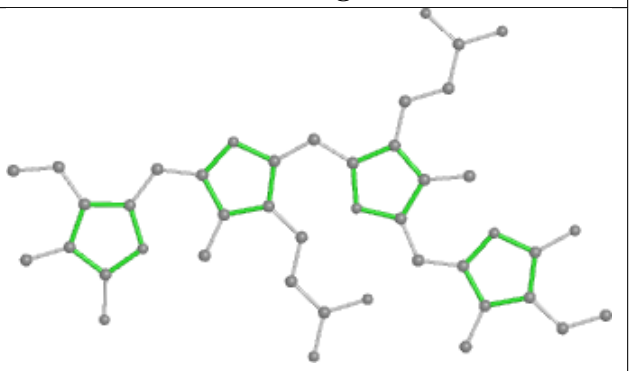
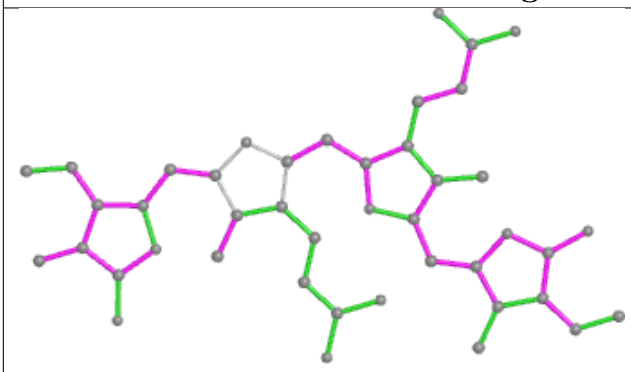


Rings

Ligand CYC G 201



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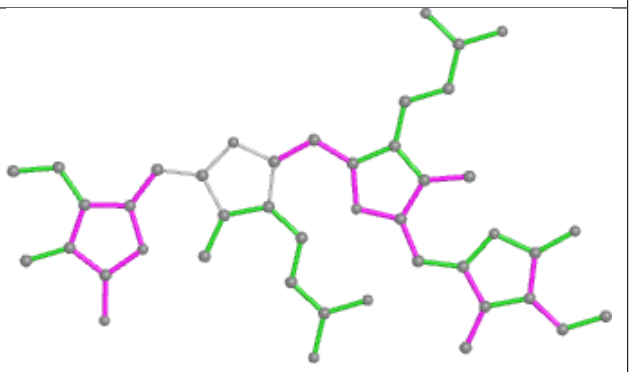
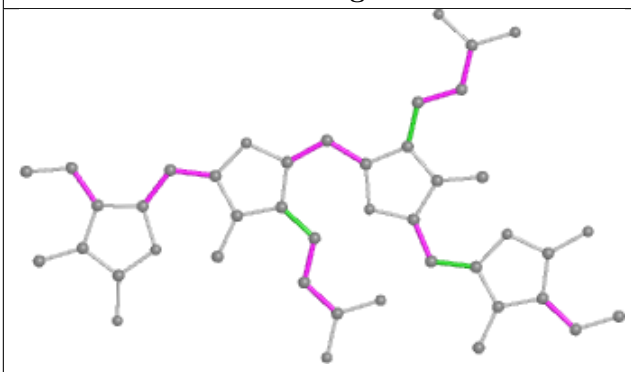


Bond angles



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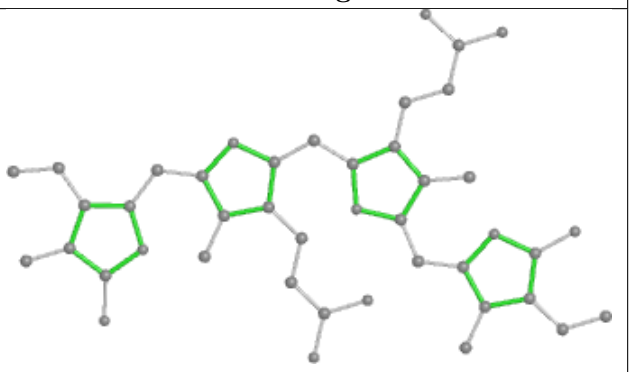
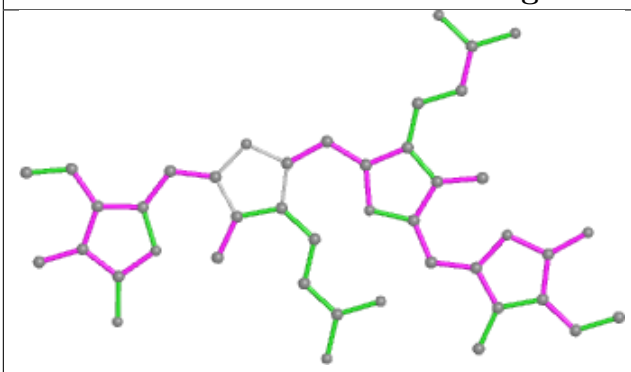


Rings

Ligand CYC U 201



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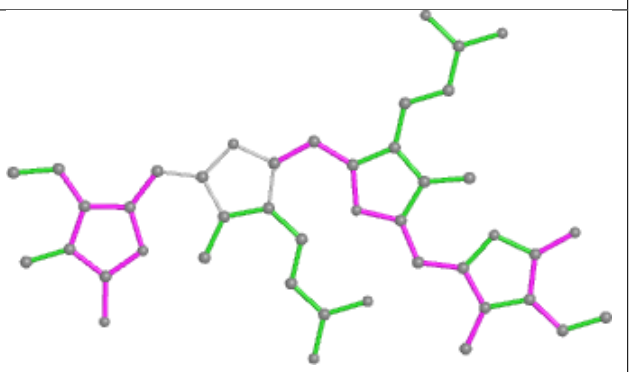
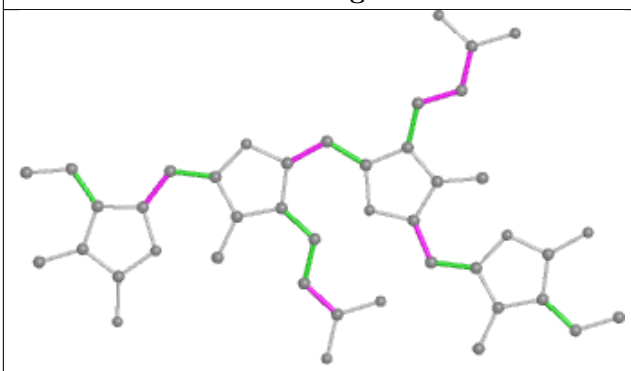
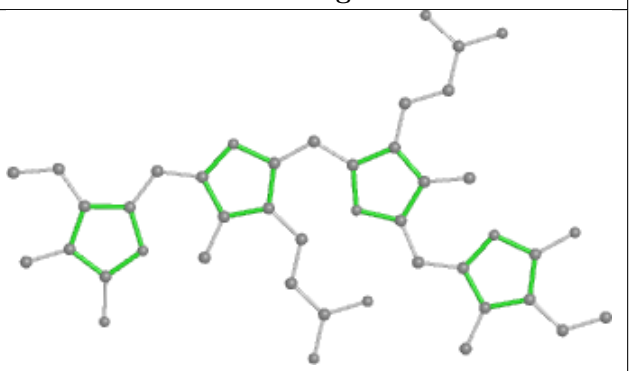


Bond angles

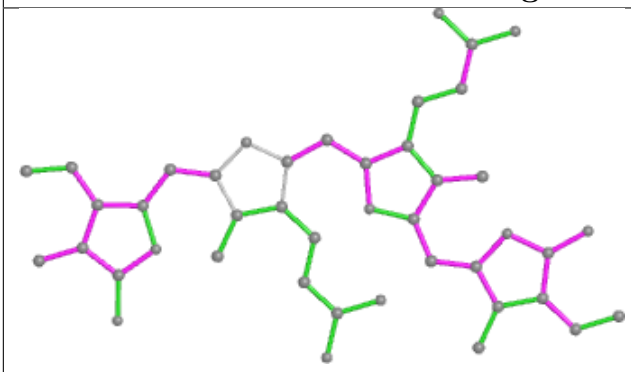


Torsions

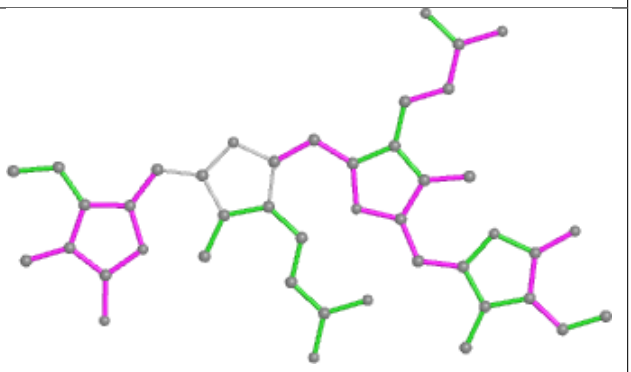


Rings

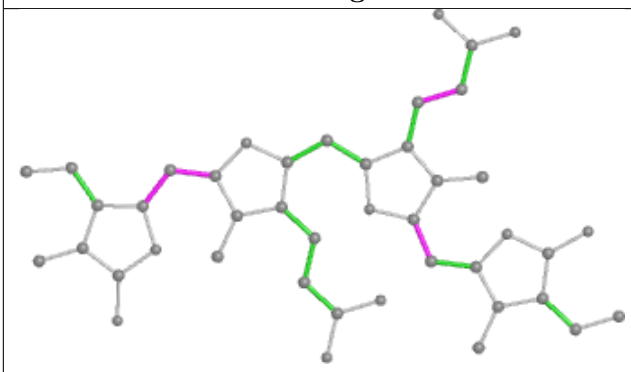
Ligand CYC Y 200



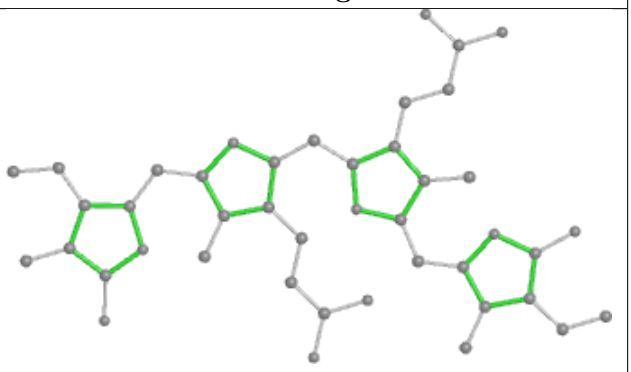
Bond lengths



Bond angles

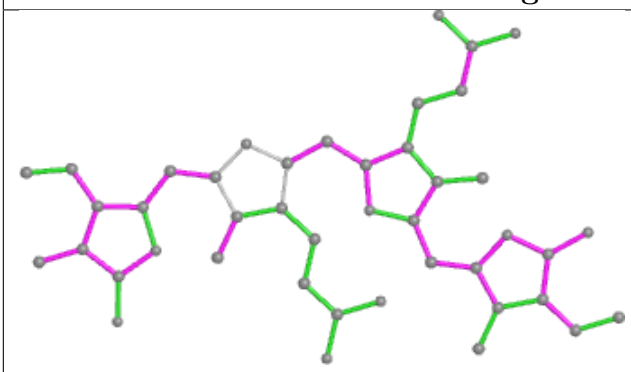


Torsions

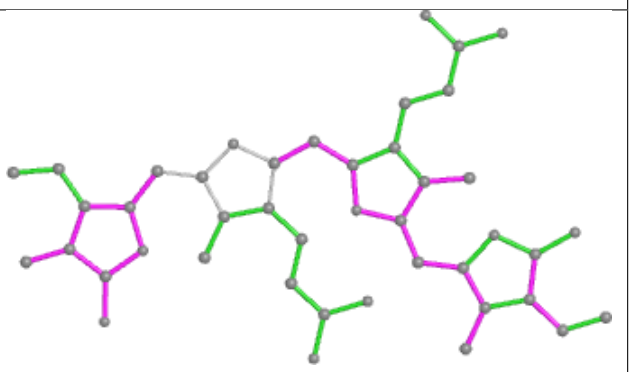


Rings

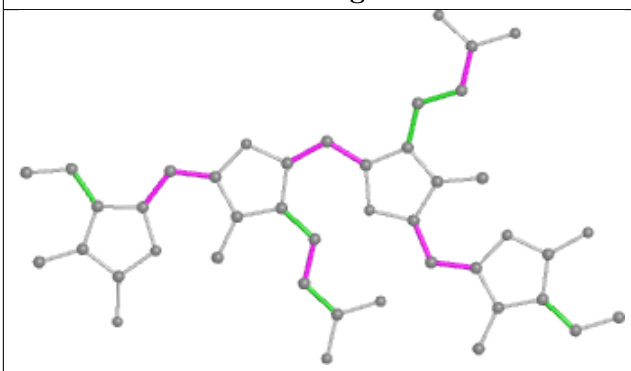
Ligand CYC X 201



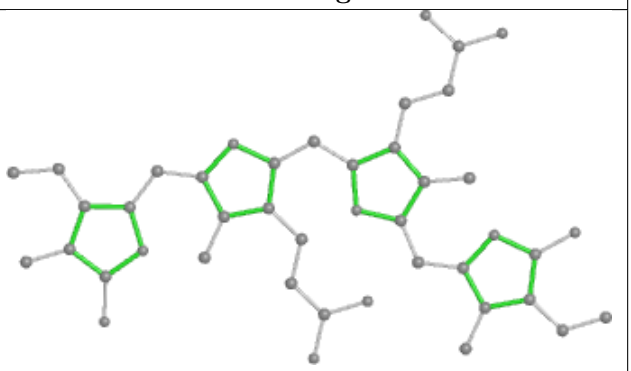
Bond lengths



Bond angles

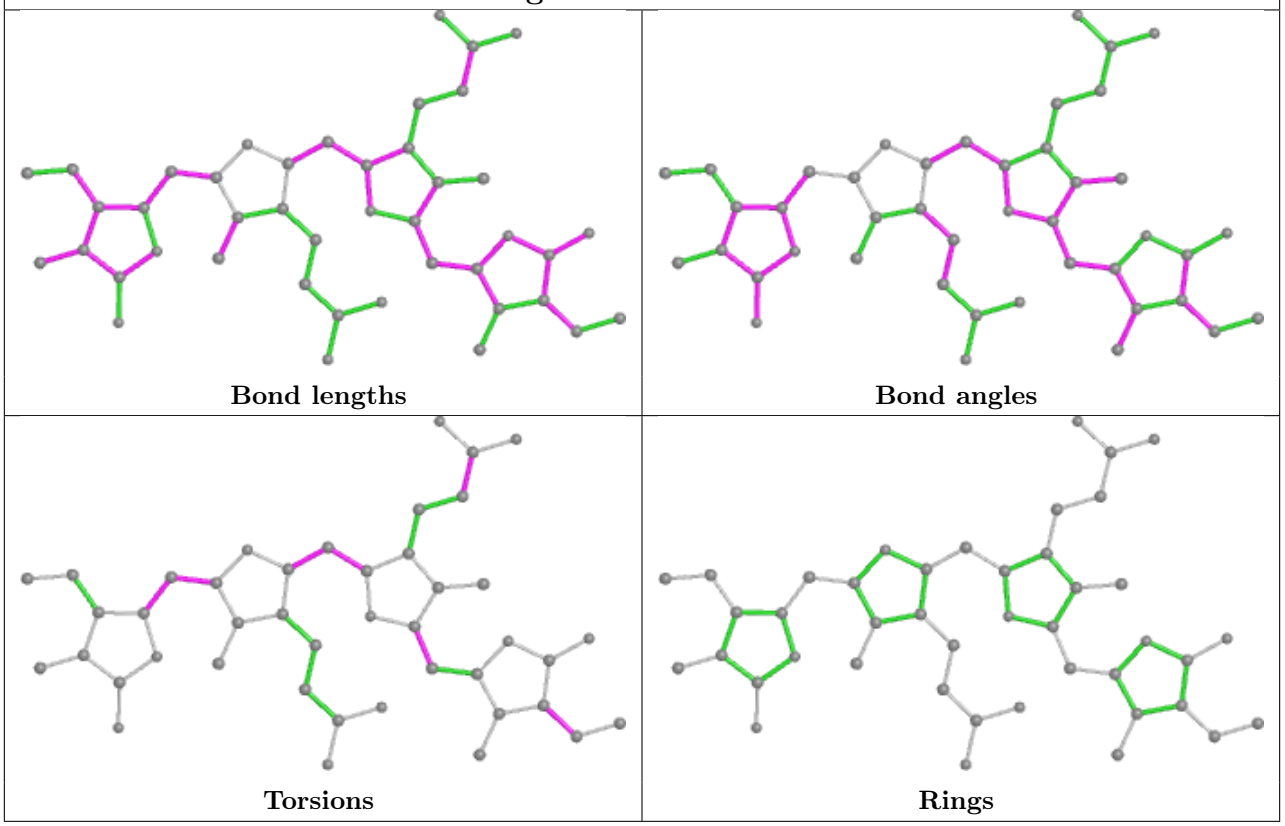


Torsions



Rings

Ligand CYC d 200



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

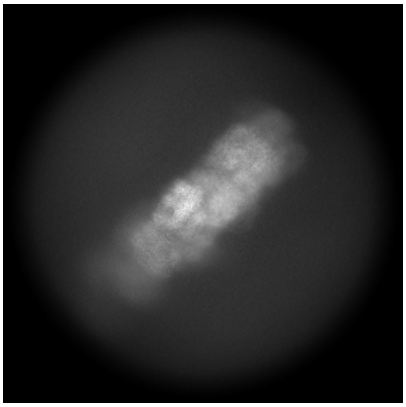
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35568. These allow visual inspection of the internal detail of the map and identification of artifacts.

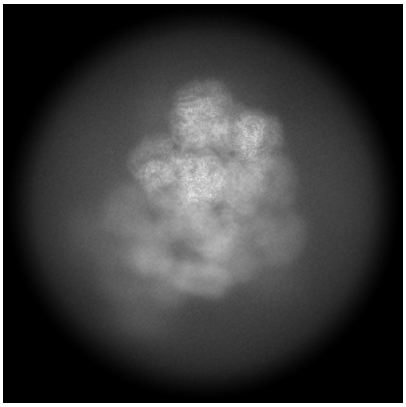
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

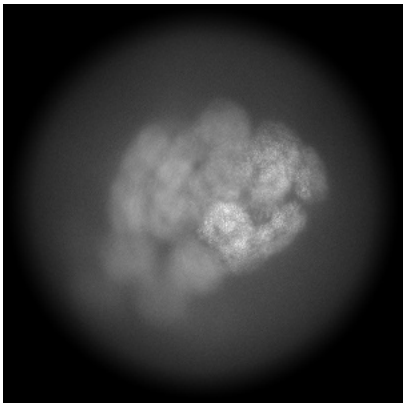
6.1.1 Primary map



X



Y

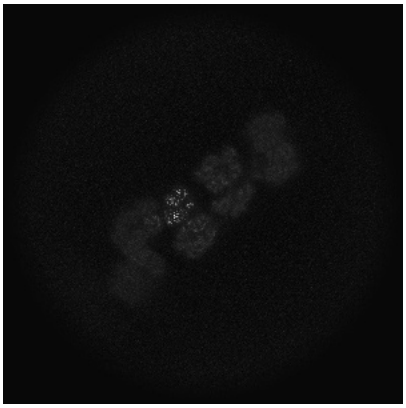


Z

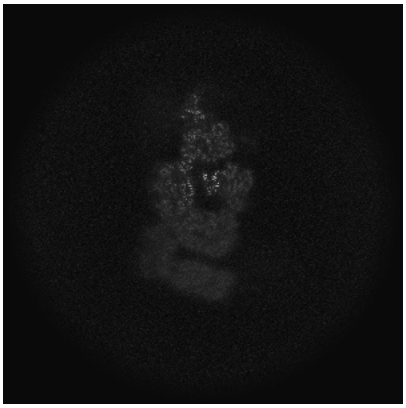
The images above show the map projected in three orthogonal directions.

6.2 Central slices

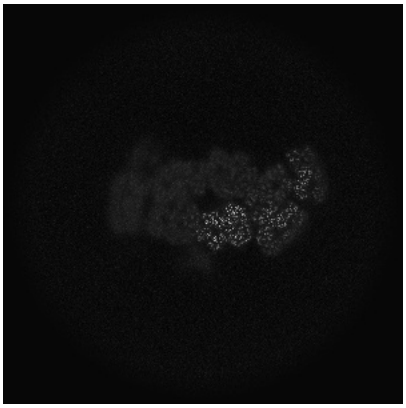
6.2.1 Primary map



X Index: 340



Y Index: 340

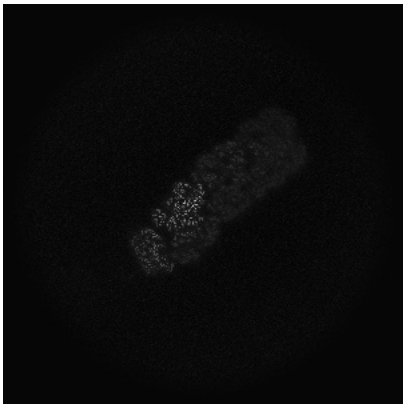


Z Index: 340

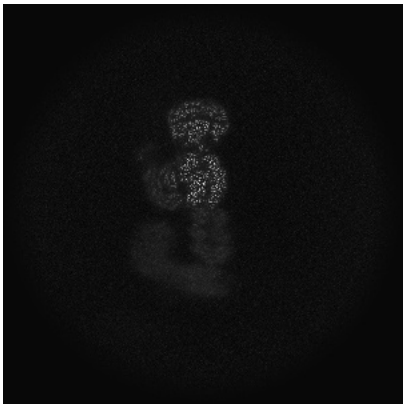
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

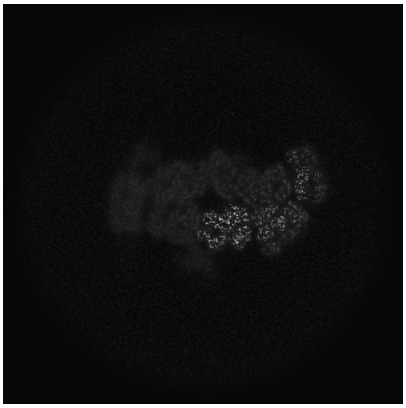
6.3.1 Primary map



X Index: 383



Y Index: 305

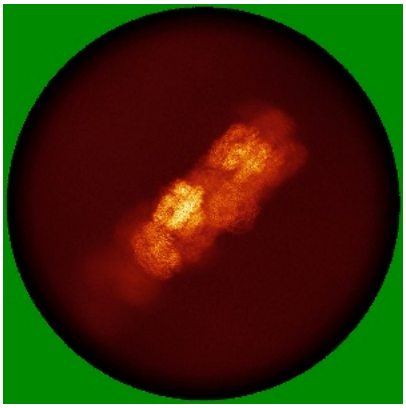


Z Index: 337

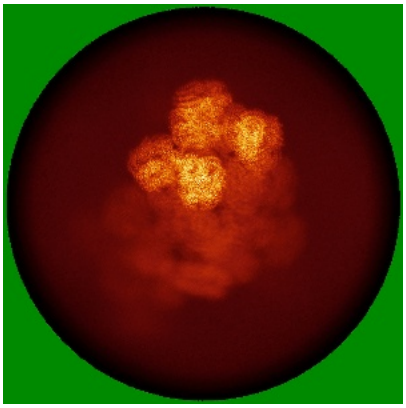
The images above show the largest variance slices of the map in three orthogonal directions.

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

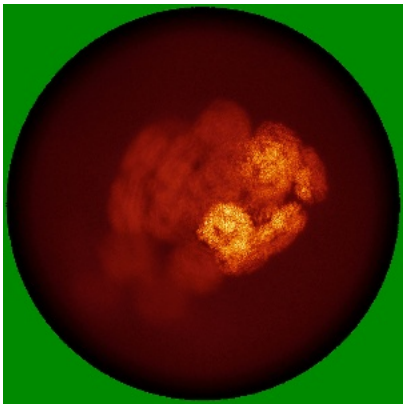
6.4.1 Primary map



X



Y

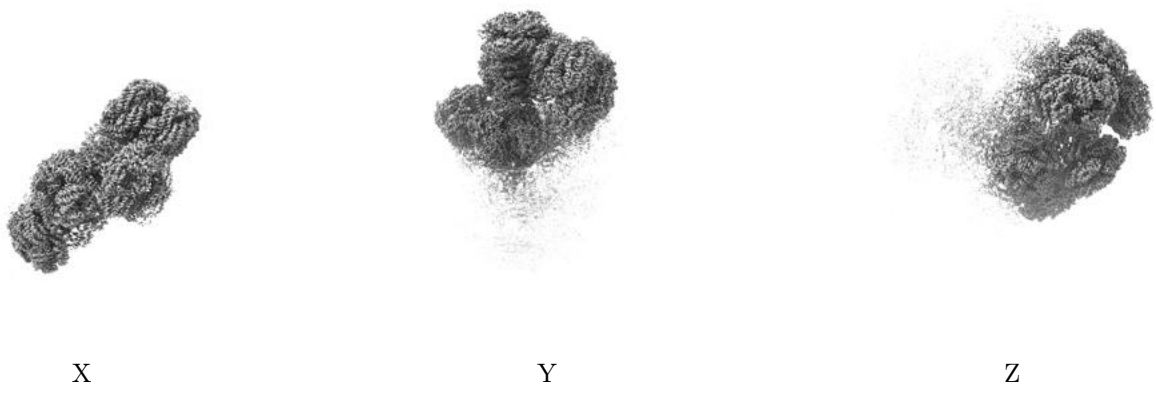


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

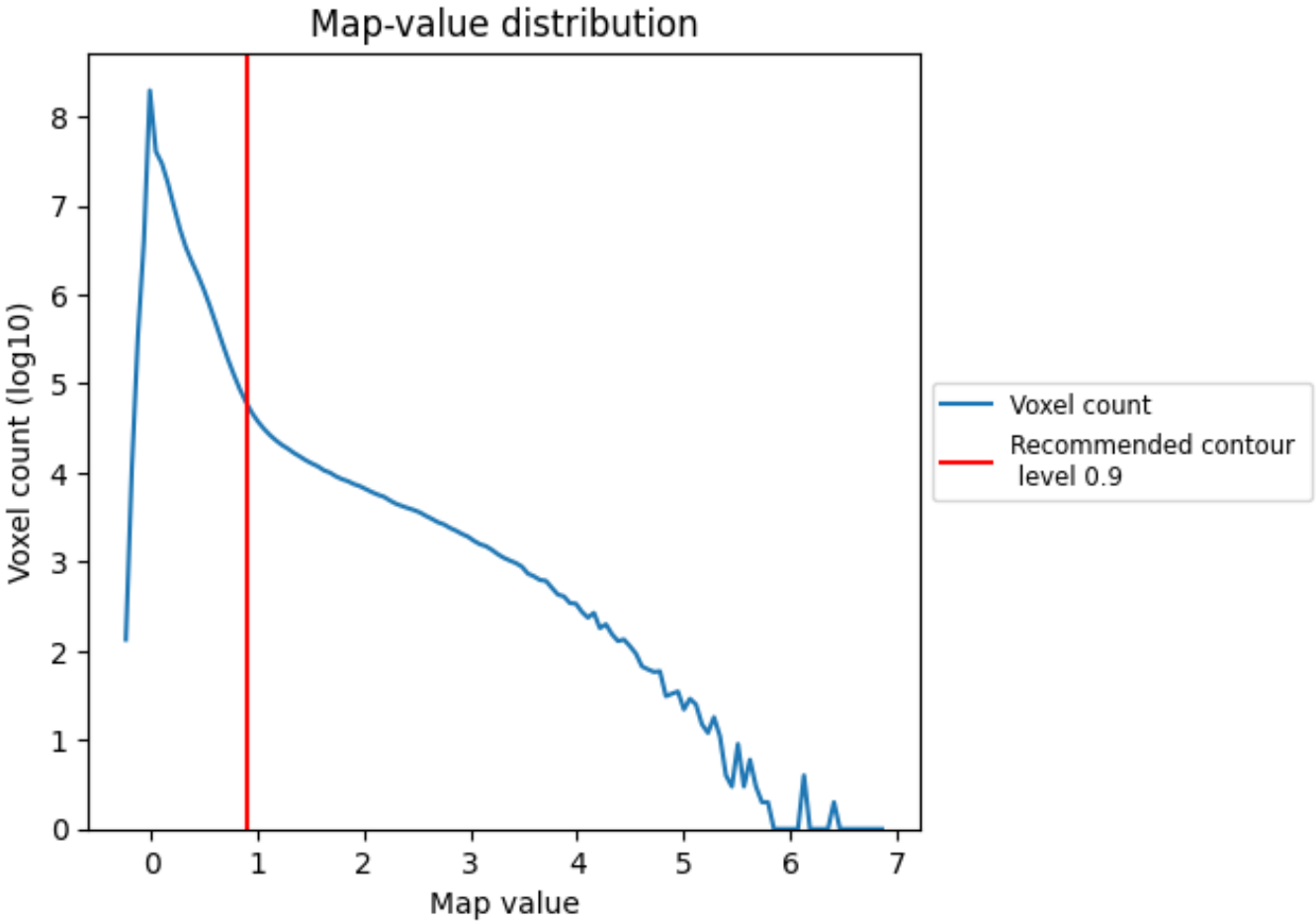
6.6 Mask visualisation (i)

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

7 Map analysis

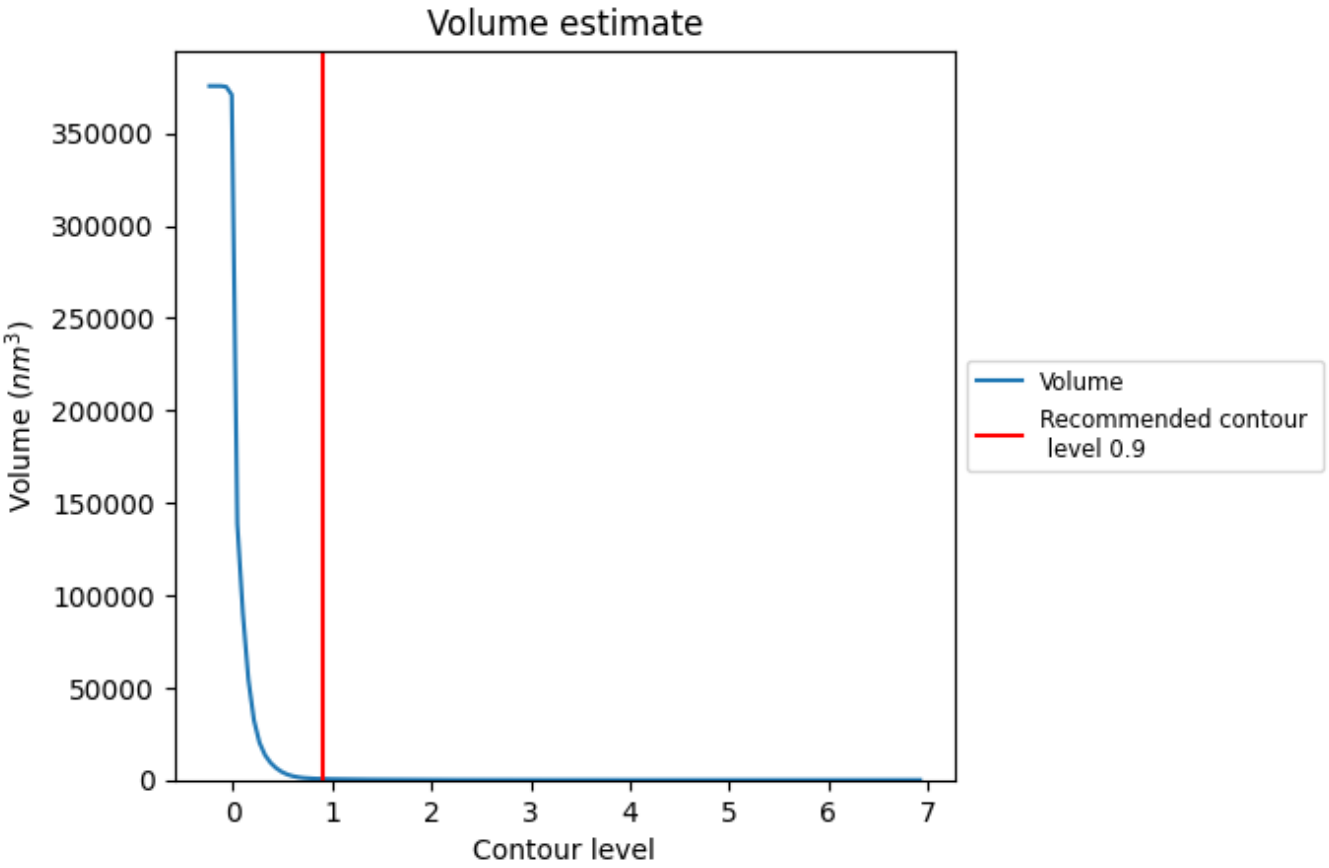
This section contains the results of statistical analysis of the map.

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.

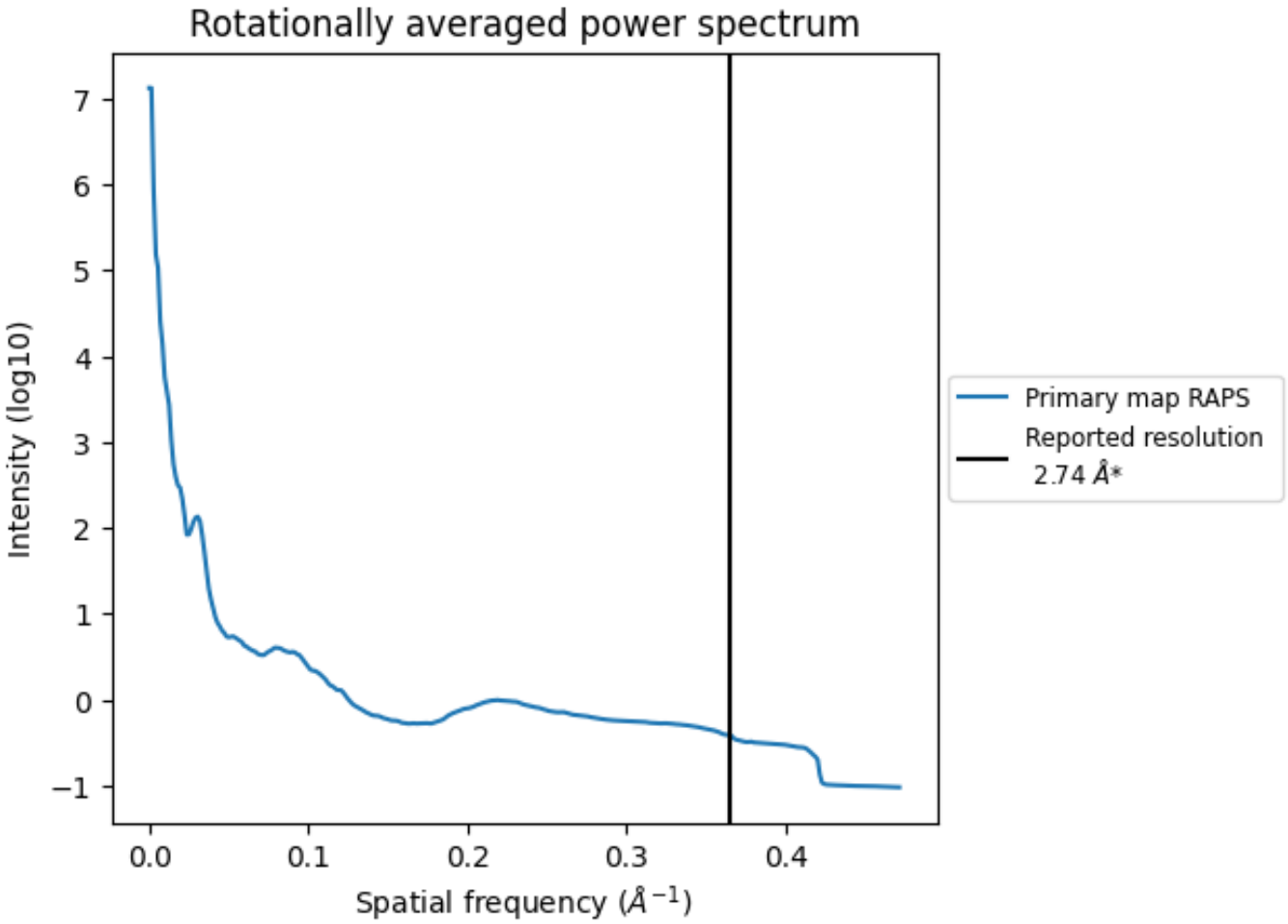
7.2 Volume estimate



The volume at the recommended contour level is 570 nm^3; this corresponds to an approximate mass of 515 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 0.365 Å^{-1}

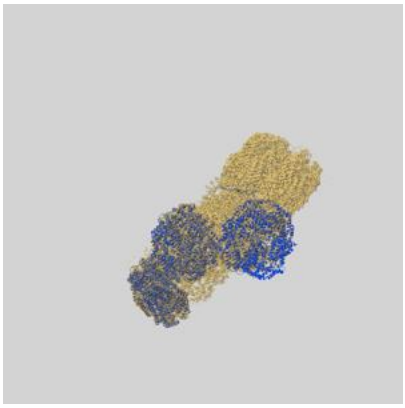
8 Fourier-Shell correlation

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

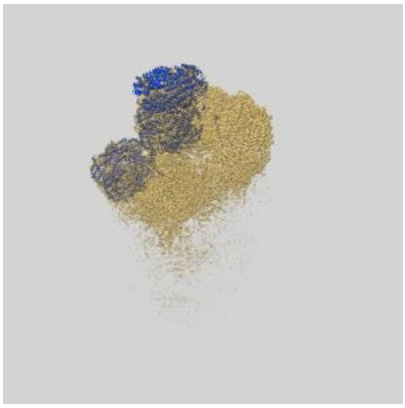
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35568 and PDB model 8IML. Per-residue inclusion information can be found in section 3 on page 11.

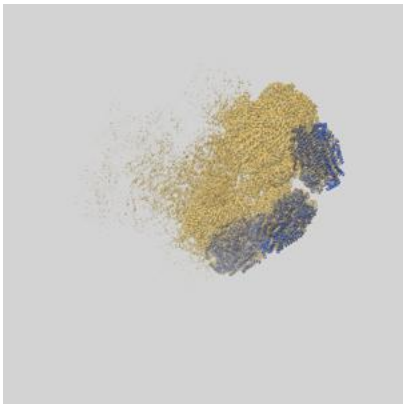
9.1 Map-model overlay



X



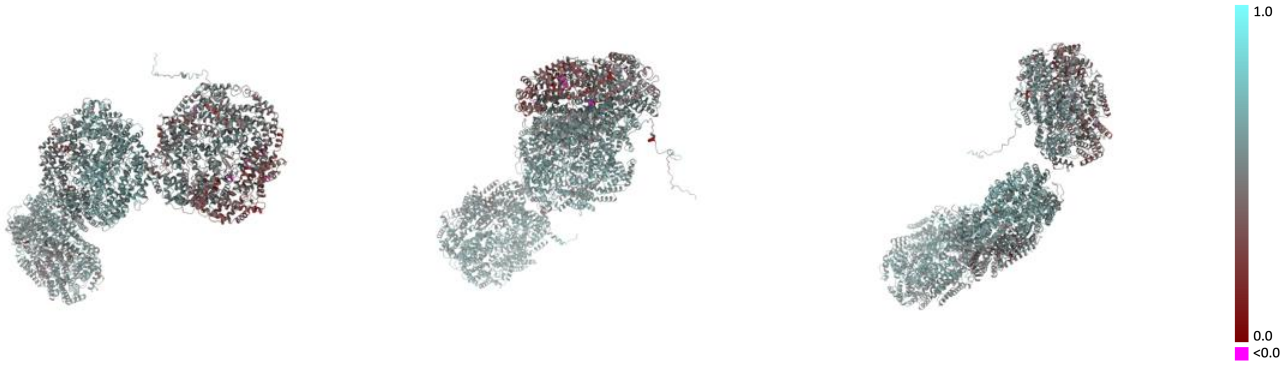
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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.

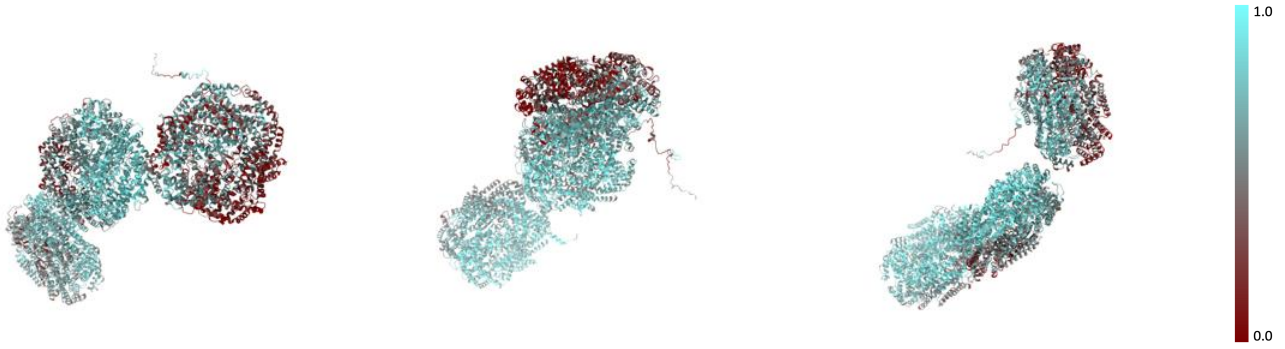
9.2 Q-score mapped to coordinate model (i)



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.

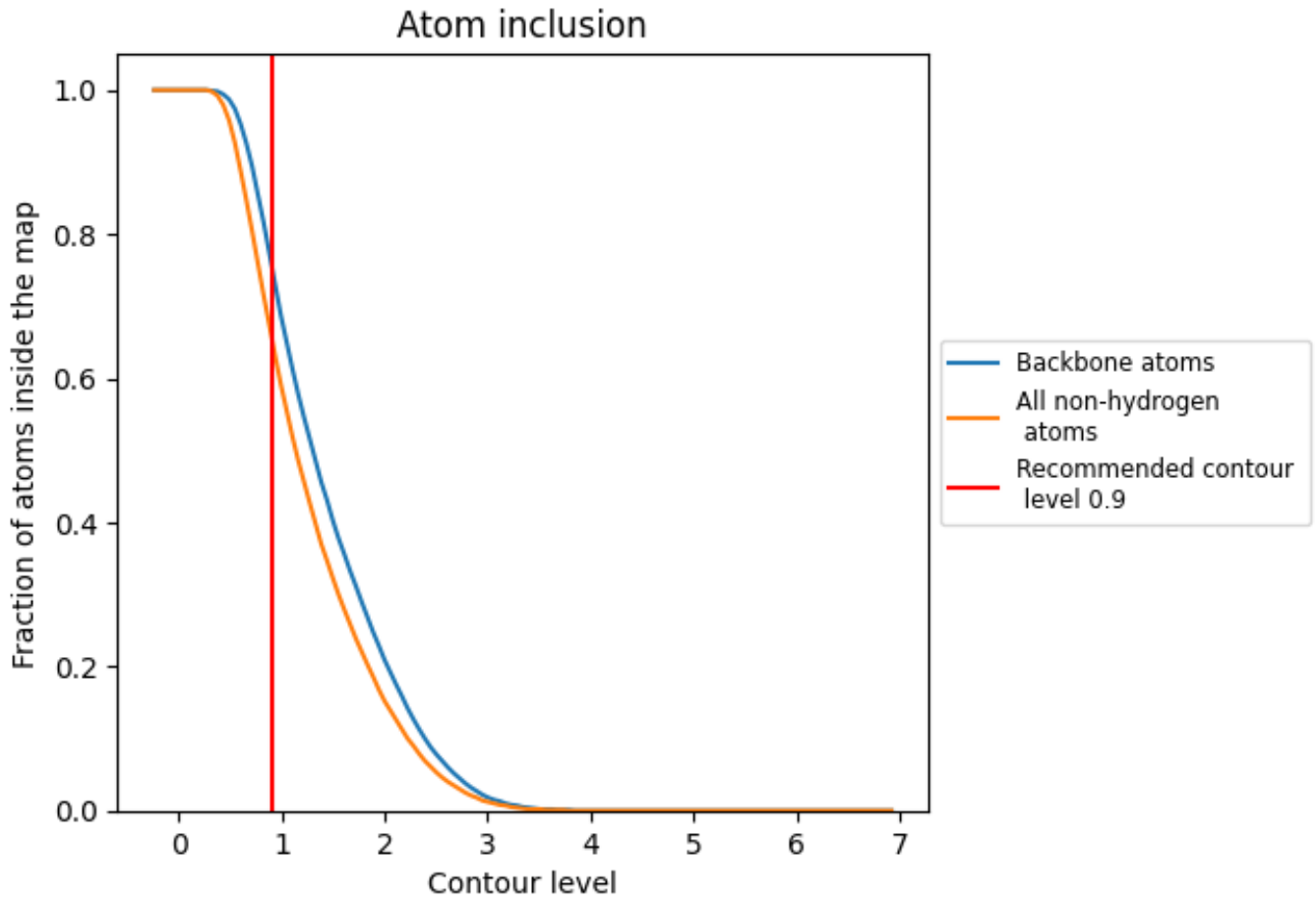
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.9).

9.4 Atom inclusion (i)



At the recommended contour level, 76% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6600	0.5410
3	0.8940	0.6220
4	0.6490	0.5440
A	0.6390	0.5270
B	0.7530	0.5540
C	0.6640	0.5640
D	0.8770	0.5930
E	0.7420	0.5660
F	0.8850	0.6070
G	0.5340	0.5160
H	0.5220	0.4940
I	0.7430	0.5540
J	0.8930	0.6070
K	0.8660	0.6010
L	0.8960	0.6110
M	0.2620	0.4860
N	0.4270	0.4940
O	0.7880	0.5770
P	0.7180	0.5890
Q	0.8820	0.6100
R	0.7090	0.5770
S	0.8600	0.5920
T	0.5080	0.5240
U	0.4880	0.4890
V	0.7260	0.5810
W	0.8340	0.5900
X	0.8870	0.6190
Y	0.8920	0.6200
Z	0.3140	0.4980
a	0.1340	0.3420
b	0.6920	0.5340
c	0.3410	0.4410
d	0.7280	0.5460
e	0.3930	0.4540
f	0.5790	0.5080

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	0.1270	0.3410
h	0.2650	0.4110
i	0.3280	0.4420
j	0.7180	0.5390
k	0.7630	0.5500
l	0.7120	0.5460
m	0.2230	0.3620