



Full wwPDB EM Validation Report ⓘ

Oct 18, 2023 – 02:10 PM JST

PDB ID : 8IMJ
EMDB ID : EMD-35566
Title : A'1-A'2, A'3-A'4, B1-B2, C1-C2 cylinder in cyanobacterial phycobilisome from Anthocerotibacter panamensis (Cluster B)
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 : 2.59 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:

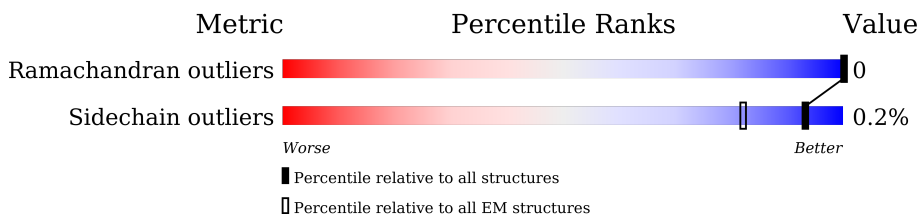
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.59 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 $\leq 5\%$. 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	0	1136	
2	A	161	
2	B	161	
2	C	161	
2	D	161	
2	E	161	
2	N	161	
2	O	161	
2	P	161	

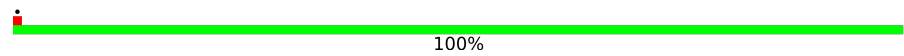
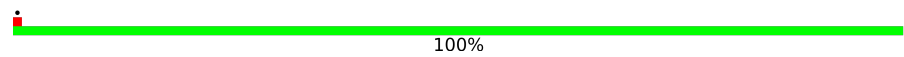
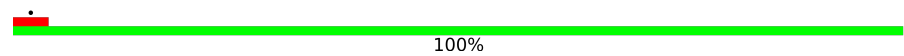
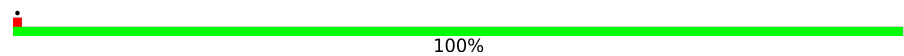
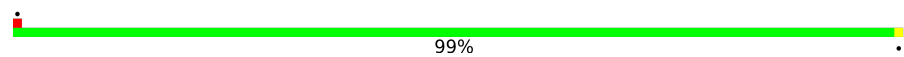

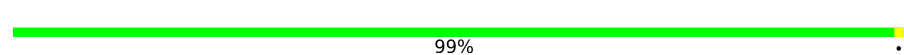



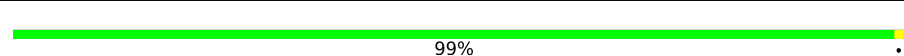
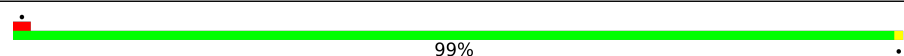
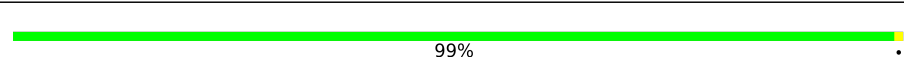
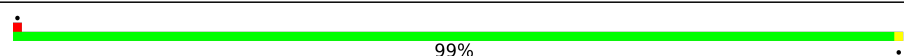
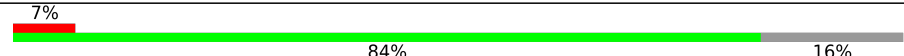
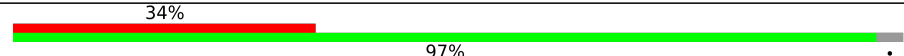
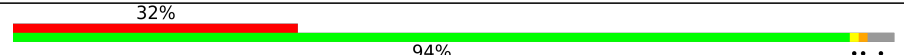
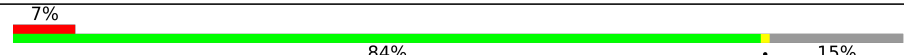
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Mol	Chain	Length	Quality of chain
2	Q	161	99%
2	R	161	99%
2	S	161	99%
2	a	161	99%
2	b	161	99%
2	c	161	99%
2	d	161	99%
2	e	161	99%
2	f	161	99%
2	n	161	99%
2	o	161	99%
2	p	161	99%
2	q	161	99%
2	r	161	99%
2	s	161	99%
3	G	161	100%
4	H	162	100%
4	I	162	100%
4	J	162	100%
4	K	162	99%
4	L	162	100%
4	T	162	100%
4	U	162	100%
4	V	162	100%
4	W	162	100%

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Mol	Chain	Length	Quality of chain
4	X	162	 100%
4	Y	162	 100%
4	g	162	 100%
4	h	162	 100%
4	i	162	 99%
4	j	162	 100%
4	k	162	 99%
4	l	162	 100%
4	t	162	 100%
4	u	162	 100%
4	v	162	 99%
4	w	162	 99%
4	x	162	 99%
4	y	162	 99%
5	M	68	 7% 84% 16%
5	Z	68	 34% 97%
5	m	68	 32% 94%
5	z	68	 7% 84% 15%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 69970 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 ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	1045	8344	5311	1451	1565	17	0	0

- Molecule 2 is a protein called ApcA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	160	1218	766	211	237	4	0	0
2	B	160	1218	766	211	237	4	0	0
2	C	160	1218	766	211	237	4	0	0
2	D	160	1218	766	211	237	4	0	0
2	E	160	1218	766	211	237	4	0	0
2	N	160	1218	766	211	237	4	0	0
2	O	160	1218	766	211	237	4	0	0
2	P	160	1218	766	211	237	4	0	0
2	Q	160	1218	766	211	237	4	0	0
2	R	160	1218	766	211	237	4	0	0
2	S	160	1218	766	211	237	4	0	0
2	a	160	1218	766	211	237	4	0	0
2	b	160	1218	766	211	237	4	0	0
2	c	160	1218	766	211	237	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	d	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		
2	e	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		
2	f	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		
2	n	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		
2	o	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		
2	p	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		
2	q	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		
2	r	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		
2	s	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		

- Molecule 3 is a protein called ApcB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	161	Total	C	N	O	S	0	0
			1242	794	211	232	5		

- Molecule 4 is a protein called ApcB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	I	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	J	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	K	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	L	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	T	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	U	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	W	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	X	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	Y	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	g	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	h	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	i	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	j	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	k	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	l	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	t	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	u	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	v	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	w	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	x	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
4	y	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		

- Molecule 5 is a protein called ApcC2.

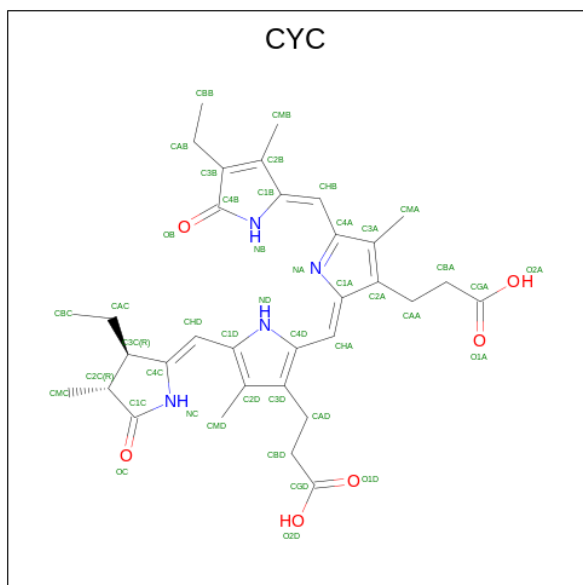
Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	57	Total	C	N	O	S	0	0
			474	307	86	80	1		
5	Z	66	Total	C	N	O	S	0	0
			532	343	97	91	1		
5	m	66	Total	C	N	O	S	0	0
			532	343	97	91	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	z	58	478	309	87	81	1	0	0

- 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
			Total	C	N	O	
6	0	1	43	33	4	6	0
6	0	1	43	33	4	6	0
6	0	1	43	33	4	6	0
6	A	1	43	33	4	6	0
6	B	1	43	33	4	6	0
6	C	1	43	33	4	6	0
6	D	1	43	33	4	6	0
6	E	1	43	33	4	6	0
6	G	1	43	33	4	6	0
6	H	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	I	1	Total 43	C 33	N 4	O 6	0
6	J	1	Total 43	C 33	N 4	O 6	0
6	L	1	Total 43	C 33	N 4	O 6	0
6	N	1	Total 43	C 33	N 4	O 6	0
6	O	1	Total 43	C 33	N 4	O 6	0
6	P	1	Total 43	C 33	N 4	O 6	0
6	Q	1	Total 43	C 33	N 4	O 6	0
6	R	1	Total 43	C 33	N 4	O 6	0
6	S	1	Total 43	C 33	N 4	O 6	0
6	T	1	Total 43	C 33	N 4	O 6	0
6	U	1	Total 43	C 33	N 4	O 6	0
6	V	1	Total 43	C 33	N 4	O 6	0
6	W	1	Total 43	C 33	N 4	O 6	0
6	Y	1	Total 43	C 33	N 4	O 6	0
6	a	1	Total 43	C 33	N 4	O 6	0
6	b	1	Total 43	C 33	N 4	O 6	0
6	c	1	Total 43	C 33	N 4	O 6	0
6	d	1	Total 43	C 33	N 4	O 6	0
6	e	1	Total 43	C 33	N 4	O 6	0
6	f	1	Total 43	C 33	N 4	O 6	0
6	h	1	Total 43	C 33	N 4	O 6	0

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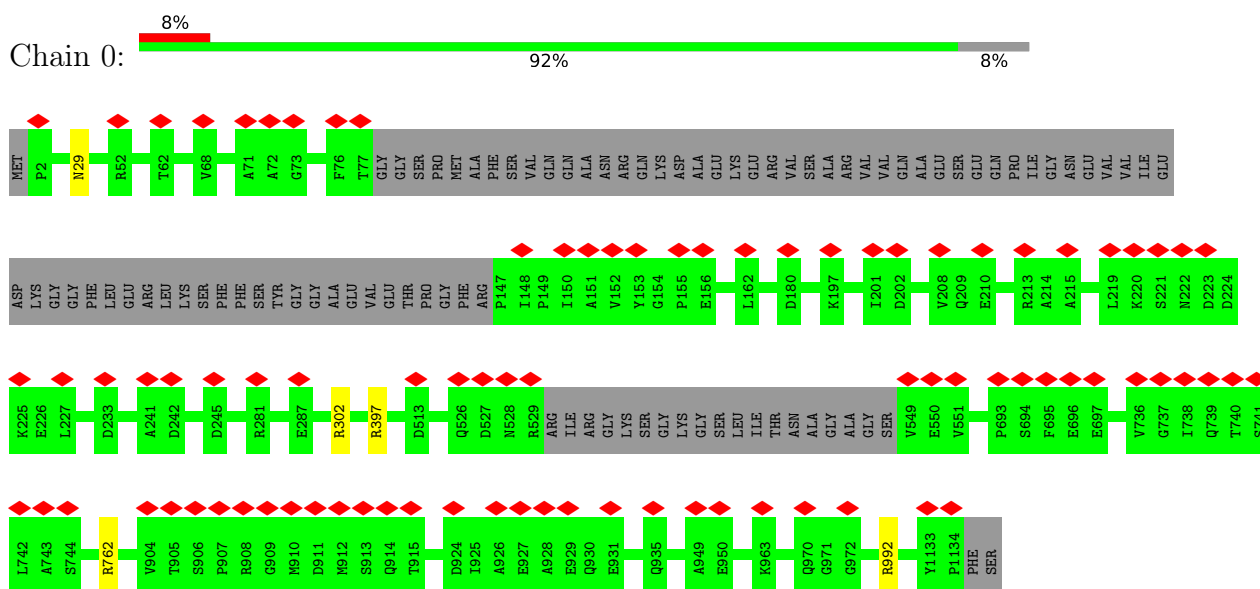
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	i	1	Total 43	C 33	N 4	O 6	0
6	j	1	Total 43	C 33	N 4	O 6	0
6	k	1	Total 43	C 33	N 4	O 6	0
6	l	1	Total 43	C 33	N 4	O 6	0
6	m	1	Total 43	C 33	N 4	O 6	0
6	n	1	Total 43	C 33	N 4	O 6	0
6	o	1	Total 43	C 33	N 4	O 6	0
6	p	1	Total 43	C 33	N 4	O 6	0
6	q	1	Total 43	C 33	N 4	O 6	0
6	r	1	Total 43	C 33	N 4	O 6	0
6	s	1	Total 43	C 33	N 4	O 6	0
6	t	1	Total 43	C 33	N 4	O 6	0
6	u	1	Total 43	C 33	N 4	O 6	0
6	v	1	Total 43	C 33	N 4	O 6	0
6	w	1	Total 43	C 33	N 4	O 6	0
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6	y	1	Total 43	C 33	N 4	O 6	0

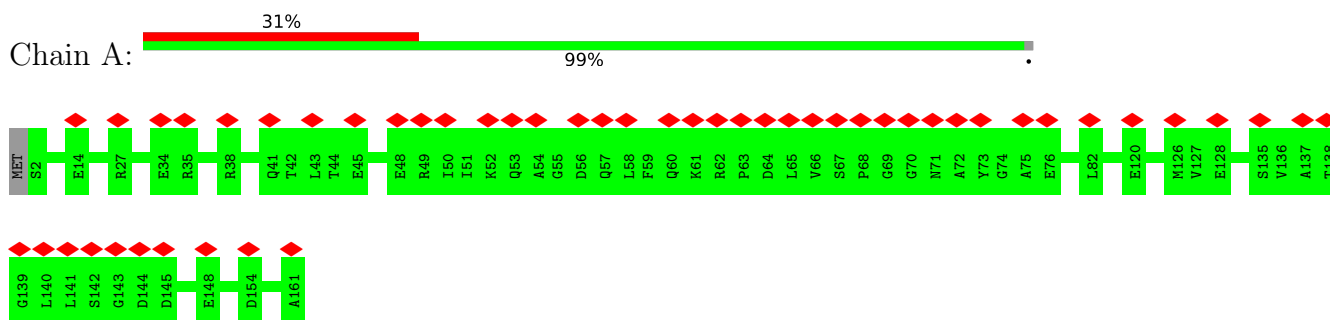
3 Residue-property plots [i](#)

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

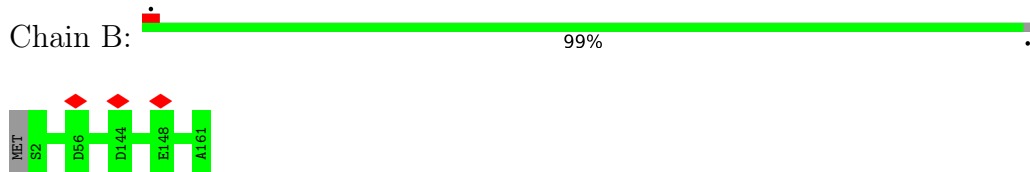
- Molecule 1: ApcE



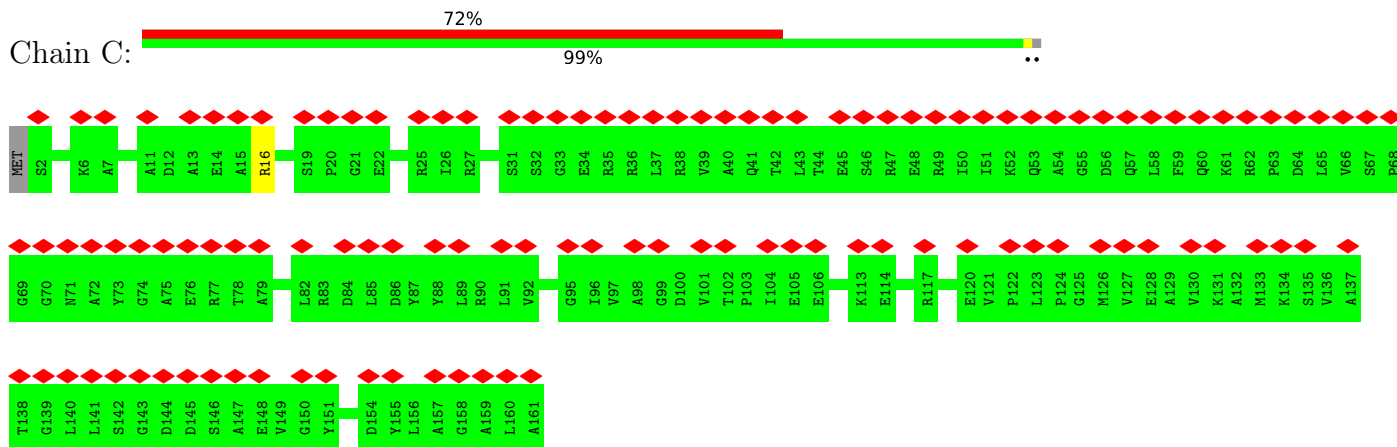
- Molecule 2: ApcA2



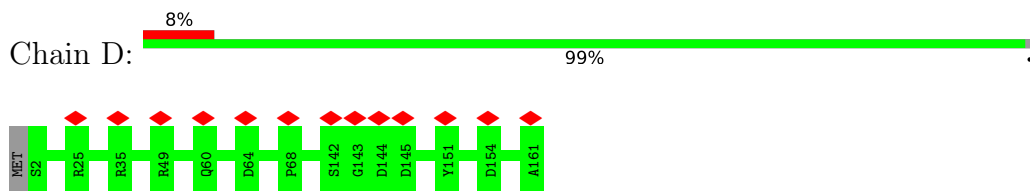
- Molecule 2: ApcA2



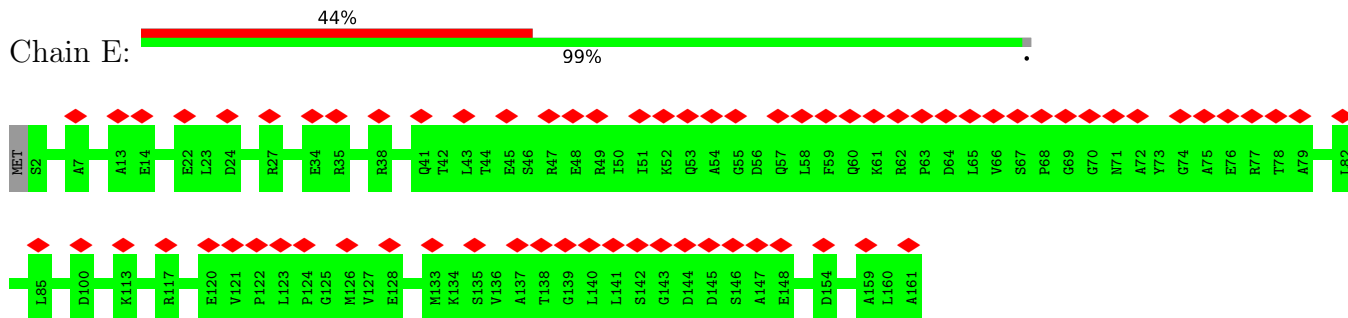
• Molecule 2: ApcA2



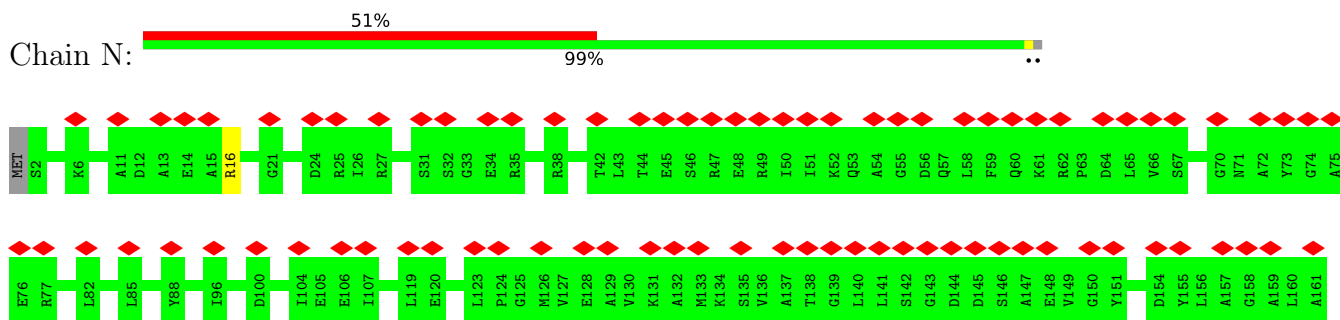
• Molecule 2: ApcA2



• Molecule 2: ApcA2

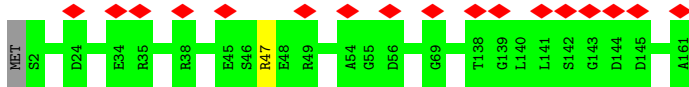


• Molecule 2: ApcA2

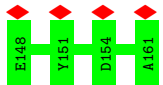
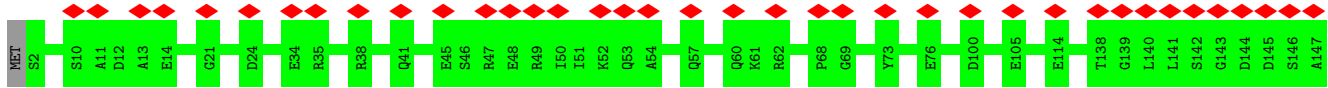


• Molecule 2: ApcA2

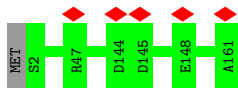




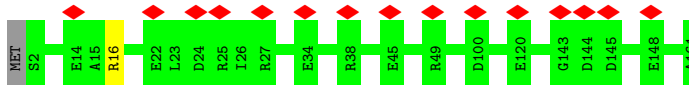
- Molecule 2: ApcA2



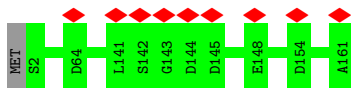
- Molecule 2: ApcA2



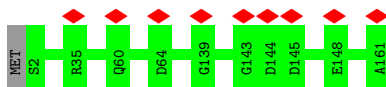
- Molecule 2: ApcA2



- Molecule 2: ApcA2

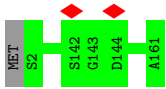


- Molecule 2: ApcA2

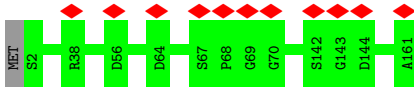


- Molecule 2: ApcA2

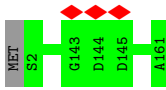




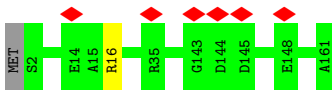
- Molecule 2: ApcA2



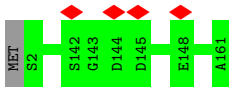
- Molecule 2: ApcA2



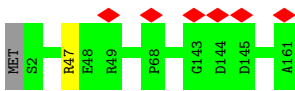
- Molecule 2: ApcA2



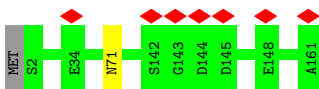
- Molecule 2: ApcA2



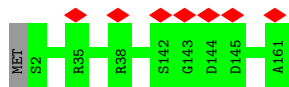
- Molecule 2: ApcA2



- Molecule 2: ApcA2



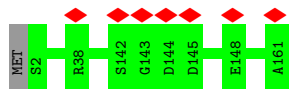
- Molecule 2: ApcA2



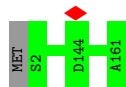
• Molecule 2: ApcA2



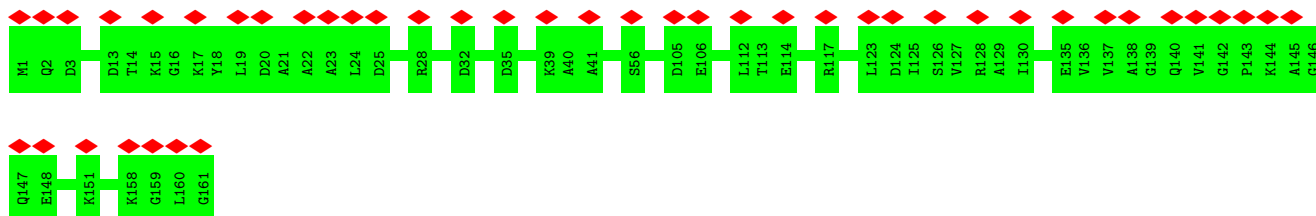
• Molecule 2: ApcA2



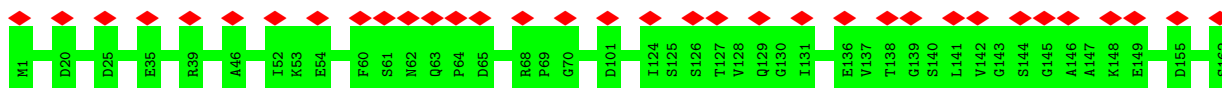
• Molecule 2: ApcA2



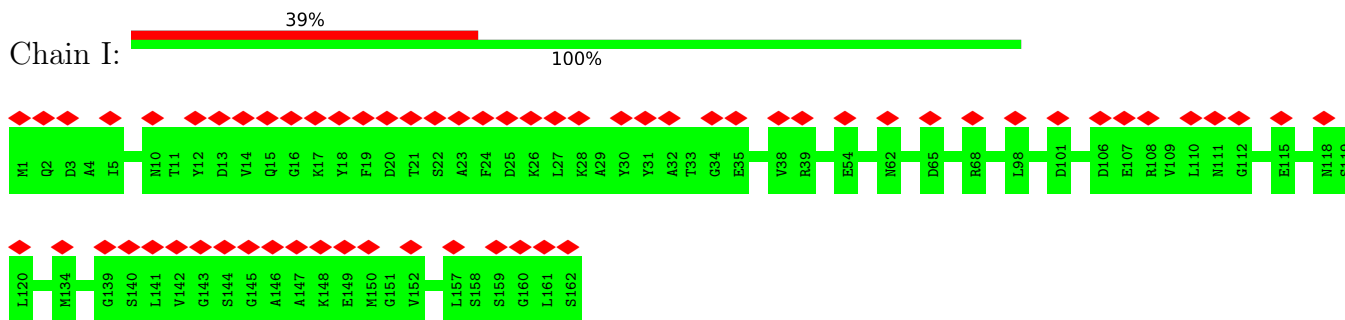
• Molecule 3: ApcB3



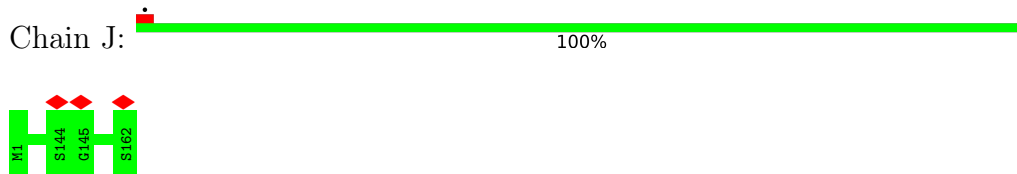
• Molecule 4: ApcB2



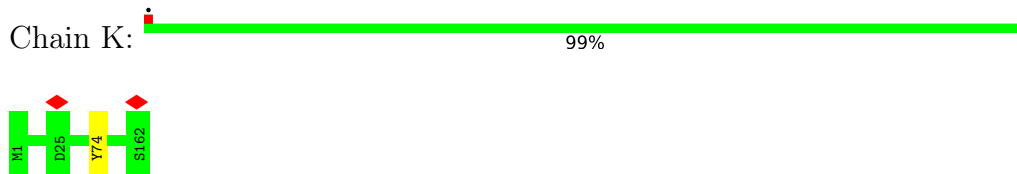
• Molecule 4: ApcB2



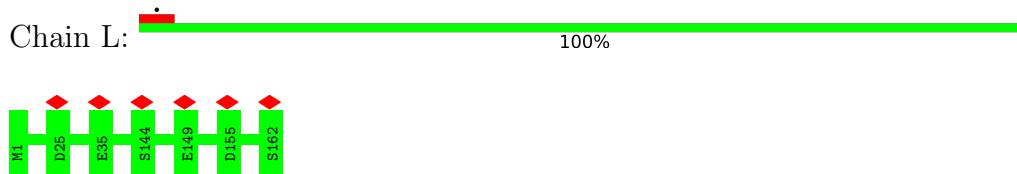
• Molecule 4: ApcB2



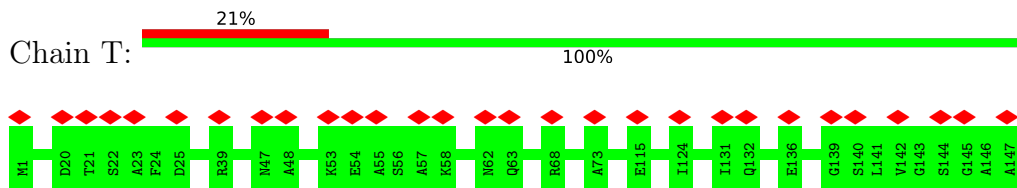
• Molecule 4: ApcB2



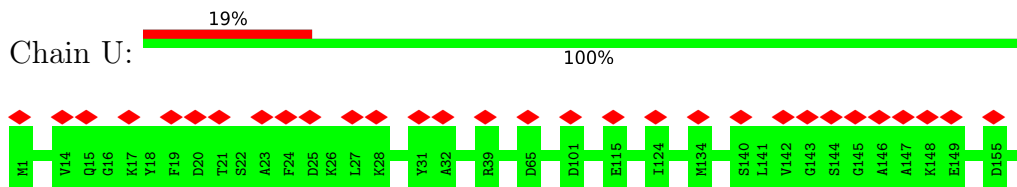
• Molecule 4: ApcB2



• Molecule 4: ApcB2

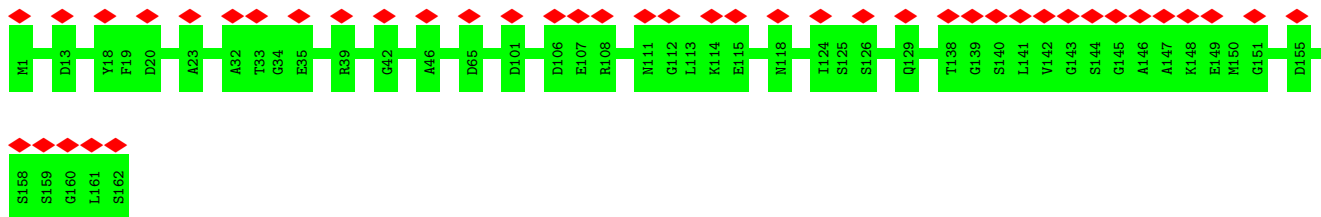


• Molecule 4: ApcB2

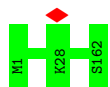


• Molecule 4: ApcB2





• Molecule 4: ApcB2



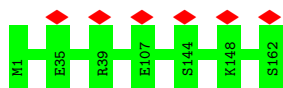
• Molecule 4: ApcB2



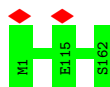
• Molecule 4: ApcB2



• Molecule 4: ApcB2

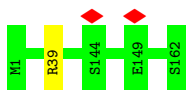


• Molecule 4: ApcB2



• Molecule 4: ApcB2





- Molecule 4: ApcB2



- Molecule 4: ApcB2



- Molecule 4: ApcB2



- Molecule 4: ApcB2



- Molecule 4: ApcB2



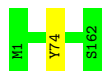
- Molecule 4: ApcB2



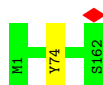
- Molecule 4: ApcB2



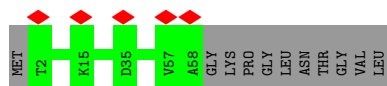
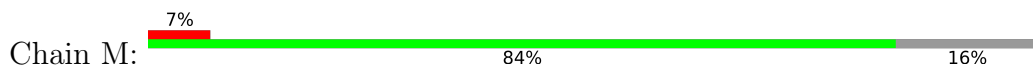
• Molecule 4: ApcB2



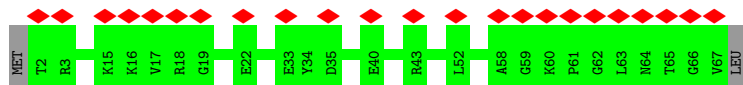
• Molecule 4: ApcB2



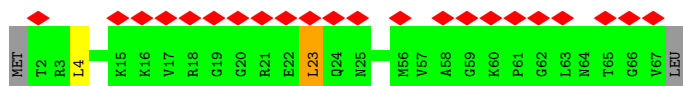
• Molecule 5: ApcC2



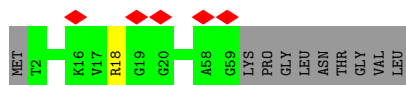
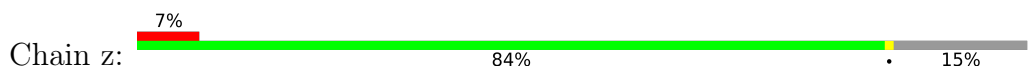
• Molecule 5: ApcC2



• Molecule 5: ApcC2



• Molecule 5: ApcC2



4 Experimental information

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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.587	Depositor
Minimum map value	-0.359	Depositor
Average map value	0.056	Depositor
Map value standard deviation	0.118	Depositor
Recommended contour level	1.0	Depositor
Map size (\AA)	721.48, 721.48, 721.48	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.061, 1.061, 1.061	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0	0.33	0/8527	0.48	0/11545
2	A	0.27	0/1235	0.46	0/1668
2	B	0.29	0/1235	0.42	0/1668
2	C	0.28	0/1235	0.45	0/1668
2	D	0.29	0/1235	0.44	0/1668
2	E	0.29	0/1235	0.48	0/1668
2	N	0.30	0/1235	0.47	0/1668
2	O	0.32	0/1235	0.51	1/1668 (0.1%)
2	P	0.28	0/1235	0.46	0/1668
2	Q	0.33	0/1235	0.49	0/1668
2	R	0.28	0/1235	0.46	0/1668
2	S	0.30	0/1235	0.46	0/1668
2	a	0.29	0/1235	0.46	0/1668
2	b	0.33	0/1235	0.47	0/1668
2	c	0.32	0/1235	0.49	0/1668
2	d	0.32	0/1235	0.44	0/1668
2	e	0.30	0/1235	0.43	0/1668
2	f	0.31	0/1235	0.45	0/1668
2	n	0.31	0/1235	0.48	1/1668 (0.1%)
2	o	0.31	0/1235	0.47	0/1668
2	p	0.30	0/1235	0.44	0/1668
2	q	0.31	0/1235	0.43	0/1668
2	r	0.29	0/1235	0.43	0/1668
2	s	0.34	0/1235	0.48	0/1668
3	G	0.30	0/1263	0.47	0/1709
4	H	0.29	0/1249	0.46	0/1688
4	I	0.27	0/1249	0.43	0/1688
4	J	0.32	0/1249	0.44	0/1688
4	K	0.33	0/1249	0.46	0/1688
4	L	0.31	0/1249	0.44	0/1688
4	T	0.29	0/1249	0.45	0/1688
4	U	0.28	0/1249	0.44	0/1688

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	V	0.29	0/1249	0.47	0/1688
4	W	0.34	0/1249	0.46	0/1688
4	X	0.36	0/1249	0.48	0/1688
4	Y	0.32	0/1249	0.45	0/1688
4	g	0.30	0/1249	0.44	0/1688
4	h	0.32	0/1249	0.47	0/1688
4	i	0.30	0/1249	0.43	0/1688
4	j	0.32	0/1249	0.49	0/1688
4	k	0.33	0/1249	0.46	0/1688
4	l	0.36	0/1249	0.48	0/1688
4	t	0.33	0/1249	0.45	0/1688
4	u	0.31	0/1249	0.45	0/1688
4	v	0.32	0/1249	0.46	0/1688
4	w	0.35	0/1249	0.48	0/1688
4	x	0.36	0/1249	0.48	0/1688
4	y	0.34	0/1249	0.48	0/1688
5	M	0.29	0/482	0.47	0/644
5	Z	0.28	0/541	0.48	0/724
5	m	0.30	0/541	0.73	3/724 (0.4%)
5	z	0.31	0/486	0.52	0/649
All	All	0.31	0/68972	0.47	5/93183 (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
4	K	0	1
4	k	0	1
4	v	0	1
4	w	0	1
4	x	0	1
4	y	0	1
5	m	0	1
All	All	0	7

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	m	23	LEU	CA-CB-CG	-8.02	96.86	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	47	ARG	CB-CG-CD	-6.37	95.03	111.60
5	m	4	LEU	CA-CB-CG	5.82	128.68	115.30
2	n	47	ARG	CB-CG-CD	-5.66	96.88	111.60
5	m	23	LEU	CB-CG-CD2	5.50	120.35	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	K	74	TYR	Peptide
4	k	74	TYR	Peptide
5	m	23	LEU	Peptide
4	v	74	TYR	Peptide
4	w	74	TYR	Peptide
4	x	74	TYR	Peptide
4	y	74	TYR	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	0	1039/1136 (92%)	1009 (97%)	30 (3%)	0	100	100
2	A	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	B	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	C	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	D	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	E	158/161 (98%)	156 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	O	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
2	P	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	Q	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	R	158/161 (98%)	158 (100%)	0	0	100	100
2	S	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	a	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	b	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	c	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	d	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	e	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	f	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	n	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	o	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	p	158/161 (98%)	158 (100%)	0	0	100	100
2	q	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	r	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	s	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
3	G	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
4	H	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
4	I	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	J	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	K	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	L	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
4	T	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	U	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
4	V	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	W	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	X	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	Y	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	g	160/162 (99%)	159 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	h	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
4	i	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
4	j	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	k	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	l	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
4	t	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	u	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
4	v	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	w	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	x	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	y	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
5	M	55/68 (81%)	51 (93%)	4 (7%)	0	100	100
5	Z	64/68 (94%)	63 (98%)	1 (2%)	0	100	100
5	m	64/68 (94%)	57 (89%)	7 (11%)	0	100	100
5	z	56/68 (82%)	54 (96%)	2 (4%)	0	100	100
All	All	8751/8998 (97%)	8590 (98%)	161 (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	0	892/962 (93%)	887 (99%)	5 (1%)	86	95
2	A	127/128 (99%)	127 (100%)	0	100	100
2	B	127/128 (99%)	127 (100%)	0	100	100
2	C	127/128 (99%)	126 (99%)	1 (1%)	81	92
2	D	127/128 (99%)	127 (100%)	0	100	100
2	E	127/128 (99%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	127/128 (99%)	126 (99%)	1 (1%)	81	92
2	O	127/128 (99%)	127 (100%)	0	100	100
2	P	127/128 (99%)	127 (100%)	0	100	100
2	Q	127/128 (99%)	127 (100%)	0	100	100
2	R	127/128 (99%)	126 (99%)	1 (1%)	81	92
2	S	127/128 (99%)	127 (100%)	0	100	100
2	a	127/128 (99%)	127 (100%)	0	100	100
2	b	127/128 (99%)	127 (100%)	0	100	100
2	c	127/128 (99%)	127 (100%)	0	100	100
2	d	127/128 (99%)	127 (100%)	0	100	100
2	e	127/128 (99%)	126 (99%)	1 (1%)	81	92
2	f	127/128 (99%)	127 (100%)	0	100	100
2	n	127/128 (99%)	127 (100%)	0	100	100
2	o	127/128 (99%)	126 (99%)	1 (1%)	81	92
2	p	127/128 (99%)	127 (100%)	0	100	100
2	q	127/128 (99%)	127 (100%)	0	100	100
2	r	127/128 (99%)	127 (100%)	0	100	100
2	s	127/128 (99%)	127 (100%)	0	100	100
3	G	124/124 (100%)	124 (100%)	0	100	100
4	H	128/128 (100%)	128 (100%)	0	100	100
4	I	128/128 (100%)	128 (100%)	0	100	100
4	J	128/128 (100%)	128 (100%)	0	100	100
4	K	128/128 (100%)	128 (100%)	0	100	100
4	L	128/128 (100%)	128 (100%)	0	100	100
4	T	128/128 (100%)	128 (100%)	0	100	100
4	U	128/128 (100%)	128 (100%)	0	100	100
4	V	128/128 (100%)	128 (100%)	0	100	100
4	W	128/128 (100%)	128 (100%)	0	100	100
4	X	128/128 (100%)	128 (100%)	0	100	100
4	Y	128/128 (100%)	128 (100%)	0	100	100
4	g	128/128 (100%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	h	128/128 (100%)	128 (100%)	0	100	100
4	i	128/128 (100%)	127 (99%)	1 (1%)	81	92
4	j	128/128 (100%)	128 (100%)	0	100	100
4	k	128/128 (100%)	128 (100%)	0	100	100
4	l	128/128 (100%)	128 (100%)	0	100	100
4	t	128/128 (100%)	128 (100%)	0	100	100
4	u	128/128 (100%)	128 (100%)	0	100	100
4	v	128/128 (100%)	128 (100%)	0	100	100
4	w	128/128 (100%)	128 (100%)	0	100	100
4	x	128/128 (100%)	128 (100%)	0	100	100
4	y	128/128 (100%)	128 (100%)	0	100	100
5	M	50/58 (86%)	50 (100%)	0	100	100
5	Z	56/58 (97%)	56 (100%)	0	100	100
5	m	56/58 (97%)	56 (100%)	0	100	100
5	z	50/58 (86%)	49 (98%)	1 (2%)	55	78
All	All	7093/7206 (98%)	7081 (100%)	12 (0%)	93	98

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	29	ASN
1	0	302	ARG
1	0	397	ARG
1	0	762	ARG
1	0	992	ARG
2	C	16	ARG
2	N	16	ARG
2	R	16	ARG
2	e	16	ARG
4	i	39	ARG
2	o	71	ASN
5	z	18	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	320	ASN
1	0	460	ASN
1	0	792	GLN
2	E	41	GLN
4	H	62	ASN
4	H	72	ASN
4	J	72	ASN
4	J	132	GLN
2	N	71	ASN
2	P	53	GLN
2	Q	71	ASN
4	T	72	ASN
4	U	2	GLN
4	U	72	ASN
4	V	2	GLN
4	V	118	ASN
4	g	118	ASN
4	j	129	GLN
4	j	132	GLN
2	p	53	GLN
2	r	71	ASN
2	s	71	ASN
4	t	2	GLN
4	t	10	ASN
4	u	47	ASN
5	z	25	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

48 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	I	200	-	42,46,46	6.55	25 (59%)	50,67,67	4.32	11 (22%)
6	CYC	h	200	-	42,46,46	6.50	25 (59%)	50,67,67	4.34	12 (24%)
6	CYC	j	200	-	42,46,46	6.48	24 (57%)	50,67,67	3.96	12 (24%)
6	CYC	i	200	-	42,46,46	6.46	24 (57%)	50,67,67	4.19	12 (24%)
6	CYC	o	200	-	42,46,46	6.45	24 (57%)	50,67,67	4.38	13 (26%)
6	CYC	O	200	-	42,46,46	6.52	25 (59%)	50,67,67	4.23	11 (22%)
6	CYC	W	200	-	42,46,46	6.37	23 (54%)	50,67,67	4.46	14 (28%)
6	CYC	l	200	-	42,46,46	6.41	24 (57%)	50,67,67	4.36	12 (24%)
6	CYC	f	200	-	42,46,46	6.49	24 (57%)	50,67,67	4.39	12 (24%)
6	CYC	T	200	-	42,46,46	6.52	25 (59%)	50,67,67	4.30	14 (28%)
6	CYC	Q	200	-	42,46,46	6.47	24 (57%)	50,67,67	4.27	13 (26%)
6	CYC	a	200	-	42,46,46	6.49	24 (57%)	50,67,67	4.32	12 (24%)
6	CYC	p	200	-	42,46,46	6.51	25 (59%)	50,67,67	4.35	15 (30%)
6	CYC	v	200	-	42,46,46	6.37	24 (57%)	50,67,67	4.39	12 (24%)
6	CYC	r	200	-	42,46,46	6.47	24 (57%)	50,67,67	4.35	13 (26%)
6	CYC	J	200	-	42,46,46	6.49	23 (54%)	50,67,67	4.25	11 (22%)
6	CYC	H	200	-	42,46,46	6.57	24 (57%)	50,67,67	4.52	14 (28%)
6	CYC	S	200	-	42,46,46	6.48	24 (57%)	50,67,67	4.41	13 (26%)
6	CYC	b	200	-	42,46,46	6.48	24 (57%)	50,67,67	4.27	15 (30%)
6	CYC	B	200	-	42,46,46	6.53	23 (54%)	50,67,67	4.33	12 (24%)
6	CYC	m	200	-	42,46,46	6.57	23 (54%)	50,67,67	4.65	15 (30%)
6	CYC	n	200	-	42,46,46	6.51	24 (57%)	50,67,67	4.40	12 (24%)
6	CYC	0	1202	-	42,46,46	6.45	24 (57%)	50,67,67	4.36	13 (26%)
6	CYC	P	200	-	42,46,46	6.61	25 (59%)	50,67,67	4.35	11 (22%)
6	CYC	x	200	-	42,46,46	6.49	24 (57%)	50,67,67	4.37	15 (30%)
6	CYC	C	200	-	42,46,46	6.53	24 (57%)	50,67,67	4.73	12 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CYC	E	200	-	42,46,46	6.59	25 (59%)	50,67,67	4.15	13 (26%)
6	CYC	u	200	-	42,46,46	6.49	24 (57%)	50,67,67	4.28	13 (26%)
6	CYC	V	200	-	42,46,46	6.51	24 (57%)	50,67,67	4.30	11 (22%)
6	CYC	0	1201	-	42,46,46	6.58	24 (57%)	50,67,67	4.51	17 (34%)
6	CYC	c	200	-	42,46,46	6.51	24 (57%)	50,67,67	4.49	13 (26%)
6	CYC	R	200	-	42,46,46	6.54	24 (57%)	50,67,67	4.29	14 (28%)
6	CYC	t	200	-	42,46,46	6.46	24 (57%)	50,67,67	4.26	15 (30%)
6	CYC	L	200	-	42,46,46	6.48	25 (59%)	50,67,67	4.34	12 (24%)
6	CYC	e	200	-	42,46,46	6.54	24 (57%)	50,67,67	4.11	14 (28%)
6	CYC	G	200	-	42,46,46	6.55	25 (59%)	50,67,67	4.33	12 (24%)
6	CYC	q	200	-	42,46,46	6.49	24 (57%)	50,67,67	4.29	12 (24%)
6	CYC	U	200	-	42,46,46	6.56	25 (59%)	50,67,67	4.31	12 (24%)
6	CYC	N	200	-	42,46,46	6.47	24 (57%)	50,67,67	4.64	12 (24%)
6	CYC	0	1203	-	42,46,46	6.48	23 (54%)	50,67,67	4.27	15 (30%)
6	CYC	D	200	-	42,46,46	6.53	24 (57%)	50,67,67	4.40	11 (22%)
6	CYC	A	200	-	42,46,46	6.54	24 (57%)	50,67,67	4.25	11 (22%)
6	CYC	d	200	-	42,46,46	6.47	24 (57%)	50,67,67	4.36	14 (28%)
6	CYC	y	200	-	42,46,46	6.49	24 (57%)	50,67,67	4.24	12 (24%)
6	CYC	w	200	-	42,46,46	6.51	27 (64%)	50,67,67	4.01	12 (24%)
6	CYC	k	200	-	42,46,46	6.43	24 (57%)	50,67,67	4.31	13 (26%)
6	CYC	Y	200	-	42,46,46	6.46	23 (54%)	50,67,67	4.16	12 (24%)
6	CYC	s	200	-	42,46,46	6.43	25 (59%)	50,67,67	4.29	13 (26%)

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	I	200	-	-	10/25/74/74	0/4/4/4
6	CYC	h	200	-	-	8/25/74/74	0/4/4/4
6	CYC	j	200	-	-	7/25/74/74	0/4/4/4
6	CYC	i	200	-	-	10/25/74/74	0/4/4/4
6	CYC	o	200	-	-	5/25/74/74	0/4/4/4
6	CYC	O	200	-	-	7/25/74/74	0/4/4/4
6	CYC	W	200	-	-	7/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	l	200	-	-	9/25/74/74	0/4/4/4
6	CYC	f	200	-	-	6/25/74/74	0/4/4/4
6	CYC	T	200	-	-	13/25/74/74	0/4/4/4
6	CYC	Q	200	-	-	7/25/74/74	0/4/4/4
6	CYC	a	200	-	-	6/25/74/74	0/4/4/4
6	CYC	p	200	-	-	10/25/74/74	0/4/4/4
6	CYC	v	200	-	-	7/25/74/74	0/4/4/4
6	CYC	r	200	-	-	8/25/74/74	0/4/4/4
6	CYC	J	200	-	-	10/25/74/74	0/4/4/4
6	CYC	H	200	-	-	11/25/74/74	0/4/4/4
6	CYC	S	200	-	-	8/25/74/74	0/4/4/4
6	CYC	b	200	-	-	8/25/74/74	0/4/4/4
6	CYC	B	200	-	-	7/25/74/74	0/4/4/4
6	CYC	m	200	-	-	14/25/74/74	0/4/4/4
6	CYC	n	200	-	-	7/25/74/74	0/4/4/4
6	CYC	0	1202	-	-	9/25/74/74	0/4/4/4
6	CYC	P	200	-	-	9/25/74/74	0/4/4/4
6	CYC	x	200	-	-	7/25/74/74	0/4/4/4
6	CYC	C	200	-	-	12/25/74/74	0/4/4/4
6	CYC	E	200	-	-	15/25/74/74	0/4/4/4
6	CYC	u	200	-	-	7/25/74/74	0/4/4/4
6	CYC	V	200	-	-	11/25/74/74	0/4/4/4
6	CYC	0	1201	-	-	16/25/74/74	0/4/4/4
6	CYC	c	200	-	-	7/25/74/74	0/4/4/4
6	CYC	R	200	-	-	7/25/74/74	0/4/4/4
6	CYC	t	200	-	-	9/25/74/74	0/4/4/4
6	CYC	L	200	-	-	11/25/74/74	0/4/4/4
6	CYC	e	200	-	-	9/25/74/74	0/4/4/4
6	CYC	G	200	-	-	10/25/74/74	0/4/4/4
6	CYC	q	200	-	-	9/25/74/74	0/4/4/4
6	CYC	U	200	-	-	7/25/74/74	0/4/4/4
6	CYC	N	200	-	-	17/25/74/74	0/4/4/4
6	CYC	0	1203	-	-	8/25/74/74	0/4/4/4
6	CYC	D	200	-	-	6/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	A	200	-	-	9/25/74/74	0/4/4/4
6	CYC	d	200	-	-	8/25/74/74	0/4/4/4
6	CYC	y	200	-	-	8/25/74/74	0/4/4/4
6	CYC	w	200	-	-	7/25/74/74	0/4/4/4
6	CYC	k	200	-	-	7/25/74/74	0/4/4/4
6	CYC	Y	200	-	-	9/25/74/74	0/4/4/4
6	CYC	s	200	-	-	5/25/74/74	0/4/4/4

All (1160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	200	CYC	CHA-C1A	26.90	1.57	1.35
6	U	200	CYC	CHA-C1A	26.63	1.57	1.35
6	I	200	CYC	CHA-C1A	26.54	1.57	1.35
6	C	200	CYC	CHA-C1A	26.52	1.57	1.35
6	H	200	CYC	CHA-C1A	26.50	1.57	1.35
6	0	1201	CYC	CHA-C1A	26.46	1.57	1.35
6	R	200	CYC	CHA-C1A	26.42	1.57	1.35
6	G	200	CYC	CHA-C1A	26.41	1.57	1.35
6	V	200	CYC	CHA-C1A	26.36	1.57	1.35
6	B	200	CYC	CHA-C1A	26.31	1.57	1.35
6	c	200	CYC	CHA-C1A	26.28	1.57	1.35
6	e	200	CYC	CHA-C1A	26.27	1.57	1.35
6	p	200	CYC	CHA-C1A	26.23	1.57	1.35
6	E	200	CYC	CHA-C1A	26.23	1.57	1.35
6	A	200	CYC	CHA-C1A	26.23	1.57	1.35
6	D	200	CYC	CHA-C1A	26.22	1.57	1.35
6	T	200	CYC	CHA-C1A	26.17	1.57	1.35
6	n	200	CYC	CHA-C1A	26.12	1.56	1.35
6	L	200	CYC	CHA-C1A	26.11	1.56	1.35
6	J	200	CYC	CHA-C1A	26.06	1.56	1.35
6	y	200	CYC	CHA-C1A	26.02	1.56	1.35
6	S	200	CYC	CHA-C1A	26.01	1.56	1.35
6	O	200	CYC	CHA-C1A	26.00	1.56	1.35
6	N	200	CYC	CHA-C1A	25.98	1.56	1.35
6	r	200	CYC	CHA-C1A	25.97	1.56	1.35
6	Q	200	CYC	CHA-C1A	25.93	1.56	1.35
6	x	200	CYC	CHA-C1A	25.91	1.56	1.35
6	w	200	CYC	CHA-C1A	25.90	1.56	1.35
6	f	200	CYC	CHA-C1A	25.90	1.56	1.35
6	h	200	CYC	CHA-C1A	25.87	1.56	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	0	1203	CYC	CHA-C1A	25.84	1.56	1.35
6	t	200	CYC	CHA-C1A	25.84	1.56	1.35
6	a	200	CYC	CHA-C1A	25.81	1.56	1.35
6	u	200	CYC	CHA-C1A	25.78	1.56	1.35
6	q	200	CYC	CHA-C1A	25.77	1.56	1.35
6	b	200	CYC	CHA-C1A	25.70	1.56	1.35
6	d	200	CYC	CHA-C1A	25.69	1.56	1.35
6	o	200	CYC	CHA-C1A	25.69	1.56	1.35
6	0	1202	CYC	CHA-C1A	25.61	1.56	1.35
6	i	200	CYC	CHA-C1A	25.56	1.56	1.35
6	Y	200	CYC	CHA-C1A	25.53	1.56	1.35
6	k	200	CYC	CHA-C1A	25.53	1.56	1.35
6	l	200	CYC	CHA-C1A	25.53	1.56	1.35
6	s	200	CYC	CHA-C1A	25.50	1.56	1.35
6	j	200	CYC	CHA-C1A	25.48	1.56	1.35
6	m	200	CYC	CHA-C1A	25.33	1.56	1.35
6	v	200	CYC	CHA-C1A	25.32	1.56	1.35
6	W	200	CYC	CHA-C1A	25.12	1.56	1.35
6	j	200	CYC	C2C-C1C	13.97	1.64	1.52
6	w	200	CYC	C2C-C1C	13.79	1.64	1.52
6	m	200	CYC	OB-C4B	13.61	1.49	1.23
6	E	200	CYC	C3C-C4C	13.44	1.70	1.50
6	m	200	CYC	C2C-C1C	13.33	1.64	1.52
6	d	200	CYC	C3C-C4C	13.22	1.70	1.50
6	T	200	CYC	C3C-C4C	13.19	1.70	1.50
6	i	200	CYC	C2C-C1C	13.18	1.63	1.52
6	R	200	CYC	C3C-C4C	13.16	1.70	1.50
6	H	200	CYC	C2C-C1C	13.15	1.63	1.52
6	C	200	CYC	C3C-C4C	13.14	1.70	1.50
6	h	200	CYC	C2C-C1C	13.13	1.63	1.52
6	b	200	CYC	C2C-C1C	13.11	1.63	1.52
6	p	200	CYC	C2C-C1C	13.11	1.63	1.52
6	0	1201	CYC	C3C-C4C	13.10	1.69	1.50
6	O	200	CYC	C3C-C4C	13.10	1.69	1.50
6	0	1203	CYC	C2C-C1C	13.10	1.63	1.52
6	a	200	CYC	C3C-C4C	13.09	1.69	1.50
6	u	200	CYC	C3C-C4C	13.09	1.69	1.50
6	H	200	CYC	C3C-C4C	13.09	1.69	1.50
6	G	200	CYC	C3C-C4C	13.09	1.69	1.50
6	V	200	CYC	C3C-C4C	13.09	1.69	1.50
6	u	200	CYC	C2C-C1C	13.09	1.63	1.52
6	b	200	CYC	C3C-C4C	13.08	1.69	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	e	200	CYC	C2C-C1C	13.08	1.63	1.52
6	G	200	CYC	C2C-C1C	13.06	1.63	1.52
6	o	200	CYC	C3C-C4C	13.06	1.69	1.50
6	f	200	CYC	C3C-C4C	13.04	1.69	1.50
6	n	200	CYC	C3C-C4C	13.03	1.69	1.50
6	k	200	CYC	C3C-C4C	13.00	1.69	1.50
6	y	200	CYC	C3C-C4C	13.00	1.69	1.50
6	0	1202	CYC	C3C-C4C	12.99	1.69	1.50
6	Y	200	CYC	C2C-C1C	12.99	1.63	1.52
6	P	200	CYC	C2C-C1C	12.99	1.63	1.52
6	B	200	CYC	C3C-C4C	12.98	1.69	1.50
6	O	200	CYC	C2C-C1C	12.97	1.63	1.52
6	0	1203	CYC	C3C-C4C	12.97	1.69	1.50
6	I	200	CYC	C2C-C1C	12.96	1.63	1.52
6	L	200	CYC	C2C-C1C	12.96	1.63	1.52
6	W	200	CYC	C3C-C4C	12.95	1.69	1.50
6	a	200	CYC	C2C-C1C	12.94	1.63	1.52
6	q	200	CYC	C3C-C4C	12.94	1.69	1.50
6	h	200	CYC	C3C-C4C	12.94	1.69	1.50
6	v	200	CYC	C3C-C4C	12.94	1.69	1.50
6	o	200	CYC	C2C-C1C	12.93	1.63	1.52
6	U	200	CYC	C2C-C1C	12.93	1.63	1.52
6	Q	200	CYC	C3C-C4C	12.92	1.69	1.50
6	y	200	CYC	C2C-C1C	12.92	1.63	1.52
6	P	200	CYC	C3C-C4C	12.92	1.69	1.50
6	0	1201	CYC	C2C-C1C	12.92	1.63	1.52
6	D	200	CYC	C2C-C1C	12.91	1.63	1.52
6	Y	200	CYC	C3C-C4C	12.91	1.69	1.50
6	V	200	CYC	C2C-C1C	12.90	1.63	1.52
6	e	200	CYC	C3C-C4C	12.89	1.69	1.50
6	U	200	CYC	C3C-C4C	12.89	1.69	1.50
6	T	200	CYC	C2C-C1C	12.88	1.63	1.52
6	i	200	CYC	C3C-C4C	12.87	1.69	1.50
6	x	200	CYC	C3C-C4C	12.86	1.69	1.50
6	S	200	CYC	C3C-C4C	12.86	1.69	1.50
6	q	200	CYC	C2C-C1C	12.85	1.63	1.52
6	J	200	CYC	C2C-C1C	12.85	1.63	1.52
6	t	200	CYC	C3C-C4C	12.85	1.69	1.50
6	x	200	CYC	C2C-C1C	12.85	1.63	1.52
6	f	200	CYC	C2C-C1C	12.85	1.63	1.52
6	k	200	CYC	C2C-C1C	12.84	1.63	1.52
6	I	200	CYC	C3C-C4C	12.82	1.69	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	200	CYC	C2C-C1C	12.82	1.63	1.52
6	0	1202	CYC	C2C-C1C	12.81	1.63	1.52
6	D	200	CYC	C3C-C4C	12.80	1.69	1.50
6	E	200	CYC	C2C-C1C	12.79	1.63	1.52
6	B	200	CYC	C2C-C1C	12.79	1.63	1.52
6	p	200	CYC	C3C-C4C	12.78	1.69	1.50
6	d	200	CYC	C2C-C1C	12.77	1.63	1.52
6	c	200	CYC	C2C-C1C	12.77	1.63	1.52
6	Q	200	CYC	C2C-C1C	12.77	1.63	1.52
6	r	200	CYC	C3C-C4C	12.75	1.69	1.50
6	c	200	CYC	C3C-C4C	12.75	1.69	1.50
6	l	200	CYC	C2C-C1C	12.73	1.63	1.52
6	A	200	CYC	C3C-C4C	12.73	1.69	1.50
6	J	200	CYC	C3C-C4C	12.73	1.69	1.50
6	l	200	CYC	C3C-C4C	12.73	1.69	1.50
6	L	200	CYC	C3C-C4C	12.72	1.69	1.50
6	n	200	CYC	C2C-C1C	12.70	1.63	1.52
6	r	200	CYC	C2C-C1C	12.70	1.63	1.52
6	s	200	CYC	C2C-C1C	12.65	1.63	1.52
6	S	200	CYC	C2C-C1C	12.65	1.63	1.52
6	s	200	CYC	C3C-C4C	12.64	1.69	1.50
6	R	200	CYC	C2C-C1C	12.62	1.63	1.52
6	m	200	CYC	C3C-C4C	12.61	1.69	1.50
6	W	200	CYC	C2C-C1C	12.58	1.63	1.52
6	E	200	CYC	C1C-NC	12.57	1.53	1.37
6	N	200	CYC	C3C-C4C	12.57	1.69	1.50
6	N	200	CYC	C2C-C1C	12.57	1.63	1.52
6	t	200	CYC	C2C-C1C	12.54	1.63	1.52
6	C	200	CYC	C2C-C1C	12.47	1.63	1.52
6	v	200	CYC	C2C-C1C	12.42	1.63	1.52
6	j	200	CYC	C3C-C4C	12.34	1.68	1.50
6	w	200	CYC	C3C-C4C	12.26	1.68	1.50
6	A	200	CYC	C1C-NC	12.13	1.53	1.37
6	H	200	CYC	C1C-NC	12.05	1.53	1.37
6	I	200	CYC	C1C-NC	11.93	1.53	1.37
6	N	200	CYC	C1C-NC	11.86	1.53	1.37
6	j	200	CYC	C1C-NC	11.86	1.53	1.37
6	x	200	CYC	C1C-NC	11.83	1.52	1.37
6	C	200	CYC	C1C-NC	11.82	1.52	1.37
6	w	200	CYC	C1C-NC	11.81	1.52	1.37
6	Y	200	CYC	C1C-NC	11.79	1.52	1.37
6	0	1201	CYC	C1C-NC	11.78	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	e	200	CYC	C1C-NC	11.78	1.52	1.37
6	s	200	CYC	C1C-NC	11.77	1.52	1.37
6	D	200	CYC	C1C-NC	11.75	1.52	1.37
6	U	200	CYC	C1C-NC	11.74	1.52	1.37
6	P	200	CYC	C1C-NC	11.73	1.52	1.37
6	O	200	CYC	C1C-NC	11.72	1.52	1.37
6	0	1202	CYC	C1C-NC	11.71	1.52	1.37
6	G	200	CYC	C1C-NC	11.70	1.52	1.37
6	q	200	CYC	C1C-NC	11.69	1.52	1.37
6	t	200	CYC	C1C-NC	11.68	1.52	1.37
6	m	200	CYC	C1C-NC	11.68	1.52	1.37
6	a	200	CYC	C1C-NC	11.67	1.52	1.37
6	T	200	CYC	C1C-NC	11.62	1.52	1.37
6	i	200	CYC	C1C-NC	11.62	1.52	1.37
6	J	200	CYC	C1C-NC	11.61	1.52	1.37
6	r	200	CYC	C1C-NC	11.60	1.52	1.37
6	u	200	CYC	C1C-NC	11.59	1.52	1.37
6	0	1203	CYC	C1C-NC	11.58	1.52	1.37
6	n	200	CYC	C1C-NC	11.57	1.52	1.37
6	b	200	CYC	C1C-NC	11.52	1.52	1.37
6	h	200	CYC	C1C-NC	11.52	1.52	1.37
6	R	200	CYC	C1C-NC	11.51	1.52	1.37
6	S	200	CYC	C1C-NC	11.48	1.52	1.37
6	c	200	CYC	C1C-NC	11.47	1.52	1.37
6	B	200	CYC	C1C-NC	11.44	1.52	1.37
6	V	200	CYC	OB-C4B	11.43	1.45	1.23
6	d	200	CYC	C1C-NC	11.42	1.52	1.37
6	k	200	CYC	C1C-NC	11.41	1.52	1.37
6	y	200	CYC	C1C-NC	11.41	1.52	1.37
6	L	200	CYC	C1C-NC	11.40	1.52	1.37
6	Q	200	CYC	C1C-NC	11.38	1.52	1.37
6	f	200	CYC	C1C-NC	11.37	1.52	1.37
6	i	200	CYC	OB-C4B	11.37	1.45	1.23
6	I	200	CYC	OB-C4B	11.34	1.45	1.23
6	p	200	CYC	C1C-NC	11.34	1.52	1.37
6	0	1201	CYC	OB-C4B	11.34	1.45	1.23
6	T	200	CYC	OB-C4B	11.33	1.45	1.23
6	R	200	CYC	OB-C4B	11.32	1.45	1.23
6	l	200	CYC	C1C-NC	11.31	1.52	1.37
6	H	200	CYC	OB-C4B	11.31	1.45	1.23
6	P	200	CYC	OB-C4B	11.31	1.45	1.23
6	h	200	CYC	OB-C4B	11.30	1.45	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	200	CYC	C1C-NC	11.28	1.52	1.37
6	U	200	CYC	OB-C4B	11.28	1.45	1.23
6	p	200	CYC	OB-C4B	11.27	1.45	1.23
6	J	200	CYC	OB-C4B	11.27	1.45	1.23
6	v	200	CYC	OB-C4B	11.26	1.45	1.23
6	B	200	CYC	OB-C4B	11.26	1.45	1.23
6	N	200	CYC	OB-C4B	11.26	1.45	1.23
6	l	200	CYC	OB-C4B	11.23	1.45	1.23
6	o	200	CYC	C1C-NC	11.23	1.52	1.37
6	0	1202	CYC	OB-C4B	11.23	1.44	1.23
6	y	200	CYC	OB-C4B	11.21	1.44	1.23
6	k	200	CYC	OB-C4B	11.20	1.44	1.23
6	A	200	CYC	OB-C4B	11.20	1.44	1.23
6	S	200	CYC	OB-C4B	11.20	1.44	1.23
6	n	200	CYC	OB-C4B	11.19	1.44	1.23
6	E	200	CYC	OB-C4B	11.19	1.44	1.23
6	u	200	CYC	OB-C4B	11.18	1.44	1.23
6	d	200	CYC	OB-C4B	11.18	1.44	1.23
6	L	200	CYC	OB-C4B	11.17	1.44	1.23
6	c	200	CYC	OB-C4B	11.17	1.44	1.23
6	e	200	CYC	OB-C4B	11.17	1.44	1.23
6	j	200	CYC	OB-C4B	11.17	1.44	1.23
6	C	200	CYC	OB-C4B	11.17	1.44	1.23
6	w	200	CYC	OB-C4B	11.16	1.44	1.23
6	Y	200	CYC	OB-C4B	11.16	1.44	1.23
6	r	200	CYC	OB-C4B	11.15	1.44	1.23
6	O	200	CYC	OB-C4B	11.15	1.44	1.23
6	q	200	CYC	OB-C4B	11.15	1.44	1.23
6	G	200	CYC	OB-C4B	11.15	1.44	1.23
6	Q	200	CYC	OB-C4B	11.15	1.44	1.23
6	a	200	CYC	OB-C4B	11.15	1.44	1.23
6	f	200	CYC	OB-C4B	11.11	1.44	1.23
6	x	200	CYC	OB-C4B	11.10	1.44	1.23
6	o	200	CYC	OB-C4B	11.09	1.44	1.23
6	D	200	CYC	OB-C4B	11.08	1.44	1.23
6	0	1203	CYC	OB-C4B	11.07	1.44	1.23
6	s	200	CYC	OB-C4B	11.07	1.44	1.23
6	b	200	CYC	OB-C4B	11.06	1.44	1.23
6	W	200	CYC	C1C-NC	11.05	1.51	1.37
6	W	200	CYC	OB-C4B	11.03	1.44	1.23
6	v	200	CYC	C1C-NC	10.96	1.51	1.37
6	t	200	CYC	OB-C4B	10.90	1.44	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	200	CYC	CHB-C4A	10.14	1.64	1.40
6	A	200	CYC	C2C-C3C	-10.00	1.26	1.54
6	m	200	CYC	CHB-C4A	9.93	1.63	1.40
6	q	200	CYC	C2C-C3C	-9.91	1.26	1.54
6	m	200	CYC	C2C-C3C	-9.90	1.26	1.54
6	J	200	CYC	C2C-C3C	-9.88	1.26	1.54
6	e	200	CYC	C2C-C3C	-9.87	1.26	1.54
6	A	200	CYC	CHB-C4A	9.86	1.63	1.40
6	t	200	CYC	C2C-C3C	-9.85	1.27	1.54
6	0	1203	CYC	C2C-C3C	-9.84	1.27	1.54
6	D	200	CYC	CHB-C4A	9.84	1.63	1.40
6	U	200	CYC	CHB-C4A	9.84	1.63	1.40
6	w	200	CYC	CHB-C4A	9.83	1.63	1.40
6	I	200	CYC	C2C-C3C	-9.83	1.27	1.54
6	0	1202	CYC	C2C-C3C	-9.83	1.27	1.54
6	B	200	CYC	CHB-C4A	9.83	1.63	1.40
6	y	200	CYC	C2C-C3C	-9.82	1.27	1.54
6	n	200	CYC	C2C-C3C	-9.82	1.27	1.54
6	U	200	CYC	C2C-C3C	-9.81	1.27	1.54
6	s	200	CYC	C2C-C3C	-9.80	1.27	1.54
6	u	200	CYC	C2C-C3C	-9.80	1.27	1.54
6	G	200	CYC	CHB-C4A	9.80	1.63	1.40
6	k	200	CYC	C2C-C3C	-9.79	1.27	1.54
6	D	200	CYC	C2C-C3C	-9.78	1.27	1.54
6	i	200	CYC	C2C-C3C	-9.78	1.27	1.54
6	J	200	CYC	CHB-C4A	9.77	1.63	1.40
6	O	200	CYC	C2C-C3C	-9.77	1.27	1.54
6	E	200	CYC	CHB-C4A	9.77	1.63	1.40
6	h	200	CYC	C2C-C3C	-9.77	1.27	1.54
6	0	1201	CYC	C2C-C3C	-9.76	1.27	1.54
6	0	1201	CYC	CHB-C4A	9.76	1.63	1.40
6	T	200	CYC	CHB-C4A	9.76	1.63	1.40
6	c	200	CYC	CHB-C4A	9.76	1.63	1.40
6	N	200	CYC	C2C-C3C	-9.76	1.27	1.54
6	Y	200	CYC	C2C-C3C	-9.74	1.27	1.54
6	R	200	CYC	C2C-C3C	-9.74	1.27	1.54
6	x	200	CYC	C2C-C3C	-9.73	1.27	1.54
6	O	200	CYC	CHB-C4A	9.73	1.63	1.40
6	W	200	CYC	CHB-C4A	9.72	1.63	1.40
6	a	200	CYC	C2C-C3C	-9.71	1.27	1.54
6	H	200	CYC	C2C-C3C	-9.71	1.27	1.54
6	W	200	CYC	C2C-C3C	-9.71	1.27	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	200	CYC	C2C-C3C	-9.71	1.27	1.54
6	b	200	CYC	C2C-C3C	-9.71	1.27	1.54
6	S	200	CYC	C2C-C3C	-9.70	1.27	1.54
6	R	200	CYC	CHB-C4A	9.70	1.63	1.40
6	r	200	CYC	C2C-C3C	-9.69	1.27	1.54
6	E	200	CYC	C2C-C3C	-9.69	1.27	1.54
6	T	200	CYC	C2C-C3C	-9.69	1.27	1.54
6	t	200	CYC	CHB-C4A	9.69	1.63	1.40
6	c	200	CYC	C2C-C3C	-9.69	1.27	1.54
6	f	200	CYC	C2C-C3C	-9.68	1.27	1.54
6	V	200	CYC	C2C-C3C	-9.68	1.27	1.54
6	C	200	CYC	C2C-C3C	-9.68	1.27	1.54
6	N	200	CYC	CHB-C4A	9.68	1.63	1.40
6	l	200	CYC	C2C-C3C	-9.68	1.27	1.54
6	G	200	CYC	C2C-C3C	-9.68	1.27	1.54
6	P	200	CYC	C2C-C3C	-9.67	1.27	1.54
6	H	200	CYC	CHB-C4A	9.66	1.63	1.40
6	I	200	CYC	CHB-C4A	9.66	1.63	1.40
6	o	200	CYC	C2C-C3C	-9.65	1.27	1.54
6	v	200	CYC	C2C-C3C	-9.65	1.27	1.54
6	0	1203	CYC	CHB-C4A	9.65	1.63	1.40
6	q	200	CYC	CHB-C4A	9.64	1.63	1.40
6	Q	200	CYC	C2C-C3C	-9.64	1.27	1.54
6	L	200	CYC	C2C-C3C	-9.63	1.27	1.54
6	e	200	CYC	CHB-C4A	9.63	1.62	1.40
6	C	200	CYC	CHB-C4A	9.62	1.62	1.40
6	p	200	CYC	C2C-C3C	-9.62	1.27	1.54
6	w	200	CYC	C2C-C3C	-9.61	1.27	1.54
6	f	200	CYC	CHB-C4A	9.61	1.62	1.40
6	j	200	CYC	C2C-C3C	-9.61	1.27	1.54
6	h	200	CYC	CHB-C4A	9.61	1.62	1.40
6	x	200	CYC	CHB-C4A	9.61	1.62	1.40
6	0	1202	CYC	CHB-C4A	9.61	1.62	1.40
6	n	200	CYC	CHB-C4A	9.60	1.62	1.40
6	u	200	CYC	CHB-C4A	9.60	1.62	1.40
6	o	200	CYC	CHB-C4A	9.59	1.62	1.40
6	L	200	CYC	CHB-C4A	9.58	1.62	1.40
6	y	200	CYC	CHB-C4A	9.58	1.62	1.40
6	a	200	CYC	CHB-C4A	9.57	1.62	1.40
6	Y	200	CYC	CHB-C4A	9.56	1.62	1.40
6	d	200	CYC	C2C-C3C	-9.55	1.27	1.54
6	i	200	CYC	CHB-C4A	9.55	1.62	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	200	CYC	CHB-C4A	9.55	1.62	1.40
6	r	200	CYC	CHB-C4A	9.54	1.62	1.40
6	j	200	CYC	CHB-C4A	9.52	1.62	1.40
6	S	200	CYC	CHB-C4A	9.52	1.62	1.40
6	d	200	CYC	CHB-C4A	9.50	1.62	1.40
6	b	200	CYC	CHB-C4A	9.50	1.62	1.40
6	p	200	CYC	CHB-C4A	9.49	1.62	1.40
6	V	200	CYC	CHB-C4A	9.45	1.62	1.40
6	s	200	CYC	CHB-C4A	9.42	1.62	1.40
6	l	200	CYC	CHB-C4A	9.41	1.62	1.40
6	v	200	CYC	CHB-C4A	9.38	1.62	1.40
6	k	200	CYC	CHB-C4A	9.31	1.62	1.40
6	P	200	CYC	CHB-C1B	6.32	1.53	1.38
6	t	200	CYC	C4B-C3B	-6.27	1.36	1.48
6	m	200	CYC	CHB-C1B	6.24	1.52	1.38
6	R	200	CYC	CHB-C1B	6.23	1.52	1.38
6	A	200	CYC	CHB-C1B	6.22	1.52	1.38
6	T	200	CYC	CHB-C1B	6.22	1.52	1.38
6	d	200	CYC	C4B-C3B	-6.20	1.36	1.48
6	b	200	CYC	C4B-C3B	-6.19	1.36	1.48
6	s	200	CYC	C4B-C3B	-6.19	1.36	1.48
6	G	200	CYC	CHB-C1B	6.18	1.52	1.38
6	I	200	CYC	CHB-C1B	6.18	1.52	1.38
6	S	200	CYC	C4B-C3B	-6.15	1.36	1.48
6	J	200	CYC	CHB-C1B	6.15	1.52	1.38
6	U	200	CYC	CHB-C1B	6.13	1.52	1.38
6	D	200	CYC	C4B-C3B	-6.12	1.36	1.48
6	f	200	CYC	C4B-C3B	-6.11	1.36	1.48
6	x	200	CYC	C4B-C3B	-6.11	1.36	1.48
6	a	200	CYC	C4B-C3B	-6.10	1.36	1.48
6	c	200	CYC	CHB-C1B	6.09	1.52	1.38
6	w	200	CYC	CHB-C1B	6.09	1.52	1.38
6	0	1201	CYC	CHB-C1B	6.09	1.52	1.38
6	c	200	CYC	C4B-C3B	-6.09	1.36	1.48
6	D	200	CYC	CHB-C1B	6.08	1.52	1.38
6	B	200	CYC	CHB-C1B	6.08	1.52	1.38
6	G	200	CYC	C4B-C3B	-6.08	1.36	1.48
6	R	200	CYC	C4B-C3B	-6.08	1.36	1.48
6	q	200	CYC	C4B-C3B	-6.08	1.36	1.48
6	E	200	CYC	CHB-C1B	6.08	1.52	1.38
6	l	200	CYC	C4B-C3B	-6.07	1.36	1.48
6	h	200	CYC	CHB-C1B	6.07	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	200	CYC	C4B-C3B	-6.07	1.36	1.48
6	n	200	CYC	CHB-C1B	6.06	1.52	1.38
6	p	200	CYC	C4B-C3B	-6.06	1.36	1.48
6	w	200	CYC	C4B-C3B	-6.05	1.36	1.48
6	f	200	CYC	CHB-C1B	6.05	1.52	1.38
6	C	200	CYC	CHB-C1B	6.05	1.52	1.38
6	e	200	CYC	CHB-C1B	6.04	1.52	1.38
6	O	200	CYC	CHB-C1B	6.03	1.52	1.38
6	Q	200	CYC	C4B-C3B	-6.03	1.36	1.48
6	O	200	CYC	C4B-C3B	-6.02	1.36	1.48
6	o	200	CYC	C4B-C3B	-6.02	1.36	1.48
6	P	200	CYC	C4B-C3B	-6.01	1.36	1.48
6	r	200	CYC	C4B-C3B	-6.01	1.36	1.48
6	y	200	CYC	C4B-C3B	-6.01	1.36	1.48
6	n	200	CYC	C4B-C3B	-5.99	1.36	1.48
6	p	200	CYC	CHB-C1B	5.99	1.52	1.38
6	L	200	CYC	C4B-C3B	-5.99	1.36	1.48
6	N	200	CYC	CHB-C1B	5.98	1.52	1.38
6	V	200	CYC	CHB-C1B	5.97	1.52	1.38
6	Y	200	CYC	CHB-C1B	5.97	1.52	1.38
6	r	200	CYC	CHB-C1B	5.97	1.52	1.38
6	v	200	CYC	C4B-C3B	-5.96	1.36	1.48
6	o	200	CYC	CHB-C1B	5.96	1.52	1.38
6	J	200	CYC	C4B-C3B	-5.96	1.36	1.48
6	j	200	CYC	C4B-C3B	-5.96	1.36	1.48
6	u	200	CYC	CHB-C1B	5.95	1.52	1.38
6	h	200	CYC	C4B-C3B	-5.95	1.36	1.48
6	x	200	CYC	CHB-C1B	5.94	1.52	1.38
6	U	200	CYC	C4B-C3B	-5.93	1.36	1.48
6	C	200	CYC	C4B-C3B	-5.93	1.36	1.48
6	Y	200	CYC	C4B-C3B	-5.93	1.36	1.48
6	T	200	CYC	C4B-C3B	-5.93	1.36	1.48
6	t	200	CYC	CHB-C1B	5.93	1.52	1.38
6	E	200	CYC	C4B-C3B	-5.92	1.37	1.48
6	0	1202	CYC	C4B-C3B	-5.92	1.37	1.48
6	a	200	CYC	CHB-C1B	5.92	1.52	1.38
6	H	200	CYC	CHB-C1B	5.91	1.52	1.38
6	0	1202	CYC	CHB-C1B	5.91	1.52	1.38
6	W	200	CYC	CHB-C1B	5.90	1.52	1.38
6	I	200	CYC	C4B-C3B	-5.90	1.37	1.48
6	u	200	CYC	C4B-C3B	-5.90	1.37	1.48
6	L	200	CYC	CHB-C1B	5.90	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	200	CYC	C4B-C3B	-5.90	1.37	1.48
6	0	1203	CYC	CHB-C1B	5.89	1.52	1.38
6	i	200	CYC	CHB-C1B	5.89	1.52	1.38
6	0	1203	CYC	C4B-C3B	-5.88	1.37	1.48
6	H	200	CYC	C4B-C3B	-5.88	1.37	1.48
6	0	1201	CYC	C4B-C3B	-5.88	1.37	1.48
6	S	200	CYC	CHB-C1B	5.87	1.52	1.38
6	e	200	CYC	C4B-C3B	-5.87	1.37	1.48
6	l	200	CYC	CHB-C1B	5.87	1.52	1.38
6	A	200	CYC	C4B-C3B	-5.86	1.37	1.48
6	Q	200	CYC	CHB-C1B	5.86	1.52	1.38
6	i	200	CYC	C4B-C3B	-5.85	1.37	1.48
6	b	200	CYC	CHB-C1B	5.85	1.51	1.38
6	d	200	CYC	CHB-C1B	5.84	1.51	1.38
6	N	200	CYC	C4B-C3B	-5.83	1.37	1.48
6	k	200	CYC	C4B-C3B	-5.83	1.37	1.48
6	j	200	CYC	CHB-C1B	5.80	1.51	1.38
6	y	200	CYC	CHB-C1B	5.80	1.51	1.38
6	s	200	CYC	CHB-C1B	5.78	1.51	1.38
6	q	200	CYC	CHB-C1B	5.76	1.51	1.38
6	v	200	CYC	CHB-C1B	5.74	1.51	1.38
6	V	200	CYC	C4B-C3B	-5.68	1.37	1.48
6	m	200	CYC	C1B-NB	-5.64	1.28	1.37
6	E	200	CYC	CHD-C4C	5.61	1.52	1.38
6	k	200	CYC	CHB-C1B	5.55	1.51	1.38
6	q	200	CYC	CHD-C4C	5.48	1.52	1.38
6	s	200	CYC	CHD-C4C	5.48	1.52	1.38
6	O	200	CYC	CHD-C4C	5.40	1.51	1.38
6	e	200	CYC	CHD-C4C	5.36	1.51	1.38
6	n	200	CYC	CHD-C4C	5.33	1.51	1.38
6	0	1201	CYC	C4D-CHA	5.32	1.61	1.41
6	Q	200	CYC	CHD-C4C	5.32	1.51	1.38
6	W	200	CYC	CHD-C4C	5.32	1.51	1.38
6	m	200	CYC	C4B-C3B	-5.32	1.38	1.48
6	e	200	CYC	C4D-CHA	5.31	1.61	1.41
6	d	200	CYC	CHD-C4C	5.31	1.51	1.38
6	y	200	CYC	C4D-CHA	5.30	1.61	1.41
6	y	200	CYC	CHD-C4C	5.29	1.51	1.38
6	D	200	CYC	CHD-C4C	5.28	1.51	1.38
6	p	200	CYC	C4D-CHA	5.28	1.61	1.41
6	j	200	CYC	CHD-C4C	5.27	1.51	1.38
6	B	200	CYC	CHD-C4C	5.27	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	200	CYC	CHD-C4C	5.27	1.51	1.38
6	n	200	CYC	C4D-CHA	5.26	1.61	1.41
6	b	200	CYC	CHD-C4C	5.26	1.51	1.38
6	E	200	CYC	C4D-CHA	5.26	1.61	1.41
6	a	200	CYC	CHD-C4C	5.26	1.51	1.38
6	P	200	CYC	C4D-CHA	5.25	1.61	1.41
6	H	200	CYC	CHD-C4C	5.24	1.51	1.38
6	r	200	CYC	CHD-C4C	5.24	1.51	1.38
6	c	200	CYC	CHD-C4C	5.24	1.51	1.38
6	T	200	CYC	CHD-C4C	5.24	1.51	1.38
6	L	200	CYC	CHD-C4C	5.23	1.51	1.38
6	i	200	CYC	CHD-C4C	5.23	1.51	1.38
6	U	200	CYC	C4D-CHA	5.23	1.61	1.41
6	r	200	CYC	C4D-CHA	5.23	1.61	1.41
6	O	200	CYC	C4D-CHA	5.23	1.61	1.41
6	p	200	CYC	CHD-C4C	5.23	1.51	1.38
6	S	200	CYC	CHD-C4C	5.23	1.51	1.38
6	f	200	CYC	CHD-C4C	5.22	1.51	1.38
6	G	200	CYC	C4D-CHA	5.22	1.61	1.41
6	C	200	CYC	CHD-C4C	5.22	1.51	1.38
6	G	200	CYC	CHD-C4C	5.22	1.51	1.38
6	a	200	CYC	C4D-CHA	5.22	1.61	1.41
6	R	200	CYC	C4D-CHA	5.22	1.61	1.41
6	A	200	CYC	C4D-CHA	5.22	1.61	1.41
6	B	200	CYC	C4D-CHA	5.22	1.61	1.41
6	A	200	CYC	CHD-C4C	5.21	1.51	1.38
6	D	200	CYC	C4D-CHA	5.21	1.61	1.41
6	i	200	CYC	C4D-CHA	5.21	1.61	1.41
6	C	200	CYC	C4D-CHA	5.21	1.61	1.41
6	P	200	CYC	CHD-C4C	5.20	1.51	1.38
6	o	200	CYC	CHD-C4C	5.20	1.51	1.38
6	H	200	CYC	C4D-CHA	5.19	1.61	1.41
6	h	200	CYC	CHD-C4C	5.19	1.51	1.38
6	t	200	CYC	C4D-CHA	5.19	1.61	1.41
6	S	200	CYC	C4D-CHA	5.19	1.61	1.41
6	L	200	CYC	C4D-CHA	5.19	1.61	1.41
6	b	200	CYC	C4D-CHA	5.19	1.61	1.41
6	t	200	CYC	CHD-C4C	5.18	1.51	1.38
6	0	1203	CYC	C4D-CHA	5.18	1.61	1.41
6	x	200	CYC	C4D-CHA	5.18	1.61	1.41
6	R	200	CYC	CHD-C4C	5.17	1.51	1.38
6	v	200	CYC	CHD-C4C	5.17	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	d	200	CYC	C4D-CHA	5.17	1.61	1.41
6	0	1202	CYC	C4D-CHA	5.16	1.61	1.41
6	V	200	CYC	CHD-C4C	5.16	1.51	1.38
6	Q	200	CYC	C4D-CHA	5.16	1.61	1.41
6	o	200	CYC	C4D-CHA	5.16	1.61	1.41
6	s	200	CYC	C4D-CHA	5.15	1.61	1.41
6	N	200	CYC	C4D-CHA	5.15	1.61	1.41
6	Y	200	CYC	C4D-CHA	5.14	1.61	1.41
6	0	1201	CYC	CHD-C4C	5.14	1.51	1.38
6	x	200	CYC	CHD-C4C	5.14	1.51	1.38
6	f	200	CYC	C4D-CHA	5.14	1.61	1.41
6	0	1203	CYC	CHD-C4C	5.13	1.51	1.38
6	l	200	CYC	CHD-C4C	5.13	1.51	1.38
6	J	200	CYC	CHD-C4C	5.13	1.51	1.38
6	N	200	CYC	CHD-C4C	5.13	1.51	1.38
6	I	200	CYC	C4D-CHA	5.13	1.61	1.41
6	V	200	CYC	C4D-CHA	5.12	1.61	1.41
6	c	200	CYC	C4D-CHA	5.12	1.61	1.41
6	d	200	CYC	C1D-CHD	5.12	1.61	1.41
6	q	200	CYC	C4D-CHA	5.12	1.61	1.41
6	T	200	CYC	C4D-CHA	5.12	1.61	1.41
6	L	200	CYC	C1D-CHD	5.12	1.61	1.41
6	k	200	CYC	CHD-C4C	5.12	1.51	1.38
6	k	200	CYC	C4D-CHA	5.11	1.61	1.41
6	m	200	CYC	C4D-CHA	5.10	1.61	1.41
6	0	1202	CYC	CHD-C4C	5.10	1.51	1.38
6	m	200	CYC	C1A-C2A	-5.09	1.37	1.45
6	h	200	CYC	C4D-CHA	5.09	1.60	1.41
6	s	200	CYC	C1D-CHD	5.08	1.60	1.41
6	j	200	CYC	C4D-CHA	5.08	1.60	1.41
6	v	200	CYC	C4D-CHA	5.08	1.60	1.41
6	u	200	CYC	C4D-CHA	5.07	1.60	1.41
6	w	200	CYC	CHD-C4C	5.07	1.51	1.38
6	q	200	CYC	C1D-CHD	5.07	1.60	1.41
6	u	200	CYC	CHD-C4C	5.06	1.50	1.38
6	Q	200	CYC	C1D-CHD	5.06	1.60	1.41
6	n	200	CYC	C1D-CHD	5.05	1.60	1.41
6	J	200	CYC	C4D-CHA	5.05	1.60	1.41
6	l	200	CYC	C1D-CHD	5.05	1.60	1.41
6	U	200	CYC	CHD-C4C	5.05	1.50	1.38
6	E	200	CYC	C1D-CHD	5.05	1.60	1.41
6	l	200	CYC	C4D-CHA	5.03	1.60	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	e	200	CYC	C1D-CHD	5.03	1.60	1.41
6	W	200	CYC	C4D-CHA	5.03	1.60	1.41
6	a	200	CYC	C1D-CHD	5.02	1.60	1.41
6	N	200	CYC	C1D-CHD	5.02	1.60	1.41
6	I	200	CYC	CHD-C4C	5.02	1.50	1.38
6	p	200	CYC	C1D-CHD	5.02	1.60	1.41
6	O	200	CYC	C1D-CHD	5.01	1.60	1.41
6	B	200	CYC	C1D-CHD	5.01	1.60	1.41
6	C	200	CYC	C1D-CHD	5.01	1.60	1.41
6	f	200	CYC	C1D-CHD	5.00	1.60	1.41
6	j	200	CYC	C1D-CHD	5.00	1.60	1.41
6	S	200	CYC	C1D-CHD	4.98	1.60	1.41
6	o	200	CYC	C1D-CHD	4.98	1.60	1.41
6	P	200	CYC	C1D-CHD	4.98	1.60	1.41
6	w	200	CYC	C4D-CHA	4.98	1.60	1.41
6	c	200	CYC	C1D-CHD	4.97	1.60	1.41
6	b	200	CYC	C1D-CHD	4.96	1.60	1.41
6	D	200	CYC	C1D-CHD	4.96	1.60	1.41
6	t	200	CYC	C1D-CHD	4.95	1.60	1.41
6	r	200	CYC	C1D-CHD	4.95	1.60	1.41
6	W	200	CYC	C1D-CHD	4.94	1.60	1.41
6	y	200	CYC	C1D-CHD	4.94	1.60	1.41
6	W	200	CYC	C1A-C2A	-4.94	1.37	1.45
6	G	200	CYC	C1D-CHD	4.93	1.60	1.41
6	T	200	CYC	C1D-CHD	4.93	1.60	1.41
6	k	200	CYC	C1D-CHD	4.91	1.60	1.41
6	J	200	CYC	C1D-CHD	4.91	1.60	1.41
6	Y	200	CYC	C1D-CHD	4.90	1.60	1.41
6	w	200	CYC	C1D-CHD	4.90	1.60	1.41
6	0	1201	CYC	C1D-CHD	4.90	1.60	1.41
6	h	200	CYC	C1D-CHD	4.89	1.60	1.41
6	R	200	CYC	C1D-CHD	4.89	1.60	1.41
6	0	1203	CYC	C1D-CHD	4.87	1.60	1.41
6	V	200	CYC	C1D-CHD	4.87	1.60	1.41
6	v	200	CYC	C1D-CHD	4.87	1.60	1.41
6	I	200	CYC	C1D-CHD	4.83	1.59	1.41
6	H	200	CYC	C1D-CHD	4.83	1.59	1.41
6	x	200	CYC	C1D-CHD	4.83	1.59	1.41
6	k	200	CYC	C1B-C2B	-4.83	1.36	1.45
6	U	200	CYC	C1D-CHD	4.82	1.59	1.41
6	i	200	CYC	C1D-CHD	4.82	1.59	1.41
6	A	200	CYC	C1D-CHD	4.82	1.59	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	m	200	CYC	CHD-C4C	4.80	1.50	1.38
6	u	200	CYC	C1D-CHD	4.78	1.59	1.41
6	0	1202	CYC	C1D-CHD	4.77	1.59	1.41
6	m	200	CYC	C1D-CHD	4.76	1.59	1.41
6	c	200	CYC	C1A-C2A	-4.73	1.38	1.45
6	r	200	CYC	C1B-C2B	-4.71	1.36	1.45
6	J	200	CYC	C1A-C2A	-4.70	1.38	1.45
6	S	200	CYC	C1A-C2A	-4.69	1.38	1.45
6	0	1202	CYC	C1A-C2A	-4.69	1.38	1.45
6	Q	200	CYC	C1B-C2B	-4.68	1.36	1.45
6	f	200	CYC	C1A-C2A	-4.66	1.38	1.45
6	d	200	CYC	C1A-C2A	-4.65	1.38	1.45
6	b	200	CYC	C1B-C2B	-4.64	1.36	1.45
6	j	200	CYC	C1A-C2A	-4.64	1.38	1.45
6	u	200	CYC	C1B-C2B	-4.63	1.36	1.45
6	D	200	CYC	C1A-C2A	-4.63	1.38	1.45
6	s	200	CYC	C1B-C2B	-4.63	1.36	1.45
6	q	200	CYC	C1A-C2A	-4.62	1.38	1.45
6	s	200	CYC	C1A-C2A	-4.61	1.38	1.45
6	e	200	CYC	C1B-C2B	-4.61	1.36	1.45
6	Y	200	CYC	C1B-C2B	-4.61	1.36	1.45
6	l	200	CYC	C1A-C2A	-4.59	1.38	1.45
6	d	200	CYC	C1B-C2B	-4.59	1.36	1.45
6	b	200	CYC	C1A-C2A	-4.59	1.38	1.45
6	x	200	CYC	C1A-C2A	-4.58	1.38	1.45
6	i	200	CYC	C1B-C2B	-4.58	1.36	1.45
6	n	200	CYC	C1B-C2B	-4.58	1.36	1.45
6	Y	200	CYC	C1A-C2A	-4.58	1.38	1.45
6	h	200	CYC	C1A-C2A	-4.57	1.38	1.45
6	v	200	CYC	C1A-C2A	-4.57	1.38	1.45
6	q	200	CYC	C1B-C2B	-4.57	1.36	1.45
6	Q	200	CYC	C1A-C2A	-4.56	1.38	1.45
6	0	1203	CYC	C1B-C2B	-4.56	1.36	1.45
6	x	200	CYC	C1B-C2B	-4.55	1.36	1.45
6	o	200	CYC	C1B-C2B	-4.55	1.36	1.45
6	A	200	CYC	C1A-C2A	-4.54	1.38	1.45
6	y	200	CYC	C1B-C2B	-4.54	1.36	1.45
6	v	200	CYC	C1B-C2B	-4.54	1.36	1.45
6	B	200	CYC	C1B-C2B	-4.53	1.37	1.45
6	0	1202	CYC	C1B-C2B	-4.53	1.37	1.45
6	j	200	CYC	C1B-C2B	-4.52	1.37	1.45
6	l	200	CYC	C1B-C2B	-4.52	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	t	200	CYC	C1A-C2A	-4.52	1.38	1.45
6	R	200	CYC	C1A-C2A	-4.51	1.38	1.45
6	a	200	CYC	C1A-C2A	-4.50	1.38	1.45
6	O	200	CYC	C1B-C2B	-4.49	1.37	1.45
6	r	200	CYC	C1A-C2A	-4.49	1.38	1.45
6	w	200	CYC	C1A-C2A	-4.48	1.38	1.45
6	B	200	CYC	C1A-C2A	-4.48	1.38	1.45
6	o	200	CYC	C1A-C2A	-4.48	1.38	1.45
6	S	200	CYC	C1B-C2B	-4.48	1.37	1.45
6	f	200	CYC	C1B-C2B	-4.47	1.37	1.45
6	i	200	CYC	C1A-C2A	-4.46	1.38	1.45
6	O	200	CYC	C1A-C2A	-4.46	1.38	1.45
6	n	200	CYC	C1A-C2A	-4.45	1.38	1.45
6	L	200	CYC	C1B-C2B	-4.45	1.37	1.45
6	W	200	CYC	C1B-C2B	-4.45	1.37	1.45
6	y	200	CYC	C1A-C2A	-4.44	1.38	1.45
6	m	200	CYC	C1B-C2B	-4.44	1.37	1.45
6	a	200	CYC	C1B-C2B	-4.43	1.37	1.45
6	h	200	CYC	C1B-C2B	-4.43	1.37	1.45
6	q	200	CYC	C1B-NB	-4.43	1.30	1.37
6	N	200	CYC	C1A-C2A	-4.40	1.38	1.45
6	E	200	CYC	C1A-C2A	-4.40	1.38	1.45
6	k	200	CYC	C1B-NB	-4.39	1.30	1.37
6	H	200	CYC	C1B-C2B	-4.39	1.37	1.45
6	p	200	CYC	C1B-C2B	-4.39	1.37	1.45
6	w	200	CYC	C1B-C2B	-4.39	1.37	1.45
6	R	200	CYC	C1B-C2B	-4.39	1.37	1.45
6	P	200	CYC	C1A-C2A	-4.38	1.38	1.45
6	k	200	CYC	C1A-C2A	-4.38	1.38	1.45
6	0	1201	CYC	C1B-NB	-4.38	1.30	1.37
6	f	200	CYC	C1B-NB	-4.37	1.30	1.37
6	u	200	CYC	C1A-C2A	-4.36	1.38	1.45
6	A	200	CYC	C1B-C2B	-4.36	1.37	1.45
6	I	200	CYC	C1A-C2A	-4.35	1.38	1.45
6	D	200	CYC	C1B-C2B	-4.35	1.37	1.45
6	0	1203	CYC	C1A-C2A	-4.35	1.38	1.45
6	e	200	CYC	C1A-C2A	-4.34	1.38	1.45
6	L	200	CYC	C1A-C2A	-4.34	1.38	1.45
6	W	200	CYC	C1B-NB	-4.32	1.30	1.37
6	V	200	CYC	C1B-C2B	-4.32	1.37	1.45
6	T	200	CYC	C1B-C2B	-4.31	1.37	1.45
6	0	1201	CYC	C1B-C2B	-4.31	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	c	200	CYC	C1B-C2B	-4.30	1.37	1.45
6	G	200	CYC	C1A-C2A	-4.30	1.38	1.45
6	b	200	CYC	C1B-NB	-4.30	1.30	1.37
6	j	200	CYC	C1B-NB	-4.29	1.30	1.37
6	t	200	CYC	C1B-NB	-4.29	1.30	1.37
6	0	1201	CYC	C1A-C2A	-4.29	1.38	1.45
6	J	200	CYC	C1B-C2B	-4.27	1.37	1.45
6	d	200	CYC	C1B-NB	-4.27	1.30	1.37
6	t	200	CYC	C1B-C2B	-4.27	1.37	1.45
6	U	200	CYC	C1A-C2A	-4.26	1.38	1.45
6	a	200	CYC	C1B-NB	-4.25	1.30	1.37
6	v	200	CYC	C1B-NB	-4.25	1.30	1.37
6	x	200	CYC	C1B-NB	-4.25	1.30	1.37
6	o	200	CYC	C1B-NB	-4.25	1.30	1.37
6	s	200	CYC	C1B-NB	-4.25	1.30	1.37
6	Y	200	CYC	C1B-NB	-4.24	1.30	1.37
6	p	200	CYC	C1A-C2A	-4.24	1.39	1.45
6	E	200	CYC	C1B-C2B	-4.24	1.37	1.45
6	w	200	CYC	C1B-NB	-4.23	1.30	1.37
6	V	200	CYC	C1A-C2A	-4.22	1.39	1.45
6	C	200	CYC	C1A-C2A	-4.22	1.39	1.45
6	S	200	CYC	C1B-NB	-4.20	1.30	1.37
6	n	200	CYC	C1B-NB	-4.20	1.30	1.37
6	u	200	CYC	C1B-NB	-4.20	1.30	1.37
6	Q	200	CYC	C1B-NB	-4.20	1.30	1.37
6	H	200	CYC	C1A-C2A	-4.20	1.39	1.45
6	U	200	CYC	C1B-C2B	-4.19	1.37	1.45
6	h	200	CYC	C1B-NB	-4.18	1.30	1.37
6	i	200	CYC	C1B-NB	-4.17	1.30	1.37
6	D	200	CYC	C1B-NB	-4.17	1.30	1.37
6	I	200	CYC	C1B-C2B	-4.17	1.37	1.45
6	N	200	CYC	C1B-C2B	-4.17	1.37	1.45
6	l	200	CYC	C1B-NB	-4.16	1.30	1.37
6	O	200	CYC	C1B-NB	-4.15	1.30	1.37
6	C	200	CYC	C1B-C2B	-4.14	1.37	1.45
6	r	200	CYC	C1B-NB	-4.14	1.30	1.37
6	p	200	CYC	C1B-NB	-4.12	1.30	1.37
6	J	200	CYC	C1B-NB	-4.11	1.30	1.37
6	R	200	CYC	C1B-NB	-4.11	1.30	1.37
6	0	1202	CYC	C1B-NB	-4.11	1.30	1.37
6	G	200	CYC	C1B-C2B	-4.10	1.37	1.45
6	B	200	CYC	C1B-NB	-4.10	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	200	CYC	C1B-C2B	-4.09	1.37	1.45
6	c	200	CYC	C1B-NB	-4.09	1.31	1.37
6	0	1203	CYC	C1B-NB	-4.09	1.31	1.37
6	U	200	CYC	C1B-NB	-4.08	1.31	1.37
6	y	200	CYC	C1B-NB	-4.07	1.31	1.37
6	G	200	CYC	C1B-NB	-4.05	1.31	1.37
6	E	200	CYC	C1B-NB	-4.04	1.31	1.37
6	e	200	CYC	C1B-NB	-4.04	1.31	1.37
6	A	200	CYC	C1B-NB	-4.01	1.31	1.37
6	L	200	CYC	C1B-NB	-4.01	1.31	1.37
6	T	200	CYC	C1A-C2A	-4.00	1.39	1.45
6	H	200	CYC	C1B-NB	-3.98	1.31	1.37
6	P	200	CYC	C1B-NB	-3.97	1.31	1.37
6	N	200	CYC	C1B-NB	-3.96	1.31	1.37
6	E	200	CYC	CBA-CGA	3.95	1.59	1.50
6	C	200	CYC	C1B-NB	-3.95	1.31	1.37
6	T	200	CYC	C1B-NB	-3.94	1.31	1.37
6	p	200	CYC	CBA-CGA	3.93	1.59	1.50
6	i	200	CYC	CBA-CGA	3.92	1.59	1.50
6	V	200	CYC	C1B-NB	-3.92	1.31	1.37
6	w	200	CYC	CBA-CGA	3.91	1.59	1.50
6	I	200	CYC	CBA-CGA	3.91	1.59	1.50
6	I	200	CYC	C1B-NB	-3.91	1.31	1.37
6	A	200	CYC	CBA-CGA	3.90	1.59	1.50
6	O	200	CYC	CBA-CGA	3.90	1.59	1.50
6	B	200	CYC	CBA-CGA	3.89	1.59	1.50
6	N	200	CYC	CBA-CGA	3.87	1.59	1.50
6	t	200	CYC	CBA-CGA	3.86	1.59	1.50
6	V	200	CYC	CBA-CGA	3.86	1.59	1.50
6	u	200	CYC	CBA-CGA	3.86	1.59	1.50
6	H	200	CYC	CBA-CGA	3.84	1.59	1.50
6	h	200	CYC	CBA-CGA	3.84	1.59	1.50
6	C	200	CYC	CBA-CGA	3.83	1.59	1.50
6	G	200	CYC	CBA-CGA	3.82	1.59	1.50
6	U	200	CYC	CBA-CGA	3.82	1.59	1.50
6	0	1201	CYC	CMC-C2C	3.82	1.61	1.53
6	D	200	CYC	CBA-CGA	3.81	1.59	1.50
6	P	200	CYC	CBA-CGA	3.81	1.59	1.50
6	0	1203	CYC	CBA-CGA	3.80	1.59	1.50
6	R	200	CYC	CBA-CGA	3.80	1.59	1.50
6	E	200	CYC	CMC-C2C	3.79	1.61	1.53
6	p	200	CYC	CMC-C2C	3.78	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	x	200	CYC	CBA-CGA	3.77	1.59	1.50
6	C	200	CYC	CMC-C2C	3.77	1.61	1.53
6	S	200	CYC	CBA-CGA	3.77	1.59	1.50
6	T	200	CYC	CBA-CGA	3.76	1.59	1.50
6	e	200	CYC	CBA-CGA	3.76	1.59	1.50
6	q	200	CYC	CBA-CGA	3.76	1.59	1.50
6	a	200	CYC	CBA-CGA	3.76	1.59	1.50
6	o	200	CYC	CBA-CGA	3.76	1.59	1.50
6	0	1201	CYC	CBA-CGA	3.76	1.59	1.50
6	r	200	CYC	CBA-CGA	3.76	1.59	1.50
6	P	200	CYC	CMC-C2C	3.75	1.61	1.53
6	f	200	CYC	CBA-CGA	3.74	1.59	1.50
6	m	200	CYC	CBA-CGA	3.73	1.59	1.50
6	Q	200	CYC	CBA-CGA	3.73	1.59	1.50
6	J	200	CYC	CBA-CGA	3.72	1.59	1.50
6	Q	200	CYC	CMC-C2C	3.72	1.61	1.53
6	d	200	CYC	CBA-CGA	3.71	1.59	1.50
6	i	200	CYC	CMC-C2C	3.71	1.61	1.53
6	c	200	CYC	CBA-CGA	3.71	1.59	1.50
6	n	200	CYC	CMC-C2C	3.71	1.61	1.53
6	b	200	CYC	CBA-CGA	3.71	1.59	1.50
6	n	200	CYC	CBA-CGA	3.71	1.59	1.50
6	A	200	CYC	CMC-C2C	3.70	1.61	1.53
6	Y	200	CYC	CBA-CGA	3.70	1.59	1.50
6	d	200	CYC	CMC-C2C	3.70	1.61	1.53
6	m	200	CYC	CMC-C2C	3.70	1.61	1.53
6	a	200	CYC	CMC-C2C	3.70	1.61	1.53
6	G	200	CYC	CMC-C2C	3.69	1.61	1.53
6	H	200	CYC	CMC-C2C	3.69	1.61	1.53
6	u	200	CYC	CMC-C2C	3.69	1.61	1.53
6	c	200	CYC	CMC-C2C	3.69	1.61	1.53
6	B	200	CYC	CMC-C2C	3.68	1.61	1.53
6	O	200	CYC	CMC-C2C	3.68	1.61	1.53
6	V	200	CYC	CMC-C2C	3.67	1.61	1.53
6	e	200	CYC	CMC-C2C	3.67	1.61	1.53
6	k	200	CYC	CBA-CGA	3.66	1.59	1.50
6	x	200	CYC	CMC-C2C	3.66	1.61	1.53
6	r	200	CYC	CMC-C2C	3.66	1.61	1.53
6	L	200	CYC	CBA-CGA	3.66	1.59	1.50
6	D	200	CYC	CMC-C2C	3.65	1.61	1.53
6	k	200	CYC	CMC-C2C	3.65	1.61	1.53
6	N	200	CYC	CMC-C2C	3.64	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	s	200	CYC	CBA-CGA	3.64	1.59	1.50
6	U	200	CYC	CMC-C2C	3.64	1.61	1.53
6	j	200	CYC	CMC-C2C	3.63	1.61	1.53
6	Y	200	CYC	CMC-C2C	3.63	1.61	1.53
6	j	200	CYC	CBA-CGA	3.62	1.59	1.50
6	v	200	CYC	CBA-CGA	3.62	1.59	1.50
6	o	200	CYC	CMC-C2C	3.62	1.61	1.53
6	q	200	CYC	CMC-C2C	3.62	1.61	1.53
6	R	200	CYC	CMC-C2C	3.61	1.61	1.53
6	l	200	CYC	CBA-CGA	3.61	1.59	1.50
6	T	200	CYC	CMC-C2C	3.61	1.60	1.53
6	0	1203	CYC	CMC-C2C	3.60	1.60	1.53
6	0	1202	CYC	CBA-CGA	3.60	1.59	1.50
6	I	200	CYC	CMC-C2C	3.60	1.60	1.53
6	s	200	CYC	CMC-C2C	3.60	1.60	1.53
6	y	200	CYC	CMC-C2C	3.59	1.60	1.53
6	b	200	CYC	CMC-C2C	3.59	1.60	1.53
6	w	200	CYC	CMC-C2C	3.59	1.60	1.53
6	f	200	CYC	CMC-C2C	3.58	1.60	1.53
6	0	1202	CYC	CMC-C2C	3.58	1.60	1.53
6	y	200	CYC	CBA-CGA	3.57	1.58	1.50
6	L	200	CYC	CMC-C2C	3.55	1.60	1.53
6	S	200	CYC	CMC-C2C	3.53	1.60	1.53
6	h	200	CYC	CMC-C2C	3.51	1.60	1.53
6	W	200	CYC	CMC-C2C	3.50	1.60	1.53
6	l	200	CYC	CMC-C2C	3.49	1.60	1.53
6	W	200	CYC	CBA-CGA	3.48	1.58	1.50
6	J	200	CYC	CMC-C2C	3.46	1.60	1.53
6	v	200	CYC	CMC-C2C	3.44	1.60	1.53
6	0	1201	CYC	CAB-C3B	3.41	1.59	1.51
6	k	200	CYC	C1A-NA	-3.30	1.31	1.38
6	s	200	CYC	C1A-NA	-3.28	1.31	1.38
6	t	200	CYC	CMC-C2C	3.28	1.60	1.53
6	x	200	CYC	C1A-NA	-3.21	1.31	1.38
6	u	200	CYC	C1A-NA	-3.20	1.31	1.38
6	j	200	CYC	C1A-NA	-3.20	1.31	1.38
6	W	200	CYC	C1A-NA	-3.19	1.31	1.38
6	v	200	CYC	C1A-NA	-3.19	1.31	1.38
6	d	200	CYC	C1A-NA	-3.11	1.31	1.38
6	y	200	CYC	C1A-NA	-3.11	1.31	1.38
6	m	200	CYC	CAB-C3B	3.10	1.59	1.51
6	q	200	CYC	C1A-NA	-3.08	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	200	CYC	CAB-C3B	3.08	1.59	1.51
6	Y	200	CYC	C1A-NA	-3.08	1.32	1.38
6	b	200	CYC	C1A-NA	-3.08	1.32	1.38
6	w	200	CYC	C1A-NA	-3.07	1.32	1.38
6	w	200	CYC	CAB-C3B	3.06	1.58	1.51
6	i	200	CYC	CAB-C3B	3.05	1.58	1.51
6	t	200	CYC	C1A-NA	-3.05	1.32	1.38
6	f	200	CYC	C1A-NA	-3.05	1.32	1.38
6	G	200	CYC	CAB-C3B	3.05	1.58	1.51
6	Q	200	CYC	C1A-NA	-3.05	1.32	1.38
6	h	200	CYC	C1A-NA	-3.05	1.32	1.38
6	V	200	CYC	CAB-C3B	3.04	1.58	1.51
6	l	200	CYC	C1A-NA	-3.04	1.32	1.38
6	r	200	CYC	C1A-NA	-3.03	1.32	1.38
6	0	1203	CYC	C1A-NA	-3.03	1.32	1.38
6	S	200	CYC	C1A-NA	-3.03	1.32	1.38
6	A	200	CYC	CAB-C3B	3.02	1.58	1.51
6	C	200	CYC	CAB-C3B	3.02	1.58	1.51
6	n	200	CYC	CAB-C3B	3.02	1.58	1.51
6	0	1201	CYC	C1A-NA	-3.01	1.32	1.38
6	J	200	CYC	CAB-C3B	3.01	1.58	1.51
6	p	200	CYC	C1A-NA	-3.01	1.32	1.38
6	0	1202	CYC	C1A-NA	-3.00	1.32	1.38
6	n	200	CYC	C1A-NA	-3.00	1.32	1.38
6	o	200	CYC	C1A-NA	-3.00	1.32	1.38
6	Y	200	CYC	C4B-NB	-3.00	1.31	1.38
6	i	200	CYC	C1A-NA	-2.99	1.32	1.38
6	r	200	CYC	CAB-C3B	2.99	1.58	1.51
6	d	200	CYC	C4B-NB	-2.99	1.31	1.38
6	q	200	CYC	C4B-NB	-2.99	1.31	1.38
6	h	200	CYC	CAB-C3B	2.98	1.58	1.51
6	H	200	CYC	C1A-NA	-2.96	1.32	1.38
6	R	200	CYC	CAB-C3B	2.96	1.58	1.51
6	f	200	CYC	CAB-C3B	2.96	1.58	1.51
6	E	200	CYC	CAB-C3B	2.96	1.58	1.51
6	N	200	CYC	CAB-C3B	2.96	1.58	1.51
6	D	200	CYC	CAB-C3B	2.96	1.58	1.51
6	L	200	CYC	CAB-C3B	2.95	1.58	1.51
6	f	200	CYC	C4B-NB	-2.95	1.31	1.38
6	x	200	CYC	CAB-C3B	2.95	1.58	1.51
6	P	200	CYC	CAB-C3B	2.95	1.58	1.51
6	e	200	CYC	C1A-NA	-2.95	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	200	CYC	CAB-C3B	2.94	1.58	1.51
6	k	200	CYC	C4B-NB	-2.94	1.31	1.38
6	c	200	CYC	CAB-C3B	2.94	1.58	1.51
6	Q	200	CYC	CAB-C3B	2.94	1.58	1.51
6	t	200	CYC	CAB-C3B	2.93	1.58	1.51
6	a	200	CYC	C1A-NA	-2.93	1.32	1.38
6	W	200	CYC	C4B-NB	-2.93	1.31	1.38
6	l	200	CYC	CAB-C3B	2.93	1.58	1.51
6	U	200	CYC	CAB-C3B	2.93	1.58	1.51
6	j	200	CYC	CAB-C3B	2.92	1.58	1.51
6	H	200	CYC	CAB-C3B	2.92	1.58	1.51
6	o	200	CYC	CAB-C3B	2.92	1.58	1.51
6	Q	200	CYC	C4B-NB	-2.92	1.31	1.38
6	u	200	CYC	CAB-C3B	2.92	1.58	1.51
6	b	200	CYC	CAB-C3B	2.91	1.58	1.51
6	O	200	CYC	CAB-C3B	2.91	1.58	1.51
6	d	200	CYC	CAB-C3B	2.90	1.58	1.51
6	t	200	CYC	C4B-NB	-2.90	1.31	1.38
6	Y	200	CYC	CAB-C3B	2.90	1.58	1.51
6	W	200	CYC	CAB-C3B	2.90	1.58	1.51
6	e	200	CYC	CAB-C3B	2.90	1.58	1.51
6	0	1202	CYC	CAB-C3B	2.89	1.58	1.51
6	q	200	CYC	CAB-C3B	2.89	1.58	1.51
6	p	200	CYC	CAB-C3B	2.89	1.58	1.51
6	L	200	CYC	C1A-NA	-2.88	1.32	1.38
6	O	200	CYC	C1A-NA	-2.88	1.32	1.38
6	j	200	CYC	CAC-C3C	2.88	1.59	1.54
6	v	200	CYC	CAC-C3C	2.88	1.59	1.54
6	B	200	CYC	CAB-C3B	2.88	1.58	1.51
6	0	1201	CYC	CAC-C3C	2.88	1.59	1.54
6	y	200	CYC	C4B-NB	-2.87	1.31	1.38
6	D	200	CYC	C1A-NA	-2.87	1.32	1.38
6	l	200	CYC	C4B-NB	-2.86	1.31	1.38
6	0	1203	CYC	CAB-C3B	2.86	1.58	1.51
6	a	200	CYC	CAB-C3B	2.86	1.58	1.51
6	s	200	CYC	CAB-C3B	2.86	1.58	1.51
6	O	200	CYC	C4B-NB	-2.85	1.31	1.38
6	U	200	CYC	C1A-NA	-2.85	1.32	1.38
6	c	200	CYC	C1A-NA	-2.85	1.32	1.38
6	w	200	CYC	CAC-C3C	2.85	1.59	1.54
6	s	200	CYC	C4B-NB	-2.84	1.32	1.38
6	v	200	CYC	CAB-C3B	2.84	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	j	200	CYC	C4B-NB	-2.84	1.32	1.38
6	a	200	CYC	C4B-NB	-2.83	1.32	1.38
6	0	1201	CYC	C4B-NB	-2.82	1.32	1.38
6	N	200	CYC	C1A-NA	-2.81	1.32	1.38
6	0	1203	CYC	C4B-NB	-2.81	1.32	1.38
6	v	200	CYC	C4B-NB	-2.81	1.32	1.38
6	y	200	CYC	CAB-C3B	2.80	1.58	1.51
6	f	200	CYC	CAC-C3C	2.80	1.59	1.54
6	S	200	CYC	CAC-C3C	2.80	1.59	1.54
6	D	200	CYC	C4B-NB	-2.80	1.32	1.38
6	B	200	CYC	C1A-NA	-2.80	1.32	1.38
6	h	200	CYC	C4B-NB	-2.79	1.32	1.38
6	x	200	CYC	C4B-NB	-2.79	1.32	1.38
6	L	200	CYC	CAC-C3C	2.79	1.59	1.54
6	R	200	CYC	C1A-NA	-2.79	1.32	1.38
6	R	200	CYC	C4B-NB	-2.79	1.32	1.38
6	S	200	CYC	CAB-C3B	2.79	1.58	1.51
6	b	200	CYC	C4B-NB	-2.79	1.32	1.38
6	B	200	CYC	C4B-NB	-2.79	1.32	1.38
6	o	200	CYC	C4B-NB	-2.78	1.32	1.38
6	S	200	CYC	C4B-NB	-2.78	1.32	1.38
6	c	200	CYC	CAC-C3C	2.77	1.59	1.54
6	r	200	CYC	CAC-C3C	2.77	1.59	1.54
6	J	200	CYC	C1A-NA	-2.77	1.32	1.38
6	E	200	CYC	C1A-NA	-2.76	1.32	1.38
6	V	200	CYC	CAC-C3C	2.76	1.59	1.54
6	d	200	CYC	CAC-C3C	2.76	1.59	1.54
6	a	200	CYC	CAC-C3C	2.76	1.59	1.54
6	c	200	CYC	C4B-NB	-2.76	1.32	1.38
6	0	1202	CYC	C4B-NB	-2.75	1.32	1.38
6	W	200	CYC	CAC-C3C	2.75	1.59	1.54
6	w	200	CYC	C4B-NB	-2.75	1.32	1.38
6	R	200	CYC	CAC-C3C	2.75	1.59	1.54
6	G	200	CYC	C4B-NB	-2.74	1.32	1.38
6	C	200	CYC	CAC-C3C	2.74	1.59	1.54
6	A	200	CYC	C1A-NA	-2.74	1.32	1.38
6	r	200	CYC	C4B-NB	-2.74	1.32	1.38
6	G	200	CYC	C1A-NA	-2.73	1.32	1.38
6	o	200	CYC	CAC-C3C	2.72	1.59	1.54
6	k	200	CYC	CAB-C3B	2.72	1.58	1.51
6	T	200	CYC	CAC-C3C	2.72	1.59	1.54
6	n	200	CYC	CAC-C3C	2.71	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	200	CYC	C4B-NB	-2.71	1.32	1.38
6	C	200	CYC	C4B-NB	-2.71	1.32	1.38
6	t	200	CYC	CAC-C3C	2.71	1.59	1.54
6	e	200	CYC	CAC-C3C	2.70	1.59	1.54
6	G	200	CYC	CAC-C3C	2.70	1.59	1.54
6	N	200	CYC	CAC-C3C	2.70	1.59	1.54
6	V	200	CYC	C4B-NB	-2.70	1.32	1.38
6	P	200	CYC	C1A-NA	-2.70	1.32	1.38
6	E	200	CYC	C4B-NB	-2.70	1.32	1.38
6	m	200	CYC	C4B-NB	-2.69	1.32	1.38
6	b	200	CYC	CAC-C3C	2.69	1.59	1.54
6	P	200	CYC	C4B-NB	-2.69	1.32	1.38
6	n	200	CYC	C4B-NB	-2.68	1.32	1.38
6	u	200	CYC	C4B-NB	-2.67	1.32	1.38
6	p	200	CYC	C4B-NB	-2.66	1.32	1.38
6	0	1202	CYC	CAC-C3C	2.66	1.59	1.54
6	0	1203	CYC	CAC-C3C	2.66	1.59	1.54
6	m	200	CYC	C4A-C3A	-2.66	1.40	1.45
6	i	200	CYC	C4B-NB	-2.65	1.32	1.38
6	I	200	CYC	C4B-NB	-2.65	1.32	1.38
6	h	200	CYC	CAC-C3C	2.65	1.59	1.54
6	m	200	CYC	CAC-C3C	2.65	1.59	1.54
6	N	200	CYC	C4B-NB	-2.65	1.32	1.38
6	e	200	CYC	C4B-NB	-2.65	1.32	1.38
6	l	200	CYC	CAC-C3C	2.65	1.59	1.54
6	V	200	CYC	C4A-C3A	-2.64	1.40	1.45
6	L	200	CYC	C4B-NB	-2.64	1.32	1.38
6	p	200	CYC	CAC-C3C	2.63	1.59	1.54
6	T	200	CYC	C1A-NA	-2.63	1.32	1.38
6	P	200	CYC	CAC-C3C	2.62	1.59	1.54
6	Y	200	CYC	CAC-C3C	2.62	1.59	1.54
6	V	200	CYC	C1A-NA	-2.62	1.33	1.38
6	T	200	CYC	C4B-NB	-2.61	1.32	1.38
6	A	200	CYC	C4B-NB	-2.60	1.32	1.38
6	B	200	CYC	CAC-C3C	2.60	1.59	1.54
6	L	200	CYC	C4A-C3A	-2.59	1.40	1.45
6	y	200	CYC	CAC-C3C	2.59	1.59	1.54
6	H	200	CYC	CAC-C3C	2.59	1.59	1.54
6	I	200	CYC	C1A-NA	-2.57	1.33	1.38
6	C	200	CYC	C1A-NA	-2.57	1.33	1.38
6	H	200	CYC	C4B-NB	-2.57	1.32	1.38
6	k	200	CYC	CAC-C3C	2.56	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	O	200	CYC	CAC-C3C	2.55	1.59	1.54
6	D	200	CYC	CAC-C3C	2.55	1.59	1.54
6	u	200	CYC	CAC-C3C	2.55	1.59	1.54
6	I	200	CYC	CAC-C3C	2.53	1.59	1.54
6	v	200	CYC	C4A-C3A	-2.53	1.40	1.45
6	Q	200	CYC	CAC-C3C	2.53	1.59	1.54
6	U	200	CYC	CAC-C3C	2.52	1.58	1.54
6	x	200	CYC	C4A-C3A	-2.52	1.40	1.45
6	s	200	CYC	CAC-C3C	2.51	1.58	1.54
6	R	200	CYC	CMD-C2D	2.51	1.56	1.51
6	x	200	CYC	CAC-C3C	2.50	1.58	1.54
6	n	200	CYC	C4A-C3A	-2.50	1.40	1.45
6	B	200	CYC	CMD-C2D	2.49	1.56	1.51
6	U	200	CYC	C4B-NB	-2.48	1.32	1.38
6	k	200	CYC	C4A-C3A	-2.48	1.40	1.45
6	v	200	CYC	CMD-C2D	2.48	1.56	1.51
6	I	200	CYC	C4A-C3A	-2.47	1.40	1.45
6	U	200	CYC	CMD-C2D	2.47	1.56	1.51
6	w	200	CYC	CMD-C2D	2.47	1.56	1.51
6	G	200	CYC	CMD-C2D	2.45	1.56	1.51
6	p	200	CYC	CMD-C2D	2.45	1.56	1.51
6	L	200	CYC	CMD-C2D	2.45	1.56	1.51
6	a	200	CYC	CMD-C2D	2.45	1.56	1.51
6	p	200	CYC	C4A-C3A	-2.45	1.40	1.45
6	Y	200	CYC	C4A-C3A	-2.45	1.40	1.45
6	E	200	CYC	CAC-C3C	2.44	1.58	1.54
6	i	200	CYC	C4A-C3A	-2.44	1.40	1.45
6	i	200	CYC	CAC-C3C	2.44	1.58	1.54
6	u	200	CYC	C4A-C3A	-2.44	1.40	1.45
6	l	200	CYC	C4A-C3A	-2.43	1.40	1.45
6	f	200	CYC	CMD-C2D	2.43	1.56	1.51
6	J	200	CYC	CAC-C3C	2.43	1.58	1.54
6	A	200	CYC	CAC-C3C	2.43	1.58	1.54
6	0	1203	CYC	CMD-C2D	2.43	1.56	1.51
6	0	1201	CYC	CMD-C2D	2.43	1.56	1.51
6	D	200	CYC	CMD-C2D	2.42	1.56	1.51
6	H	200	CYC	C4A-C3A	-2.42	1.40	1.45
6	y	200	CYC	C4A-C3A	-2.42	1.40	1.45
6	b	200	CYC	CMD-C2D	2.42	1.56	1.51
6	T	200	CYC	CMD-C2D	2.41	1.56	1.51
6	S	200	CYC	C4A-C3A	-2.41	1.40	1.45
6	Q	200	CYC	CMD-C2D	2.41	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	200	CYC	C4A-C3A	-2.41	1.40	1.45
6	c	200	CYC	CMD-C2D	2.41	1.56	1.51
6	S	200	CYC	CMD-C2D	2.40	1.56	1.51
6	l	200	CYC	CMD-C2D	2.40	1.56	1.51
6	r	200	CYC	CMD-C2D	2.40	1.56	1.51
6	D	200	CYC	C4A-C3A	-2.40	1.40	1.45
6	n	200	CYC	CMD-C2D	2.39	1.56	1.51
6	R	200	CYC	C4A-C3A	-2.39	1.40	1.45
6	e	200	CYC	CMD-C2D	2.39	1.56	1.51
6	G	200	CYC	C4A-C3A	-2.38	1.40	1.45
6	r	200	CYC	C4A-C3A	-2.38	1.40	1.45
6	U	200	CYC	C4A-C3A	-2.38	1.40	1.45
6	u	200	CYC	CMD-C2D	2.38	1.56	1.51
6	C	200	CYC	C4A-C3A	-2.38	1.40	1.45
6	h	200	CYC	CMD-C2D	2.37	1.56	1.51
6	j	200	CYC	CMD-C2D	2.37	1.56	1.51
6	0	1201	CYC	C4A-C3A	-2.37	1.40	1.45
6	I	200	CYC	CMD-C2D	2.37	1.56	1.51
6	0	1202	CYC	CMD-C2D	2.37	1.56	1.51
6	e	200	CYC	C4A-C3A	-2.37	1.40	1.45
6	O	200	CYC	CMD-C2D	2.37	1.56	1.51
6	0	1203	CYC	C4A-C3A	-2.37	1.40	1.45
6	N	200	CYC	CMD-C2D	2.36	1.56	1.51
6	0	1202	CYC	C4A-C3A	-2.36	1.40	1.45
6	J	200	CYC	C4A-C3A	-2.35	1.40	1.45
6	A	200	CYC	CMD-C2D	2.35	1.56	1.51
6	N	200	CYC	C4A-C3A	-2.35	1.40	1.45
6	E	200	CYC	CMD-C2D	2.34	1.56	1.51
6	m	200	CYC	C1A-NA	-2.34	1.33	1.38
6	Q	200	CYC	C4A-C3A	-2.33	1.40	1.45
6	J	200	CYC	CMD-C2D	2.33	1.56	1.51
6	q	200	CYC	CMD-C2D	2.33	1.56	1.51
6	P	200	CYC	CMD-C2D	2.32	1.56	1.51
6	d	200	CYC	CMD-C2D	2.32	1.56	1.51
6	a	200	CYC	C4A-C3A	-2.32	1.40	1.45
6	x	200	CYC	CMD-C2D	2.32	1.56	1.51
6	t	200	CYC	C4A-C3A	-2.32	1.40	1.45
6	d	200	CYC	C4A-C3A	-2.32	1.40	1.45
6	V	200	CYC	CMD-C2D	2.32	1.56	1.51
6	o	200	CYC	C4A-C3A	-2.31	1.40	1.45
6	k	200	CYC	CMD-C2D	2.31	1.56	1.51
6	C	200	CYC	CMD-C2D	2.30	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	b	200	CYC	C4A-C3A	-2.30	1.40	1.45
6	c	200	CYC	C4A-C3A	-2.30	1.40	1.45
6	H	200	CYC	CMD-C2D	2.29	1.56	1.51
6	o	200	CYC	CMD-C2D	2.29	1.56	1.51
6	W	200	CYC	C4A-C3A	-2.29	1.40	1.45
6	s	200	CYC	C4A-C3A	-2.29	1.40	1.45
6	q	200	CYC	CAC-C3C	2.29	1.58	1.54
6	s	200	CYC	CMD-C2D	2.29	1.56	1.51
6	y	200	CYC	CMD-C2D	2.29	1.56	1.51
6	f	200	CYC	C4A-C3A	-2.29	1.40	1.45
6	B	200	CYC	C4A-C3A	-2.28	1.40	1.45
6	h	200	CYC	C4A-C3A	-2.27	1.40	1.45
6	m	200	CYC	CMD-C2D	2.26	1.56	1.51
6	V	200	CYC	CMA-C3A	2.26	1.55	1.50
6	j	200	CYC	C4A-C3A	-2.25	1.41	1.45
6	i	200	CYC	CMD-C2D	2.25	1.56	1.51
6	Y	200	CYC	CMD-C2D	2.25	1.56	1.51
6	A	200	CYC	C4A-C3A	-2.24	1.41	1.45
6	q	200	CYC	C4A-C3A	-2.24	1.41	1.45
6	t	200	CYC	CMD-C2D	2.24	1.56	1.51
6	O	200	CYC	C4A-C3A	-2.23	1.41	1.45
6	q	200	CYC	CMA-C3A	2.23	1.55	1.50
6	w	200	CYC	C4A-C3A	-2.22	1.41	1.45
6	C	200	CYC	CMA-C3A	2.20	1.55	1.50
6	S	200	CYC	CMA-C3A	2.20	1.55	1.50
6	a	200	CYC	CMA-C3A	2.20	1.55	1.50
6	E	200	CYC	C4A-C3A	-2.19	1.41	1.45
6	s	200	CYC	CMA-C3A	2.19	1.55	1.50
6	G	200	CYC	CMA-C3A	2.19	1.55	1.50
6	I	200	CYC	CMA-C3A	2.18	1.55	1.50
6	N	200	CYC	CMA-C3A	2.18	1.55	1.50
6	f	200	CYC	CMA-C3A	2.18	1.55	1.50
6	0	1201	CYC	CMA-C3A	2.17	1.55	1.50
6	L	200	CYC	CMA-C3A	2.17	1.55	1.50
6	W	200	CYC	CMD-C2D	2.15	1.56	1.51
6	t	200	CYC	CMA-C3A	2.15	1.55	1.50
6	u	200	CYC	CMA-C3A	2.15	1.55	1.50
6	h	200	CYC	CMA-C3A	2.15	1.55	1.50
6	o	200	CYC	CMA-C3A	2.15	1.55	1.50
6	r	200	CYC	CMA-C3A	2.15	1.55	1.50
6	c	200	CYC	CMA-C3A	2.14	1.55	1.50
6	A	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	w	200	CYC	CMA-C3A	2.14	1.55	1.50
6	p	200	CYC	CMA-C3A	2.13	1.55	1.50
6	D	200	CYC	CMA-C3A	2.12	1.55	1.50
6	P	200	CYC	CMA-C3A	2.12	1.55	1.50
6	v	200	CYC	CMA-C3A	2.12	1.55	1.50
6	H	200	CYC	CMA-C3A	2.12	1.55	1.50
6	b	200	CYC	CMA-C3A	2.12	1.55	1.50
6	w	200	CYC	CBA-CAA	2.12	1.58	1.52
6	w	200	CYC	C4C-NC	-2.11	1.32	1.37
6	U	200	CYC	CMA-C3A	2.11	1.55	1.50
6	Q	200	CYC	CMA-C3A	2.11	1.55	1.50
6	k	200	CYC	CMA-C3A	2.11	1.55	1.50
6	i	200	CYC	CMA-C3A	2.11	1.55	1.50
6	E	200	CYC	CMA-C3A	2.10	1.55	1.50
6	T	200	CYC	CBA-CAA	2.09	1.58	1.52
6	e	200	CYC	CMA-C3A	2.09	1.55	1.50
6	d	200	CYC	CMA-C3A	2.08	1.55	1.50
6	R	200	CYC	CMA-C3A	2.08	1.55	1.50
6	j	200	CYC	CMA-C3A	2.08	1.55	1.50
6	P	200	CYC	C4A-C3A	-2.08	1.41	1.45
6	y	200	CYC	CMA-C3A	2.06	1.55	1.50
6	O	200	CYC	CMA-C3A	2.05	1.55	1.50
6	E	200	CYC	CBA-CAA	2.05	1.58	1.52
6	0	1202	CYC	CMA-C3A	2.05	1.55	1.50
6	I	200	CYC	CBA-CAA	2.04	1.58	1.52
6	L	200	CYC	C4C-NC	-2.04	1.33	1.37
6	U	200	CYC	CBA-CAA	2.03	1.58	1.52
6	p	200	CYC	CBA-CAA	2.03	1.58	1.52
6	x	200	CYC	CMA-C3A	2.02	1.55	1.50
6	O	200	CYC	CBA-CAA	2.02	1.58	1.52
6	T	200	CYC	CMA-C3A	2.01	1.55	1.50
6	n	200	CYC	CMA-C3A	2.01	1.55	1.50
6	G	200	CYC	CBA-CAA	2.01	1.58	1.52
6	w	200	CYC	O2D-CGD	-2.01	1.24	1.30
6	s	200	CYC	C4A-NA	-2.01	1.32	1.36
6	l	200	CYC	C4C-NC	-2.00	1.33	1.37
6	P	200	CYC	CBA-CAA	2.00	1.58	1.52
6	h	200	CYC	CBA-CAA	2.00	1.58	1.52

All (614) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	x	200	CYC	OC-C1C-C2C	-21.64	108.97	126.17
6	C	200	CYC	OC-C1C-C2C	-21.59	109.00	126.17
6	m	200	CYC	OC-C1C-C2C	-21.16	109.35	126.17
6	0	1202	CYC	OC-C1C-C2C	-21.00	109.48	126.17
6	D	200	CYC	OC-C1C-C2C	-20.97	109.50	126.17
6	N	200	CYC	OC-C1C-C2C	-20.75	109.68	126.17
6	A	200	CYC	OC-C1C-C2C	-20.72	109.70	126.17
6	W	200	CYC	OC-C1C-C2C	-20.70	109.71	126.17
6	I	200	CYC	OC-C1C-C2C	-20.61	109.79	126.17
6	H	200	CYC	OC-C1C-C2C	-20.60	109.80	126.17
6	c	200	CYC	OC-C1C-C2C	-20.54	109.84	126.17
6	0	1203	CYC	OC-C1C-C2C	-20.43	109.93	126.17
6	S	200	CYC	OC-C1C-C2C	-20.35	109.99	126.17
6	n	200	CYC	OC-C1C-C2C	-20.33	110.01	126.17
6	G	200	CYC	OC-C1C-C2C	-20.28	110.05	126.17
6	J	200	CYC	OC-C1C-C2C	-20.26	110.07	126.17
6	f	200	CYC	OC-C1C-C2C	-20.11	110.18	126.17
6	k	200	CYC	OC-C1C-C2C	-20.08	110.21	126.17
6	U	200	CYC	OC-C1C-C2C	-20.08	110.21	126.17
6	Y	200	CYC	OC-C1C-C2C	-20.06	110.22	126.17
6	q	200	CYC	OC-C1C-C2C	-20.02	110.26	126.17
6	L	200	CYC	OC-C1C-C2C	-19.98	110.29	126.17
6	y	200	CYC	OC-C1C-C2C	-19.92	110.33	126.17
6	v	200	CYC	OC-C1C-C2C	-19.88	110.36	126.17
6	i	200	CYC	OC-C1C-C2C	-19.87	110.37	126.17
6	o	200	CYC	OC-C1C-C2C	-19.84	110.39	126.17
6	t	200	CYC	OC-C1C-C2C	-19.81	110.42	126.17
6	u	200	CYC	OC-C1C-C2C	-19.80	110.43	126.17
6	r	200	CYC	OC-C1C-C2C	-19.79	110.44	126.17
6	s	200	CYC	OC-C1C-C2C	-19.69	110.51	126.17
6	l	200	CYC	OC-C1C-C2C	-19.69	110.52	126.17
6	P	200	CYC	OC-C1C-C2C	-19.68	110.53	126.17
6	O	200	CYC	OC-C1C-C2C	-19.66	110.54	126.17
6	T	200	CYC	OC-C1C-C2C	-19.63	110.57	126.17
6	Q	200	CYC	OC-C1C-C2C	-19.55	110.63	126.17
6	R	200	CYC	OC-C1C-C2C	-19.55	110.63	126.17
6	h	200	CYC	OC-C1C-C2C	-19.55	110.63	126.17
6	b	200	CYC	OC-C1C-C2C	-19.53	110.65	126.17
6	B	200	CYC	OC-C1C-C2C	-19.52	110.65	126.17
6	a	200	CYC	OC-C1C-C2C	-19.51	110.66	126.17
6	0	1201	CYC	OC-C1C-C2C	-19.45	110.71	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	200	CYC	OC-C1C-C2C	-19.37	110.77	126.17
6	V	200	CYC	OC-C1C-C2C	-19.32	110.81	126.17
6	p	200	CYC	OC-C1C-C2C	-19.32	110.81	126.17
6	e	200	CYC	OC-C1C-C2C	-19.03	111.04	126.17
6	d	200	CYC	OC-C1C-C2C	-18.92	111.13	126.17
6	w	200	CYC	OC-C1C-C2C	-18.56	111.42	126.17
6	j	200	CYC	OC-C1C-C2C	-18.41	111.54	126.17
6	N	200	CYC	C4D-CHA-C1A	-15.05	110.83	128.81
6	0	1201	CYC	CHD-C4C-NC	-14.19	108.33	125.20
6	C	200	CYC	C4D-CHA-C1A	-13.96	112.13	128.81
6	k	200	CYC	OC-C1C-NC	-13.05	109.14	124.94
6	m	200	CYC	C4D-CHA-C1A	-12.95	113.33	128.81
6	h	200	CYC	OC-C1C-NC	-12.89	109.33	124.94
6	P	200	CYC	CHD-C4C-NC	-12.81	109.98	125.20
6	H	200	CYC	C4D-CHA-C1A	-12.80	113.52	128.81
6	y	200	CYC	OC-C1C-NC	-12.77	109.47	124.94
6	c	200	CYC	CHD-C4C-NC	-12.65	110.17	125.20
6	0	1203	CYC	OC-C1C-NC	-12.64	109.63	124.94
6	Q	200	CYC	OC-C1C-NC	-12.64	109.64	124.94
6	m	200	CYC	OC-C1C-NC	-12.62	109.66	124.94
6	o	200	CYC	OC-C1C-NC	-12.56	109.73	124.94
6	f	200	CYC	OC-C1C-NC	-12.54	109.75	124.94
6	p	200	CYC	CHD-C4C-NC	-12.49	110.35	125.20
6	B	200	CYC	CHD-C4C-NC	-12.47	110.38	125.20
6	N	200	CYC	CHD-C4C-NC	-12.47	110.38	125.20
6	G	200	CYC	OC-C1C-NC	-12.46	109.85	124.94
6	l	200	CYC	OC-C1C-NC	-12.42	109.90	124.94
6	C	200	CYC	CHD-C4C-NC	-12.42	110.44	125.20
6	b	200	CYC	OC-C1C-NC	-12.39	109.93	124.94
6	n	200	CYC	OC-C1C-NC	-12.37	109.96	124.94
6	T	200	CYC	CHD-C4C-NC	-12.36	110.51	125.20
6	L	200	CYC	OC-C1C-NC	-12.34	109.99	124.94
6	R	200	CYC	CHD-C4C-NC	-12.34	110.54	125.20
6	B	200	CYC	OC-C1C-NC	-12.32	110.02	124.94
6	V	200	CYC	CHD-C4C-NC	-12.31	110.57	125.20
6	a	200	CYC	OC-C1C-NC	-12.30	110.04	124.94
6	e	200	CYC	OC-C1C-NC	-12.28	110.07	124.94
6	d	200	CYC	CHD-C4C-NC	-12.27	110.61	125.20
6	h	200	CYC	CHD-C4C-NC	-12.27	110.61	125.20
6	r	200	CYC	CHD-C4C-NC	-12.27	110.61	125.20
6	p	200	CYC	OC-C1C-NC	-12.27	110.08	124.94
6	U	200	CYC	OC-C1C-NC	-12.27	110.09	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	200	CYC	OC-C1C-NC	-12.25	110.11	124.94
6	d	200	CYC	OC-C1C-NC	-12.21	110.15	124.94
6	x	200	CYC	OC-C1C-NC	-12.19	110.19	124.94
6	I	200	CYC	OC-C1C-NC	-12.16	110.22	124.94
6	S	200	CYC	OC-C1C-NC	-12.15	110.23	124.94
6	W	200	CYC	OC-C1C-NC	-12.14	110.24	124.94
6	v	200	CYC	CHD-C4C-NC	-12.14	110.78	125.20
6	P	200	CYC	OC-C1C-NC	-12.11	110.28	124.94
6	i	200	CYC	OC-C1C-NC	-12.10	110.28	124.94
6	H	200	CYC	CHD-C4C-NC	-12.09	110.83	125.20
6	T	200	CYC	OC-C1C-NC	-12.08	110.31	124.94
6	u	200	CYC	OC-C1C-NC	-12.06	110.34	124.94
6	c	200	CYC	OC-C1C-NC	-12.04	110.36	124.94
6	v	200	CYC	OC-C1C-NC	-12.00	110.41	124.94
6	l	200	CYC	CHD-C4C-NC	-11.99	110.95	125.20
6	S	200	CYC	CHD-C4C-NC	-11.98	110.96	125.20
6	f	200	CYC	CHD-C4C-NC	-11.96	110.98	125.20
6	0	1202	CYC	OC-C1C-NC	-11.95	110.46	124.94
6	W	200	CYC	CHD-C4C-NC	-11.95	111.00	125.20
6	D	200	CYC	CHD-C4C-NC	-11.93	111.02	125.20
6	0	1201	CYC	OC-C1C-NC	-11.93	110.50	124.94
6	s	200	CYC	OC-C1C-NC	-11.92	110.50	124.94
6	r	200	CYC	OC-C1C-NC	-11.91	110.52	124.94
6	t	200	CYC	OC-C1C-NC	-11.91	110.52	124.94
6	V	200	CYC	OC-C1C-NC	-11.90	110.53	124.94
6	m	200	CYC	CHD-C4C-NC	-11.89	111.06	125.20
6	O	200	CYC	OC-C1C-NC	-11.88	110.55	124.94
6	Y	200	CYC	OC-C1C-NC	-11.88	110.55	124.94
6	A	200	CYC	OC-C1C-NC	-11.87	110.57	124.94
6	a	200	CYC	CHD-C4C-NC	-11.86	111.10	125.20
6	q	200	CYC	OC-C1C-NC	-11.86	110.58	124.94
6	C	200	CYC	OC-C1C-NC	-11.83	110.62	124.94
6	D	200	CYC	OC-C1C-NC	-11.81	110.64	124.94
6	H	200	CYC	OC-C1C-NC	-11.80	110.65	124.94
6	G	200	CYC	CHD-C4C-NC	-11.76	111.23	125.20
6	R	200	CYC	OC-C1C-NC	-11.74	110.72	124.94
6	0	1201	CYC	C4D-CHA-C1A	-11.70	114.83	128.81
6	o	200	CYC	CHD-C4C-NC	-11.65	111.36	125.20
6	I	200	CYC	CHD-C4C-NC	-11.62	111.39	125.20
6	u	200	CYC	CHD-C4C-NC	-11.59	111.43	125.20
6	b	200	CYC	CHD-C4C-NC	-11.51	111.52	125.20
6	w	200	CYC	C4D-CHA-C1A	-11.50	115.07	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	200	CYC	CHD-C4C-NC	-11.47	111.57	125.20
6	w	200	CYC	OC-C1C-NC	-11.28	111.28	124.94
6	t	200	CYC	CHD-C4C-NC	-11.26	111.82	125.20
6	n	200	CYC	CHD-C4C-NC	-11.24	111.85	125.20
6	L	200	CYC	C4D-CHA-C1A	-11.14	115.50	128.81
6	U	200	CYC	CHD-C4C-NC	-11.13	111.97	125.20
6	j	200	CYC	OC-C1C-NC	-11.11	111.48	124.94
6	o	200	CYC	C4D-CHA-C1A	-11.08	115.57	128.81
6	q	200	CYC	CHD-C4C-NC	-11.02	112.10	125.20
6	E	200	CYC	C4D-CHA-C1A	-11.01	115.65	128.81
6	S	200	CYC	C4D-CHA-C1A	-11.00	115.67	128.81
6	0	1202	CYC	CHD-C4C-NC	-10.88	112.27	125.20
6	A	200	CYC	CHD-C4C-NC	-10.85	112.30	125.20
6	y	200	CYC	CHD-C4C-NC	-10.82	112.34	125.20
6	E	200	CYC	CHD-C4C-NC	-10.80	112.36	125.20
6	Q	200	CYC	CHD-C4C-NC	-10.79	112.37	125.20
6	s	200	CYC	CHD-C4C-NC	-10.79	112.37	125.20
6	a	200	CYC	C4D-CHA-C1A	-10.79	115.92	128.81
6	N	200	CYC	OC-C1C-NC	-10.76	111.91	124.94
6	E	200	CYC	OC-C1C-NC	-10.72	111.96	124.94
6	c	200	CYC	C4D-CHA-C1A	-10.70	116.02	128.81
6	e	200	CYC	CHD-C4C-NC	-10.64	112.56	125.20
6	h	200	CYC	C4D-CHA-C1A	-10.62	116.13	128.81
6	U	200	CYC	C4D-CHA-C1A	-10.61	116.13	128.81
6	d	200	CYC	C4D-CHA-C1A	-10.61	116.14	128.81
6	f	200	CYC	C4D-CHA-C1A	-10.58	116.18	128.81
6	r	200	CYC	C4D-CHA-C1A	-10.56	116.19	128.81
6	k	200	CYC	CHD-C4C-NC	-10.52	112.70	125.20
6	s	200	CYC	C4D-CHA-C1A	-10.49	116.27	128.81
6	0	1203	CYC	CHD-C4C-NC	-10.47	112.75	125.20
6	j	200	CYC	C4D-CHA-C1A	-10.46	116.31	128.81
6	L	200	CYC	CHD-C4C-NC	-10.42	112.82	125.20
6	W	200	CYC	C4D-CHA-C1A	-10.38	116.41	128.81
6	b	200	CYC	C4D-CHA-C1A	-10.38	116.41	128.81
6	x	200	CYC	CHD-C4C-NC	-10.36	112.89	125.20
6	n	200	CYC	C4D-CHA-C1A	-10.35	116.44	128.81
6	i	200	CYC	CHD-C4C-NC	-10.17	113.11	125.20
6	D	200	CYC	C4D-CHA-C1A	-10.14	116.69	128.81
6	v	200	CYC	C4D-CHA-C1A	-10.10	116.74	128.81
6	t	200	CYC	C4D-CHA-C1A	-10.09	116.75	128.81
6	q	200	CYC	C4D-CHA-C1A	-10.09	116.76	128.81
6	i	200	CYC	C4D-CHA-C1A	-10.08	116.77	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	200	CYC	C4D-CHA-C1A	-10.00	116.86	128.81
6	G	200	CYC	C4D-CHA-C1A	-9.93	116.95	128.81
6	P	200	CYC	C4D-CHA-C1A	-9.90	116.98	128.81
6	Y	200	CYC	CHD-C4C-NC	-9.87	113.47	125.20
6	J	200	CYC	CHD-C4C-NC	-9.76	113.60	125.20
6	0	1202	CYC	C4D-CHA-C1A	-9.72	117.19	128.81
6	Y	200	CYC	C4D-CHA-C1A	-9.67	117.25	128.81
6	l	200	CYC	C4D-CHA-C1A	-9.66	117.26	128.81
6	R	200	CYC	C4D-CHA-C1A	-9.65	117.28	128.81
6	I	200	CYC	C4D-CHA-C1A	-9.57	117.37	128.81
6	p	200	CYC	C4D-CHA-C1A	-9.57	117.38	128.81
6	u	200	CYC	C4D-CHA-C1A	-9.53	117.43	128.81
6	y	200	CYC	C4D-CHA-C1A	-9.46	117.51	128.81
6	x	200	CYC	C4D-CHA-C1A	-9.39	117.59	128.81
6	k	200	CYC	C4D-CHA-C1A	-9.38	117.60	128.81
6	T	200	CYC	C4D-CHA-C1A	-9.35	117.64	128.81
6	Q	200	CYC	C4D-CHA-C1A	-9.27	117.74	128.81
6	B	200	CYC	C4D-CHA-C1A	-9.25	117.76	128.81
6	A	200	CYC	C4D-CHA-C1A	-9.23	117.78	128.81
6	V	200	CYC	C4D-CHA-C1A	-9.18	117.84	128.81
6	O	200	CYC	C4D-CHA-C1A	-9.09	117.95	128.81
6	0	1203	CYC	C4D-CHA-C1A	-8.90	118.18	128.81
6	e	200	CYC	C4D-CHA-C1A	-7.74	119.56	128.81
6	j	200	CYC	CHD-C4C-NC	-7.63	116.13	125.20
6	v	200	CYC	C2C-C1C-NC	-7.46	101.85	108.27
6	w	200	CYC	CHD-C4C-NC	-7.24	116.60	125.20
6	p	200	CYC	C2C-C1C-NC	-7.19	102.08	108.27
6	l	200	CYC	C2C-C1C-NC	-7.15	102.11	108.27
6	d	200	CYC	C2C-C1C-NC	-7.07	102.17	108.27
6	L	200	CYC	C2C-C1C-NC	-6.95	102.28	108.27
6	V	200	CYC	C1B-CHB-C4A	-6.88	111.26	128.08
6	V	200	CYC	C2C-C1C-NC	-6.73	102.47	108.27
6	Q	200	CYC	C2C-C1C-NC	-6.72	102.48	108.27
6	w	200	CYC	C2C-C1C-NC	-6.56	102.62	108.27
6	W	200	CYC	C2C-C1C-NC	-6.52	102.65	108.27
6	n	200	CYC	C2C-C1C-NC	-6.18	102.94	108.27
6	j	200	CYC	C2C-C1C-NC	-6.09	103.02	108.27
6	o	200	CYC	C2C-C1C-NC	-6.09	103.02	108.27
6	c	200	CYC	C2C-C1C-NC	-6.00	103.10	108.27
6	B	200	CYC	C2C-C1C-NC	-5.84	103.24	108.27
6	A	200	CYC	C2C-C3C-C4C	5.70	109.88	101.34
6	C	200	CYC	C1B-CHB-C4A	-5.64	114.30	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	200	CYC	C2C-C1C-NC	-5.52	103.52	108.27
6	C	200	CYC	C2C-C1C-NC	-5.51	103.52	108.27
6	s	200	CYC	C2C-C1C-NC	-5.41	103.61	108.27
6	q	200	CYC	C2C-C3C-C4C	5.41	109.44	101.34
6	f	200	CYC	C2C-C1C-NC	-5.38	103.64	108.27
6	E	200	CYC	C2C-C3C-C4C	5.37	109.39	101.34
6	b	200	CYC	C2C-C3C-C4C	5.37	109.38	101.34
6	r	200	CYC	C2C-C1C-NC	-5.34	103.67	108.27
6	e	200	CYC	C2C-C3C-C4C	5.31	109.30	101.34
6	N	200	CYC	C2C-C1C-NC	-5.26	103.74	108.27
6	e	200	CYC	C2C-C1C-NC	-5.24	103.75	108.27
6	P	200	CYC	C2C-C1C-NC	-5.23	103.76	108.27
6	n	200	CYC	C2C-C3C-C4C	5.23	109.17	101.34
6	h	200	CYC	C2C-C3C-C4C	5.23	109.17	101.34
6	R	200	CYC	C2C-C1C-NC	-5.19	103.80	108.27
6	I	200	CYC	C1B-CHB-C4A	-5.19	115.40	128.08
6	T	200	CYC	C2C-C1C-NC	-5.17	103.82	108.27
6	s	200	CYC	C2C-C3C-C4C	5.12	109.01	101.34
6	y	200	CYC	C2C-C3C-C4C	5.05	108.91	101.34
6	J	200	CYC	C2C-C1C-NC	-5.05	103.92	108.27
6	r	200	CYC	C2C-C3C-C4C	5.04	108.89	101.34
6	u	200	CYC	C2C-C1C-NC	-5.04	103.93	108.27
6	a	200	CYC	C2C-C3C-C4C	5.02	108.86	101.34
6	C	200	CYC	C2C-C3C-C4C	5.02	108.85	101.34
6	t	200	CYC	C2C-C3C-C4C	4.95	108.75	101.34
6	D	200	CYC	C2C-C3C-C4C	4.94	108.74	101.34
6	0	1203	CYC	C2C-C3C-C4C	4.92	108.71	101.34
6	i	200	CYC	C2C-C3C-C4C	4.91	108.69	101.34
6	a	200	CYC	C2C-C1C-NC	-4.91	104.04	108.27
6	O	200	CYC	C2C-C3C-C4C	4.87	108.64	101.34
6	O	200	CYC	C2C-C1C-NC	-4.86	104.08	108.27
6	H	200	CYC	C2C-C3C-C4C	4.86	108.62	101.34
6	x	200	CYC	C2C-C3C-C4C	4.85	108.61	101.34
6	G	200	CYC	C2C-C3C-C4C	4.81	108.55	101.34
6	U	200	CYC	C2C-C1C-NC	-4.80	104.14	108.27
6	B	200	CYC	C2C-C3C-C4C	4.78	108.49	101.34
6	T	200	CYC	C2C-C3C-C4C	4.76	108.47	101.34
6	0	1202	CYC	C2C-C3C-C4C	4.70	108.39	101.34
6	c	200	CYC	C2C-C3C-C4C	4.70	108.38	101.34
6	I	200	CYC	C2C-C3C-C4C	4.69	108.36	101.34
6	D	200	CYC	C2C-C1C-NC	-4.68	104.24	108.27
6	N	200	CYC	C1B-CHB-C4A	-4.68	116.66	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	d	200	CYC	C2C-C3C-C4C	4.64	108.29	101.34
6	k	200	CYC	C2C-C3C-C4C	4.63	108.28	101.34
6	Y	200	CYC	C2C-C3C-C4C	4.60	108.23	101.34
6	S	200	CYC	C2C-C3C-C4C	4.60	108.23	101.34
6	f	200	CYC	C2C-C3C-C4C	4.58	108.20	101.34
6	o	200	CYC	C2C-C3C-C4C	4.55	108.15	101.34
6	J	200	CYC	C2C-C3C-C4C	4.53	108.12	101.34
6	0	1201	CYC	C2C-C3C-C4C	4.52	108.11	101.34
6	R	200	CYC	C2C-C3C-C4C	4.51	108.10	101.34
6	u	200	CYC	C2C-C3C-C4C	4.51	108.09	101.34
6	k	200	CYC	CMA-C3A-C4A	4.50	132.00	125.06
6	W	200	CYC	C2C-C3C-C4C	4.48	108.06	101.34
6	N	200	CYC	C2C-C3C-C4C	4.47	108.03	101.34
6	P	200	CYC	C2C-C3C-C4C	4.45	108.00	101.34
6	q	200	CYC	CMA-C3A-C4A	4.44	131.90	125.06
6	v	200	CYC	C1B-CHB-C4A	-4.43	117.26	128.08
6	0	1202	CYC	CMA-C3A-C4A	4.41	131.86	125.06
6	p	200	CYC	C2C-C3C-C4C	4.38	107.90	101.34
6	q	200	CYC	C2C-C1C-NC	-4.37	104.50	108.27
6	L	200	CYC	C1B-CHB-C4A	-4.37	117.40	128.08
6	U	200	CYC	C2C-C3C-C4C	4.36	107.87	101.34
6	Q	200	CYC	C2C-C3C-C4C	4.32	107.80	101.34
6	O	200	CYC	CMA-C3A-C4A	4.28	131.66	125.06
6	k	200	CYC	C2C-C1C-NC	-4.28	104.58	108.27
6	c	200	CYC	CMA-C3A-C4A	4.23	131.58	125.06
6	l	200	CYC	C2C-C3C-C4C	4.22	107.66	101.34
6	m	200	CYC	C1B-NB-C4B	4.21	116.02	110.67
6	B	200	CYC	CMA-C3A-C4A	4.15	131.45	125.06
6	R	200	CYC	CMA-C3A-C4A	4.13	131.42	125.06
6	i	200	CYC	CAB-C3B-C4B	4.11	127.87	121.38
6	j	200	CYC	CMA-C3A-C4A	4.11	131.39	125.06
6	V	200	CYC	C2C-C3C-C4C	4.11	107.49	101.34
6	0	1202	CYC	CAB-C3B-C4B	4.08	127.83	121.38
6	0	1203	CYC	CMA-C3A-C4A	4.08	131.35	125.06
6	d	200	CYC	CMA-C3A-C4A	4.06	131.31	125.06
6	H	200	CYC	CAB-C3B-C4B	4.04	127.75	121.38
6	e	200	CYC	CAB-C3B-C4B	4.01	127.71	121.38
6	n	200	CYC	CAB-C3B-C4B	4.00	127.69	121.38
6	v	200	CYC	C2C-C3C-C4C	3.99	107.32	101.34
6	y	200	CYC	C1B-CHB-C4A	-3.97	118.38	128.08
6	0	1201	CYC	C2C-C1C-NC	-3.97	104.85	108.27
6	r	200	CYC	CAB-C3B-C4B	3.96	127.64	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	m	200	CYC	C2C-C3C-C4C	3.96	107.27	101.34
6	t	200	CYC	CMA-C3A-C4A	3.94	131.12	125.06
6	P	200	CYC	CMA-C3A-C4A	3.94	131.12	125.06
6	V	200	CYC	CAB-C3B-C4B	3.93	127.59	121.38
6	G	200	CYC	C2C-C1C-NC	-3.93	104.88	108.27
6	l	200	CYC	C1B-CHB-C4A	-3.93	118.47	128.08
6	l	200	CYC	CAB-C3B-C4B	3.90	127.55	121.38
6	G	200	CYC	C1B-CHB-C4A	-3.90	118.56	128.08
6	J	200	CYC	CMA-C3A-C4A	3.90	131.06	125.06
6	U	200	CYC	CAB-C3B-C4B	3.89	127.52	121.38
6	O	200	CYC	CAB-C3B-C4B	3.89	127.52	121.38
6	s	200	CYC	CAB-C3B-C4B	3.88	127.50	121.38
6	v	200	CYC	CAB-C3B-C4B	3.88	127.50	121.38
6	m	200	CYC	C1B-CHB-C4A	-3.88	118.61	128.08
6	T	200	CYC	C1B-CHB-C4A	-3.84	118.69	128.08
6	u	200	CYC	CMA-C3A-C4A	3.82	130.95	125.06
6	n	200	CYC	CMA-C3A-C4A	3.80	130.92	125.06
6	c	200	CYC	CAB-C3B-C4B	3.80	127.39	121.38
6	f	200	CYC	CMA-C3A-C4A	3.80	130.92	125.06
6	N	200	CYC	CAB-C3B-C4B	3.79	127.36	121.38
6	T	200	CYC	CAB-C3B-C4B	3.79	127.36	121.38
6	R	200	CYC	CAB-C3B-C4B	3.79	127.36	121.38
6	W	200	CYC	CAB-C3B-C4B	3.78	127.36	121.38
6	y	200	CYC	CAB-C3B-C4B	3.78	127.35	121.38
6	W	200	CYC	CMA-C3A-C4A	3.78	130.88	125.06
6	A	200	CYC	CAB-C3B-C4B	3.78	127.35	121.38
6	J	200	CYC	CAB-C3B-C4B	3.78	127.34	121.38
6	p	200	CYC	CMA-C3A-C4A	3.77	130.87	125.06
6	m	200	CYC	CMA-C3A-C4A	3.77	130.87	125.06
6	Q	200	CYC	CMA-C3A-C4A	3.76	130.85	125.06
6	Y	200	CYC	C2C-C1C-NC	-3.75	105.04	108.27
6	I	200	CYC	C2C-C1C-NC	-3.74	105.05	108.27
6	j	200	CYC	CAB-C3B-C4B	3.74	127.29	121.38
6	D	200	CYC	CMA-C3A-C4A	3.74	130.82	125.06
6	Y	200	CYC	CAB-C3B-C4B	3.74	127.28	121.38
6	w	200	CYC	CMA-C3A-C4A	3.74	130.82	125.06
6	0	1201	CYC	CMA-C3A-C4A	3.74	130.82	125.06
6	b	200	CYC	CAB-C3B-C4B	3.73	127.27	121.38
6	e	200	CYC	CMA-C3A-C4A	3.71	130.77	125.06
6	u	200	CYC	CAB-C3B-C4B	3.70	127.22	121.38
6	G	200	CYC	CAB-C3B-C4B	3.70	127.22	121.38
6	k	200	CYC	CAB-C3B-C4B	3.69	127.20	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	200	CYC	CAB-C3B-C4B	3.68	127.20	121.38
6	j	200	CYC	CHB-C4A-C3A	3.67	134.34	124.90
6	x	200	CYC	CMA-C3A-C4A	3.67	130.71	125.06
6	E	200	CYC	CAB-C3B-C4B	3.67	127.17	121.38
6	Q	200	CYC	CAB-C3B-C4B	3.67	127.17	121.38
6	I	200	CYC	CAB-C3B-C4B	3.66	127.16	121.38
6	S	200	CYC	CAB-C3B-C4B	3.66	127.16	121.38
6	p	200	CYC	CAB-C3B-C4B	3.66	127.16	121.38
6	0	1203	CYC	C2C-C1C-NC	-3.66	105.12	108.27
6	f	200	CYC	CAB-C3B-C4B	3.65	127.15	121.38
6	B	200	CYC	CAB-C3B-C4B	3.65	127.14	121.38
6	o	200	CYC	CAB-C3B-C4B	3.65	127.14	121.38
6	i	200	CYC	C1B-CHB-C4A	-3.63	119.22	128.08
6	o	200	CYC	CMA-C3A-C4A	3.62	130.65	125.06
6	q	200	CYC	CAB-C3B-C4B	3.62	127.10	121.38
6	P	200	CYC	CAB-C3B-C4B	3.62	127.09	121.38
6	0	1203	CYC	CAB-C3B-C4B	3.60	127.06	121.38
6	E	200	CYC	CMA-C3A-C4A	3.59	130.59	125.06
6	b	200	CYC	CMA-C3A-C4A	3.59	130.59	125.06
6	S	200	CYC	CMA-C3A-C4A	3.59	130.59	125.06
6	t	200	CYC	C2C-C1C-NC	-3.58	105.19	108.27
6	a	200	CYC	CAB-C3B-C4B	3.57	127.01	121.38
6	0	1202	CYC	C2C-C1C-NC	-3.56	105.20	108.27
6	u	200	CYC	CHB-C4A-C3A	3.56	134.05	124.90
6	D	200	CYC	CAB-C3B-C4B	3.55	126.98	121.38
6	L	200	CYC	CAB-C3B-C4B	3.54	126.97	121.38
6	a	200	CYC	CMA-C3A-C4A	3.53	130.50	125.06
6	Y	200	CYC	CMA-C3A-C4A	3.53	130.50	125.06
6	m	200	CYC	CAB-C3B-C4B	3.53	126.95	121.38
6	h	200	CYC	CAB-C3B-C4B	3.50	126.91	121.38
6	i	200	CYC	C2C-C1C-NC	-3.50	105.26	108.27
6	t	200	CYC	CAB-C3B-C4B	3.48	126.87	121.38
6	s	200	CYC	CMA-C3A-C4A	3.47	130.41	125.06
6	h	200	CYC	CMA-C3A-C4A	3.45	130.38	125.06
6	0	1202	CYC	CHB-C4A-C3A	3.45	133.77	124.90
6	H	200	CYC	CHB-C4A-C3A	3.44	133.74	124.90
6	x	200	CYC	CAB-C3B-C4B	3.43	126.80	121.38
6	h	200	CYC	CHB-C4A-C3A	3.43	133.72	124.90
6	s	200	CYC	CHB-C4A-C3A	3.42	133.69	124.90
6	w	200	CYC	CAB-C3B-C4B	3.41	126.77	121.38
6	q	200	CYC	CHB-C4A-C3A	3.40	133.64	124.90
6	k	200	CYC	CHB-C4A-C3A	3.40	133.63	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	200	CYC	CHB-C4A-C3A	3.39	133.61	124.90
6	x	200	CYC	CHB-C4A-C3A	3.37	133.56	124.90
6	H	200	CYC	C2C-C1C-NC	-3.36	105.37	108.27
6	t	200	CYC	C1B-CHB-C4A	-3.35	119.90	128.08
6	P	200	CYC	CHB-C4A-C3A	3.35	133.50	124.90
6	Q	200	CYC	CHB-C4A-C3A	3.34	133.48	124.90
6	d	200	CYC	CAB-C3B-C4B	3.34	126.65	121.38
6	A	200	CYC	CMA-C3A-C4A	3.32	130.17	125.06
6	l	200	CYC	CMA-C3A-C4A	3.31	130.17	125.06
6	m	200	CYC	C3B-C4B-NB	-3.28	104.12	106.78
6	w	200	CYC	CHB-C4A-C3A	3.28	133.33	124.90
6	x	200	CYC	C2C-C1C-NC	-3.26	105.47	108.27
6	U	200	CYC	CMA-C3A-C4A	3.25	130.07	125.06
6	y	200	CYC	CMA-C3A-C4A	3.25	130.07	125.06
6	0	1201	CYC	CHB-C4A-C3A	3.24	133.24	124.90
6	d	200	CYC	CHB-C4A-C3A	3.23	133.20	124.90
6	r	200	CYC	CMA-C3A-C4A	3.22	130.03	125.06
6	U	200	CYC	CHB-C4A-C3A	3.20	133.13	124.90
6	i	200	CYC	CMA-C3A-C4A	3.19	129.98	125.06
6	0	1201	CYC	C1A-NA-C4A	3.17	112.48	106.51
6	b	200	CYC	CHB-C4A-C3A	3.15	133.00	124.90
6	T	200	CYC	CMA-C3A-C4A	3.14	129.90	125.06
6	G	200	CYC	CMA-C3A-C4A	3.09	129.82	125.06
6	f	200	CYC	CHB-C4A-C3A	3.08	132.82	124.90
6	P	200	CYC	C1A-NA-C4A	3.08	112.31	106.51
6	L	200	CYC	C2C-C3C-C4C	3.08	105.95	101.34
6	a	200	CYC	C1B-CHB-C4A	-3.08	120.56	128.08
6	v	200	CYC	CMA-C3A-C4A	3.06	129.77	125.06
6	j	200	CYC	CHB-C4A-NA	-3.05	118.56	124.93
6	0	1203	CYC	CHB-C4A-C3A	3.03	132.69	124.90
6	u	200	CYC	CHB-C4A-NA	-3.03	118.60	124.93
6	k	200	CYC	CHB-C1B-C2B	-3.02	120.97	126.95
6	c	200	CYC	CHB-C4A-C3A	3.01	132.65	124.90
6	H	200	CYC	CMA-C3A-C4A	3.00	129.68	125.06
6	H	200	CYC	C1A-NA-C4A	2.99	112.14	106.51
6	W	200	CYC	CHB-C4A-C3A	2.98	132.57	124.90
6	W	200	CYC	C1B-CHB-C4A	-2.97	120.83	128.08
6	k	200	CYC	CHB-C4A-NA	-2.95	118.75	124.93
6	E	200	CYC	CHB-C4A-C3A	2.95	132.49	124.90
6	e	200	CYC	CHB-C4A-C3A	2.95	132.49	124.90
6	D	200	CYC	CHB-C4A-C3A	2.94	132.46	124.90
6	H	200	CYC	CHB-C1B-C2B	-2.93	121.15	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	p	200	CYC	CHB-C4A-C3A	2.92	132.42	124.90
6	x	200	CYC	C1A-NA-C4A	2.92	112.00	106.51
6	U	200	CYC	C1A-NA-C4A	2.90	111.98	106.51
6	u	200	CYC	CHB-C1B-C2B	-2.90	121.20	126.95
6	I	200	CYC	CMA-C3A-C4A	2.89	129.52	125.06
6	0	1202	CYC	CHB-C1B-C2B	-2.89	121.23	126.95
6	B	200	CYC	CHB-C4A-C3A	2.89	132.32	124.90
6	S	200	CYC	CHB-C4A-C3A	2.88	132.32	124.90
6	e	200	CYC	C1A-NA-C4A	2.88	111.94	106.51
6	j	200	CYC	C1A-NA-C4A	2.88	111.94	106.51
6	o	200	CYC	CHB-C4A-C3A	2.88	132.30	124.90
6	R	200	CYC	CHB-C4A-C3A	2.87	132.28	124.90
6	c	200	CYC	C1A-NA-C4A	2.86	111.91	106.51
6	m	200	CYC	OB-C4B-C3B	2.86	131.15	128.04
6	h	200	CYC	C1A-NA-C4A	2.86	111.89	106.51
6	Y	200	CYC	C1B-CHB-C4A	-2.86	121.10	128.08
6	u	200	CYC	C1A-NA-C4A	2.85	111.89	106.51
6	Y	200	CYC	CHB-C4A-C3A	2.85	132.23	124.90
6	r	200	CYC	CHB-C4A-C3A	2.85	132.22	124.90
6	n	200	CYC	C1A-NA-C4A	2.83	111.85	106.51
6	w	200	CYC	C1A-NA-C4A	2.83	111.84	106.51
6	m	200	CYC	C1A-NA-C4A	2.82	111.83	106.51
6	C	200	CYC	CMA-C3A-C4A	2.81	129.40	125.06
6	e	200	CYC	CHB-C1B-C2B	-2.81	121.38	126.95
6	0	1201	CYC	CAB-C3B-C2B	2.81	132.33	127.53
6	s	200	CYC	CHB-C4A-NA	-2.81	119.06	124.93
6	D	200	CYC	C1A-NA-C4A	2.80	111.78	106.51
6	E	200	CYC	C1B-CHB-C4A	-2.80	121.25	128.08
6	R	200	CYC	C1A-NA-C4A	2.79	111.78	106.51
6	s	200	CYC	C1A-NA-C4A	2.79	111.77	106.51
6	0	1202	CYC	CHB-C4A-NA	-2.79	119.11	124.93
6	n	200	CYC	CHB-C4A-C3A	2.79	132.06	124.90
6	q	200	CYC	C1A-NA-C4A	2.78	111.75	106.51
6	J	200	CYC	C1B-CHB-C4A	-2.78	121.30	128.08
6	0	1203	CYC	C1A-NA-C4A	2.77	111.73	106.51
6	O	200	CYC	C1A-NA-C4A	2.77	111.73	106.51
6	d	200	CYC	C1A-NA-C4A	2.76	111.72	106.51
6	p	200	CYC	C1A-NA-C4A	2.76	111.72	106.51
6	t	200	CYC	C1A-NA-C4A	2.76	111.71	106.51
6	N	200	CYC	CMA-C3A-C4A	2.76	129.31	125.06
6	t	200	CYC	CHB-C4A-C3A	2.76	131.99	124.90
6	a	200	CYC	CHB-C4A-C3A	2.75	131.97	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	200	CYC	CHB-C4A-NA	-2.75	119.19	124.93
6	H	200	CYC	CHB-C4A-NA	-2.74	119.19	124.93
6	r	200	CYC	CHB-C1B-C2B	-2.74	121.51	126.95
6	b	200	CYC	C1A-NA-C4A	2.74	111.67	106.51
6	Q	200	CYC	CHB-C1B-C2B	-2.74	121.52	126.95
6	S	200	CYC	C1B-CHB-C4A	-2.73	121.41	128.08
6	o	200	CYC	C1A-NA-C4A	2.72	111.64	106.51
6	S	200	CYC	C1A-NA-C4A	2.72	111.63	106.51
6	B	200	CYC	C1A-NA-C4A	2.71	111.62	106.51
6	q	200	CYC	CHB-C4A-NA	-2.70	119.29	124.93
6	f	200	CYC	C1A-NA-C4A	2.70	111.59	106.51
6	G	200	CYC	C1A-NA-C4A	2.69	111.59	106.51
6	Q	200	CYC	C1A-NA-C4A	2.69	111.57	106.51
6	E	200	CYC	C1A-NA-C4A	2.69	111.57	106.51
6	r	200	CYC	C1A-NA-C4A	2.68	111.57	106.51
6	A	200	CYC	C1A-NA-C4A	2.68	111.56	106.51
6	A	200	CYC	C1B-CHB-C4A	-2.67	121.57	128.08
6	Y	200	CYC	C1A-NA-C4A	2.67	111.53	106.51
6	J	200	CYC	C1A-NA-C4A	2.66	111.52	106.51
6	0	1202	CYC	C1A-NA-C4A	2.66	111.51	106.51
6	h	200	CYC	CHB-C4A-NA	-2.65	119.39	124.93
6	C	200	CYC	C1A-NA-C4A	2.64	111.49	106.51
6	q	200	CYC	C1B-CHB-C4A	-2.64	121.63	128.08
6	d	200	CYC	C1B-CHB-C4A	-2.64	121.63	128.08
6	y	200	CYC	C1A-NA-C4A	2.64	111.48	106.51
6	T	200	CYC	C1A-NA-C4A	2.63	111.47	106.51
6	a	200	CYC	C1A-NA-C4A	2.63	111.47	106.51
6	x	200	CYC	CHB-C4A-NA	-2.63	119.43	124.93
6	J	200	CYC	CHB-C4A-C3A	2.62	131.63	124.90
6	k	200	CYC	C1A-NA-C4A	2.61	111.44	106.51
6	W	200	CYC	C1A-NA-C4A	2.61	111.43	106.51
6	N	200	CYC	C1A-NA-C4A	2.61	111.42	106.51
6	0	1201	CYC	CBB-CAB-C3B	2.61	119.62	112.43
6	E	200	CYC	C2C-C1C-NC	-2.60	106.03	108.27
6	f	200	CYC	C1B-CHB-C4A	-2.60	121.73	128.08
6	L	200	CYC	C1A-NA-C4A	2.60	111.41	106.51
6	0	1201	CYC	C3B-C4B-NB	2.60	108.88	106.78
6	m	200	CYC	C2C-C1C-NC	-2.60	106.03	108.27
6	D	200	CYC	C1B-CHB-C4A	-2.59	121.74	128.08
6	y	200	CYC	CHB-C4A-C3A	2.59	131.56	124.90
6	R	200	CYC	CMC-C2C-C1C	-2.58	106.84	112.40
6	y	200	CYC	C2C-C1C-NC	-2.58	106.05	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	200	CYC	CHB-C4A-NA	-2.58	119.55	124.93
6	i	200	CYC	C1A-NA-C4A	2.57	111.35	106.51
6	d	200	CYC	CHB-C4A-NA	-2.56	119.58	124.93
6	n	200	CYC	C1B-CHB-C4A	-2.55	121.86	128.08
6	j	200	CYC	CHB-C1B-C2B	-2.54	121.91	126.95
6	h	200	CYC	C2C-C1C-NC	-2.54	106.08	108.27
6	0	1201	CYC	C1B-CHB-C4A	-2.54	121.87	128.08
6	L	200	CYC	CMA-C3A-C4A	2.54	128.98	125.06
6	V	200	CYC	CMA-C3A-C4A	2.54	128.97	125.06
6	p	200	CYC	CHB-C1B-C2B	-2.54	121.92	126.95
6	o	200	CYC	C1B-CHB-C4A	-2.53	121.91	128.08
6	b	200	CYC	CHB-C1B-C2B	-2.51	121.97	126.95
6	w	200	CYC	CHB-C4A-NA	-2.51	119.68	124.93
6	A	200	CYC	CHB-C4A-C3A	2.51	131.35	124.90
6	x	200	CYC	CHB-C1B-C2B	-2.51	121.98	126.95
6	v	200	CYC	CMC-C2C-C1C	-2.49	107.05	112.40
6	B	200	CYC	C1B-CHB-C4A	-2.47	122.06	128.08
6	G	200	CYC	CMB-C2B-C1B	2.46	127.24	124.17
6	b	200	CYC	CHB-C4A-NA	-2.46	119.79	124.93
6	i	200	CYC	CHB-C4A-C3A	2.46	131.22	124.90
6	v	200	CYC	C1A-NA-C4A	2.45	111.13	106.51
6	t	200	CYC	OB-C4B-C3B	-2.44	125.39	128.04
6	U	200	CYC	CHB-C4A-NA	-2.40	119.91	124.93
6	l	200	CYC	C1A-NA-C4A	2.40	111.02	106.51
6	e	200	CYC	CHB-C1B-NB	2.39	131.18	126.06
6	l	200	CYC	CHB-C4A-C3A	2.38	131.02	124.90
6	L	200	CYC	CMC-C2C-C1C	-2.37	107.30	112.40
6	E	200	CYC	CAC-C3C-C2C	-2.37	108.35	114.26
6	I	200	CYC	C1A-NA-C4A	2.36	110.96	106.51
6	C	200	CYC	CMB-C2B-C1B	2.35	127.10	124.17
6	f	200	CYC	CHB-C4A-NA	-2.34	120.05	124.93
6	r	200	CYC	CHB-C1B-NB	2.32	131.05	126.06
6	0	1201	CYC	CHB-C4A-NA	-2.32	120.07	124.93
6	0	1202	CYC	CHB-C1B-NB	2.32	131.04	126.06
6	H	200	CYC	OB-C4B-C3B	-2.32	125.52	128.04
6	0	1201	CYC	CMC-C2C-C1C	-2.32	107.41	112.40
6	H	200	CYC	CHB-C1B-NB	2.31	131.03	126.06
6	b	200	CYC	C2C-C1C-NC	-2.31	106.28	108.27
6	m	200	CYC	C3A-C4A-NA	-2.30	105.60	110.53
6	n	200	CYC	CHB-C1B-C2B	-2.30	122.39	126.95
6	V	200	CYC	C1A-NA-C4A	2.30	110.84	106.51
6	u	200	CYC	CHB-C1B-NB	2.29	130.97	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	b	200	CYC	C1B-CHB-C4A	-2.29	122.49	128.08
6	0	1201	CYC	OB-C4B-C3B	-2.28	125.56	128.04
6	t	200	CYC	CMB-C2B-C1B	2.27	127.00	124.17
6	s	200	CYC	CHB-C1B-C2B	-2.27	122.46	126.95
6	P	200	CYC	CHB-C4A-NA	-2.26	120.20	124.93
6	p	200	CYC	CHB-C4A-NA	-2.26	120.20	124.93
6	R	200	CYC	C1B-CHB-C4A	-2.25	122.57	128.08
6	v	200	CYC	CHB-C4A-C3A	2.25	130.69	124.90
6	0	1203	CYC	CHB-C1B-C2B	-2.24	122.51	126.95
6	d	200	CYC	CHB-C1B-C2B	-2.24	122.52	126.95
6	N	200	CYC	CMB-C2B-C1B	2.24	126.96	124.17
6	k	200	CYC	CHB-C1B-NB	2.23	130.85	126.06
6	w	200	CYC	CHB-C1B-C2B	-2.22	122.56	126.95
6	S	200	CYC	CHB-C4A-NA	-2.21	120.32	124.93
6	m	200	CYC	O2A-CGA-CBA	2.19	121.08	114.03
6	R	200	CYC	CHB-C1B-C2B	-2.19	122.61	126.95
6	A	200	CYC	C2C-C1C-NC	-2.19	106.39	108.27
6	y	200	CYC	CMB-C2B-C1B	2.19	126.90	124.17
6	W	200	CYC	CMC-C2C-C1C	-2.19	107.69	112.40
6	T	200	CYC	CAA-C2A-C1A	2.19	128.87	125.01
6	0	1201	CYC	CHB-C1B-C2B	-2.18	122.63	126.95
6	b	200	CYC	CHB-C1B-NB	2.17	130.72	126.06
6	L	200	CYC	CMD-C2D-C3D	-2.16	120.87	124.94
6	l	200	CYC	CMB-C2B-C1B	2.16	126.86	124.17
6	h	200	CYC	CHB-C1B-C2B	-2.15	122.69	126.95
6	Q	200	CYC	CHB-C1B-NB	2.14	130.66	126.06
6	G	200	CYC	CHB-C4A-C3A	2.14	130.41	124.90
6	V	200	CYC	CMC-C2C-C1C	-2.14	107.78	112.40
6	U	200	CYC	CHB-C1B-C2B	-2.13	122.72	126.95
6	0	1203	CYC	CHB-C4A-NA	-2.13	120.48	124.93
6	c	200	CYC	C1B-CHB-C4A	-2.13	122.88	128.08
6	W	200	CYC	CHB-C4A-NA	-2.13	120.48	124.93
6	r	200	CYC	CHB-C4A-NA	-2.12	120.49	124.93
6	x	200	CYC	CHB-C1B-NB	2.12	130.61	126.06
6	e	200	CYC	C1B-CHB-C4A	-2.12	122.91	128.08
6	W	200	CYC	CMB-C2B-C1B	2.11	126.80	124.17
6	j	200	CYC	CHB-C1B-NB	2.11	130.58	126.06
6	E	200	CYC	CHB-C4A-NA	-2.11	120.53	124.93
6	d	200	CYC	OB-C4B-C3B	-2.10	125.76	128.04
6	B	200	CYC	CHB-C1B-C2B	-2.10	122.78	126.95
6	o	200	CYC	CHB-C4A-NA	-2.10	120.54	124.93
6	I	200	CYC	CAC-C3C-C2C	-2.09	109.03	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	p	200	CYC	CHB-C1B-NB	2.09	130.55	126.06
6	0	1203	CYC	C1B-CHB-C4A	-2.09	122.98	128.08
6	T	200	CYC	CHB-C4A-C3A	2.08	130.25	124.90
6	s	200	CYC	C1B-CHB-C4A	-2.08	123.00	128.08
6	b	200	CYC	OB-C4B-C3B	-2.08	125.79	128.04
6	t	200	CYC	C3B-C4B-NB	2.07	108.45	106.78
6	e	200	CYC	CHB-C4A-NA	-2.06	120.62	124.93
6	C	200	CYC	CMC-C2C-C1C	-2.06	107.96	112.40
6	T	200	CYC	CMB-C2B-C1B	2.06	126.74	124.17
6	N	200	CYC	CHB-C4A-C3A	2.05	130.18	124.90
6	c	200	CYC	CHB-C4A-NA	-2.05	120.64	124.93
6	0	1203	CYC	CAA-CBA-CGA	-2.05	109.19	113.60
6	Y	200	CYC	CHB-C4A-NA	-2.05	120.64	124.93
6	w	200	CYC	CHB-C1B-NB	2.04	130.44	126.06
6	T	200	CYC	CMC-C2C-C1C	-2.04	108.01	112.40
6	i	200	CYC	CHB-C1B-C2B	-2.03	122.92	126.95
6	t	200	CYC	CMC-C2C-C1C	-2.02	108.04	112.40
6	o	200	CYC	CHB-C1B-C2B	-2.02	122.94	126.95
6	c	200	CYC	CHB-C1B-C2B	-2.02	122.95	126.95
6	p	200	CYC	OB-C4B-C3B	-2.02	125.85	128.04
6	a	200	CYC	CHB-C4A-NA	-2.02	120.71	124.93
6	x	200	CYC	CMC-C2C-C1C	-2.02	108.06	112.40
6	R	200	CYC	CHB-C1B-NB	2.01	130.38	126.06
6	x	200	CYC	CBD-CAD-C3D	-2.01	109.19	112.62
6	0	1203	CYC	O2A-CGA-CBA	2.01	120.48	114.03
6	p	200	CYC	C1B-CHB-C4A	-2.00	123.19	128.08
6	S	200	CYC	CHB-C1B-C2B	-2.00	122.98	126.95

There are no chirality outliers.

All (424) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	0	1201	CYC	NA-C1A-CHA-C4D
6	0	1201	CYC	C2A-C1A-CHA-C4D
6	0	1201	CYC	ND-C4D-CHA-C1A
6	0	1201	CYC	C3D-C4D-CHA-C1A
6	0	1201	CYC	NA-C4A-CHB-C1B
6	0	1201	CYC	C3A-C4A-CHB-C1B
6	0	1201	CYC	C2C-C3C-CAC-CBC
6	0	1201	CYC	NC-C4C-CHD-C1D
6	0	1201	CYC	ND-C1D-CHD-C4C
6	0	1201	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
6	0	1202	CYC	NC-C4C-CHD-C1D
6	0	1202	CYC	ND-C1D-CHD-C4C
6	0	1202	CYC	C2D-C1D-CHD-C4C
6	0	1203	CYC	NC-C4C-CHD-C1D
6	0	1203	CYC	ND-C1D-CHD-C4C
6	0	1203	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	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-C4A-CHB-C1B
6	B	200	CYC	NC-C4C-CHD-C1D
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	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-C4A-CHB-C1B
6	D	200	CYC	NC-C4C-CHD-C1D
6	E	200	CYC	ND-C4D-CHA-C1A
6	E	200	CYC	C3D-C4D-CHA-C1A
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	E	200	CYC	C3D-CAD-CBD-CGD
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	H	200	CYC	ND-C4D-CHA-C1A
6	H	200	CYC	C3D-C4D-CHA-C1A
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

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Mol	Chain	Res	Type	Atoms
6	I	200	CYC	NA-C4A-CHB-C1B
6	I	200	CYC	C3A-C4A-CHB-C1B
6	I	200	CYC	C4C-C3C-CAC-CBC
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	J	200	CYC	NA-C4A-CHB-C1B
6	J	200	CYC	C3A-C4A-CHB-C1B
6	J	200	CYC	NC-C4C-CHD-C1D
6	J	200	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	C2C-C3C-CAC-CBC
6	L	200	CYC	C4C-C3C-CAC-CBC
6	L	200	CYC	NC-C4C-CHD-C1D
6	L	200	CYC	ND-C1D-CHD-C4C
6	L	200	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	C2C-C3C-CAC-CBC
6	N	200	CYC	C4C-C3C-CAC-CBC
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	C3A-C4A-CHB-C1B
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-C4A-CHB-C1B
6	P	200	CYC	C3A-C4A-CHB-C1B
6	P	200	CYC	NC-C4C-CHD-C1D
6	Q	200	CYC	NC-C4C-CHD-C1D
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-C4A-CHB-C1B
6	S	200	CYC	C2C-C3C-CAC-CBC
6	S	200	CYC	NC-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
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	U	200	CYC	NC-C4C-CHD-C1D
6	U	200	CYC	ND-C1D-CHD-C4C
6	U	200	CYC	C2D-C1D-CHD-C4C
6	V	200	CYC	NA-C4A-CHB-C1B
6	V	200	CYC	C3A-C4A-CHB-C1B
6	V	200	CYC	C2A-CAA-CBA-CGA
6	V	200	CYC	C4B-C3B-CAB-CBB
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	W	200	CYC	NA-C4A-CHB-C1B
6	W	200	CYC	C3A-C4A-CHB-C1B
6	W	200	CYC	C2C-C3C-CAC-CBC
6	W	200	CYC	NC-C4C-CHD-C1D
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	ND-C1D-CHD-C4C
6	Y	200	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	NC-C4C-CHD-C1D
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	C2C-C3C-CAC-CBC
6	c	200	CYC	NC-C4C-CHD-C1D
6	d	200	CYC	NA-C4A-CHB-C1B
6	d	200	CYC	NC-C4C-CHD-C1D
6	e	200	CYC	NC-C4C-CHD-C1D
6	e	200	CYC	C2D-C1D-CHD-C4C
6	f	200	CYC	NA-C4A-CHB-C1B
6	f	200	CYC	C2C-C3C-CAC-CBC
6	f	200	CYC	NC-C4C-CHD-C1D
6	h	200	CYC	NC-C4C-CHD-C1D
6	h	200	CYC	ND-C1D-CHD-C4C
6	h	200	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
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	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	k	200	CYC	NA-C4A-CHB-C1B
6	k	200	CYC	C3A-C4A-CHB-C1B
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	l	200	CYC	NA-C4A-CHB-C1B
6	l	200	CYC	C3A-C4A-CHB-C1B
6	l	200	CYC	C2C-C3C-CAC-CBC
6	l	200	CYC	NC-C4C-CHD-C1D
6	l	200	CYC	ND-C1D-CHD-C4C
6	m	200	CYC	NA-C1A-CHA-C4D
6	m	200	CYC	C2A-C1A-CHA-C4D
6	m	200	CYC	ND-C4D-CHA-C1A
6	m	200	CYC	C3D-C4D-CHA-C1A
6	m	200	CYC	NA-C4A-CHB-C1B
6	m	200	CYC	C3A-C4A-CHB-C1B
6	m	200	CYC	NC-C4C-CHD-C1D
6	m	200	CYC	ND-C1D-CHD-C4C
6	m	200	CYC	C2D-C1D-CHD-C4C
6	n	200	CYC	NA-C4A-CHB-C1B
6	n	200	CYC	NC-C4C-CHD-C1D
6	o	200	CYC	NA-C4A-CHB-C1B
6	o	200	CYC	NC-C4C-CHD-C1D
6	p	200	CYC	NA-C4A-CHB-C1B
6	p	200	CYC	C2C-C3C-CAC-CBC
6	p	200	CYC	NC-C4C-CHD-C1D
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-C4A-CHB-C1B
6	r	200	CYC	NC-C4C-CHD-C1D
6	s	200	CYC	NC-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
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	C2D-C1D-CHD-C4C
6	u	200	CYC	C3A-C4A-CHB-C1B
6	u	200	CYC	NC-C4C-CHD-C1D
6	u	200	CYC	ND-C1D-CHD-C4C
6	u	200	CYC	C2D-C1D-CHD-C4C
6	v	200	CYC	NA-C4A-CHB-C1B
6	v	200	CYC	C3A-C4A-CHB-C1B
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	w	200	CYC	C2C-C3C-CAC-CBC
6	w	200	CYC	C4C-C3C-CAC-CBC
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	x	200	CYC	NC-C4C-CHD-C1D
6	x	200	CYC	ND-C1D-CHD-C4C
6	x	200	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	ND-C1D-CHD-C4C
6	y	200	CYC	C2D-C1D-CHD-C4C
6	V	200	CYC	C2B-C3B-CAB-CBB
6	0	1201	CYC	C2B-C3B-CAB-CBB
6	C	200	CYC	C2A-CAA-CBA-CGA
6	E	200	CYC	C2A-CAA-CBA-CGA
6	I	200	CYC	C2A-CAA-CBA-CGA
6	S	200	CYC	C3A-C4A-CHB-C1B
6	f	200	CYC	C3A-C4A-CHB-C1B
6	n	200	CYC	C3A-C4A-CHB-C1B
6	o	200	CYC	C3A-C4A-CHB-C1B
6	p	200	CYC	C3A-C4A-CHB-C1B
6	r	200	CYC	C3A-C4A-CHB-C1B
6	J	200	CYC	C2B-C3B-CAB-CBB
6	I	200	CYC	C2B-C3B-CAB-CBB
6	D	200	CYC	C3D-CAD-CBD-CGD
6	H	200	CYC	C3D-CAD-CBD-CGD
6	N	200	CYC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
6	T	200	CYC	C3D-CAD-CBD-CGD
6	E	200	CYC	NA-C1A-CHA-C4D
6	L	200	CYC	NA-C1A-CHA-C4D
6	S	200	CYC	NA-C1A-CHA-C4D
6	n	200	CYC	NA-C1A-CHA-C4D
6	0	1201	CYC	C4B-C3B-CAB-CBB
6	G	200	CYC	C2B-C3B-CAB-CBB
6	m	200	CYC	NB-C1B-CHB-C4A
6	0	1202	CYC	C3A-C4A-CHB-C1B
6	j	200	CYC	C3A-C4A-CHB-C1B
6	0	1202	CYC	NA-C4A-CHB-C1B
6	0	1203	CYC	NA-C4A-CHB-C1B
6	E	200	CYC	NA-C4A-CHB-C1B
6	H	200	CYC	NA-C4A-CHB-C1B
6	O	200	CYC	NA-C4A-CHB-C1B
6	Q	200	CYC	NA-C4A-CHB-C1B
6	R	200	CYC	NA-C4A-CHB-C1B
6	U	200	CYC	NA-C4A-CHB-C1B
6	b	200	CYC	NA-C4A-CHB-C1B
6	c	200	CYC	NA-C4A-CHB-C1B
6	e	200	CYC	NA-C4A-CHB-C1B
6	h	200	CYC	NA-C4A-CHB-C1B
6	j	200	CYC	NA-C4A-CHB-C1B
6	q	200	CYC	NA-C4A-CHB-C1B
6	s	200	CYC	NA-C4A-CHB-C1B
6	u	200	CYC	NA-C4A-CHB-C1B
6	w	200	CYC	NA-C4A-CHB-C1B
6	x	200	CYC	NA-C4A-CHB-C1B
6	0	1203	CYC	C3A-C4A-CHB-C1B
6	B	200	CYC	C3A-C4A-CHB-C1B
6	D	200	CYC	C3A-C4A-CHB-C1B
6	E	200	CYC	C3A-C4A-CHB-C1B
6	H	200	CYC	C3A-C4A-CHB-C1B
6	Q	200	CYC	C3A-C4A-CHB-C1B
6	R	200	CYC	C3A-C4A-CHB-C1B
6	U	200	CYC	C3A-C4A-CHB-C1B
6	b	200	CYC	C3A-C4A-CHB-C1B
6	c	200	CYC	C3A-C4A-CHB-C1B
6	d	200	CYC	C3A-C4A-CHB-C1B
6	e	200	CYC	C3A-C4A-CHB-C1B
6	h	200	CYC	C3A-C4A-CHB-C1B
6	q	200	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
6	s	200	CYC	C3A-C4A-CHB-C1B
6	w	200	CYC	C3A-C4A-CHB-C1B
6	x	200	CYC	C3A-C4A-CHB-C1B
6	Y	200	CYC	C3D-CAD-CBD-CGD
6	A	200	CYC	NA-C1A-CHA-C4D
6	a	200	CYC	NA-C1A-CHA-C4D
6	T	200	CYC	C1A-C2A-CAA-CBA
6	T	200	CYC	C2B-C3B-CAB-CBB
6	T	200	CYC	C3A-C2A-CAA-CBA
6	P	200	CYC	C2C-C3C-CAC-CBC
6	m	200	CYC	C2B-C1B-CHB-C4A
6	r	200	CYC	NA-C1A-CHA-C4D
6	N	200	CYC	C2A-CAA-CBA-CGA
6	Q	200	CYC	C2A-CAA-CBA-CGA
6	E	200	CYC	C2A-C1A-CHA-C4D
6	L	200	CYC	C2A-C1A-CHA-C4D
6	n	200	CYC	C2A-C1A-CHA-C4D
6	Y	200	CYC	NB-C1B-CHB-C4A
6	P	200	CYC	C2A-CAA-CBA-CGA
6	p	200	CYC	C2A-CAA-CBA-CGA
6	y	200	CYC	C2A-CAA-CBA-CGA
6	l	200	CYC	NA-C1A-CHA-C4D
6	f	200	CYC	C4C-C3C-CAC-CBC
6	p	200	CYC	C4C-C3C-CAC-CBC
6	e	200	CYC	C2A-CAA-CBA-CGA
6	d	200	CYC	NA-C1A-CHA-C4D
6	I	200	CYC	C4B-C3B-CAB-CBB
6	J	200	CYC	C4B-C3B-CAB-CBB
6	A	200	CYC	C3D-CAD-CBD-CGD
6	G	200	CYC	C2C-C3C-CAC-CBC
6	b	200	CYC	C2C-C3C-CAC-CBC
6	i	200	CYC	NA-C1A-CHA-C4D
6	l	200	CYC	C2A-CAA-CBA-CGA
6	r	200	CYC	C2A-CAA-CBA-CGA
6	G	200	CYC	C4B-C3B-CAB-CBB
6	h	200	CYC	NB-C1B-CHB-C4A
6	T	200	CYC	CAD-CBD-CGD-O2D
6	l	200	CYC	CAD-CBD-CGD-O1D
6	t	200	CYC	CAD-CBD-CGD-O1D
6	Q	200	CYC	CAD-CBD-CGD-O1D
6	D	200	CYC	CAD-CBD-CGD-O1D
6	H	200	CYC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
6	N	200	CYC	CAA-CBA-CGA-O2A
6	B	200	CYC	C2B-C3B-CAB-CBB
6	E	200	CYC	CAD-CBD-CGD-O2D
6	V	200	CYC	CAA-CBA-CGA-O1A
6	J	200	CYC	CAA-CBA-CGA-O2A
6	N	200	CYC	CAA-CBA-CGA-O1A
6	T	200	CYC	CAD-CBD-CGD-O1D
6	x	200	CYC	CAD-CBD-CGD-O2D
6	c	200	CYC	CAA-CBA-CGA-O2A
6	i	200	CYC	CAD-CBD-CGD-O1D
6	E	200	CYC	CAA-CBA-CGA-O1A
6	J	200	CYC	CAA-CBA-CGA-O1A
6	J	200	CYC	CAD-CBD-CGD-O1D
6	m	200	CYC	CAD-CBD-CGD-O1D
6	l	200	CYC	CAD-CBD-CGD-O2D
6	x	200	CYC	CAD-CBD-CGD-O1D
6	0	1203	CYC	CAA-CBA-CGA-O1A
6	C	200	CYC	CAD-CBD-CGD-O1D
6	Q	200	CYC	CAD-CBD-CGD-O2D
6	r	200	CYC	CAA-CBA-CGA-O1A
6	E	200	CYC	CAA-CBA-CGA-O2A
6	S	200	CYC	CAD-CBD-CGD-O1D
6	c	200	CYC	CAA-CBA-CGA-O1A
6	m	200	CYC	CAD-CBD-CGD-O2D
6	p	200	CYC	CAA-CBA-CGA-O1A
6	t	200	CYC	CAD-CBD-CGD-O2D
6	H	200	CYC	CAD-CBD-CGD-O2D
6	T	200	CYC	CAA-CBA-CGA-O2A
6	V	200	CYC	CAA-CBA-CGA-O2A
6	O	200	CYC	CAD-CBD-CGD-O2D
6	T	200	CYC	CAA-CBA-CGA-O1A
6	n	200	CYC	CAA-CBA-CGA-O1A
6	0	1202	CYC	CAA-CBA-CGA-O2A
6	J	200	CYC	CAD-CBD-CGD-O2D
6	D	200	CYC	CAD-CBD-CGD-O2D
6	I	200	CYC	C2C-C3C-CAC-CBC
6	E	200	CYC	CAD-CBD-CGD-O1D
6	r	200	CYC	CAA-CBA-CGA-O2A
6	0	1202	CYC	CAA-CBA-CGA-O1A
6	0	1203	CYC	CAA-CBA-CGA-O2A
6	p	200	CYC	CAA-CBA-CGA-O2A
6	b	200	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
6	q	200	CYC	CAA-CBA-CGA-O2A
6	n	200	CYC	CAA-CBA-CGA-O2A
6	q	200	CYC	CAA-CBA-CGA-O1A
6	O	200	CYC	CAD-CBD-CGD-O1D
6	0	1201	CYC	CAA-CBA-CGA-O2A
6	P	200	CYC	CAD-CBD-CGD-O2D
6	e	200	CYC	CAA-CBA-CGA-O2A
6	L	200	CYC	CAD-CBD-CGD-O1D
6	i	200	CYC	CAD-CBD-CGD-O2D
6	0	1201	CYC	CAA-CBA-CGA-O1A
6	d	200	CYC	CAA-CBA-CGA-O2A
6	B	200	CYC	CAA-CBA-CGA-O2A
6	W	200	CYC	CAA-CBA-CGA-O1A
6	W	200	CYC	CAA-CBA-CGA-O2A
6	G	200	CYC	CAD-CBD-CGD-O1D
6	v	200	CYC	CAA-CBA-CGA-O2A
6	e	200	CYC	CAA-CBA-CGA-O1A
6	0	1201	CYC	CAD-CBD-CGD-O2D
6	i	200	CYC	CAA-CBA-CGA-O2A
6	y	200	CYC	CAA-CBA-CGA-O1A
6	y	200	CYC	CAA-CBA-CGA-O2A
6	B	200	CYC	CAA-CBA-CGA-O1A
6	b	200	CYC	CAD-CBD-CGD-O1D
6	P	200	CYC	NA-C1A-CHA-C4D
6	P	200	CYC	CAD-CBD-CGD-O1D
6	a	200	CYC	CAD-CBD-CGD-O1D
6	d	200	CYC	CAA-CBA-CGA-O1A
6	o	200	CYC	CAD-CBD-CGD-O1D
6	h	200	CYC	CAD-CBD-CGD-O1D
6	p	200	CYC	CAD-CBD-CGD-O1D
6	v	200	CYC	CAA-CBA-CGA-O1A
6	0	1201	CYC	CAD-CBD-CGD-O1D
6	C	200	CYC	CAD-CBD-CGD-O2D
6	S	200	CYC	CAD-CBD-CGD-O2D
6	Y	200	CYC	C2B-C1B-CHB-C4A
6	s	200	CYC	C3A-C2A-CAA-CBA
6	i	200	CYC	CAA-CBA-CGA-O1A
6	G	200	CYC	CAD-CBD-CGD-O2D
6	a	200	CYC	CAD-CBD-CGD-O2D
6	o	200	CYC	CAD-CBD-CGD-O2D
6	p	200	CYC	CAD-CBD-CGD-O2D
6	U	200	CYC	CAD-CBD-CGD-O1D

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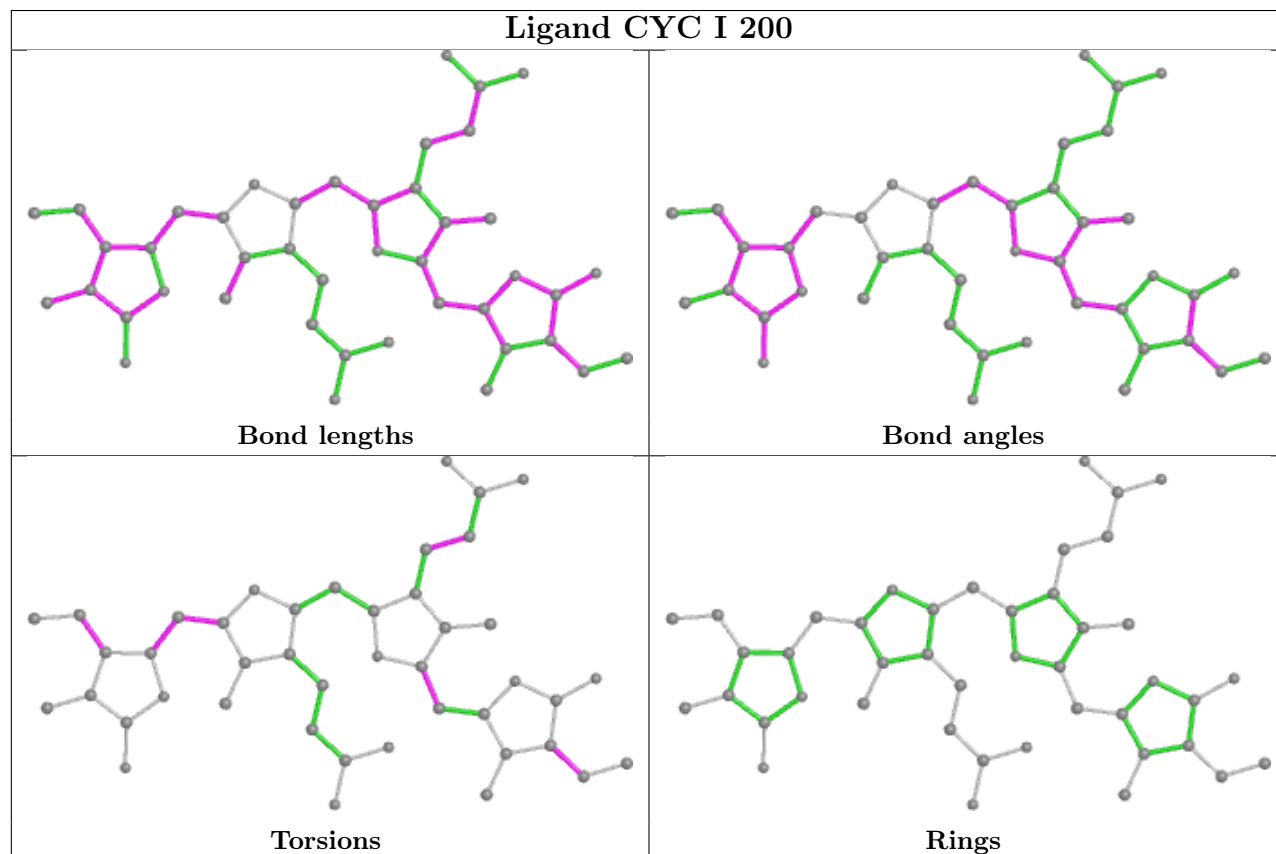
Mol	Chain	Res	Type	Atoms
6	d	200	CYC	C2B-C3B-CAB-CBB
6	h	200	CYC	CAD-CBD-CGD-O2D
6	t	200	CYC	C2B-C3B-CAB-CBB
6	t	200	CYC	CAA-CBA-CGA-O2A
6	L	200	CYC	CAD-CBD-CGD-O2D
6	k	200	CYC	CAD-CBD-CGD-O1D
6	R	200	CYC	CAA-CBA-CGA-O2A
6	A	200	CYC	CAD-CBD-CGD-O2D
6	V	200	CYC	CAD-CBD-CGD-O2D
6	f	200	CYC	CAD-CBD-CGD-O2D
6	A	200	CYC	C2A-C1A-CHA-C4D
6	S	200	CYC	C2A-C1A-CHA-C4D
6	q	200	CYC	CAD-CBD-CGD-O2D
6	W	200	CYC	CAD-CBD-CGD-O2D
6	m	200	CYC	CAA-CBA-CGA-O2A
6	t	200	CYC	CAA-CBA-CGA-O1A
6	q	200	CYC	CAD-CBD-CGD-O1D
6	0	1203	CYC	CAD-CBD-CGD-O2D
6	U	200	CYC	CAD-CBD-CGD-O2D
6	P	200	CYC	C3D-CAD-CBD-CGD
6	Q	200	CYC	C2C-C3C-CAC-CBC
6	d	200	CYC	C2C-C3C-CAC-CBC
6	0	1202	CYC	CAD-CBD-CGD-O2D
6	Y	200	CYC	CAD-CBD-CGD-O2D
6	r	200	CYC	CAD-CBD-CGD-O2D
6	u	200	CYC	CAD-CBD-CGD-O2D
6	0	1202	CYC	CAD-CBD-CGD-O1D
6	R	200	CYC	CAA-CBA-CGA-O1A
6	s	200	CYC	C1A-C2A-CAA-CBA
6	N	200	CYC	CAD-CBD-CGD-O1D
6	N	200	CYC	CAD-CBD-CGD-O2D
6	c	200	CYC	CAD-CBD-CGD-O2D
6	e	200	CYC	CAD-CBD-CGD-O2D
6	e	200	CYC	CAD-CBD-CGD-O1D
6	k	200	CYC	CAD-CBD-CGD-O2D
6	u	200	CYC	CAD-CBD-CGD-O1D

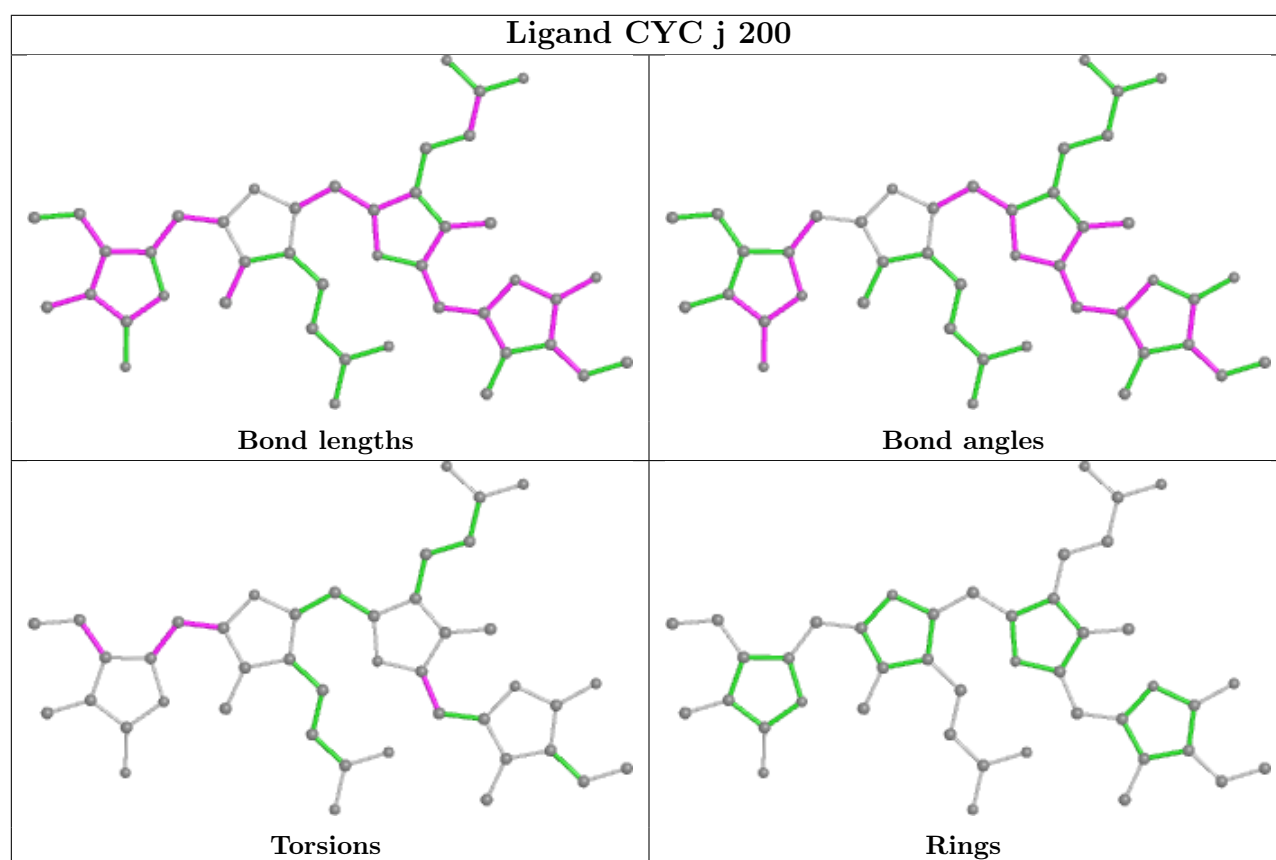
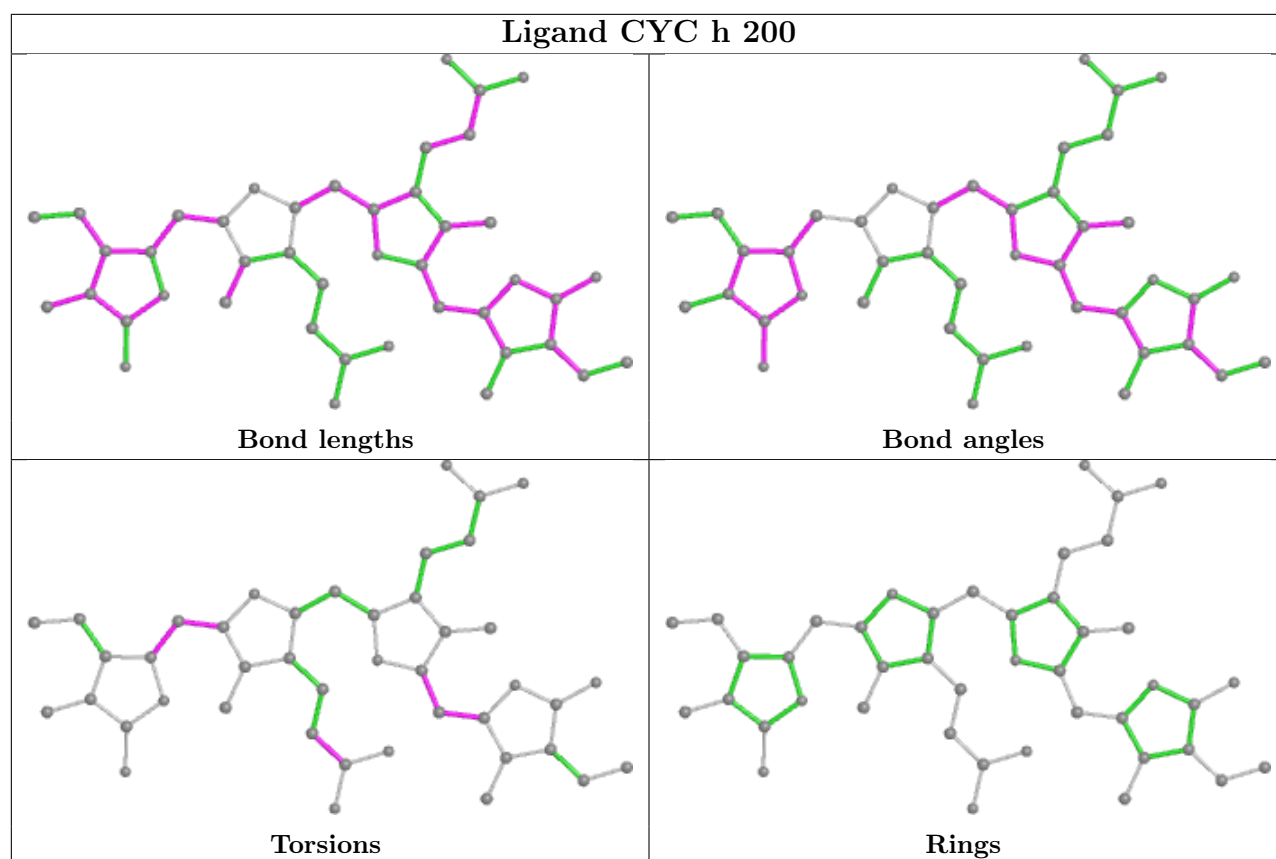
There are no ring outliers.

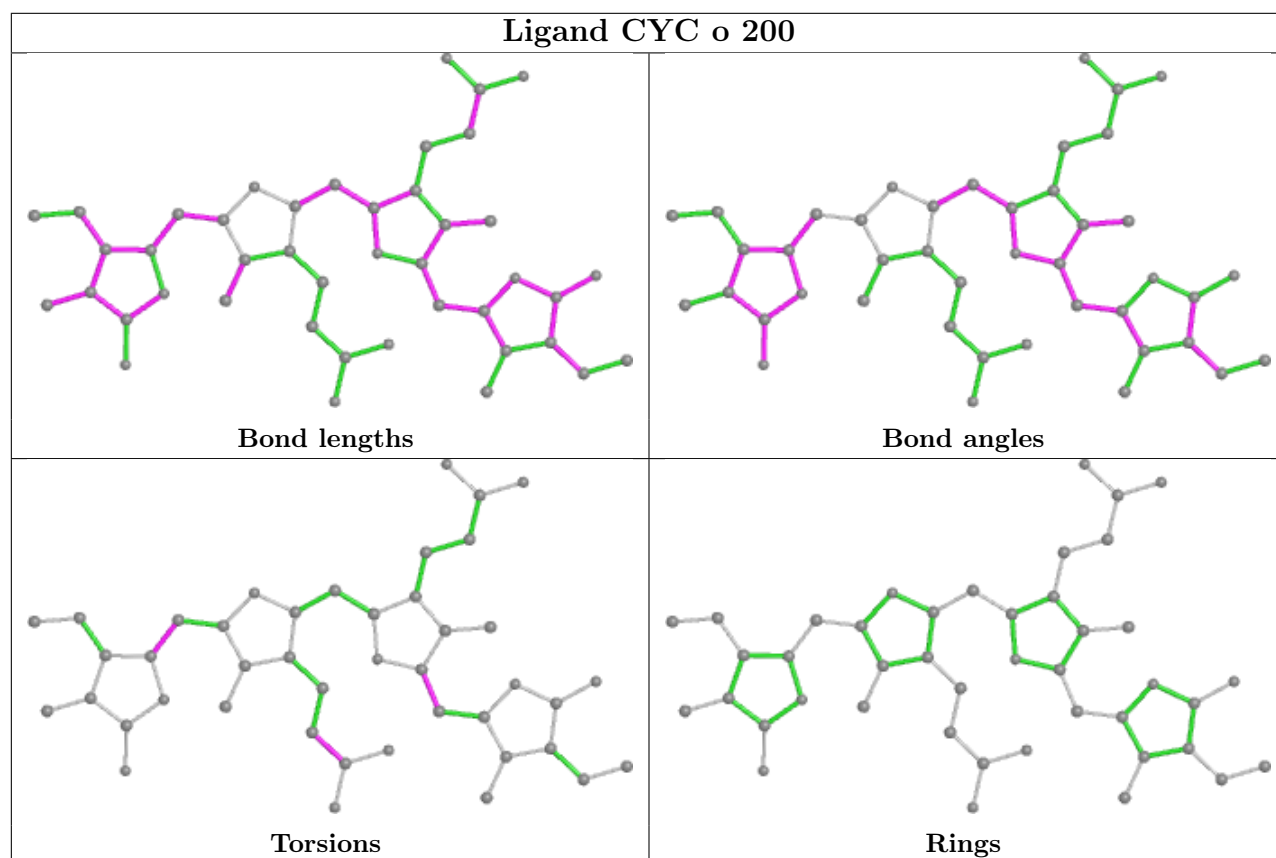
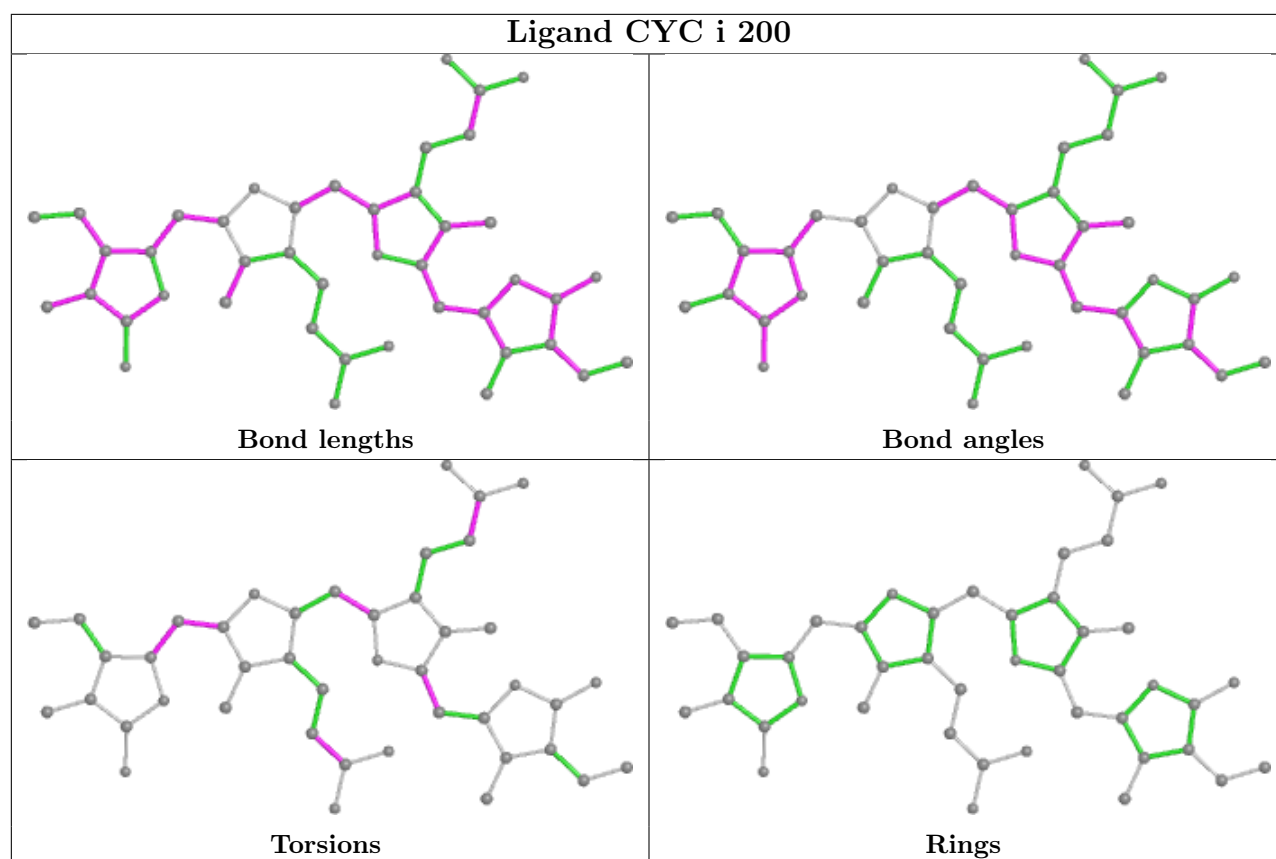
No monomer is involved in short contacts.

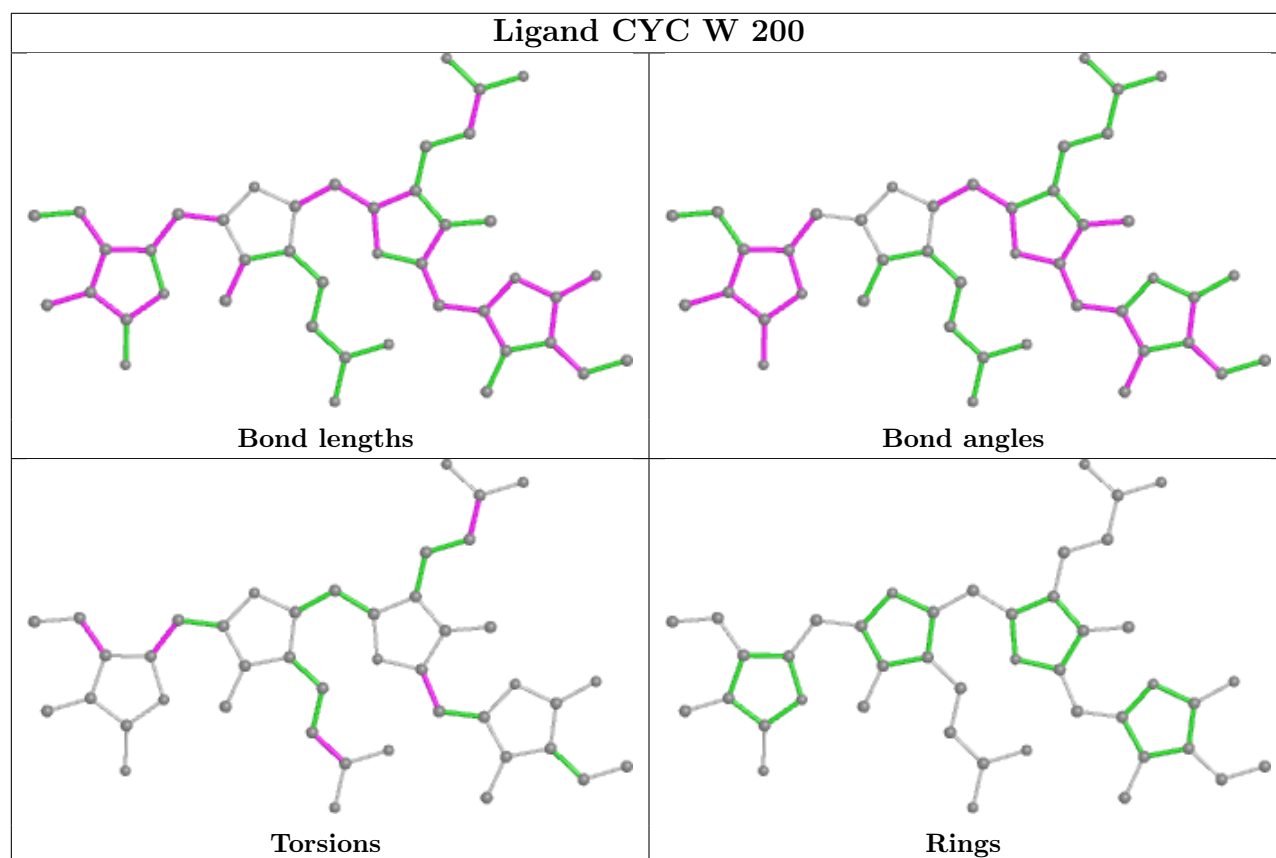
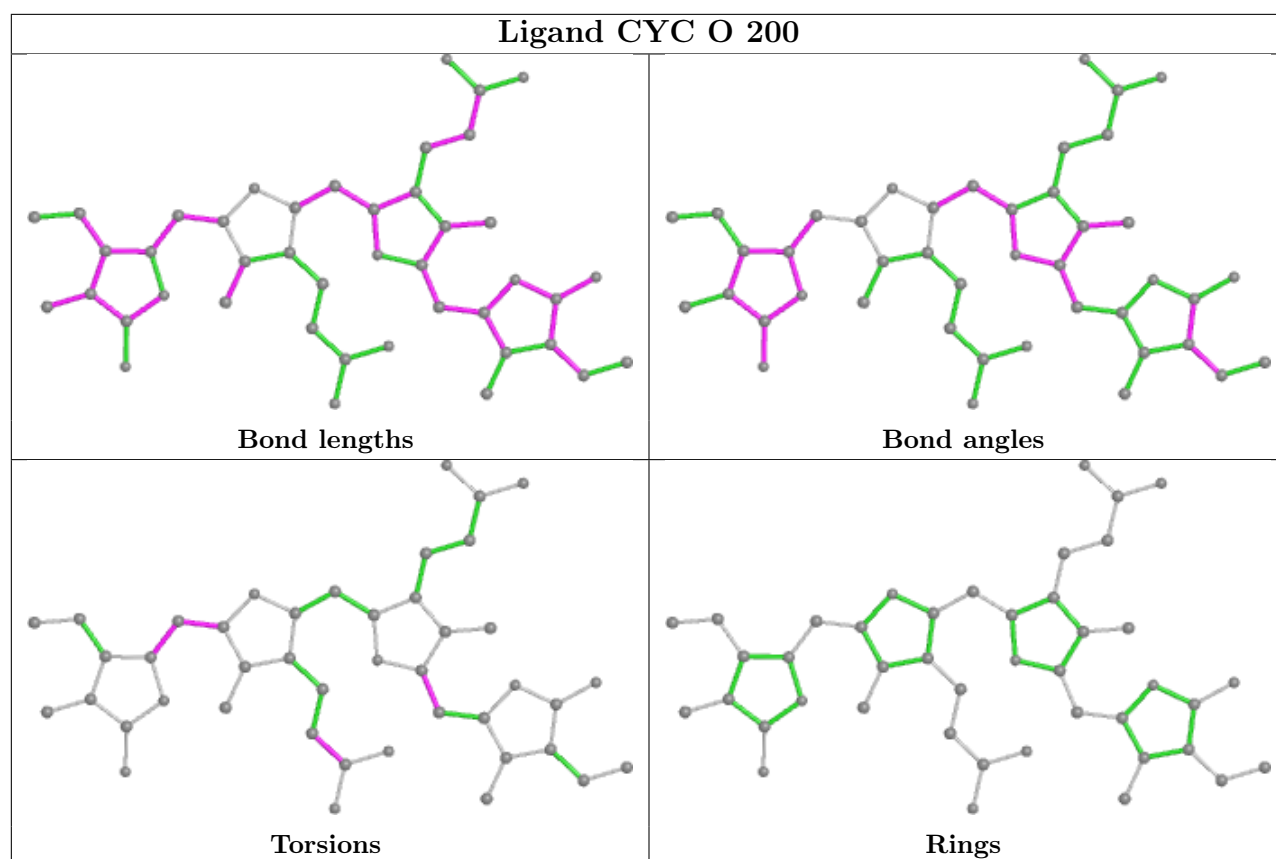
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

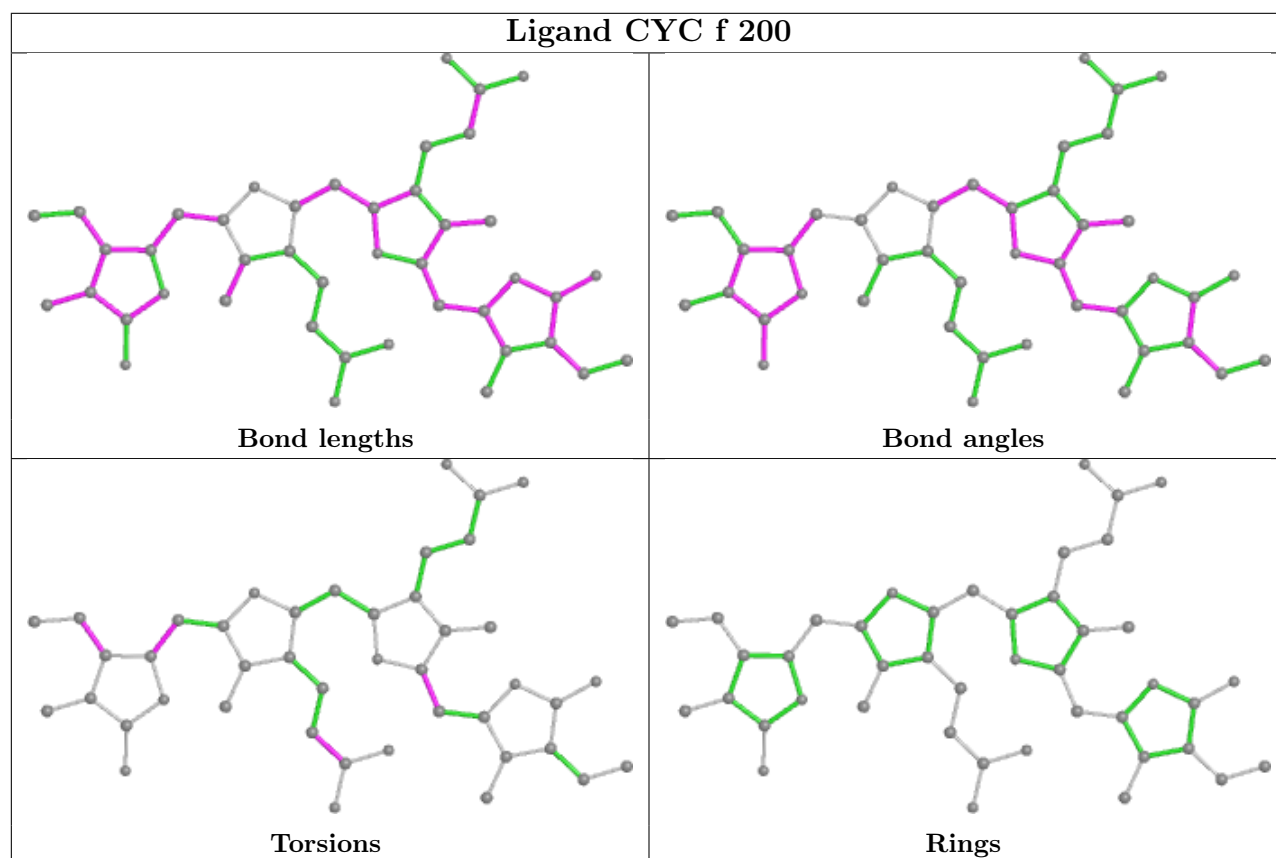
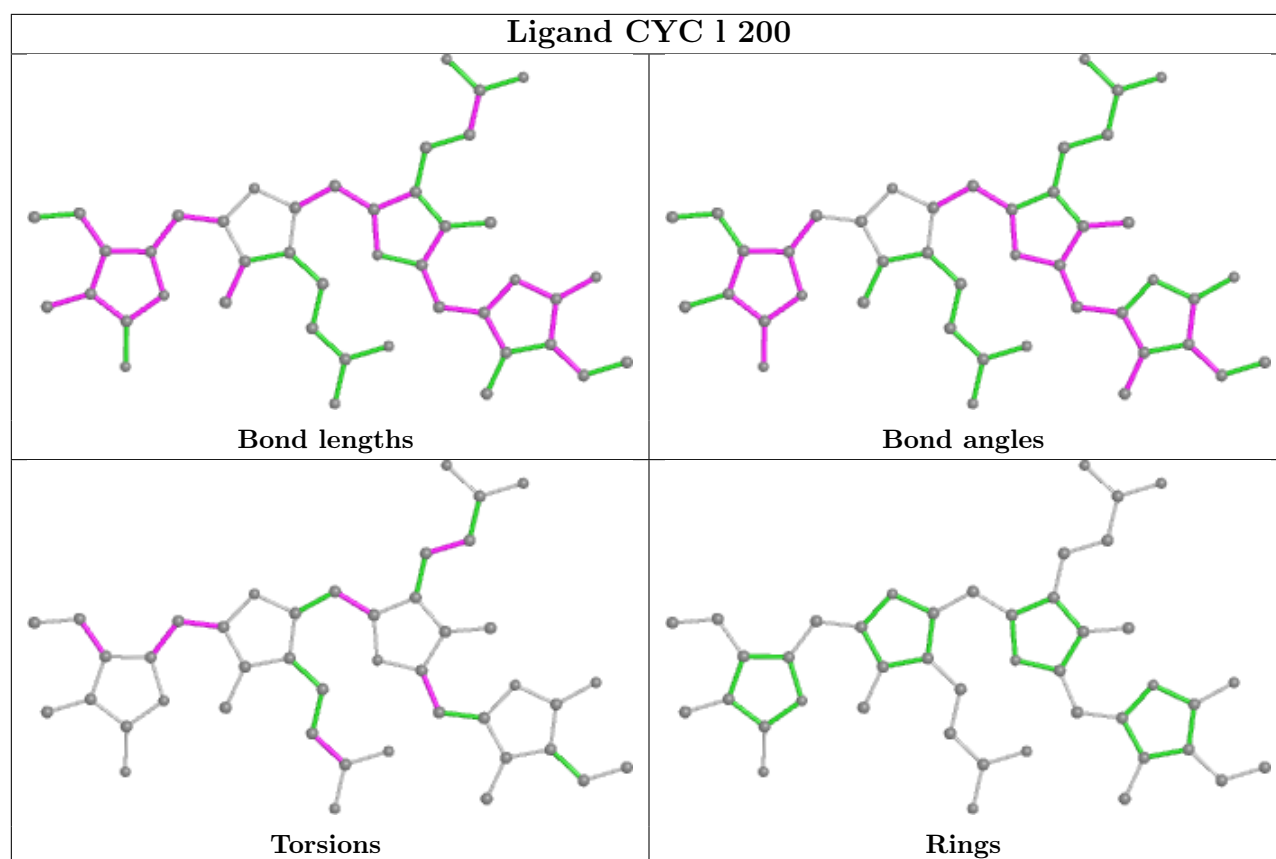
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

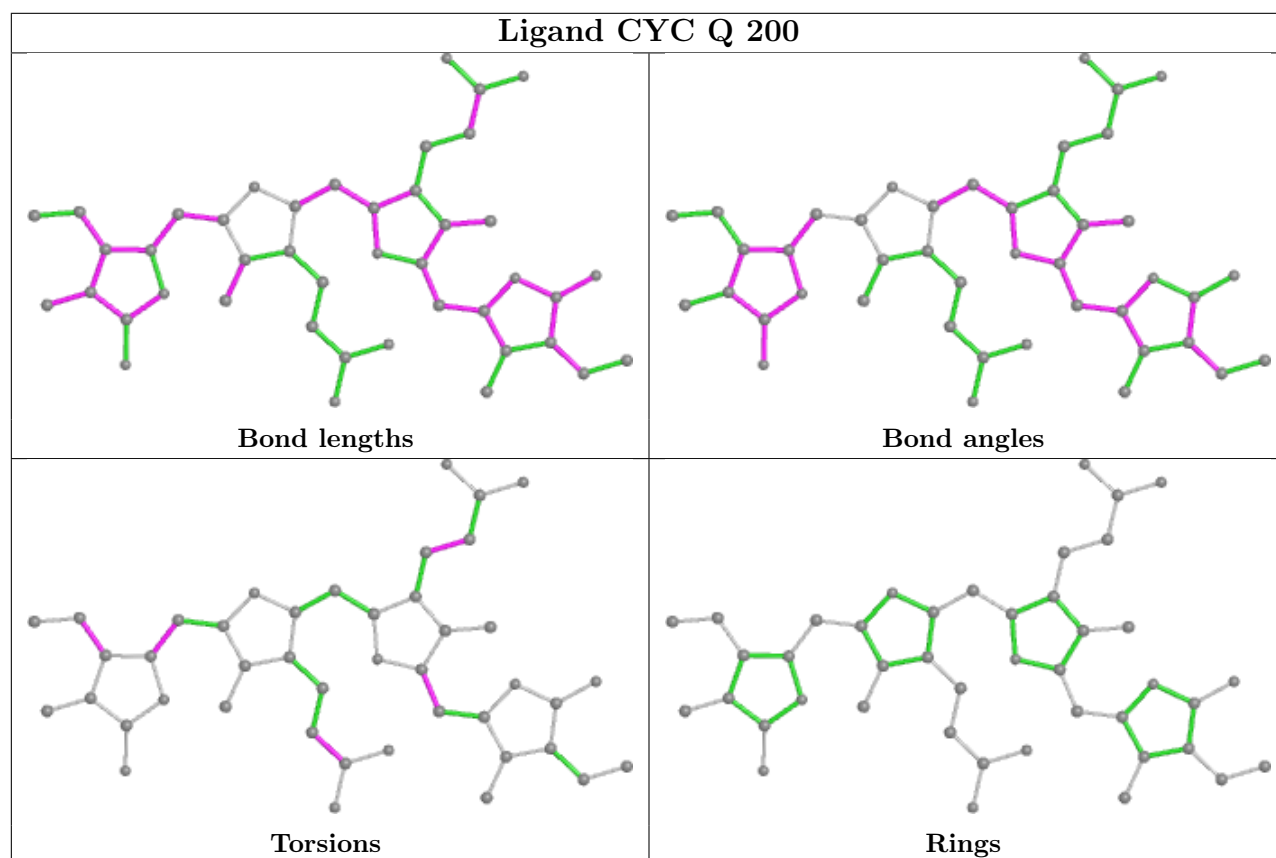
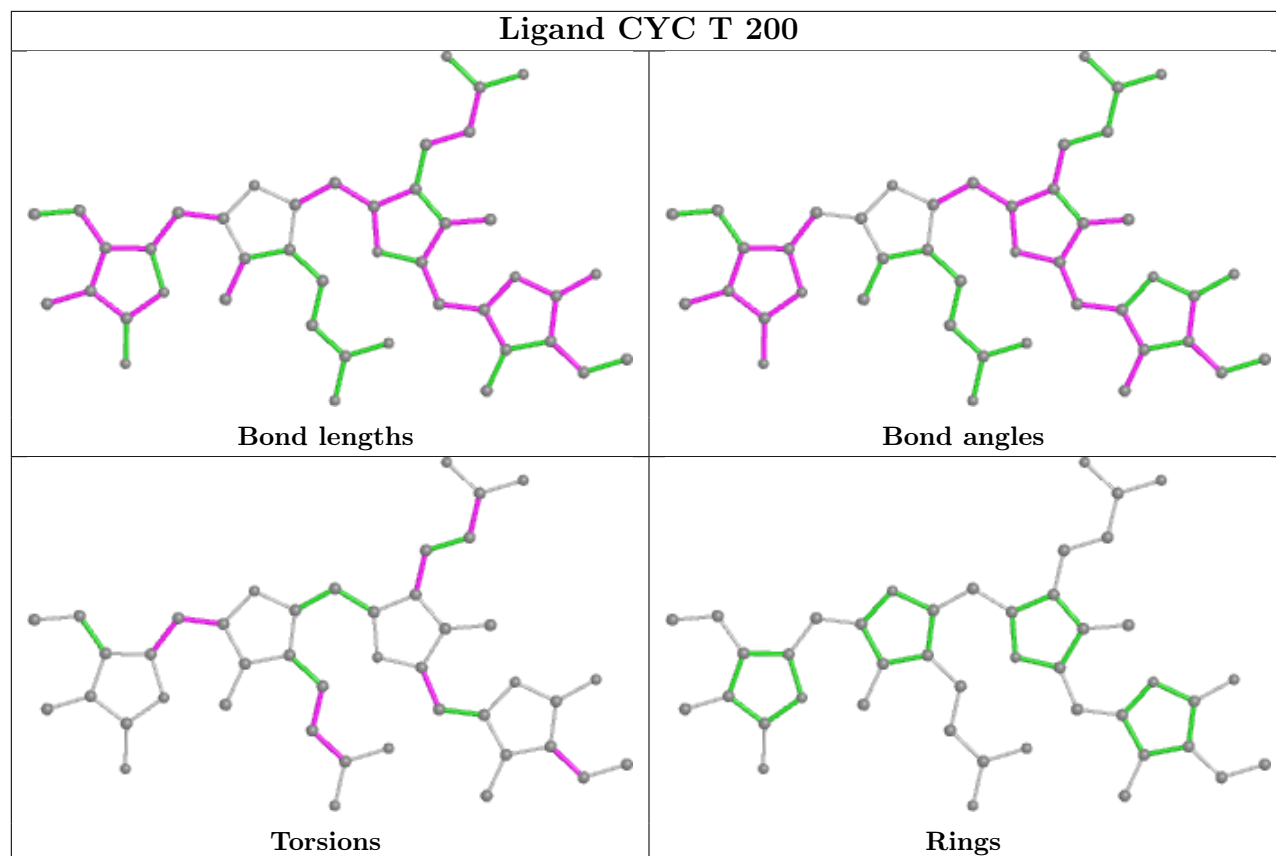


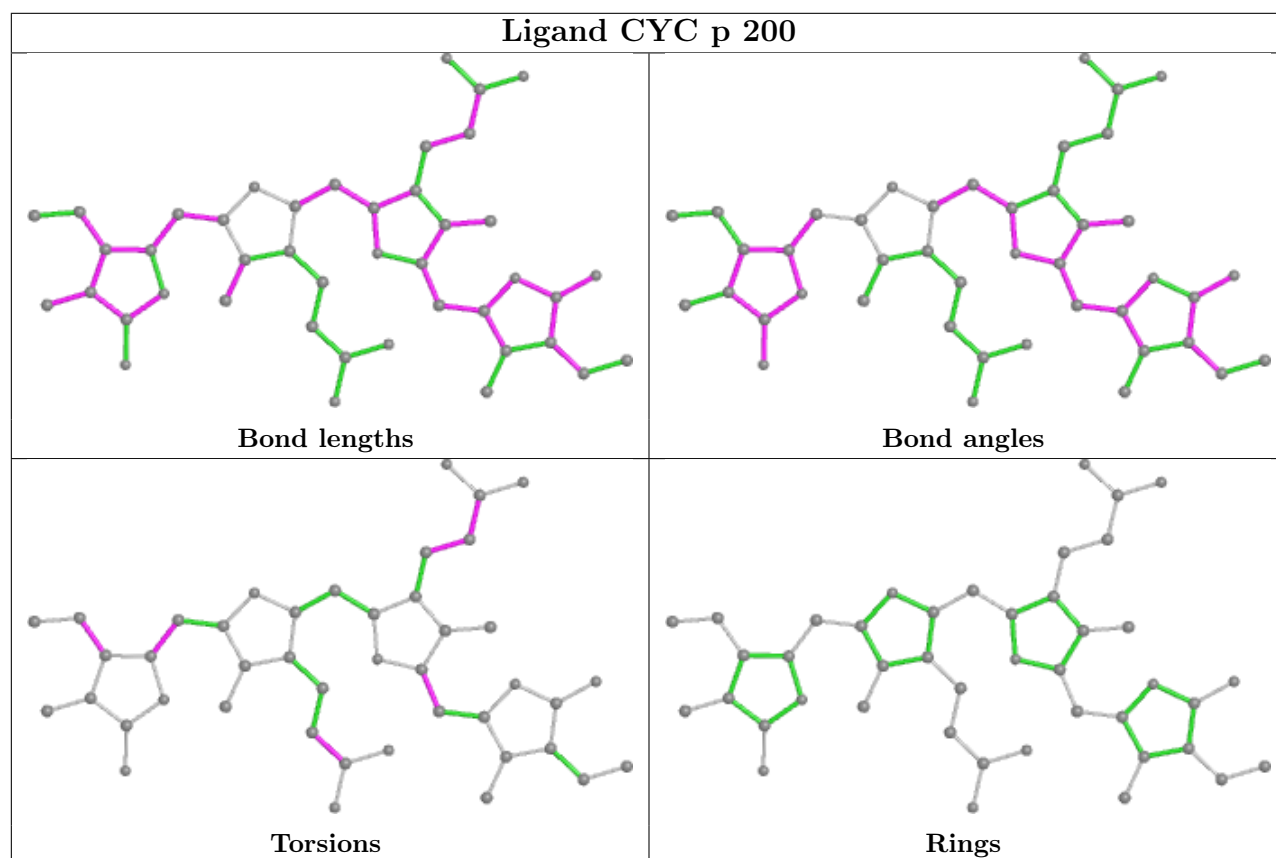
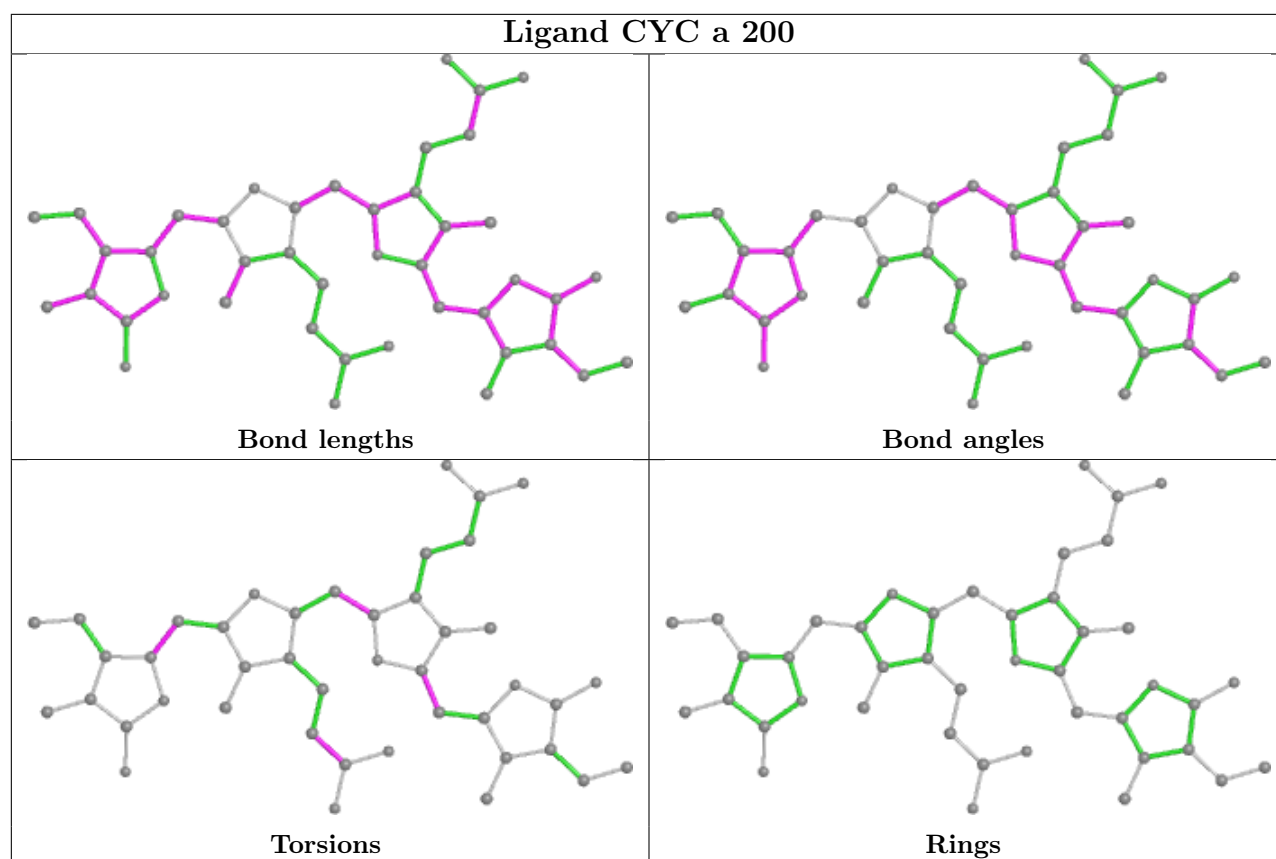


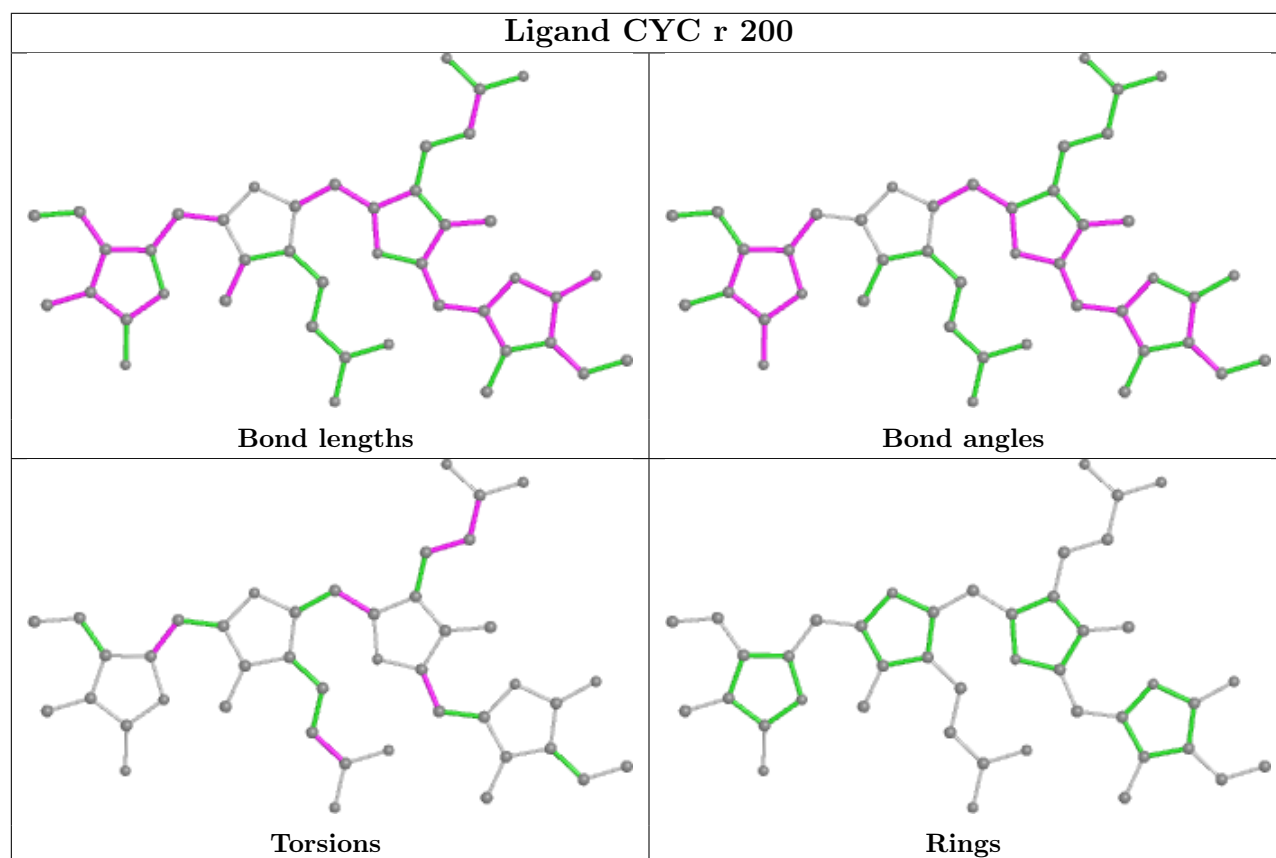
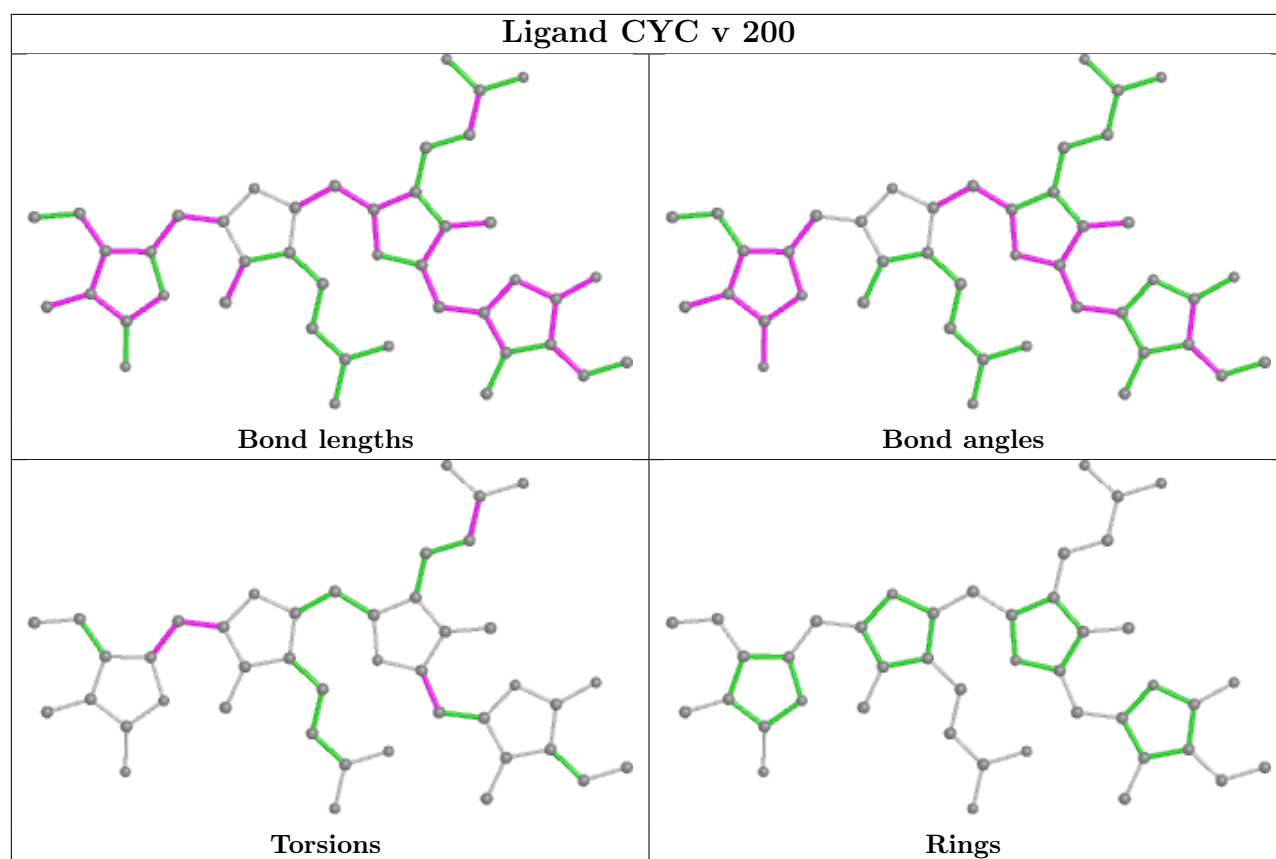


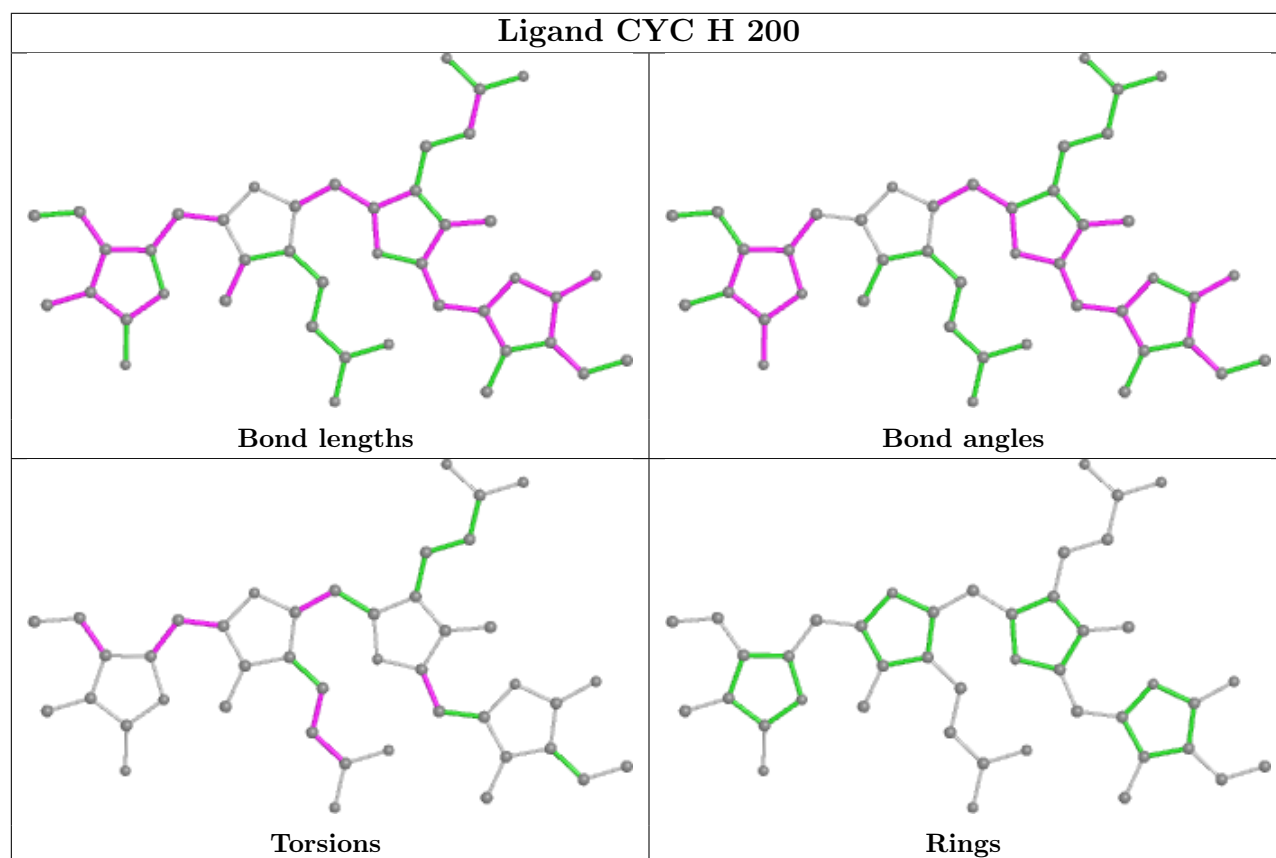
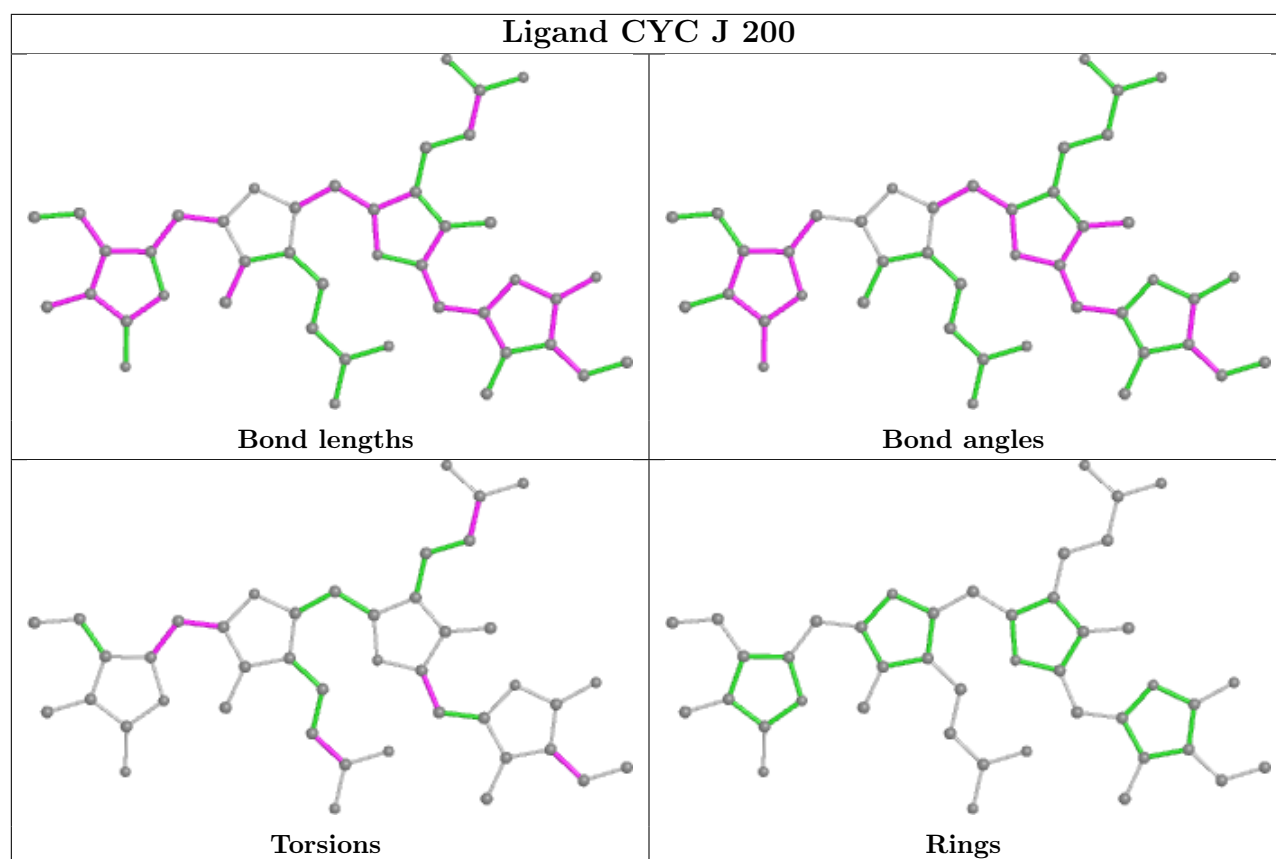


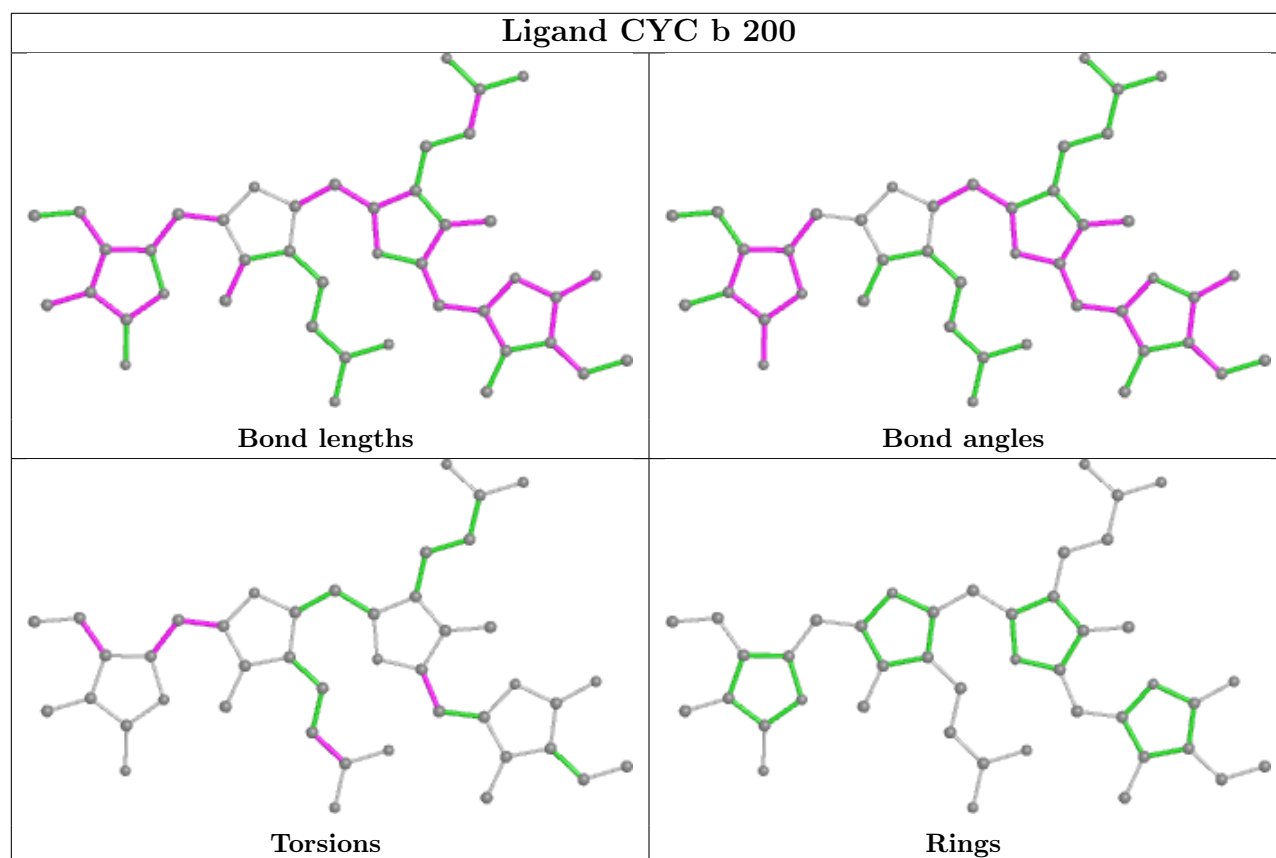
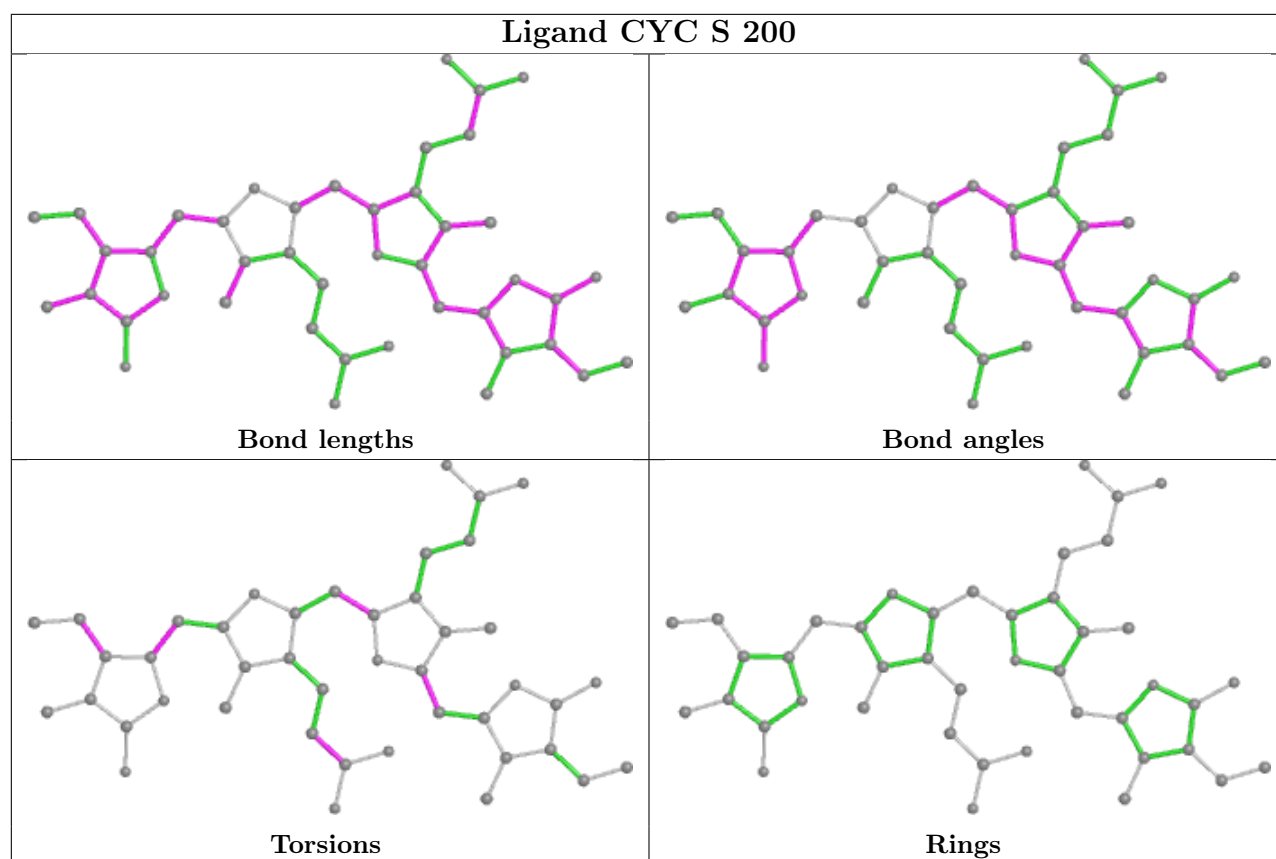


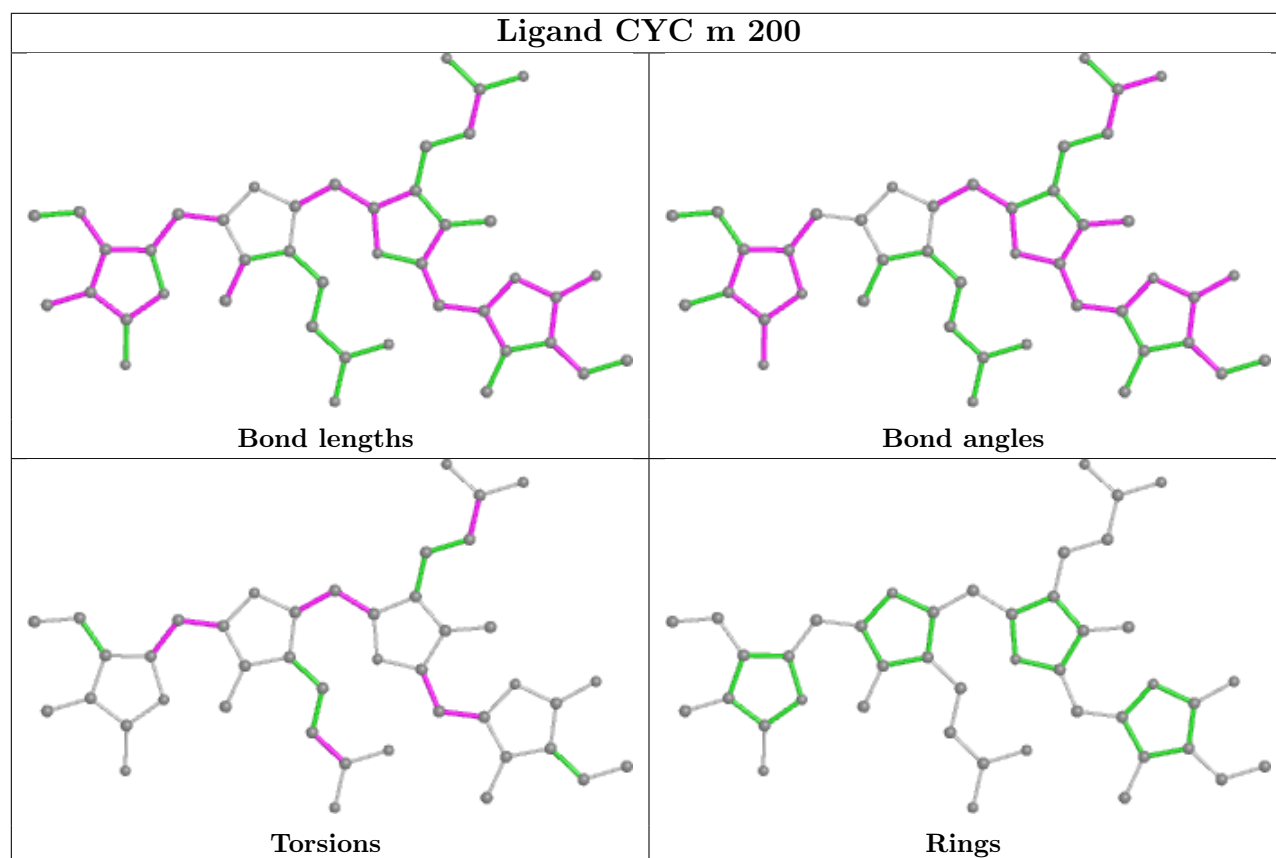
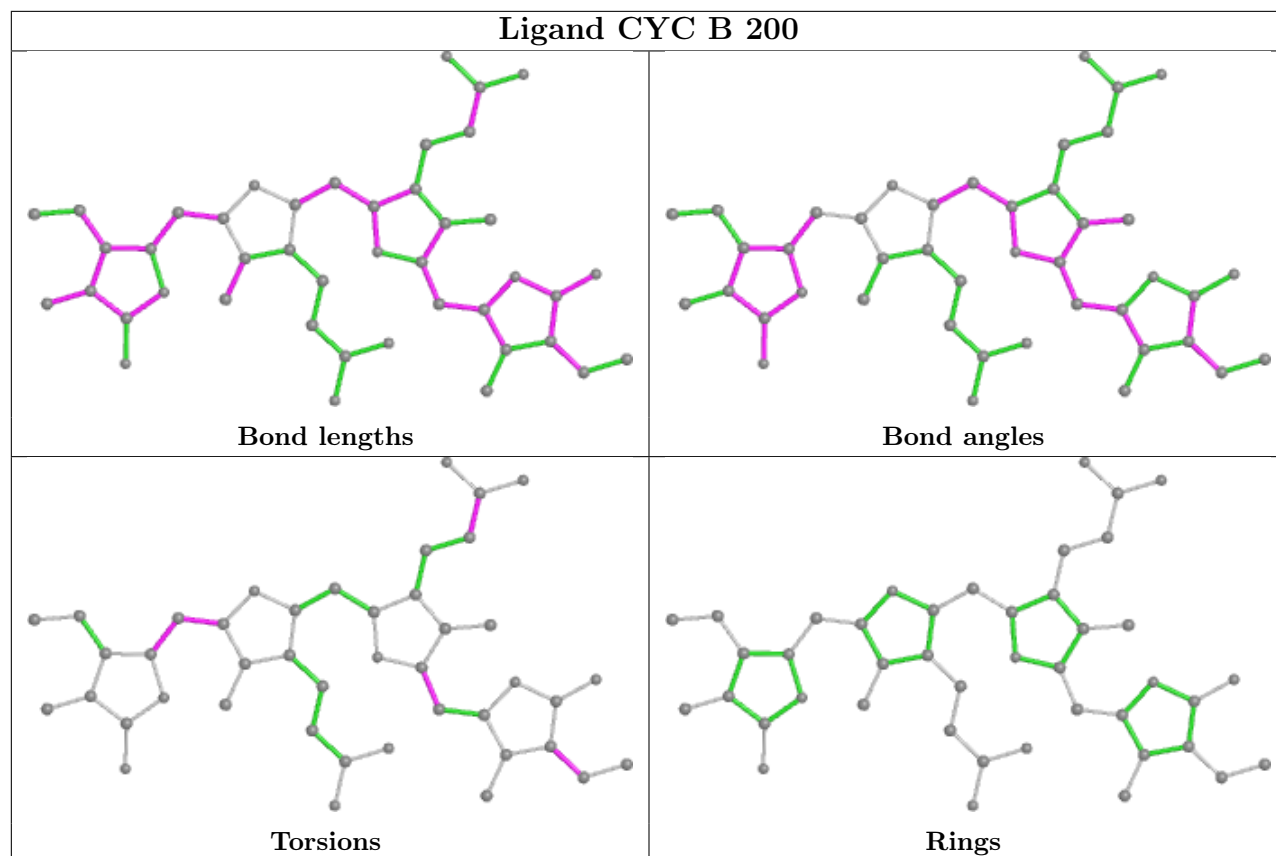


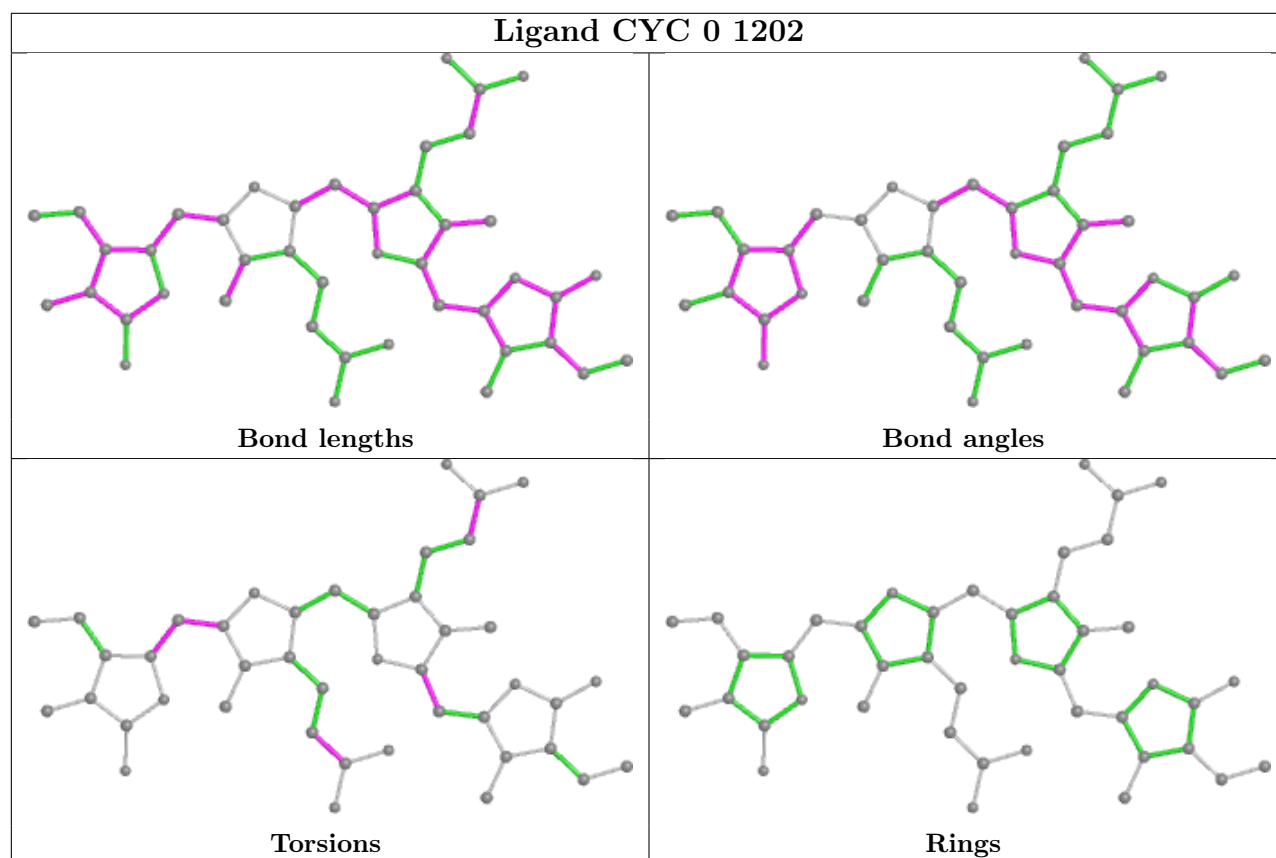
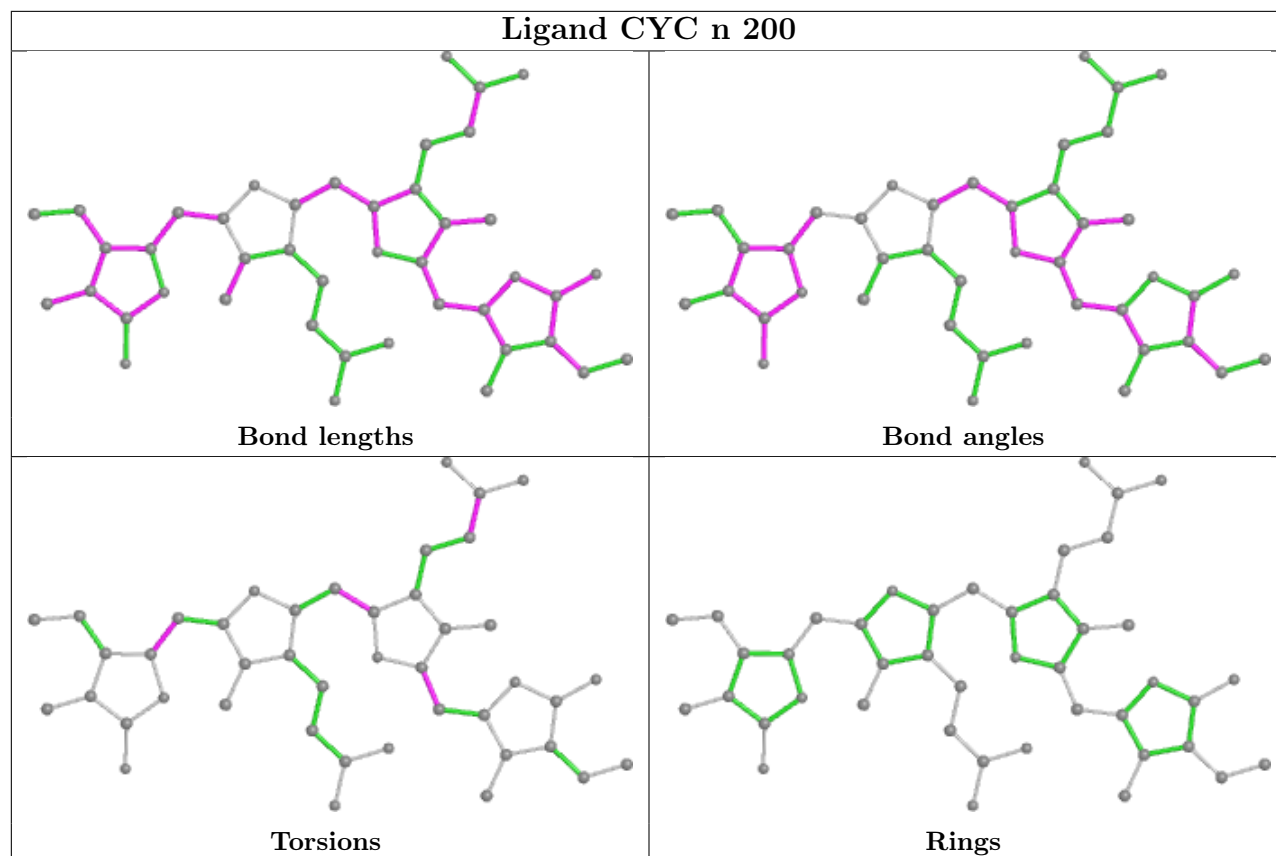


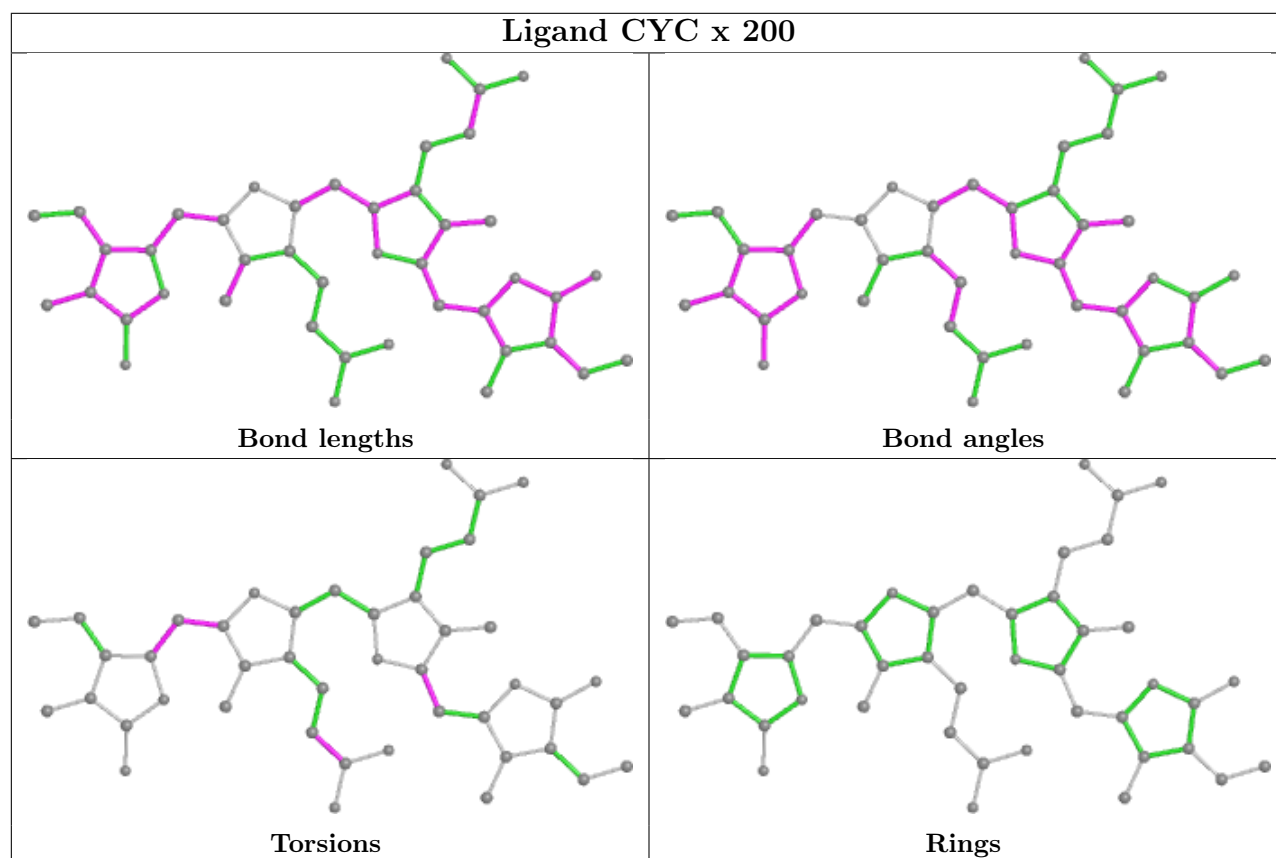
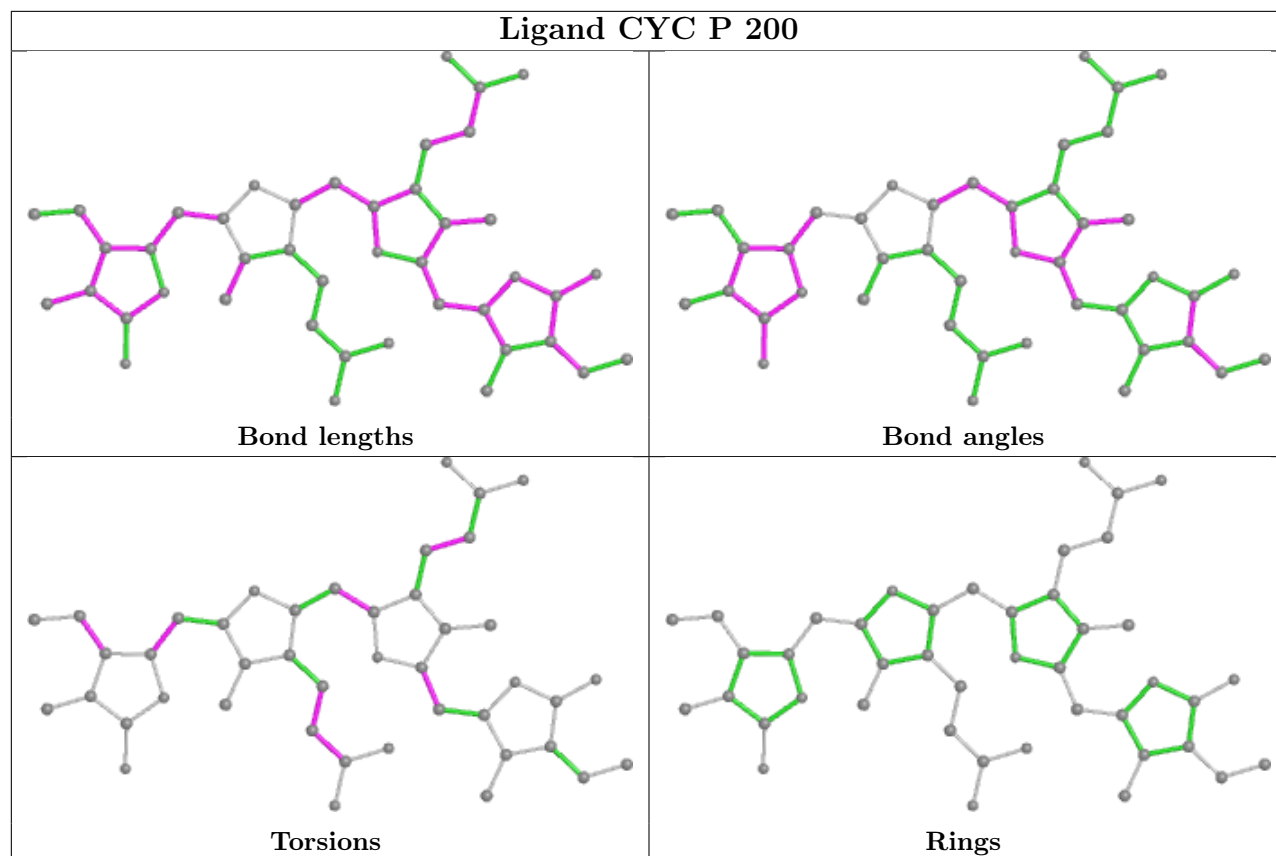


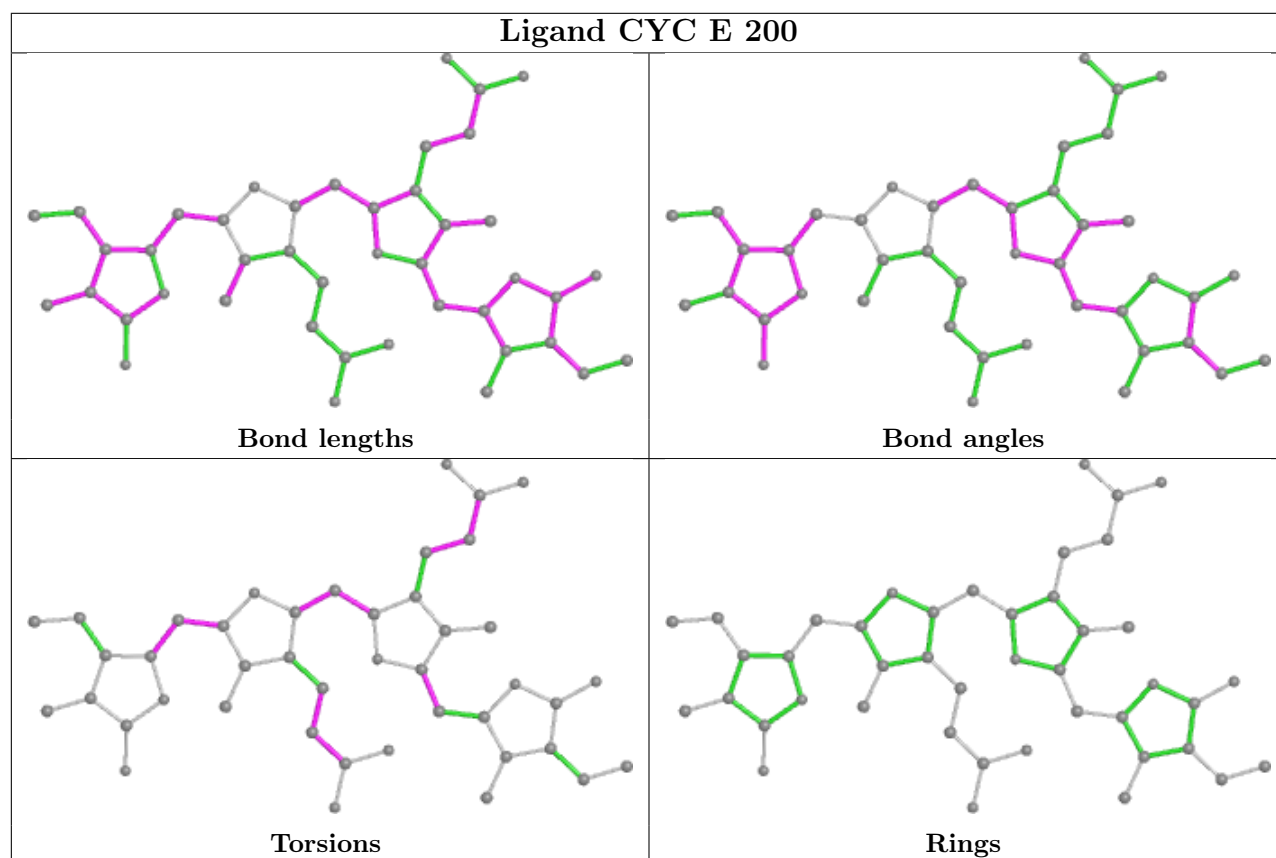
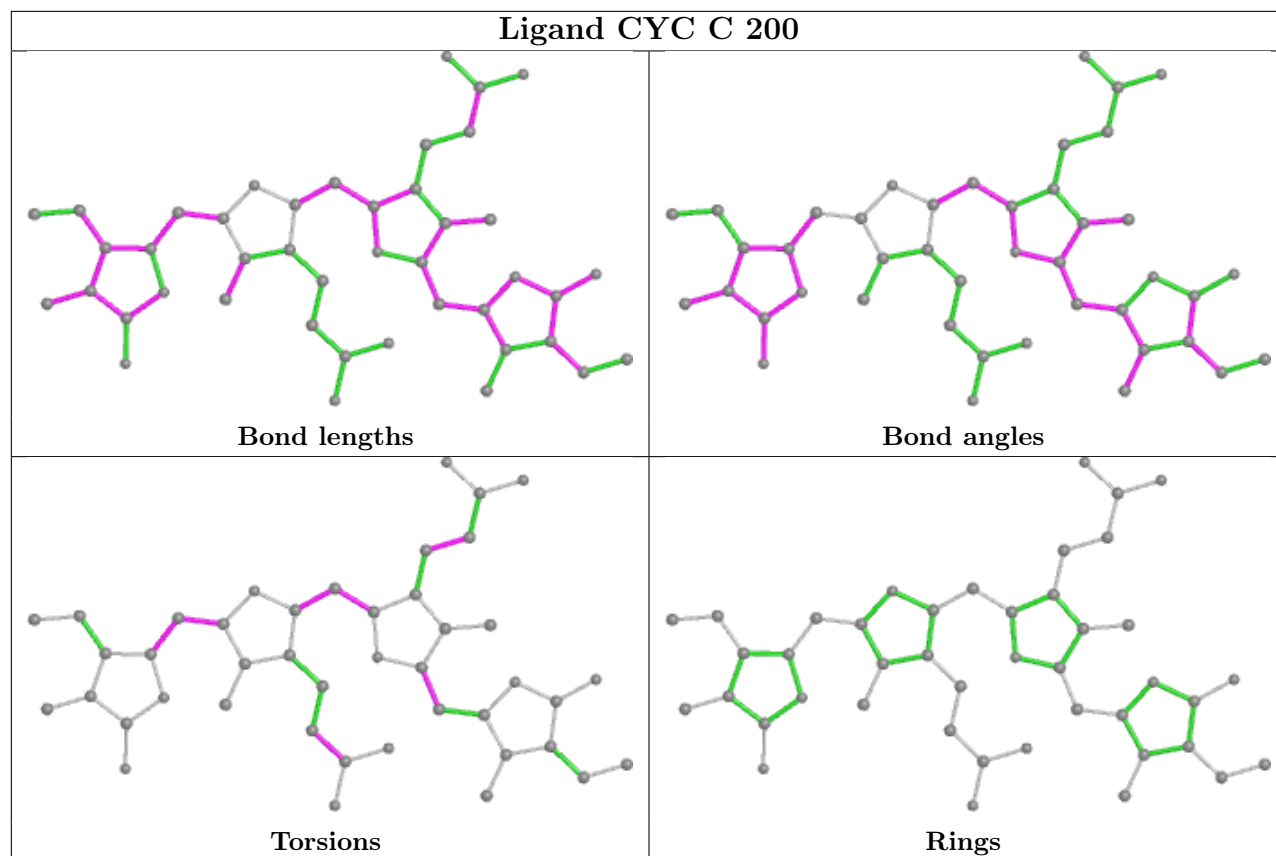


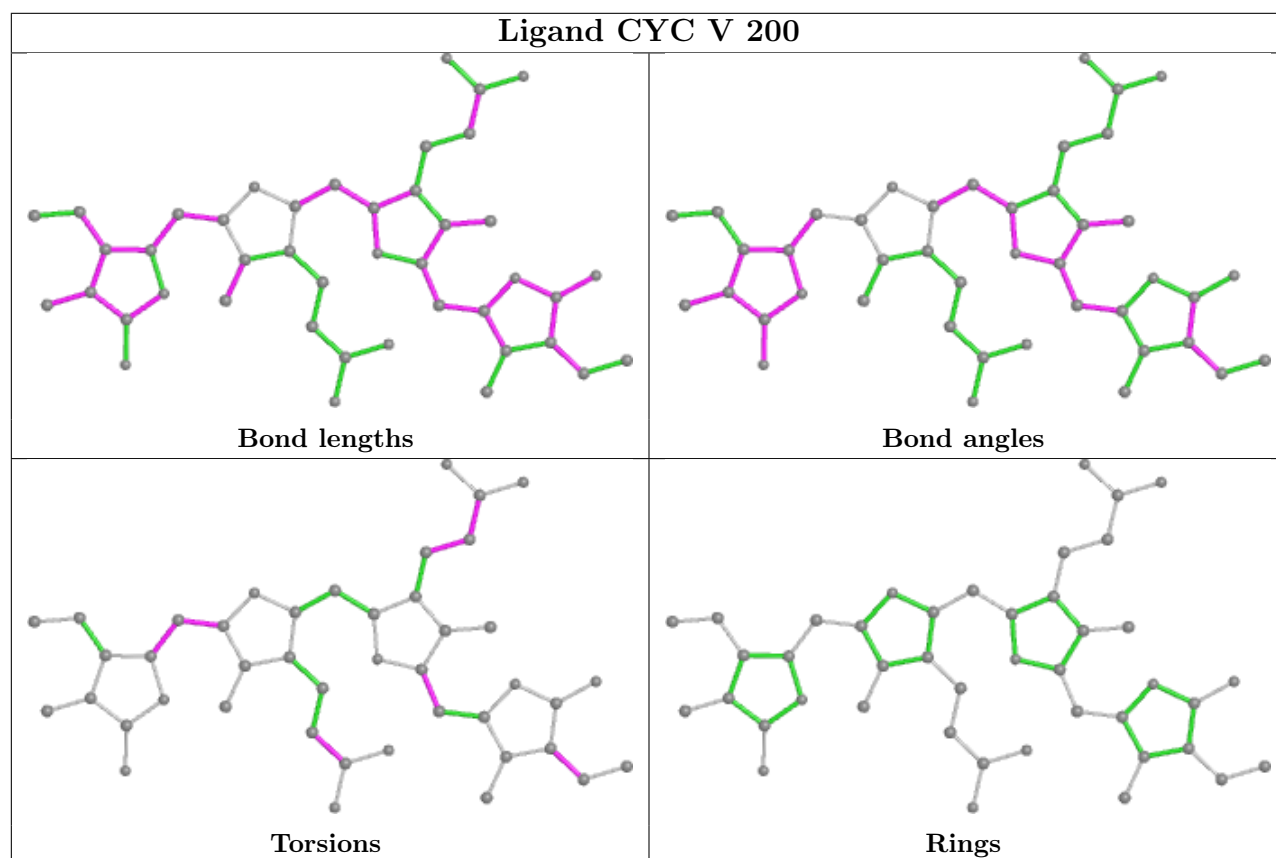
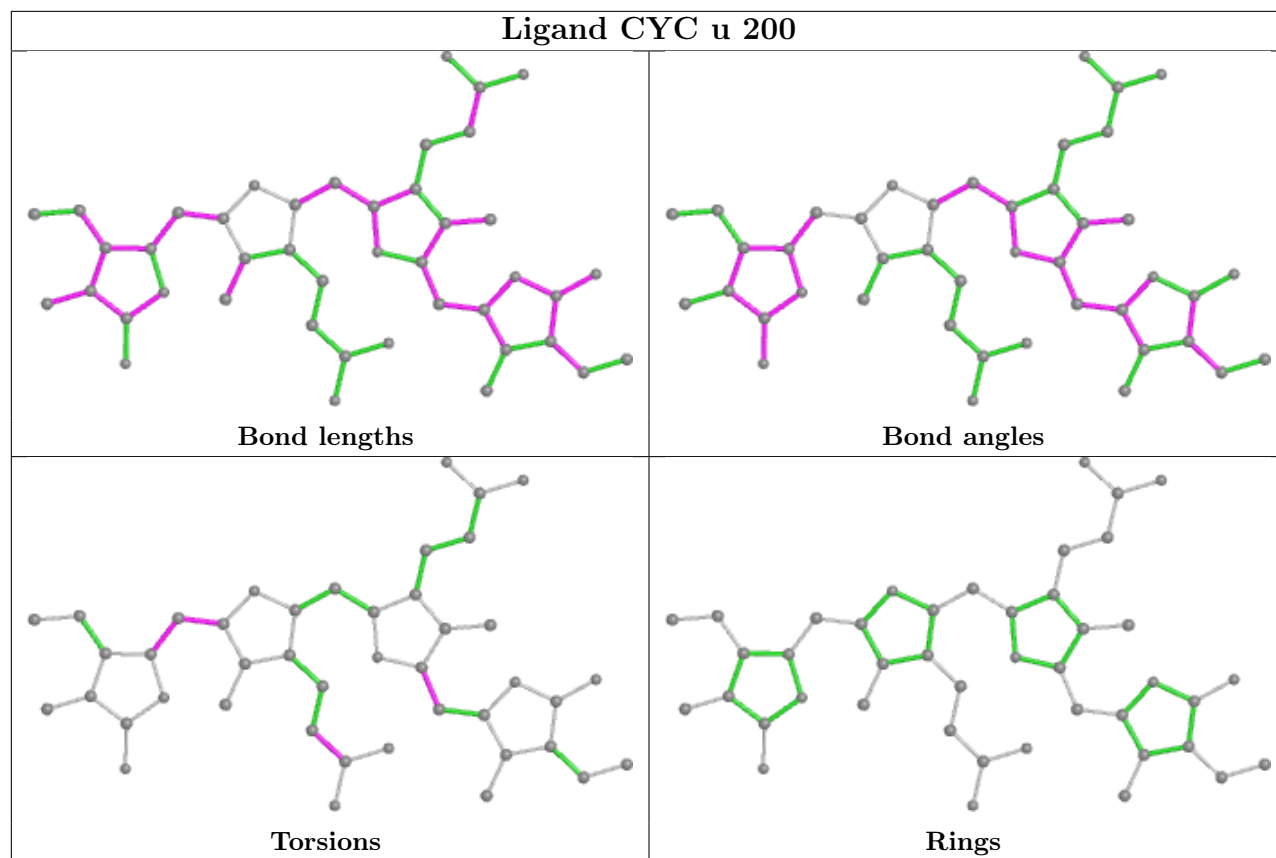


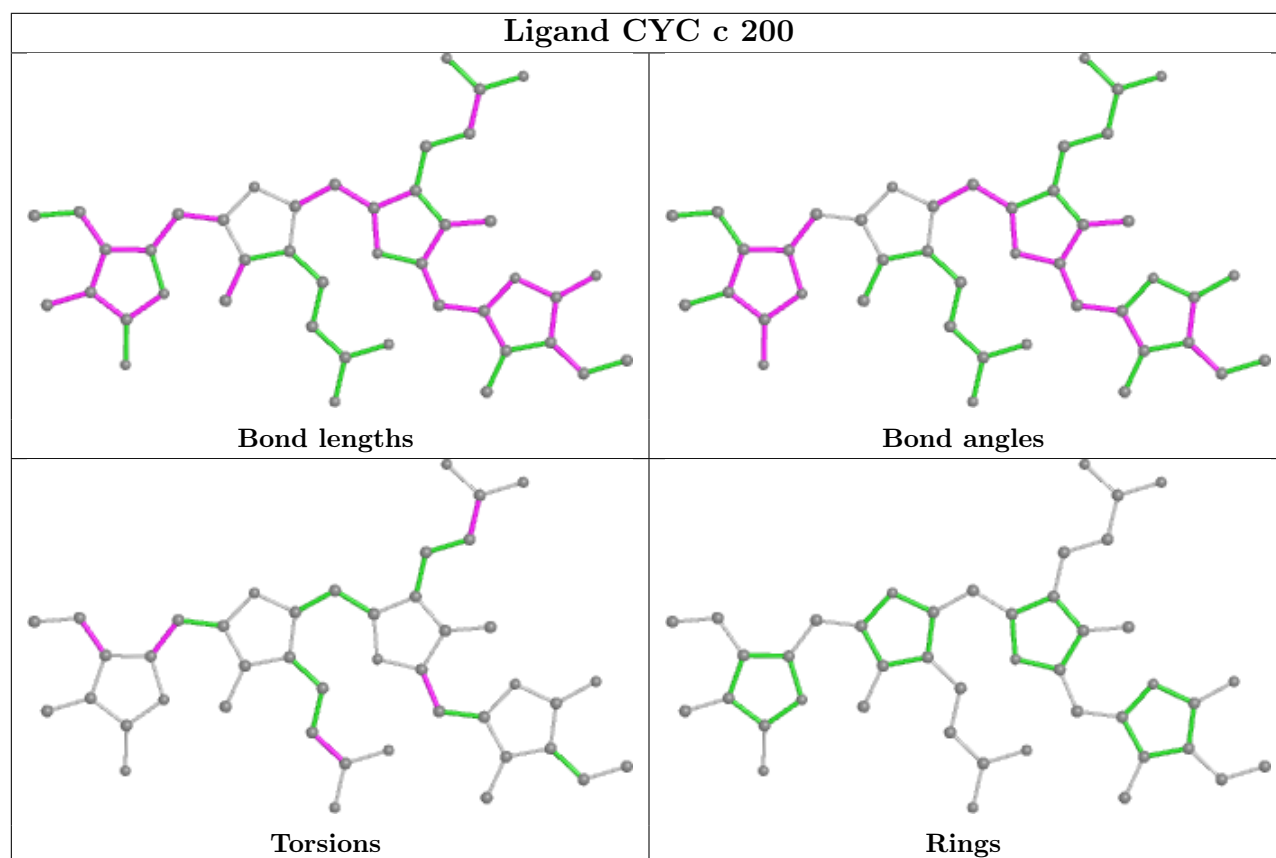
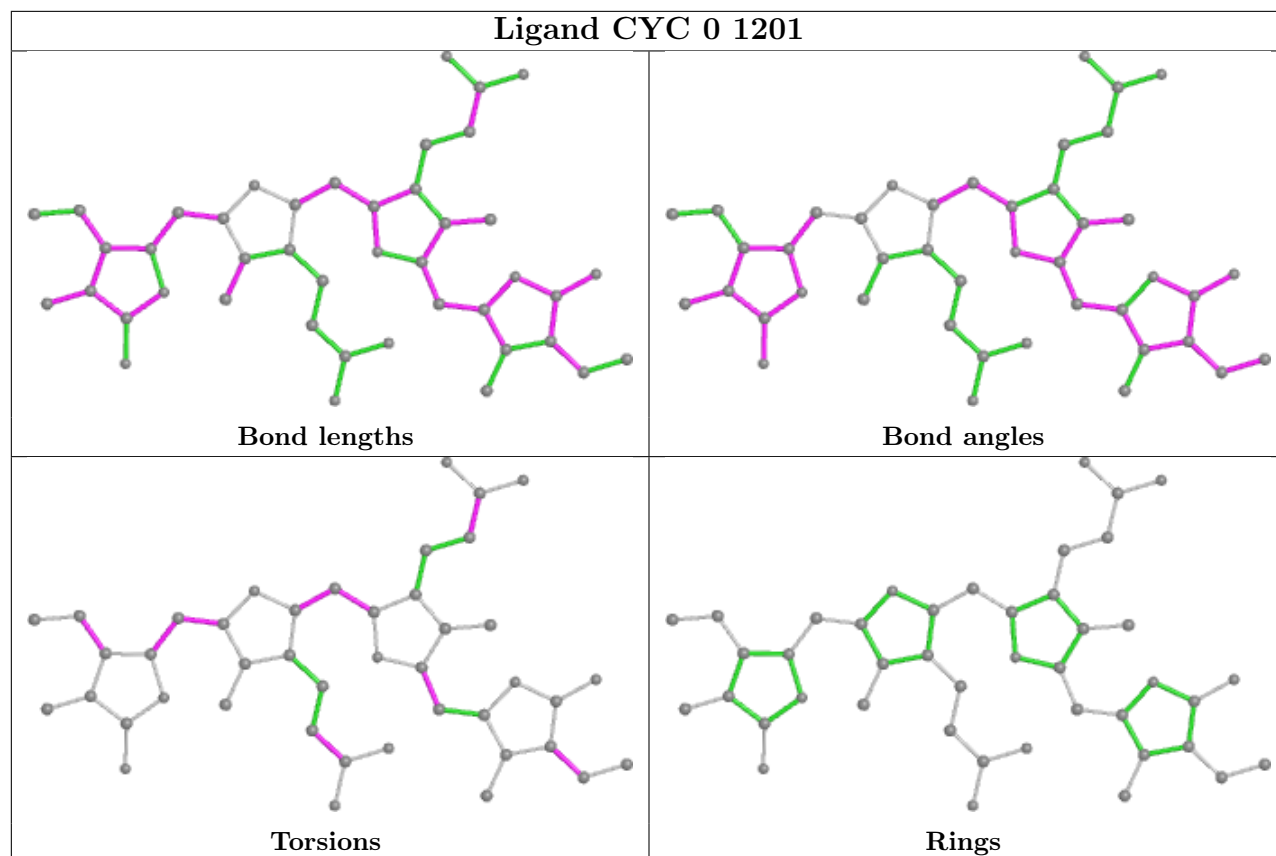


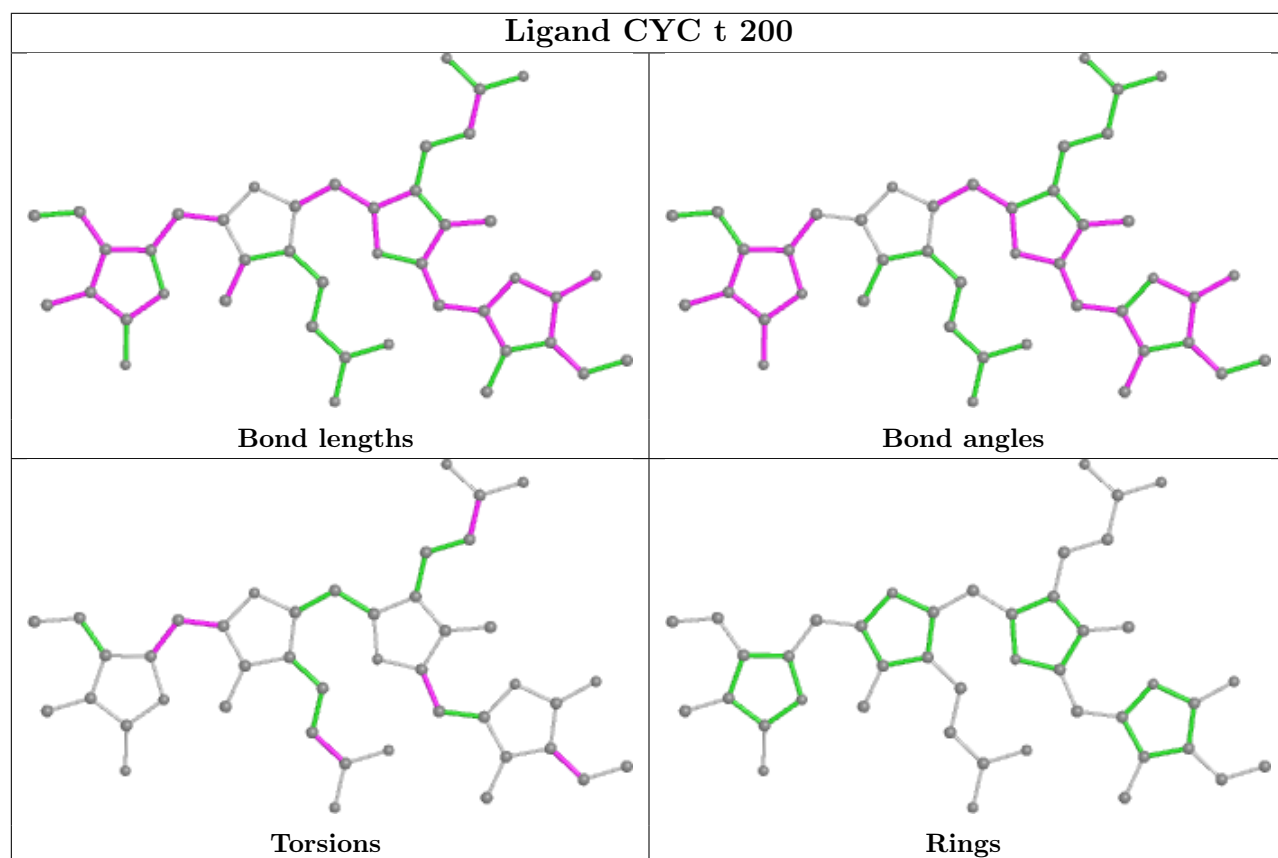
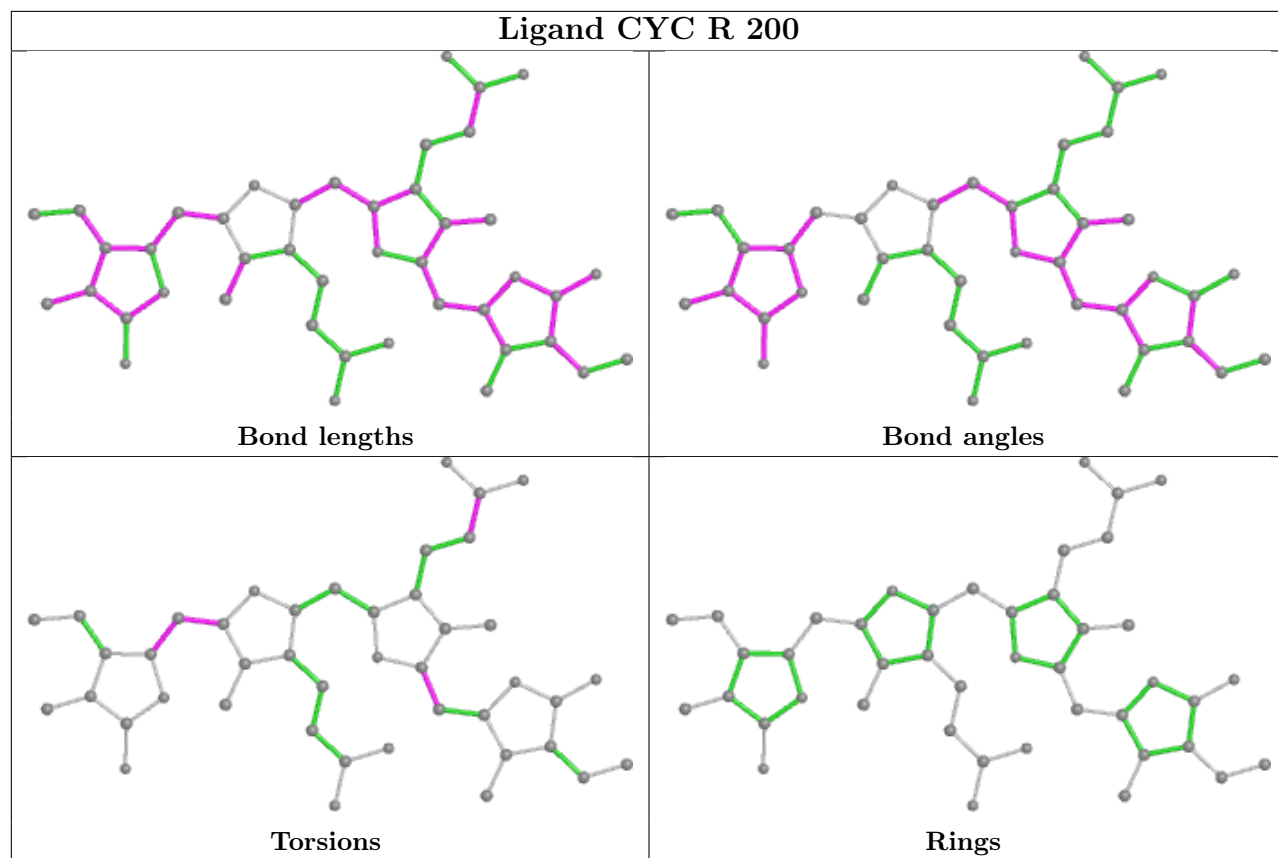


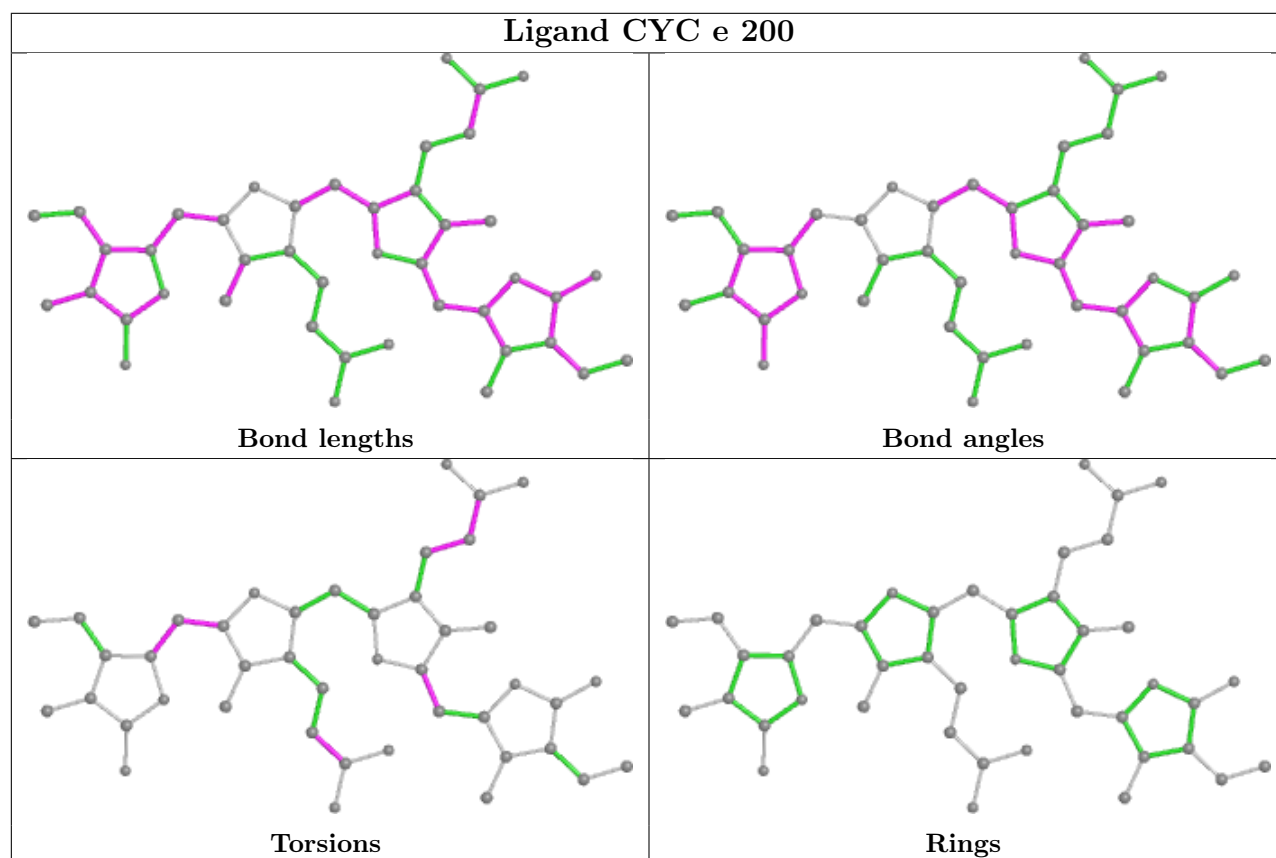
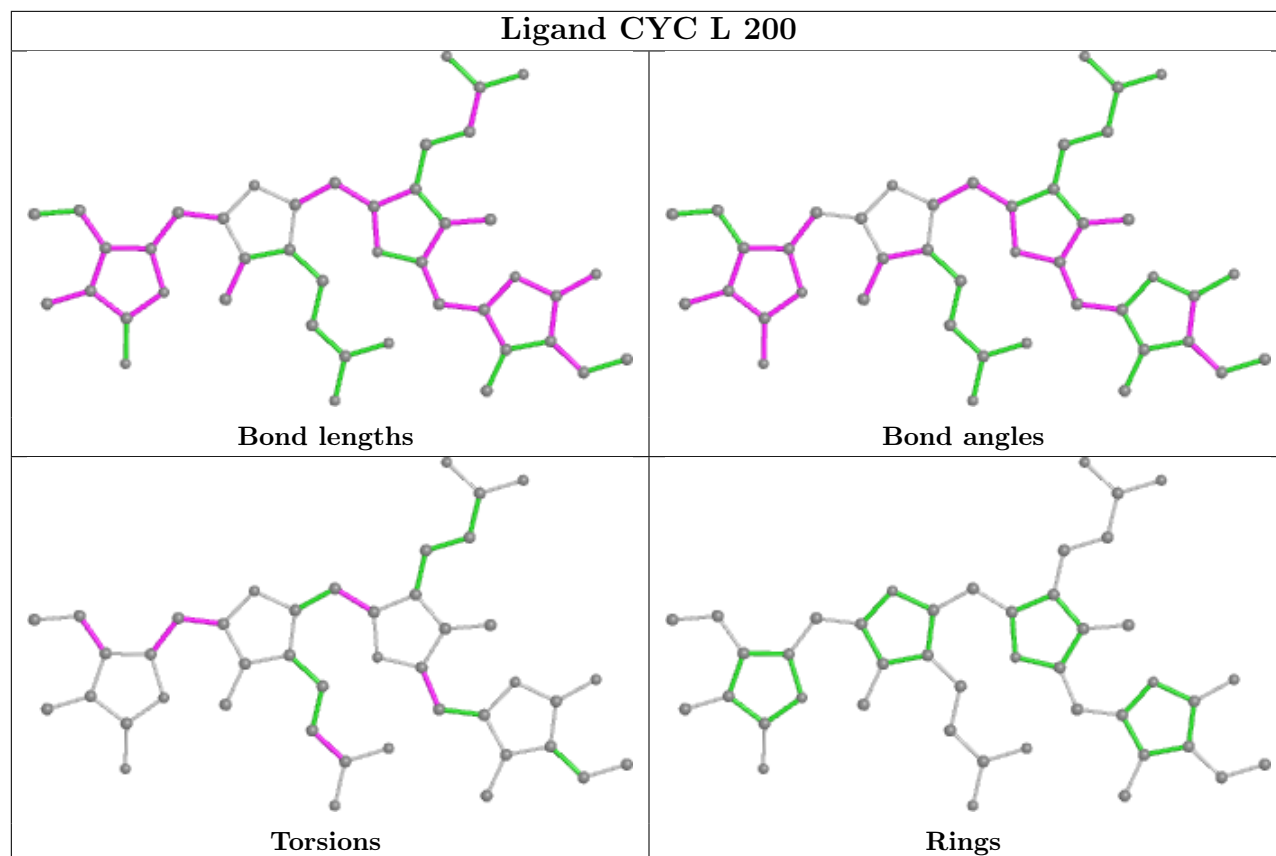


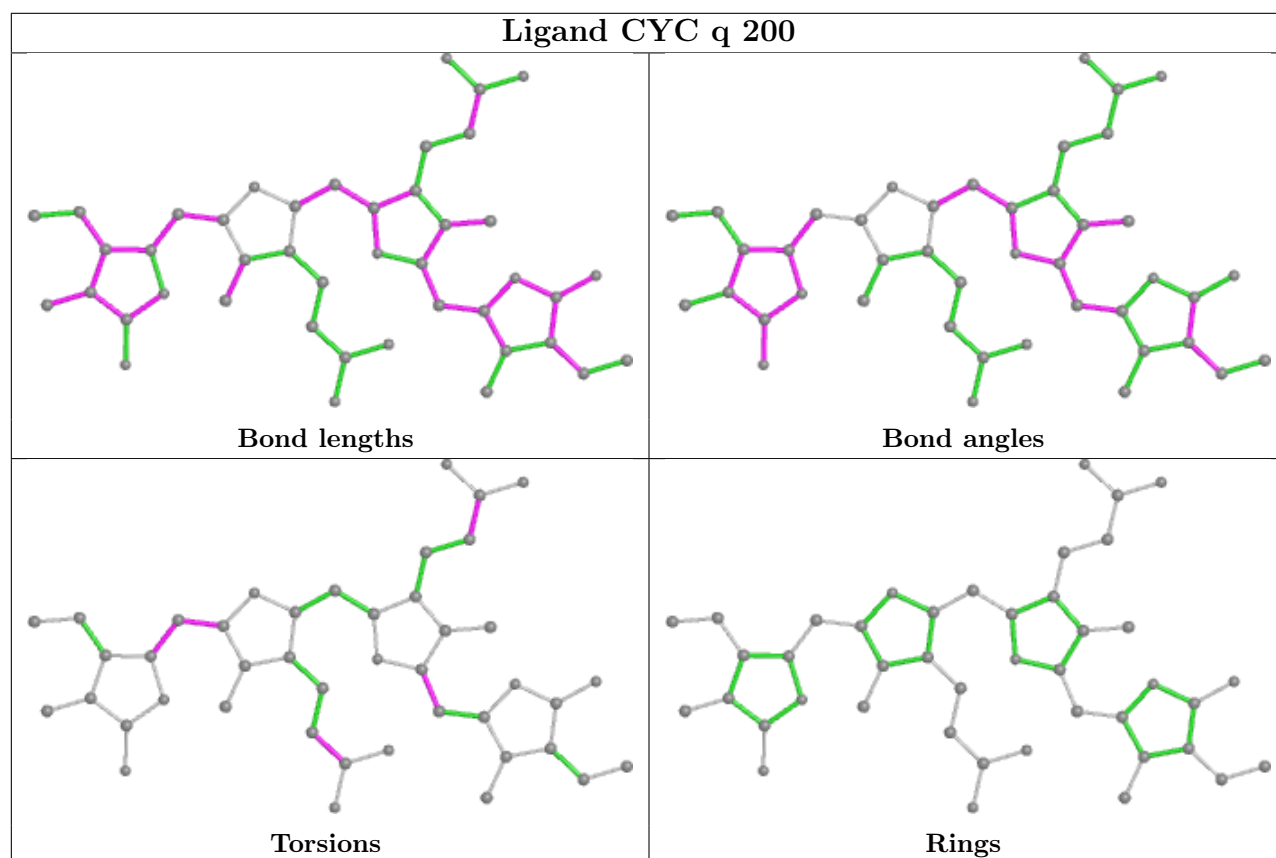
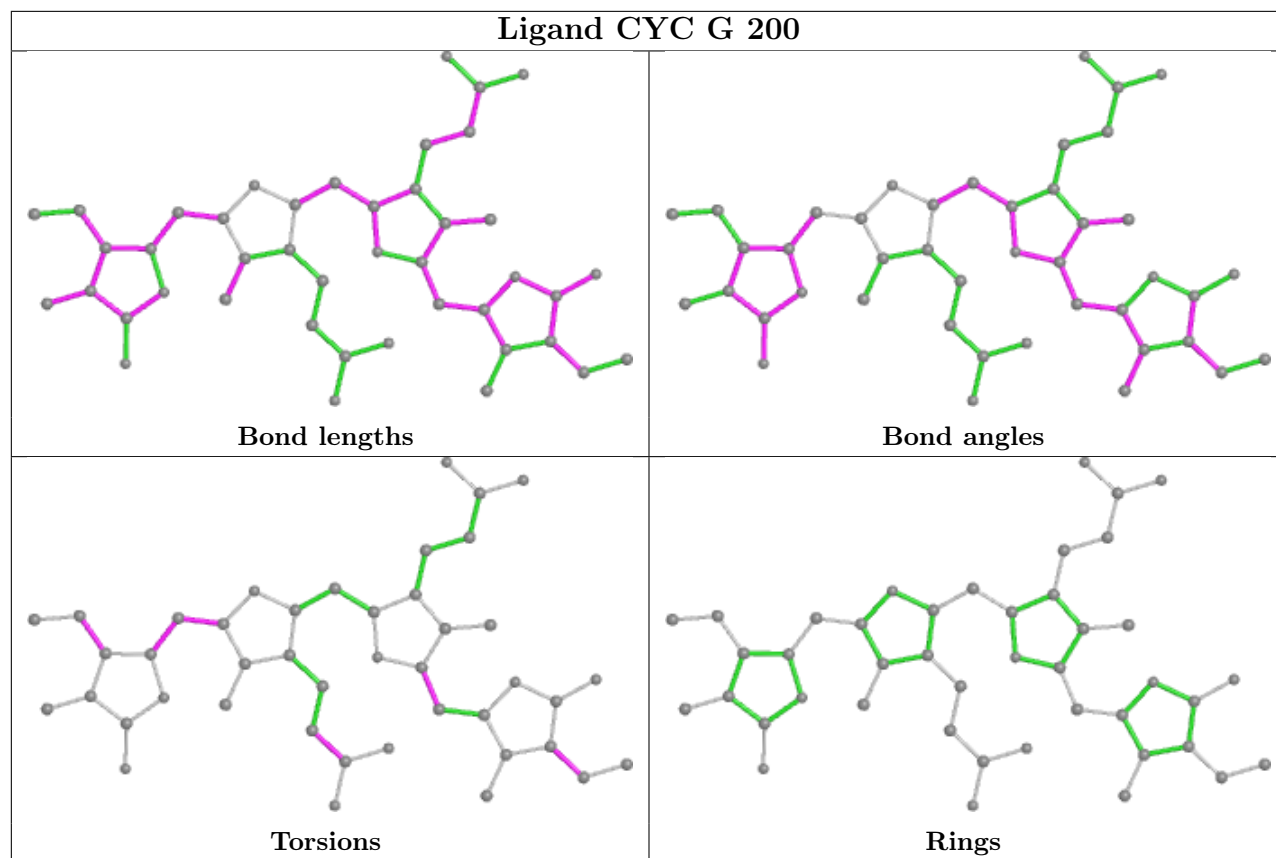


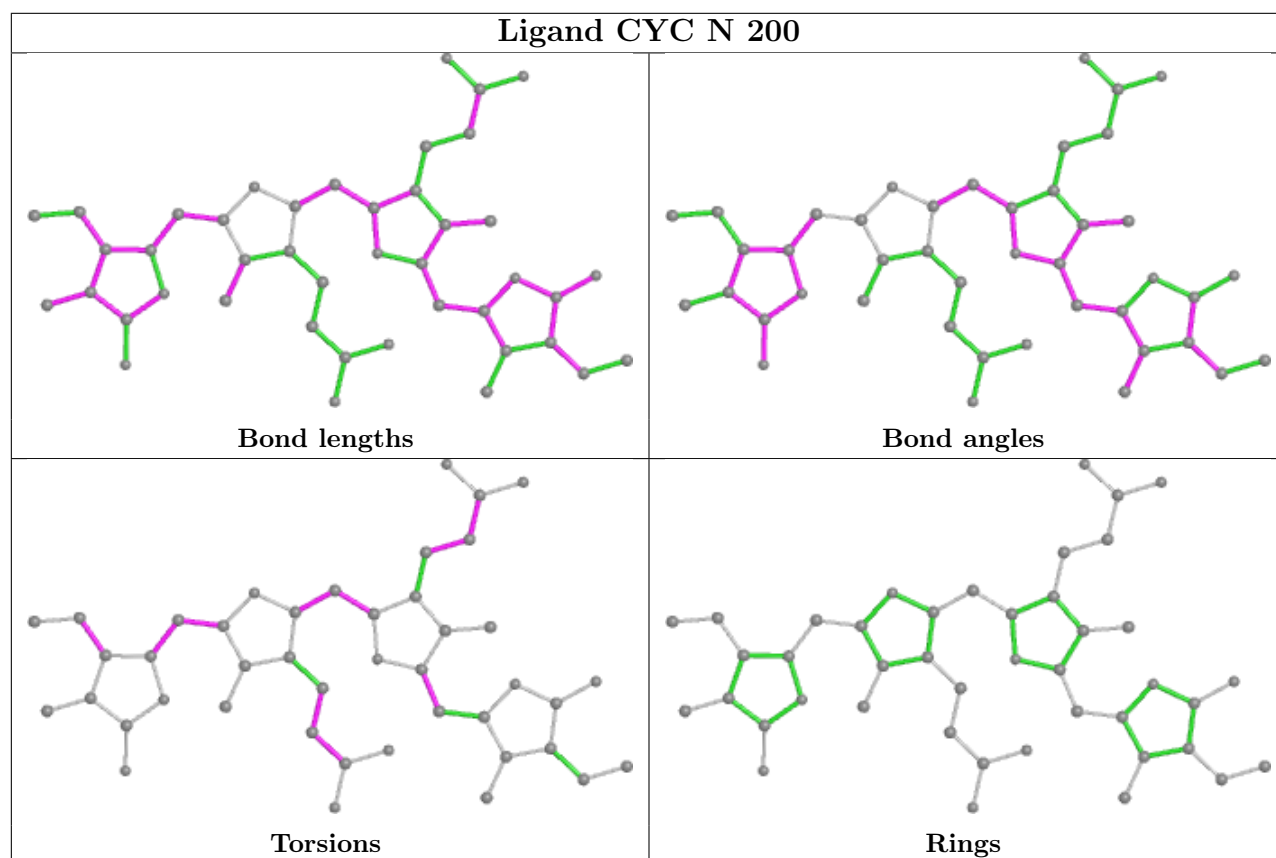
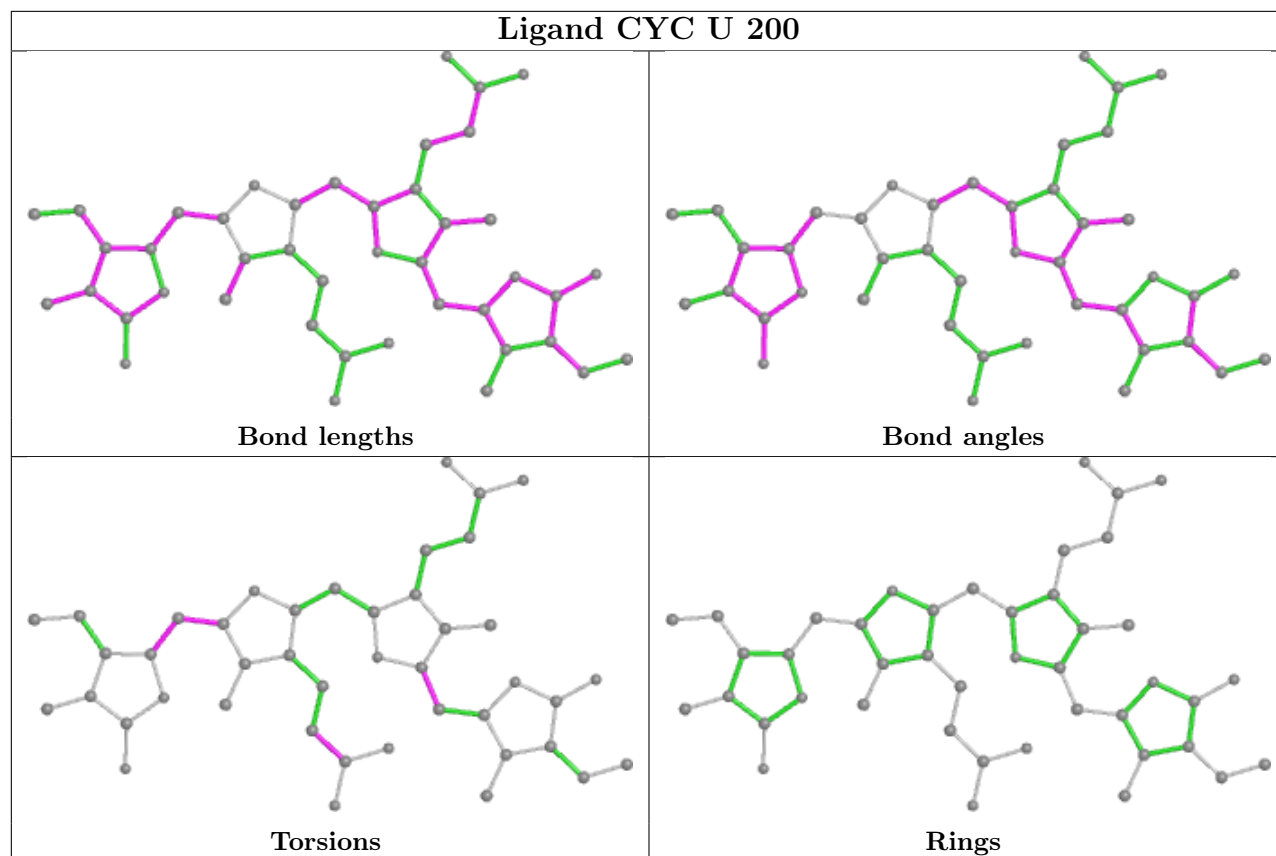


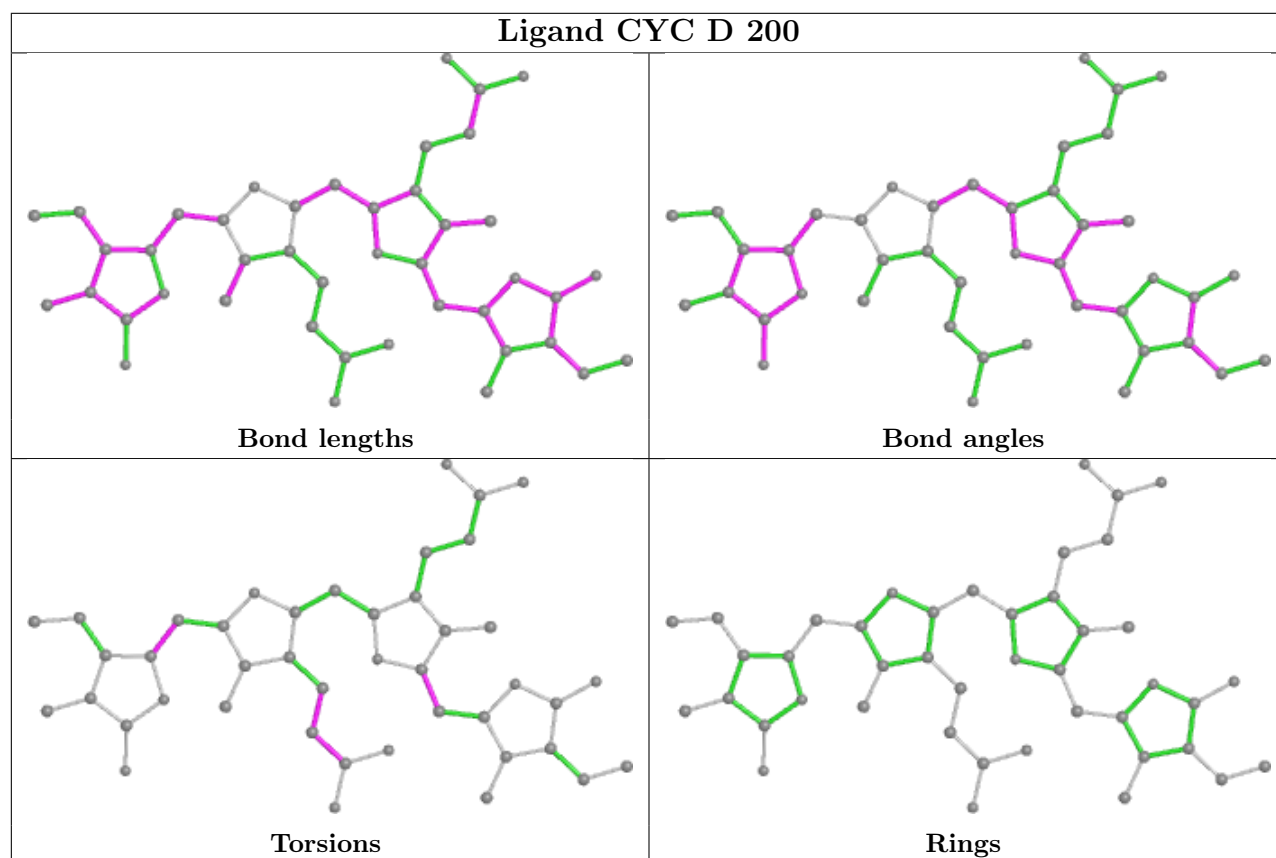
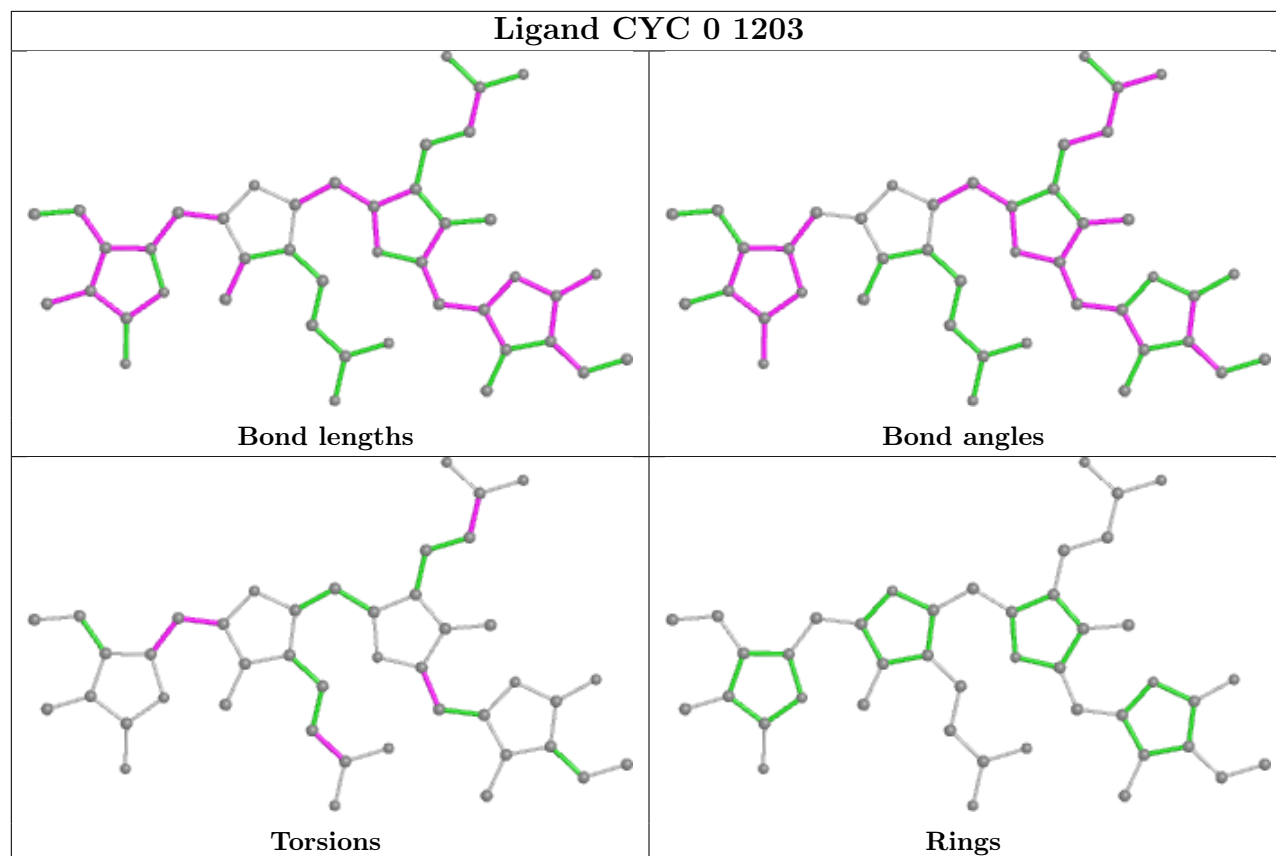


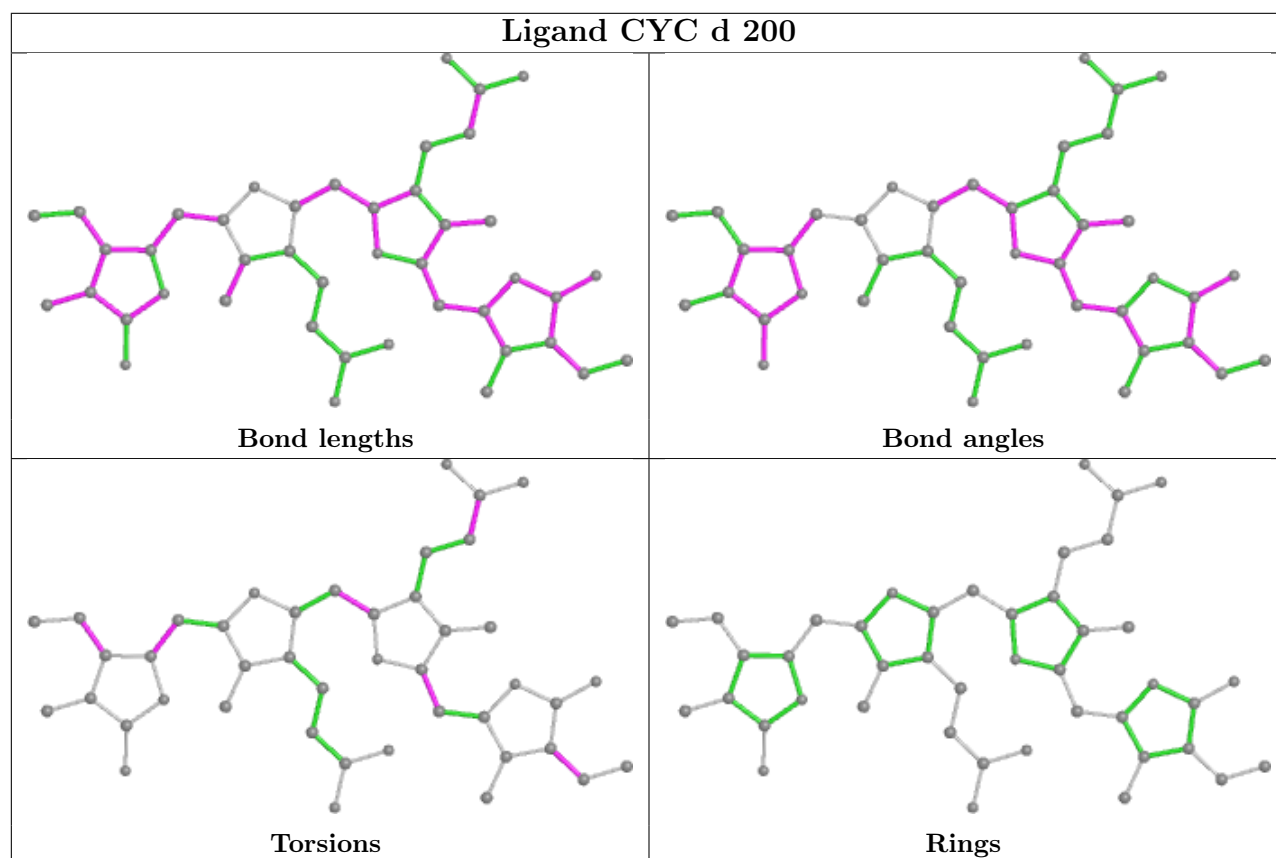
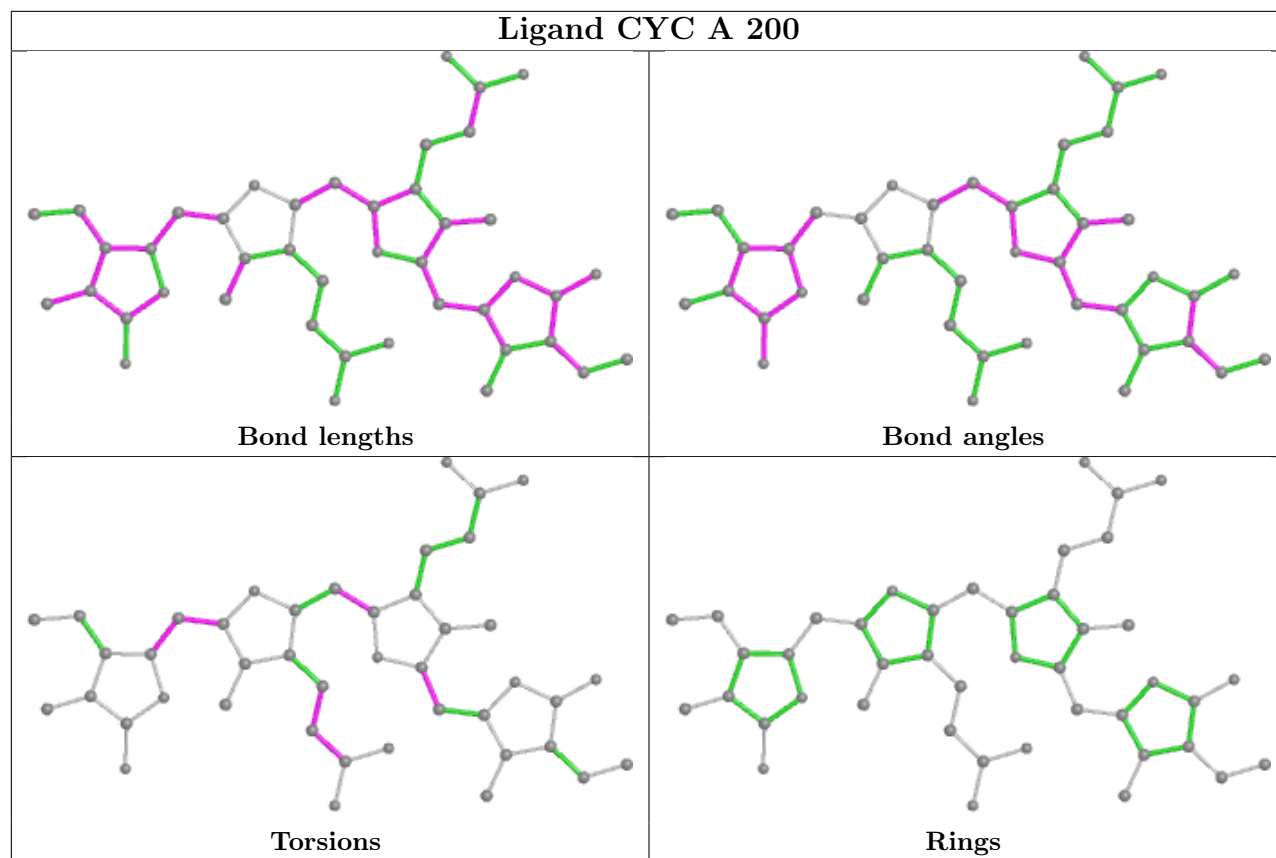


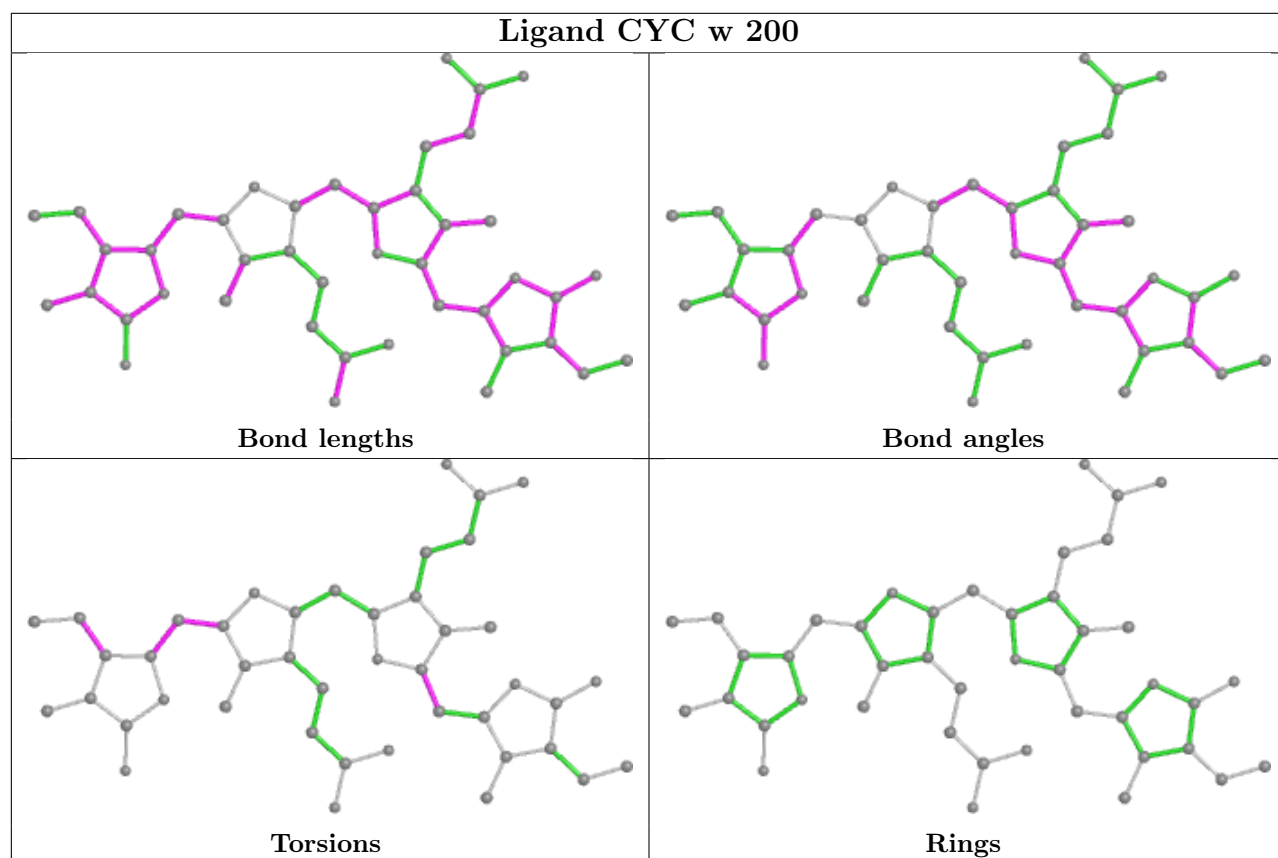
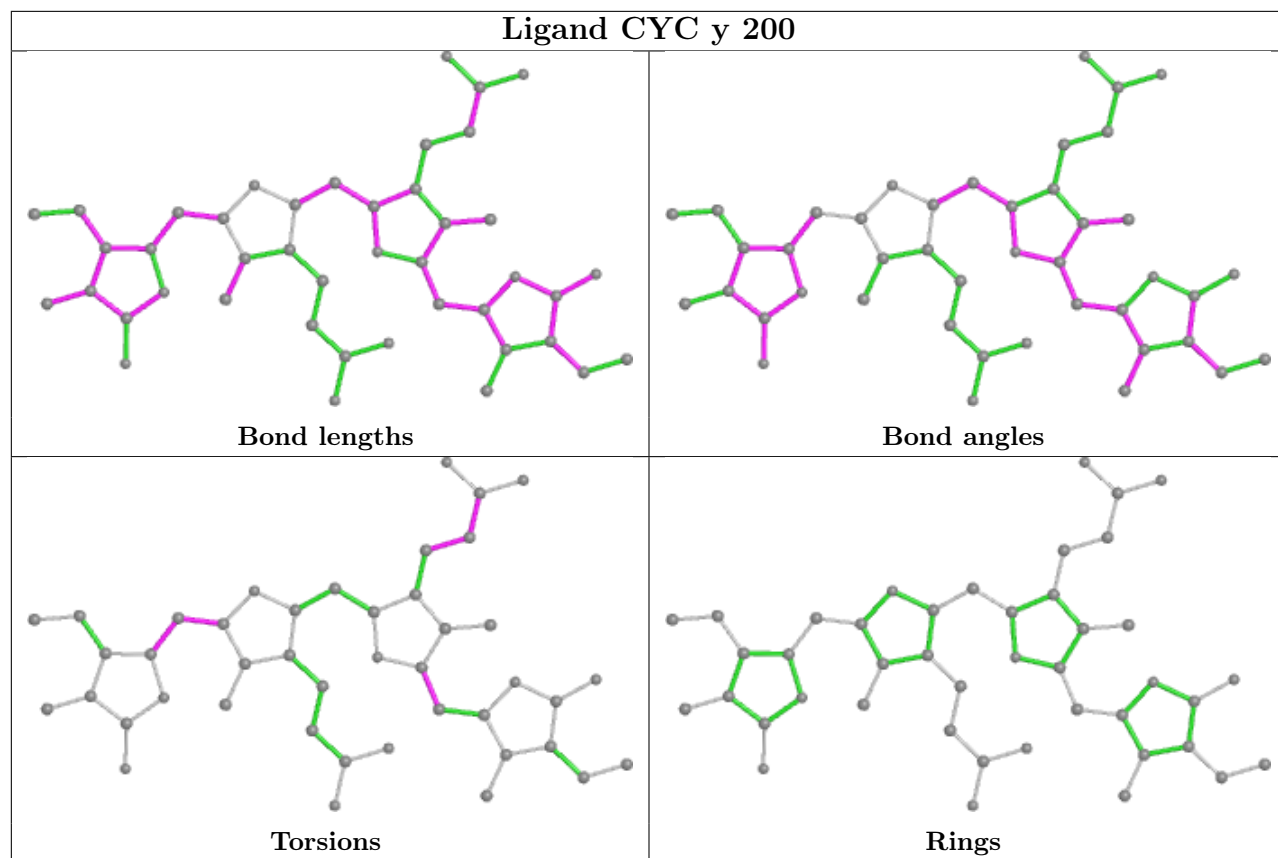


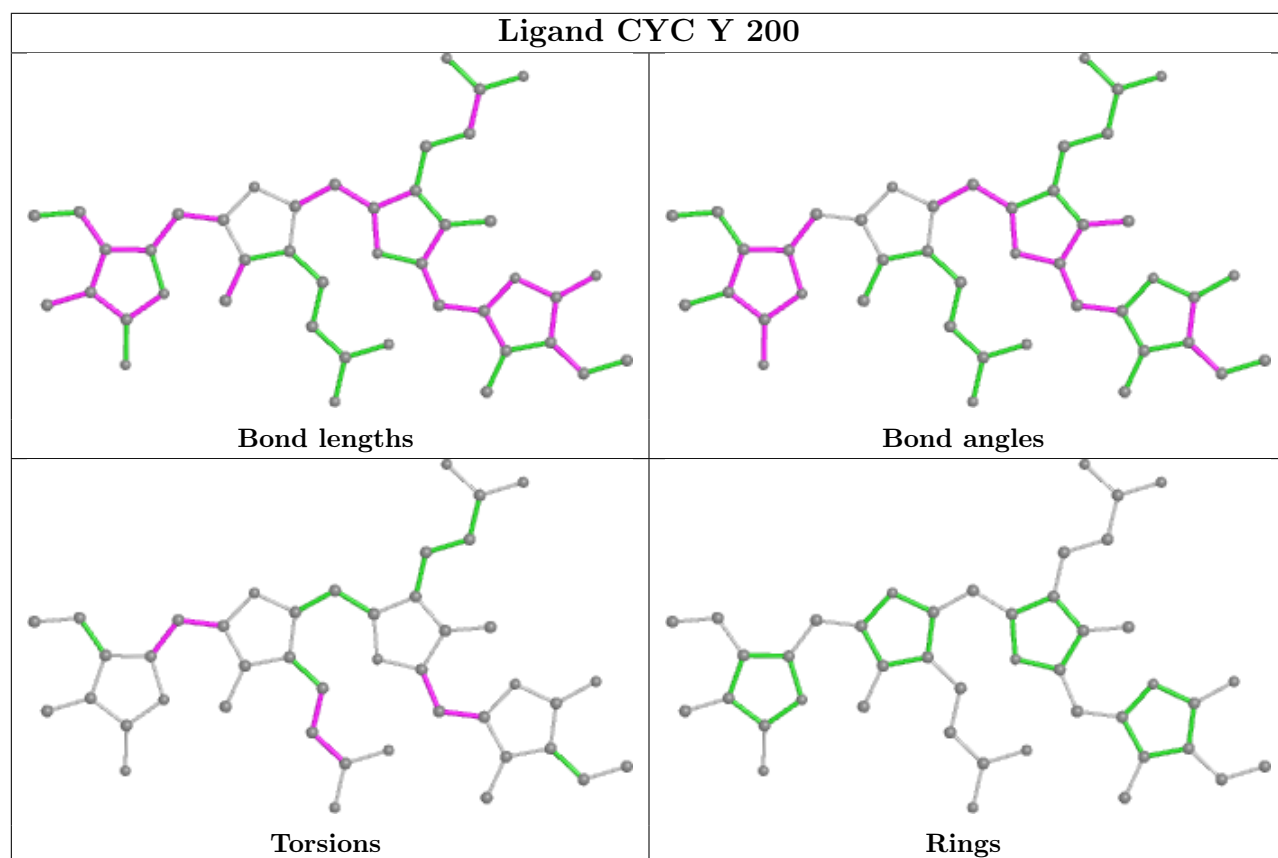
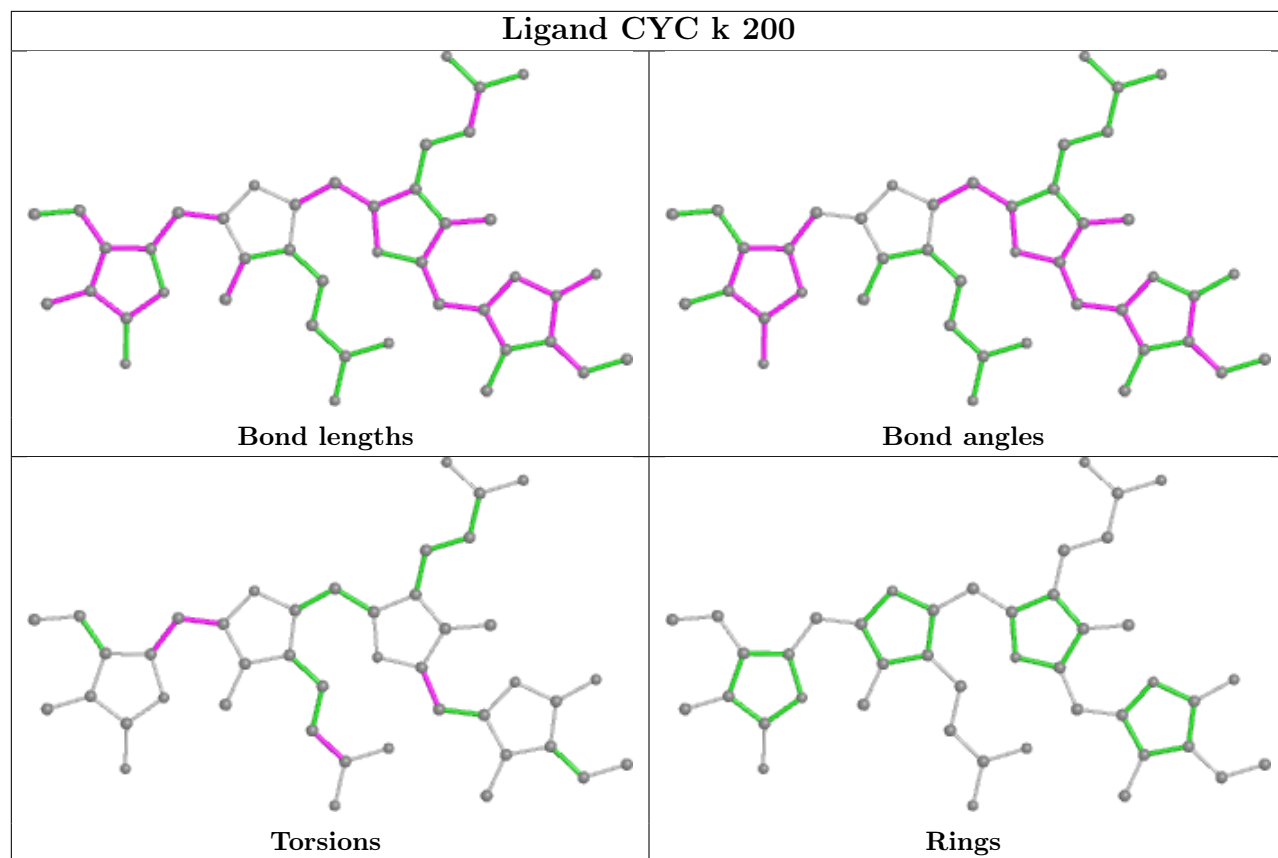


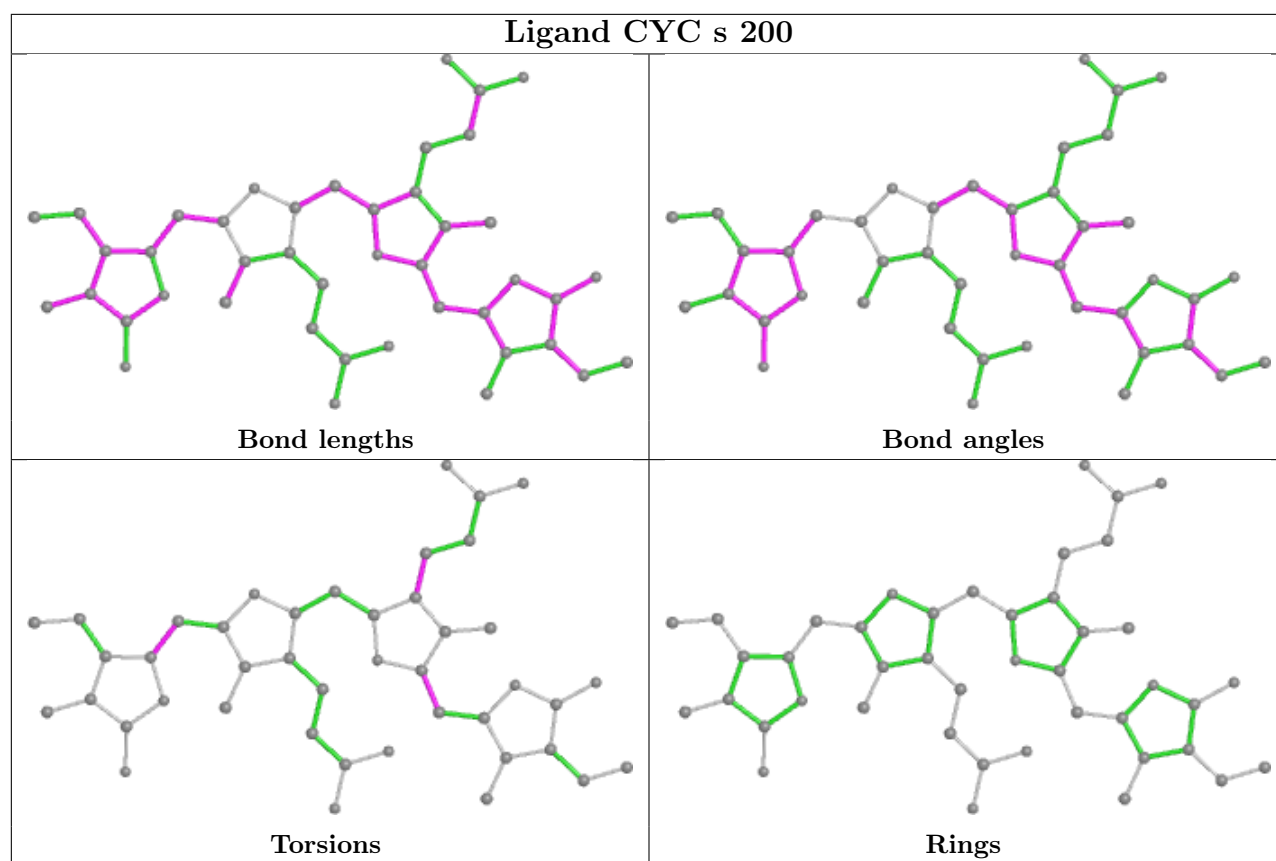












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

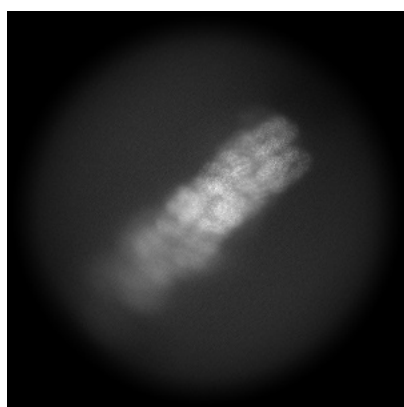
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35566. These allow visual inspection of the internal detail of the map and identification of artifacts.

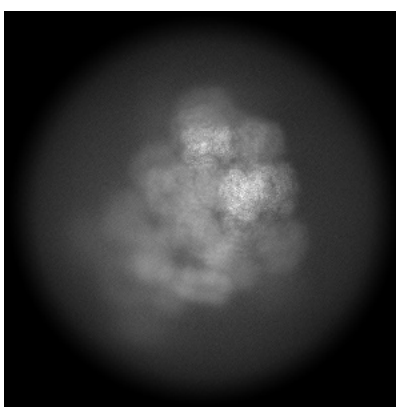
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

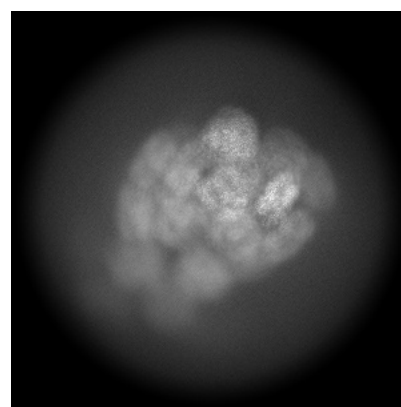
6.1.1 Primary map



X



Y

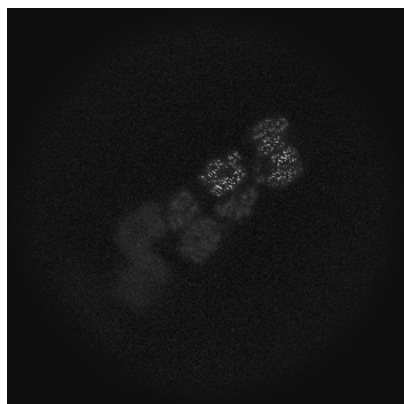


Z

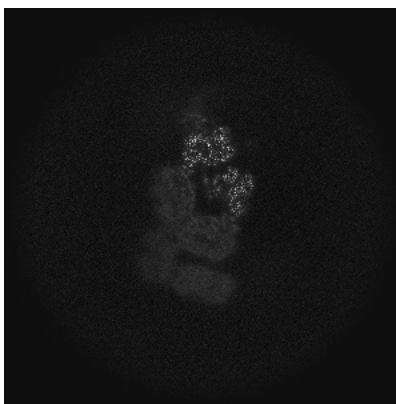
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

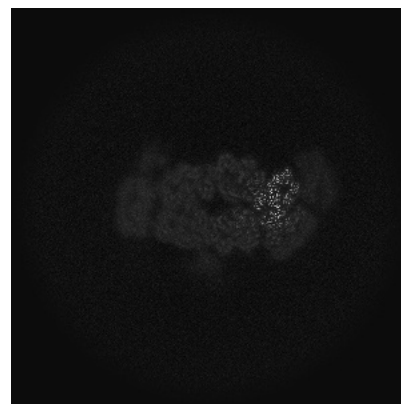
6.2.1 Primary map



X Index: 340



Y Index: 340

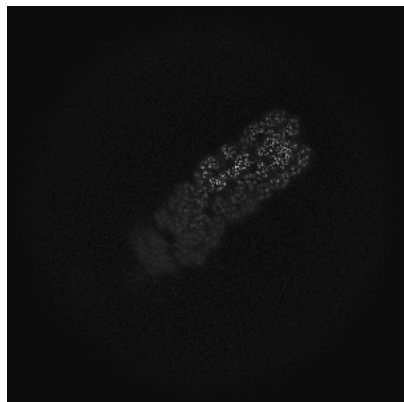


Z Index: 340

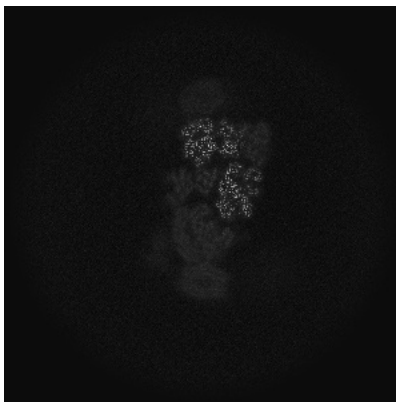
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

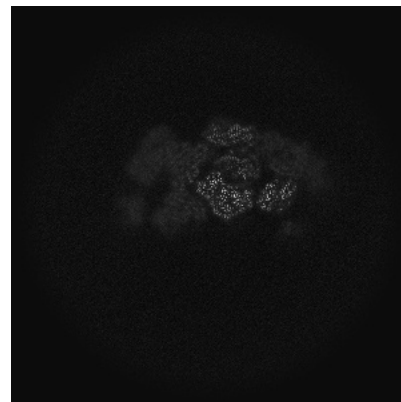
6.3.1 Primary map



X Index: 379



Y Index: 361

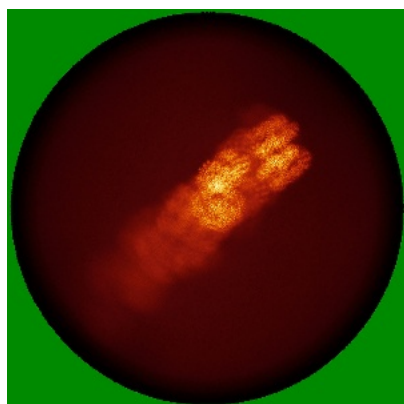


Z Index: 383

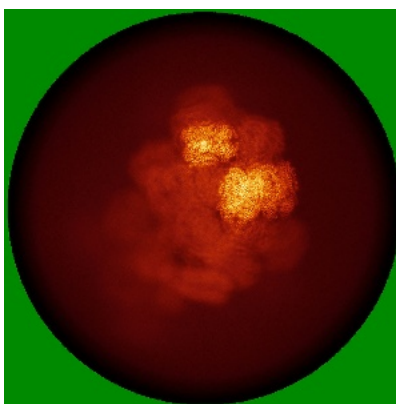
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

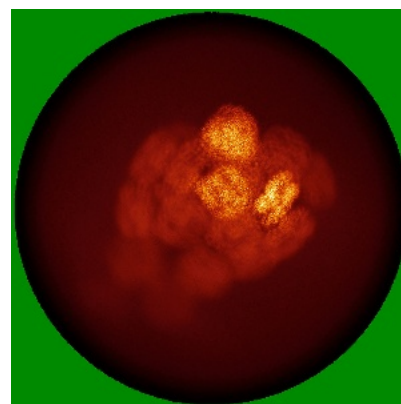
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

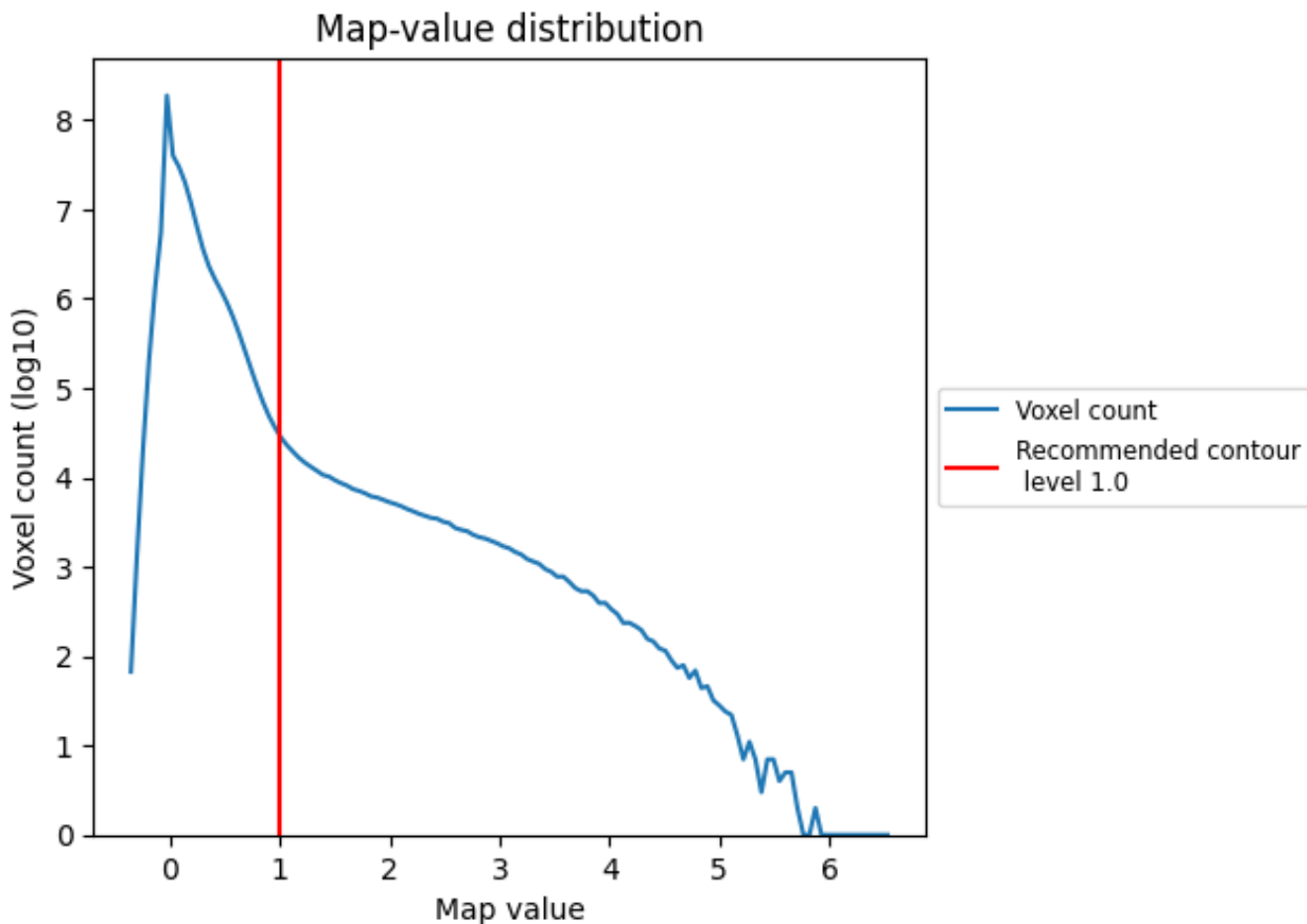
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

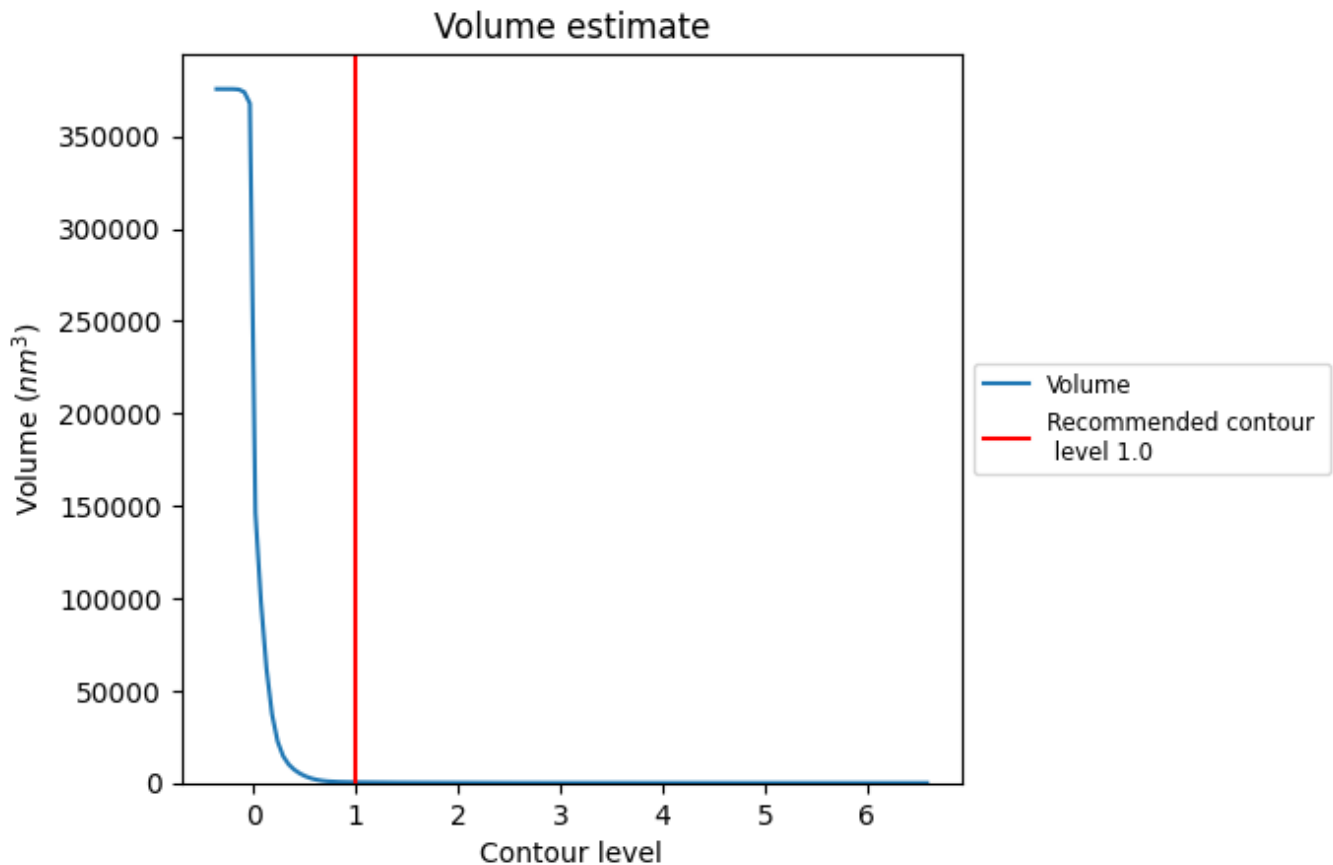
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

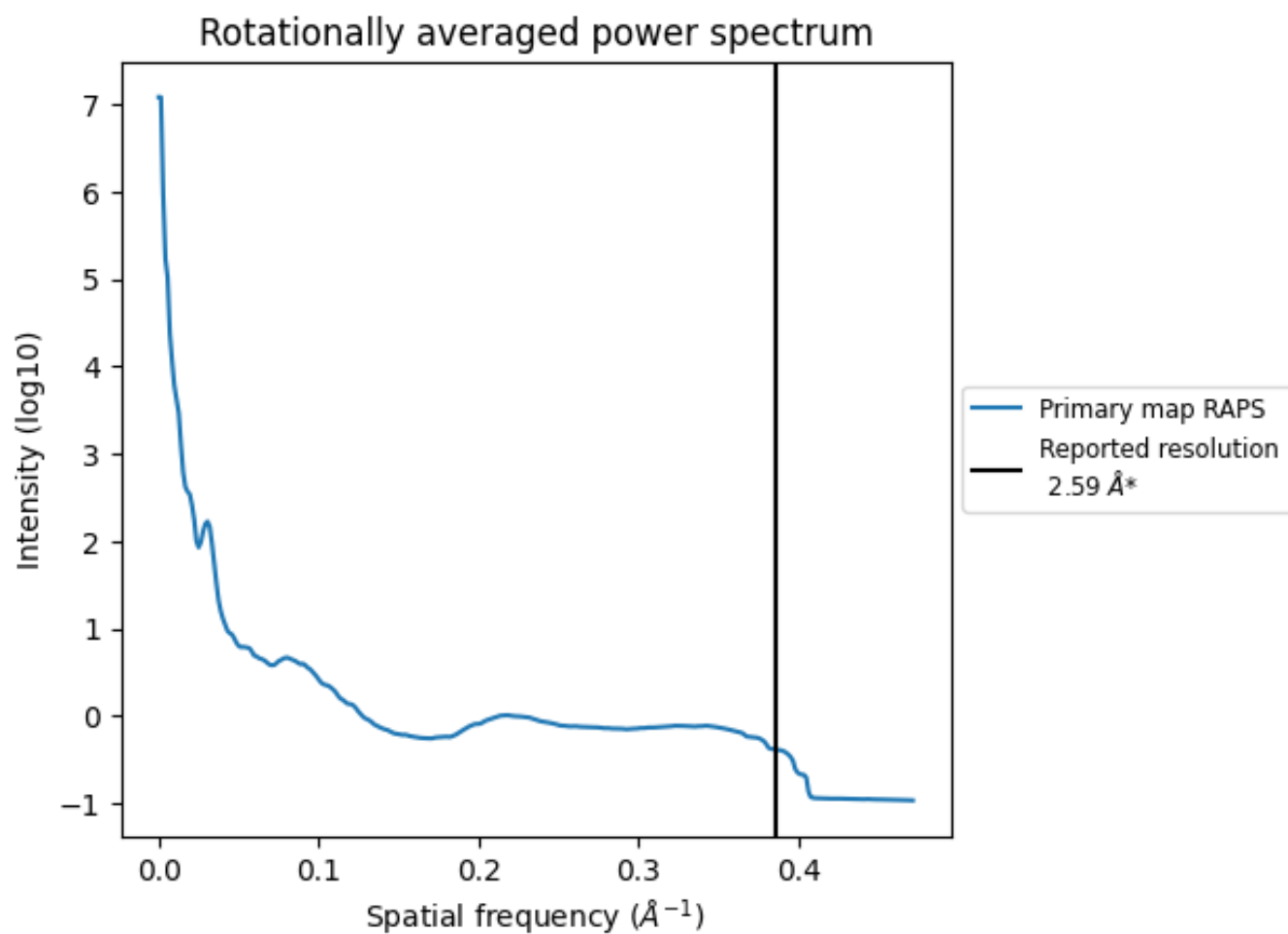
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 357 nm^3 ; this corresponds to an approximate mass of 322 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 0.386 \AA^{-1}

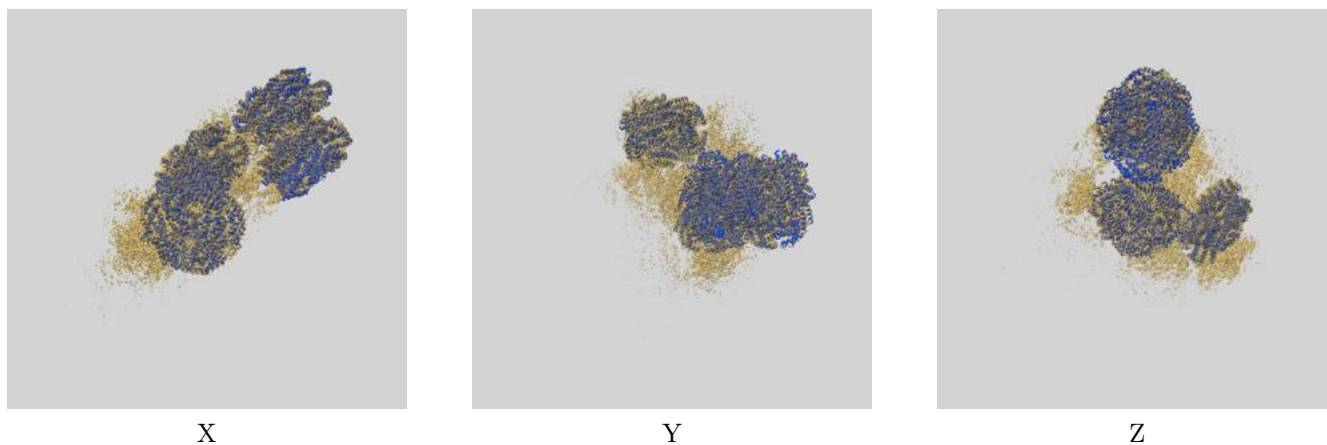
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

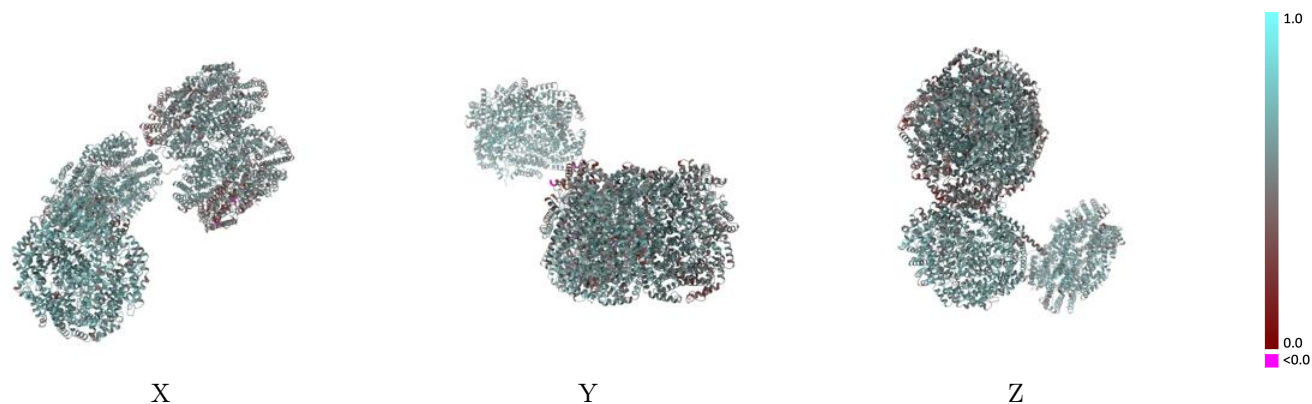
This section contains information regarding the fit between EMDB map EMD-35566 and PDB model 8IMJ. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



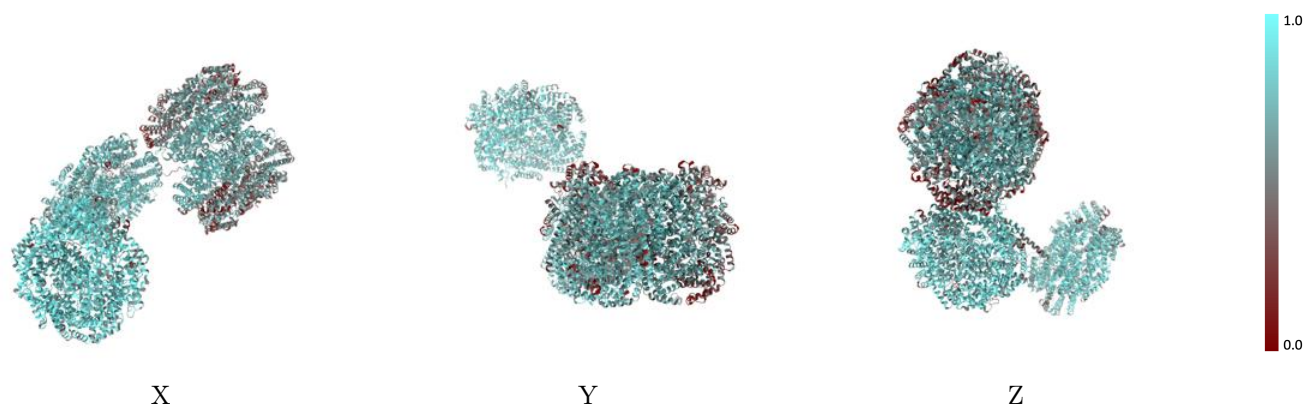
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



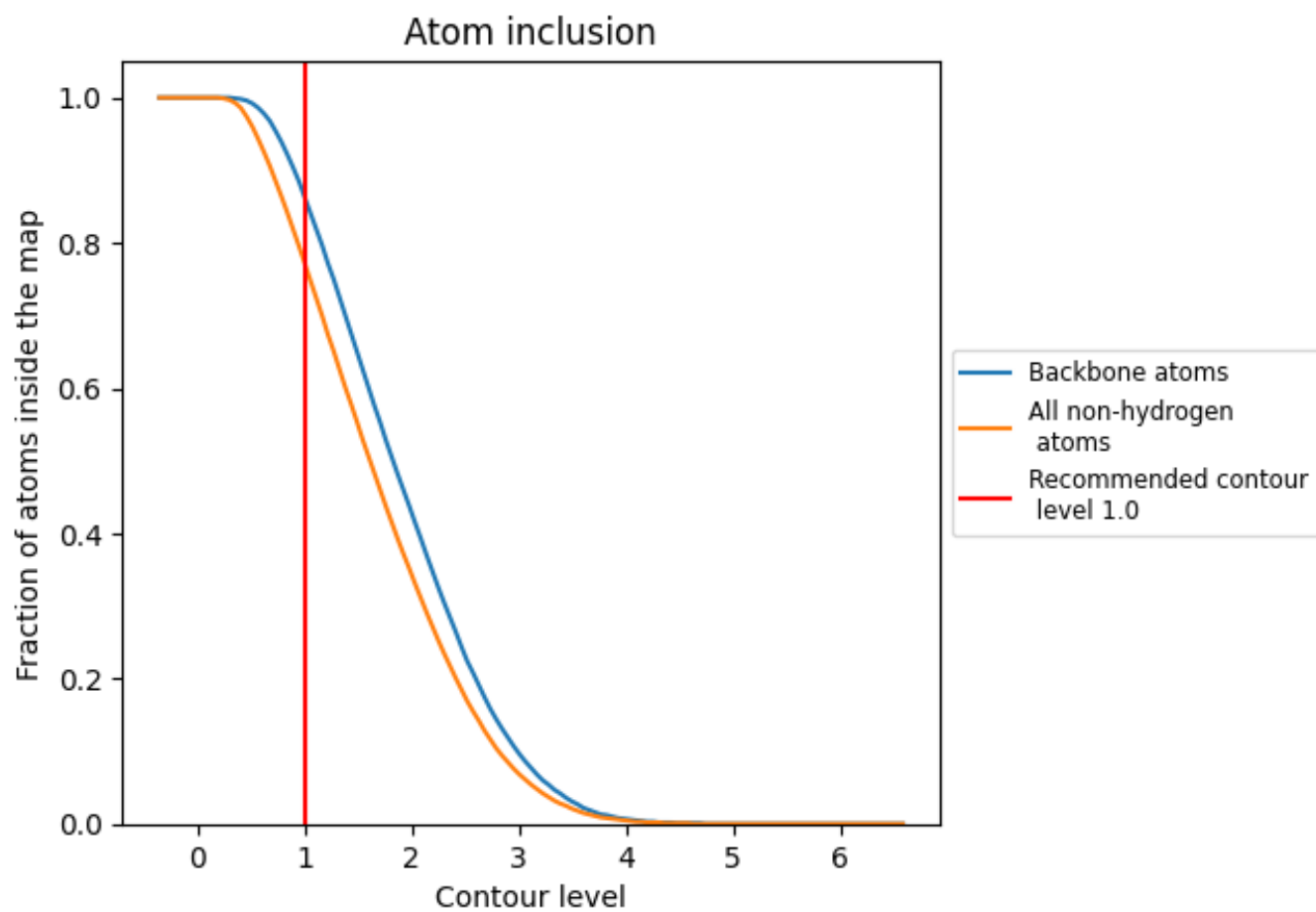
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 77% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7710	 0.5880
0	 0.8190	 0.6170
A	 0.5440	 0.5210
B	 0.7770	 0.5740
C	 0.3020	 0.4110
D	 0.7300	 0.5540
E	 0.4590	 0.4610
G	 0.5690	 0.5350
H	 0.5890	 0.5100
I	 0.4570	 0.4460
J	 0.8190	 0.5890
K	 0.8460	 0.6090
L	 0.7790	 0.5880
M	 0.6800	 0.5500
N	 0.4180	 0.4150
O	 0.7260	 0.5550
P	 0.5840	 0.5220
Q	 0.8200	 0.5910
R	 0.7440	 0.5770
S	 0.8250	 0.5970
T	 0.6220	 0.5170
U	 0.6230	 0.5280
V	 0.5760	 0.5080
W	 0.8720	 0.6210
X	 0.8660	 0.6150
Y	 0.8860	 0.6290
Z	 0.5330	 0.5270
a	 0.7800	 0.5910
b	 0.8870	 0.6280
c	 0.7850	 0.5900
d	 0.8800	 0.6360
e	 0.8250	 0.6110
f	 0.8790	 0.6390
g	 0.7850	 0.5970
h	 0.8470	 0.6240



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Chain	Atom inclusion	Q-score
i	 0.8650	 0.6390
j	 0.9150	 0.6600
k	 0.9210	 0.6660
l	 0.9200	 0.6650
m	 0.5790	 0.5130
n	 0.8290	 0.5980
o	 0.8240	 0.6010
p	 0.8240	 0.6020
q	 0.8610	 0.6220
r	 0.8340	 0.6080
s	 0.8950	 0.6370
t	 0.8820	 0.6310
u	 0.8440	 0.6200
v	 0.9030	 0.6430
w	 0.8870	 0.6440
x	 0.9200	 0.6590
y	 0.9050	 0.6500
z	 0.7440	 0.5810