Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 12:03 AM JST

PDB ID	:	7VEA
EMDB ID	:	EMD-31944
Title	:	Pentacylindrical allophycocyanin core from Thermosynechococcus vulcanus
Authors	:	Kawakami, K.; Hamaguchi, T.; Hirose, Y.; Kosumi, D.; Miyata, M.; Kamiya, N.; Yonekura, K.
Deposited on	:	2021-09-08
Resolution	:	3.70 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:

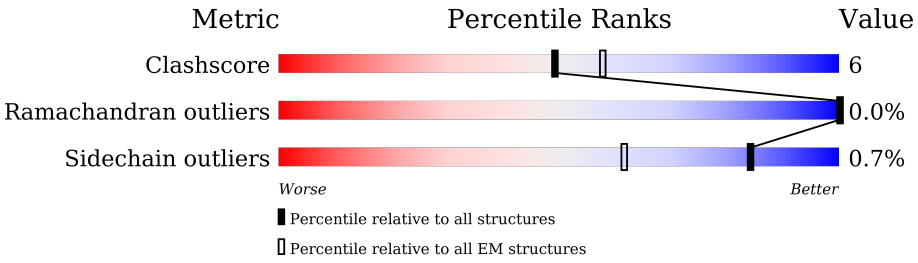
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	aA	161	99%
1	aC	161	6% 99%
1	aE	161	6% 99%
1	aG	161	99%
1	aI	161	99%
1	aK	161	99%
1	aO	161	99%
1	aQ	161	99%

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Mol	Chain	Length	Quality of chain
1	bM	161	99%
1	bO	161	98%
1	bQ	161	98%
1	bS	161	99%
1	bU	161	99%
1	bW	161	99%
1	cA	161	99%
1	cC	161	99%
1	cE	161	99%
1	cG	161	7% 99%
1	cI	161	99%
1	cK	161	99%
1	dA	161	99%
1	dC	161	7% 99%
1	dE	161	5% 99%
1	dG	161	99%
1	dI	161	99%
1	dK	161	99%
1	dO	161	99%
1	dQ	161	99%
1	eM	161	99%
1	eO	161	98%
1	eQ	161	98%
1	eS	161	99%
1	eU	161	99%

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Mol	Chain	Length	Quality of chain
1	eW	161	99%
1	fA	161	99%
1	fC	161	16% 99%
1	fE	161	99%
1	fG	161	12% 99%
1	fI	161	99%
1	fK	161	15% 99%
2	aB	161	99%
2	aD	161	99%
2	aF	161	99%
2	aH	161	98%
2	aJ	161	99%
2	aL	161	99%
2	aN	161	99%
2	aP	161	98%
2	bN	161	99%
2	bP	161	99%
2	bR	161	99%
2	bT	161	98%
2	bV	161	98%
2	bX	161	99%
2	cB	161	100%
2	cD	161	99%
2	cF	161	100%
2	cH	161	100%

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Mol	Chain	Length	Quality of chain
2	cJ	161	100%
2	cL	161	100%
2	dB	161	99%
2	dD	161	99%
2	dF	161	99%
2	dH	161	98%
2	dJ	161	99%
2	dL	161	99%
2	dN	161	99%
2	dP	161	98%
2	eN	161	99%
2	eP	161	99%
2	eR	161	99%
2	eT	161	98%
2	eV	161	98%
2	eX	161	99%
2	fB	161	100%
2	fD	161	99%
2	fF	161	100%
2	fH	161	100%
2	fJ	161	100%
2	fL	161	100%
3	aM	1139	89% 10%
3	dM	1139	89% 10%
4	aR	169	98%

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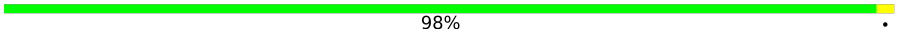
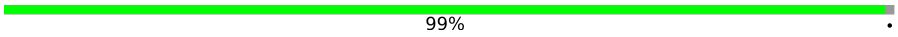
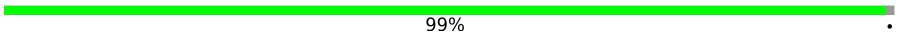
Mol	Chain	Length	Quality of chain
4	dR	169	
5	aS	67	
5	bY	67	
5	cM	67	
5	dS	67	
5	eY	67	
5	fM	67	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 111542 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 Allophycocyanin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aA	160	Total	C	N	O	S	0	0
			1193	749	206	232	6		
1	aC	159	Total	C	N	O	S	0	0
			982	605	177	197	3		
1	aE	160	Total	C	N	O	S	0	0
			1196	750	205	235	6		
1	aG	160	Total	C	N	O	S	0	0
			1202	753	209	234	6		
1	aI	160	Total	C	N	O	S	0	0
			1217	761	212	238	6		
1	aK	160	Total	C	N	O	S	0	0
			1182	742	200	234	6		
1	aO	160	Total	C	N	O	S	0	0
			1191	745	212	229	5		
1	aQ	160	Total	C	N	O	S	0	0
			1216	760	212	238	6		
1	bM	160	Total	C	N	O	S	0	0
			1220	762	212	240	6		
1	bO	160	Total	C	N	O	S	0	0
			1220	762	212	240	6		
1	bQ	160	Total	C	N	O	S	0	0
			1216	760	212	238	6		
1	bS	160	Total	C	N	O	S	0	0
			1202	753	209	234	6		
1	bU	160	Total	C	N	O	S	0	0
			1212	758	212	236	6		
1	bW	160	Total	C	N	O	S	0	0
			1198	751	208	233	6		
1	cA	160	Total	C	N	O		0	0
			809	487	160	162			
1	cC	160	Total	C	N	O		0	0
			843	505	176	162			
1	cE	160	Total	C	N	O	S	0	0
			948	586	187	173	2		

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	cG	160	Total C N O 786 466 160 160	0	0
1	cI	160	Total C N O 800 478 160 162	0	0
1	cK	160	Total C N O 824 494 165 165	0	0
1	dA	160	Total C N O S 1193 749 206 232 6	0	0
1	dC	159	Total C N O S 982 605 177 197 3	0	0
1	dE	160	Total C N O S 1196 750 205 235 6	0	0
1	dG	160	Total C N O S 1202 753 209 234 6	0	0
1	dI	160	Total C N O S 1217 761 212 238 6	0	0
1	dK	160	Total C N O S 1182 742 200 234 6	0	0
1	dO	160	Total C N O S 1191 745 212 229 5	0	0
1	dQ	160	Total C N O S 1216 760 212 238 6	0	0
1	eM	160	Total C N O S 1220 762 212 240 6	0	0
1	eO	160	Total C N O S 1220 762 212 240 6	0	0
1	eQ	160	Total C N O S 1216 760 212 238 6	0	0
1	eS	160	Total C N O S 1202 753 209 234 6	0	0
1	eU	160	Total C N O S 1212 758 212 236 6	0	0
1	eW	160	Total C N O S 1198 751 208 233 6	0	0
1	fA	160	Total C N O 809 487 160 162	0	0
1	fC	160	Total C N O 843 505 176 162	0	0
1	fE	160	Total C N O S 948 586 187 173 2	0	0
1	fG	160	Total C N O 786 466 160 160	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	fI	160	Total C N O 800 478 160 162	0	0
1	fK	160	Total C N O 824 494 165 165	0	0

- Molecule 2 is a protein called Allophycocyanin beta chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	aB	161	Total C N O S 1174 741 196 231 6	0	0
2	aD	160	Total C N O S 1176 742 195 232 7	0	0
2	aF	160	Total C N O S 1179 744 198 230 7	0	0
2	aH	161	Total C N O S 1216 768 203 237 8	0	0
2	aJ	161	Total C N O S 1208 764 203 233 8	0	0
2	aL	161	Total C N O S 1216 768 203 237 8	0	0
2	aN	161	Total C N O S 1208 764 203 233 8	0	0
2	aP	161	Total C N O S 1216 768 203 237 8	0	0
2	bN	161	Total C N O S 1216 768 203 237 8	0	0
2	bP	161	Total C N O S 1216 768 203 237 8	0	0
2	bR	161	Total C N O S 1206 763 200 235 8	0	0
2	bT	161	Total C N O S 1207 762 203 235 7	0	0
2	bV	161	Total C N O S 1195 754 200 235 6	0	0
2	bX	161	Total C N O S 1198 756 202 233 7	0	0
2	cB	161	Total C N O 808 484 161 163	0	0
2	cD	161	Total C N O S 985 620 180 182 3	0	0
2	cF	161	Total C N O S 983 612 188 182 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	cH	161	Total	C	N	O		0	0
			794	472	161	161			
2	cJ	161	Total	C	N	O		0	0
			808	484	161	163			
2	cL	161	Total	C	N	O		0	0
			800	475	164	161			
2	dB	161	Total	C	N	O	S	0	0
			1174	741	196	231	6		
2	dD	160	Total	C	N	O	S	0	0
			1176	742	195	232	7		
2	dF	160	Total	C	N	O	S	0	0
			1179	744	198	230	7		
2	dH	161	Total	C	N	O	S	0	0
			1216	768	203	237	8		
2	dJ	161	Total	C	N	O	S	0	0
			1208	764	203	233	8		
2	dL	161	Total	C	N	O	S	0	0
			1216	768	203	237	8		
2	dN	161	Total	C	N	O	S	0	0
			1208	764	203	233	8		
2	dP	161	Total	C	N	O	S	0	0
			1216	768	203	237	8		
2	eN	161	Total	C	N	O	S	0	0
			1216	768	203	237	8		
2	eP	161	Total	C	N	O	S	0	0
			1216	768	203	237	8		
2	eR	161	Total	C	N	O	S	0	0
			1206	763	200	235	8		
2	eT	161	Total	C	N	O	S	0	0
			1207	762	203	235	7		
2	eV	161	Total	C	N	O	S	0	0
			1195	754	200	235	6		
2	eX	161	Total	C	N	O	S	0	0
			1198	756	202	233	7		
2	fB	161	Total	C	N	O		0	0
			808	484	161	163			
2	fD	161	Total	C	N	O	S	0	0
			985	620	180	182	3		
2	fF	161	Total	C	N	O	S	0	0
			983	612	188	182	1		
2	fH	161	Total	C	N	O		0	0
			794	472	161	161			

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	fJ	161	Total	C	N	O	0	0
			808	484	161	163		
2	fL	161	Total	C	N	O	0	0
			800	475	164	161		

- Molecule 3 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aM	1020	Total	C	N	O	S	0	0
			7856	4993	1409	1443	11		
3	dM	1020	Total	C	N	O	S	0	0
			7856	4993	1409	1443	11		

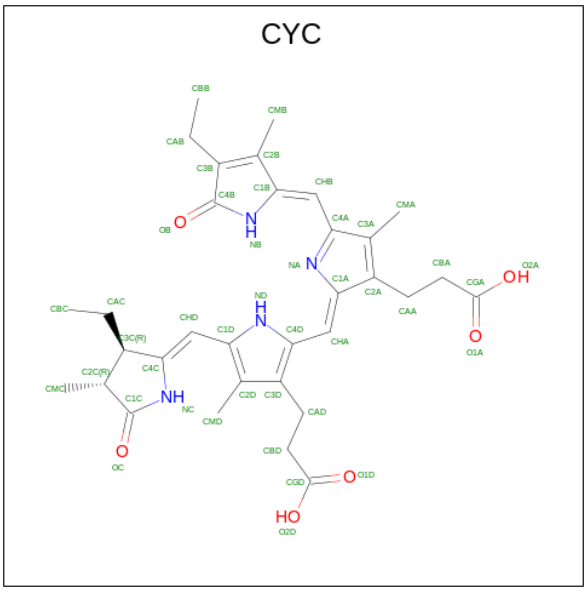
- Molecule 4 is a protein called Phycobilisome core component.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aR	169	Total	C	N	O	S	0	0
			1313	820	234	253	6		
4	dR	169	Total	C	N	O	S	0	0
			1313	820	234	253	6		

- Molecule 5 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	aS	66	Total	C	N	O		0	0
			325	193	66	66			
5	bY	66	Total	C	N	O	S	0	0
			513	328	95	88	2		
5	cM	59	Total	C	N	O		0	0
			292	174	59	59			
5	dS	66	Total	C	N	O		0	0
			325	193	66	66			
5	eY	66	Total	C	N	O	S	0	0
			513	328	95	88	2		
5	fM	59	Total	C	N	O		0	0
			292	174	59	59			

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



Mol	Chain	Residues	Atoms				AltConf
6	aA	1	Total	C	N	O	0
			43	33	4	6	
6	aB	1	Total	C	N	O	0
			43	33	4	6	
6	aC	1	Total	C	N	O	0
			43	33	4	6	
6	aD	1	Total	C	N	O	0
			43	33	4	6	
6	aE	1	Total	C	N	O	0
			43	33	4	6	
6	aF	1	Total	C	N	O	0
			43	33	4	6	
6	aG	1	Total	C	N	O	0
			43	33	4	6	
6	aH	1	Total	C	N	O	0
			43	33	4	6	
6	aI	1	Total	C	N	O	0
			43	33	4	6	
6	aJ	1	Total	C	N	O	0
			43	33	4	6	
6	aK	1	Total	C	N	O	0
			43	33	4	6	
6	aL	1	Total	C	N	O	0
			43	33	4	6	
6	aM	1	Total	C	N	O	0
			172	132	16	24	
6	aM	1	Total	C	N	O	0
			172	132	16	24	

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Mol	Chain	Residues	Atoms				AltConf
6	aM	1	Total	C	N	O	0
			172	132	16	24	
6	aM	1	Total	C	N	O	0
			172	132	16	24	
6	aN	1	Total	C	N	O	0
			43	33	4	6	
6	aO	1	Total	C	N	O	0
			43	33	4	6	
6	aP	1	Total	C	N	O	0
			43	33	4	6	
6	aQ	1	Total	C	N	O	0
			43	33	4	6	
6	bM	1	Total	C	N	O	0
			43	33	4	6	
6	bN	1	Total	C	N	O	0
			43	33	4	6	
6	bO	1	Total	C	N	O	0
			43	33	4	6	
6	bP	1	Total	C	N	O	0
			43	33	4	6	
6	bQ	1	Total	C	N	O	0
			43	33	4	6	
6	bR	1	Total	C	N	O	0
			43	33	4	6	
6	bS	1	Total	C	N	O	0
			43	33	4	6	
6	bT	1	Total	C	N	O	0
			43	33	4	6	
6	bU	1	Total	C	N	O	0
			43	33	4	6	
6	bV	1	Total	C	N	O	0
			43	33	4	6	
6	bW	1	Total	C	N	O	0
			43	33	4	6	
6	bX	1	Total	C	N	O	0
			43	33	4	6	
6	cB	1	Total	C	N	O	0
			43	33	4	6	
6	cD	1	Total	C	N	O	0
			86	66	8	12	
6	cD	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
6	cF	1	Total	C	N	O	0
			86	66	8	12	
6	cF	1	Total	C	N	O	0
			86	66	8	12	
6	cG	1	Total	C	N	O	0
			43	33	4	6	
6	cI	1	Total	C	N	O	0
			43	33	4	6	
6	cJ	1	Total	C	N	O	0
			43	33	4	6	
6	cL	1	Total	C	N	O	0
			43	33	4	6	
6	cM	1	Total	C	N	O	0
			43	33	4	6	
6	dA	1	Total	C	N	O	0
			43	33	4	6	
6	dB	1	Total	C	N	O	0
			43	33	4	6	
6	dC	1	Total	C	N	O	0
			43	33	4	6	
6	dD	1	Total	C	N	O	0
			43	33	4	6	
6	dE	1	Total	C	N	O	0
			43	33	4	6	
6	dF	1	Total	C	N	O	0
			43	33	4	6	
6	dG	1	Total	C	N	O	0
			43	33	4	6	
6	dH	1	Total	C	N	O	0
			43	33	4	6	
6	dI	1	Total	C	N	O	0
			43	33	4	6	
6	dJ	1	Total	C	N	O	0
			43	33	4	6	
6	dK	1	Total	C	N	O	0
			43	33	4	6	
6	dL	1	Total	C	N	O	0
			43	33	4	6	
6	dM	1	Total	C	N	O	0
			129	99	12	18	
6	dM	1	Total	C	N	O	0
			129	99	12	18	

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Mol	Chain	Residues	Atoms				AltConf
6	dM	1	Total	C	N	O	0
			129	99	12	18	
6	dN	1	Total	C	N	O	0
			43	33	4	6	
6	dO	1	Total	C	N	O	0
			43	33	4	6	
6	dP	1	Total	C	N	O	0
			43	33	4	6	
6	dQ	1	Total	C	N	O	0
			43	33	4	6	
6	dR	1	Total	C	N	O	0
			43	33	4	6	
6	eM	1	Total	C	N	O	0
			43	33	4	6	
6	eN	1	Total	C	N	O	0
			43	33	4	6	
6	eO	1	Total	C	N	O	0
			43	33	4	6	
6	eP	1	Total	C	N	O	0
			43	33	4	6	
6	eQ	1	Total	C	N	O	0
			43	33	4	6	
6	eR	1	Total	C	N	O	0
			43	33	4	6	
6	eS	1	Total	C	N	O	0
			43	33	4	6	
6	eT	1	Total	C	N	O	0
			43	33	4	6	
6	eU	1	Total	C	N	O	0
			43	33	4	6	
6	eV	1	Total	C	N	O	0
			43	33	4	6	
6	eW	1	Total	C	N	O	0
			43	33	4	6	
6	eX	1	Total	C	N	O	0
			43	33	4	6	
6	fB	1	Total	C	N	O	0
			43	33	4	6	
6	fD	1	Total	C	N	O	0
			86	66	8	12	
6	fD	1	Total	C	N	O	0
			86	66	8	12	

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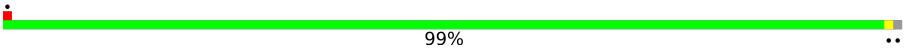
Mol	Chain	Residues	Atoms				AltConf
6	fF	1	Total	C	N	O	0
			86	66	8	12	
6	fF	1	Total	C	N	O	0
			86	66	8	12	
6	fG	1	Total	C	N	O	0
			43	33	4	6	
6	fI	1	Total	C	N	O	0
			43	33	4	6	
6	fJ	1	Total	C	N	O	0
			43	33	4	6	
6	fL	1	Total	C	N	O	0
			43	33	4	6	
6	fM	1	Total	C	N	O	0
			43	33	4	6	

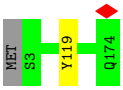
3 Residue-property plots (i)

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

• Molecule 1: Allophycocyanin alpha chain

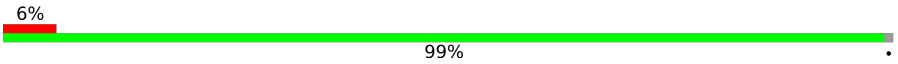
Chain aA:

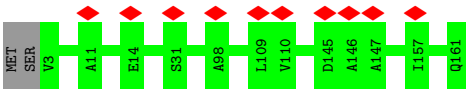




• Molecule 1: Allophycocyanin alpha chain

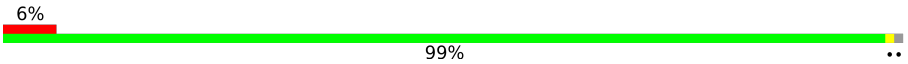
Chain aC:

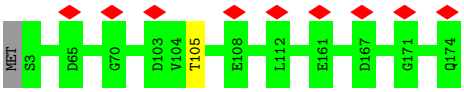




• Molecule 1: Allophycocyanin alpha chain

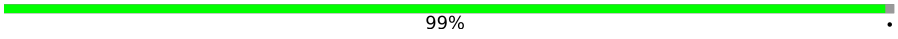
Chain aE:





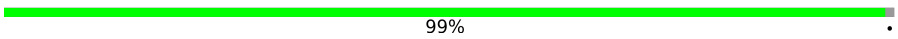
• Molecule 1: Allophycocyanin alpha chain

Chain aG:



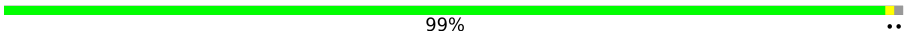
• Molecule 1: Allophycocyanin alpha chain

Chain aI:



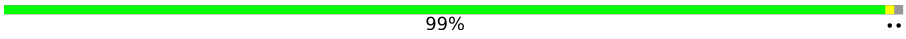
• Molecule 1: Allophycocyanin alpha chain

Chain aK:



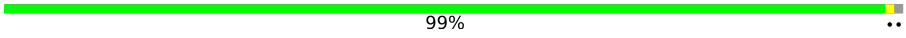
• Molecule 1: Allophycocyanin alpha chain

Chain aO:



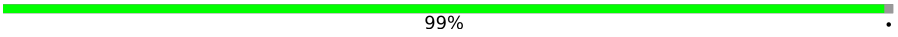
• Molecule 1: Allophycocyanin alpha chain

Chain aQ:



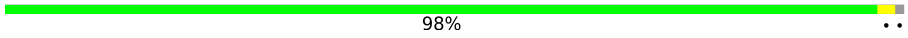
• Molecule 1: Allophycocyanin alpha chain

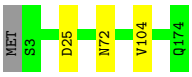
Chain bM:



• Molecule 1: Allophycocyanin alpha chain

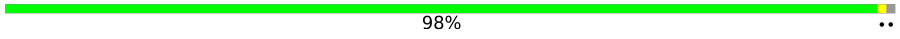
Chain bO:





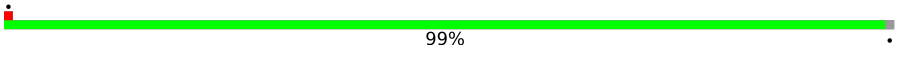
• Molecule 1: Allophycocyanin alpha chain

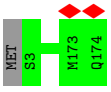
Chain bQ:



• Molecule 1: Allophycocyanin alpha chain

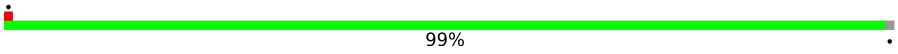
Chain bS:





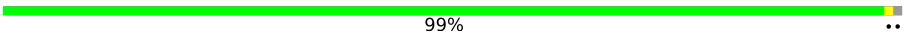
• Molecule 1: Allophycocyanin alpha chain

Chain bU:



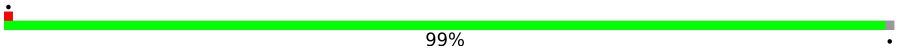
• Molecule 1: Allophycocyanin alpha chain

Chain bW:



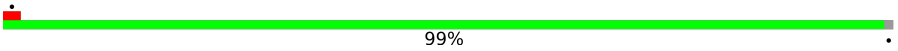
• Molecule 1: Allophycocyanin alpha chain

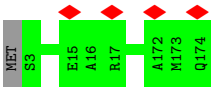
Chain cA:



• Molecule 1: Allophycocyanin alpha chain

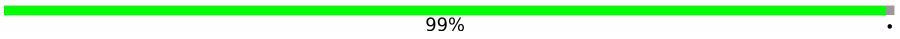
Chain cC:





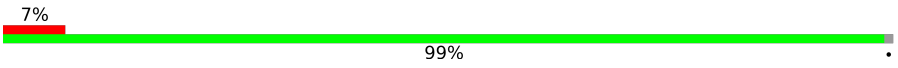
• Molecule 1: Allophycocyanin alpha chain

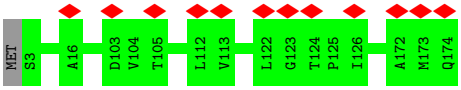
Chain cE:



• Molecule 1: Allophycocyanin alpha chain

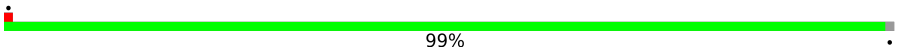
Chain cG:

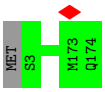




• Molecule 1: Allophycocyanin alpha chain

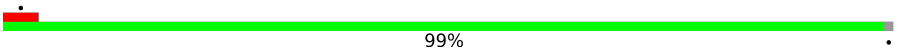
Chain cI:

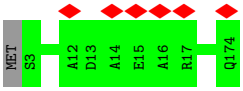




• Molecule 1: Allophycocyanin alpha chain

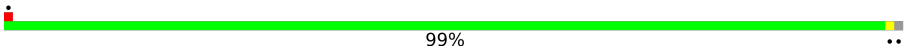
Chain cK:

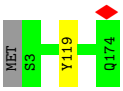




• Molecule 1: Allophycocyanin alpha chain

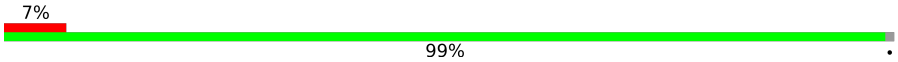
Chain dA:

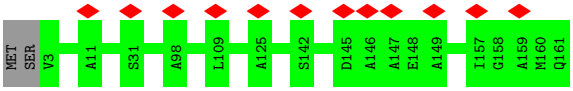




• Molecule 1: Allophycocyanin alpha chain

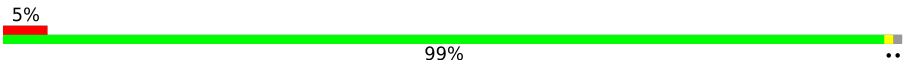
Chain dC:

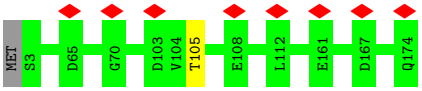




• Molecule 1: Allophycocyanin alpha chain

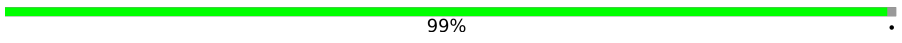
Chain dE:





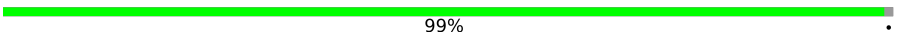
• Molecule 1: Allophycocyanin alpha chain

Chain dG:



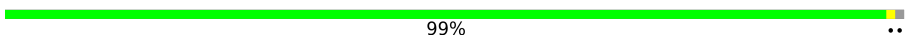
• Molecule 1: Allophycocyanin alpha chain

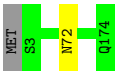
Chain dI:



• Molecule 1: Allophycocyanin alpha chain

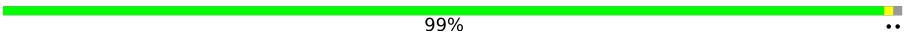
Chain dK:

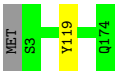




• Molecule 1: Allophycocyanin alpha chain

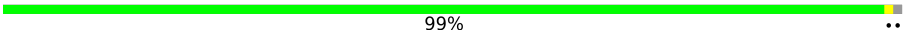
Chain dO:

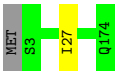




• Molecule 1: Allophycocyanin alpha chain

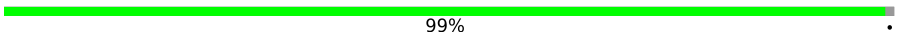
Chain dQ:





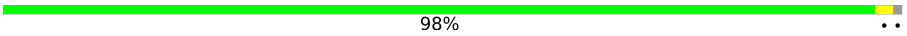
• Molecule 1: Allophycocyanin alpha chain

Chain eM:



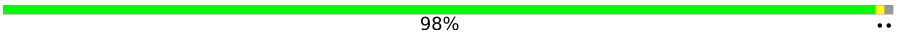
• Molecule 1: Allophycocyanin alpha chain

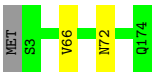
Chain eO:



• Molecule 1: Allophycocyanin alpha chain

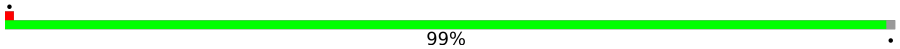
Chain eQ:

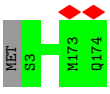




• Molecule 1: Allophycocyanin alpha chain

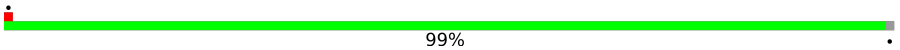
Chain eS:





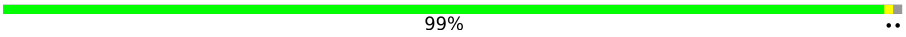
• Molecule 1: Allophycocyanin alpha chain

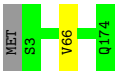
Chain eU:



• Molecule 1: Allophycocyanin alpha chain

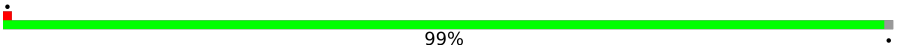
Chain eW:





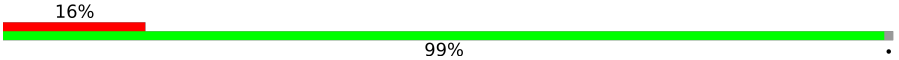
• Molecule 1: Allophycocyanin alpha chain

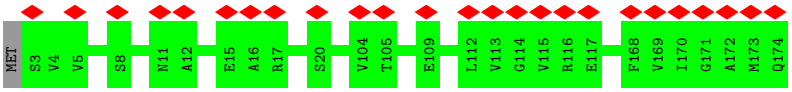
Chain fA:



• Molecule 1: Allophycocyanin alpha chain

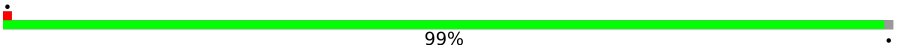
Chain fC:

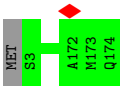




• Molecule 1: Allophycocyanin alpha chain

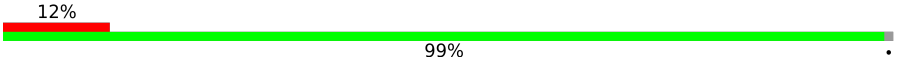
Chain fE:

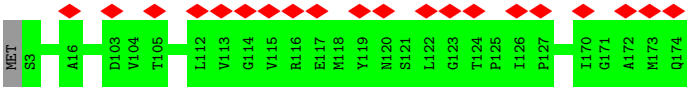




• Molecule 1: Allophycocyanin alpha chain

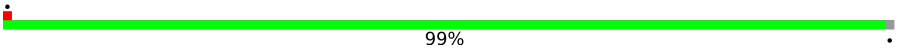
Chain fG:

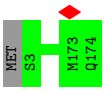




• Molecule 1: Allophycocyanin alpha chain

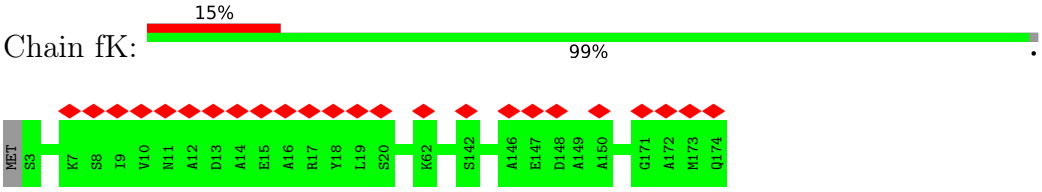
Chain fI:





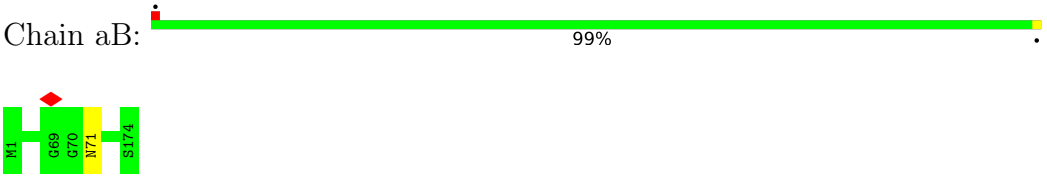
• Molecule 1: Allophycocyanin alpha chain

Chain fK:



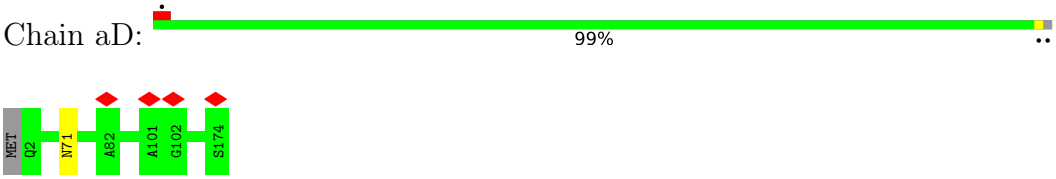
• Molecule 2: Allophycocyanin beta chain

Chain aB:



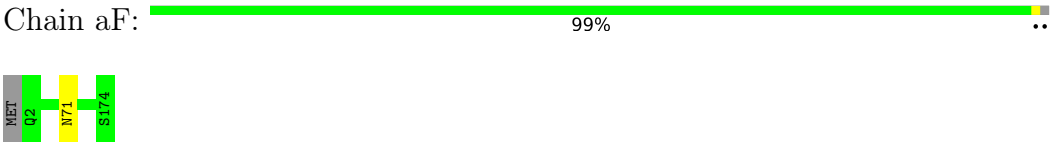
• Molecule 2: Allophycocyanin beta chain

Chain aD:



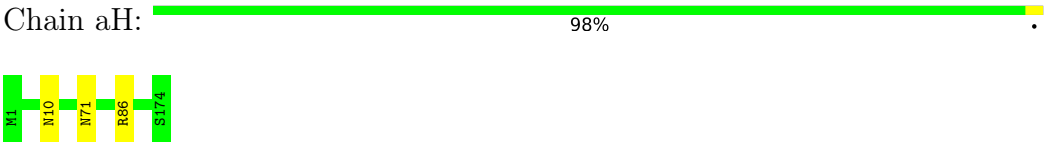
• Molecule 2: Allophycocyanin beta chain

Chain aF:



• Molecule 2: Allophycocyanin beta chain

Chain aH:

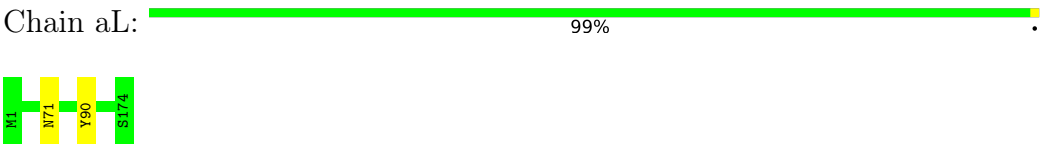


• Molecule 2: Allophycocyanin beta chain

Chain aJ:

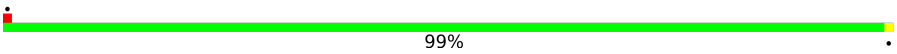
• Molecule 2: Allophycocyanin beta chain

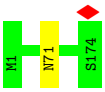
Chain aL:



• Molecule 2: Allophycocyanin beta chain

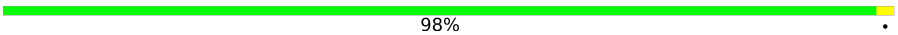
Chain aN:

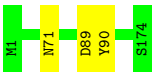




• Molecule 2: Allophycocyanin beta chain

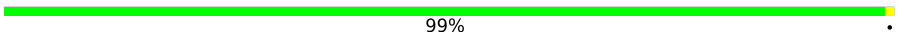
Chain aP:

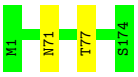




• Molecule 2: Allophycocyanin beta chain

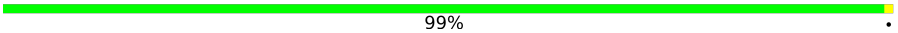
Chain bN:





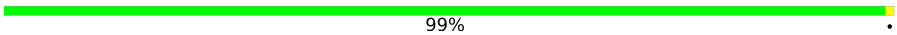
• Molecule 2: Allophycocyanin beta chain

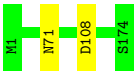
Chain bP:



• Molecule 2: Allophycocyanin beta chain

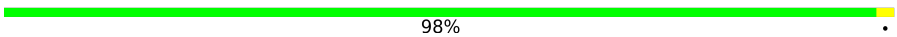
Chain bR:

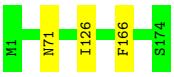




• Molecule 2: Allophycocyanin beta chain

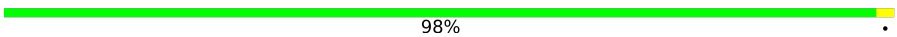
Chain bT:



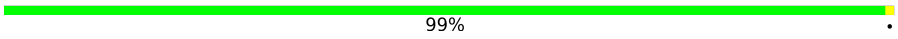


• Molecule 2: Allophycocyanin beta chain

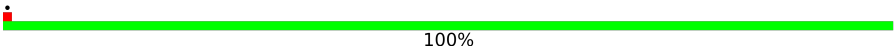
Chain bV:



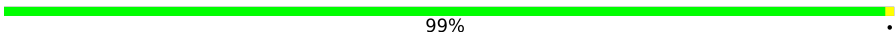
• Molecule 2: Allophycocyanin beta chain

Chain bX: 

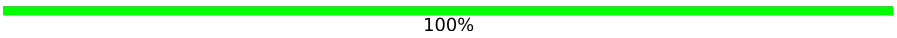
• Molecule 2: Allophycocyanin beta chain

Chain cB: 

• Molecule 2: Allophycocyanin beta chain

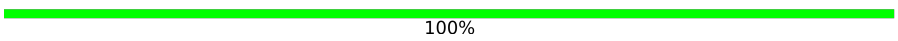
Chain cD: 

• Molecule 2: Allophycocyanin beta chain

Chain cF: 

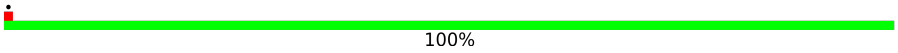
There are no outlier residues recorded for this chain.

• Molecule 2: Allophycocyanin beta chain

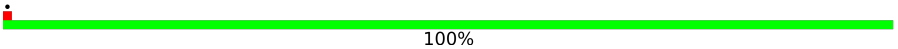
Chain cH: 

There are no outlier residues recorded for this chain.

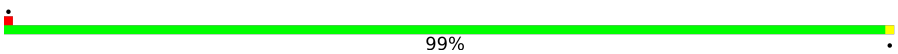
• Molecule 2: Allophycocyanin beta chain

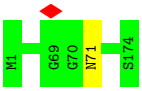
Chain cJ: 

• Molecule 2: Allophycocyanin beta chain

Chain cL: 

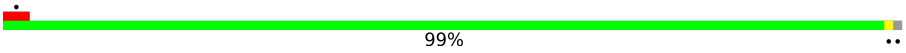
• Molecule 2: Allophycocyanin beta chain

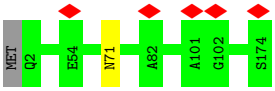
Chain dB: 



• Molecule 2: Allophycocyanin beta chain

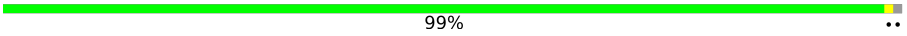
Chain dD:

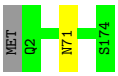




• Molecule 2: Allophycocyanin beta chain

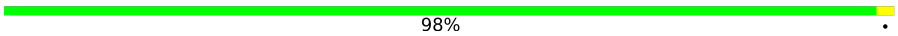
Chain dF:

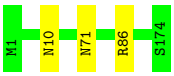




• Molecule 2: Allophycocyanin beta chain

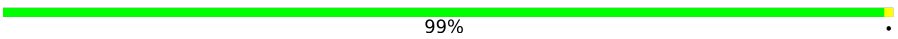
Chain dH:





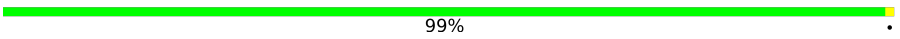
• Molecule 2: Allophycocyanin beta chain

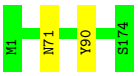
Chain dJ:



• Molecule 2: Allophycocyanin beta chain

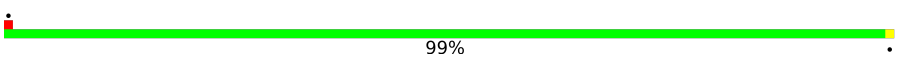
Chain dL:

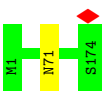




• Molecule 2: Allophycocyanin beta chain

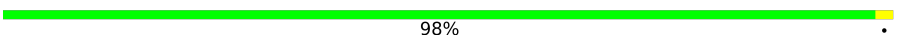
Chain dN:

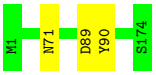




• Molecule 2: Allophycocyanin beta chain

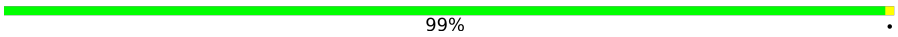
Chain dP:

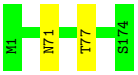




• Molecule 2: Allophycocyanin beta chain

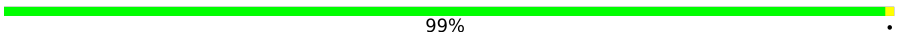
Chain eN:





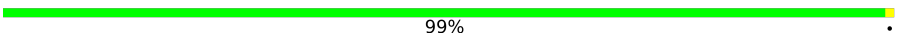
• Molecule 2: Allophycocyanin beta chain

Chain eP:



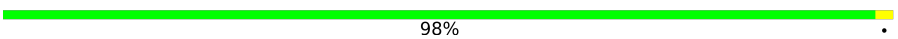
• Molecule 2: Allophycocyanin beta chain

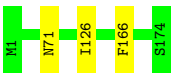
Chain eR:



• Molecule 2: Allophycocyanin beta chain

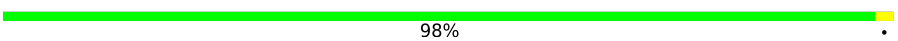
Chain eT:





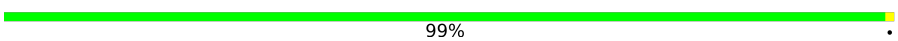
• Molecule 2: Allophycocyanin beta chain

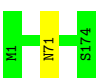
Chain eV:



• Molecule 2: Allophycocyanin beta chain

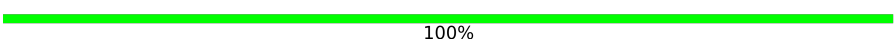
Chain eX:





• Molecule 2: Allophycocyanin beta chain

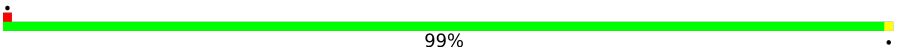
Chain fB:

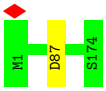


There are no outlier residues recorded for this chain.

• Molecule 2: Allophycocyanin beta chain

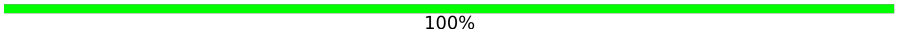
Chain fD:





• Molecule 2: Allophycocyanin beta chain

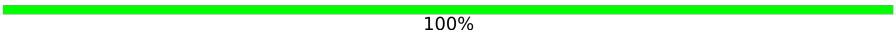
Chain fF:



There are no outlier residues recorded for this chain.

• Molecule 2: Allophycocyanin beta chain

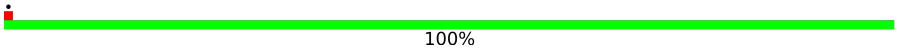
Chain fH:



There are no outlier residues recorded for this chain.

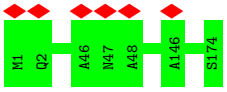
• Molecule 2: Allophycocyanin beta chain

Chain fJ:



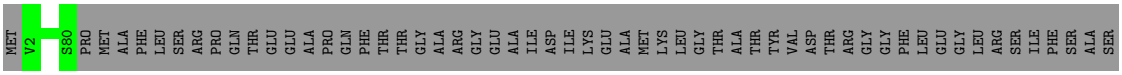
• Molecule 2: Allophycocyanin beta chain

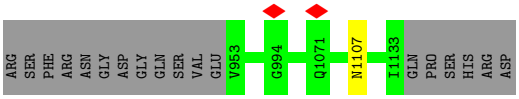
Chain fL:



• Molecule 3: Phycobiliprotein ApcE

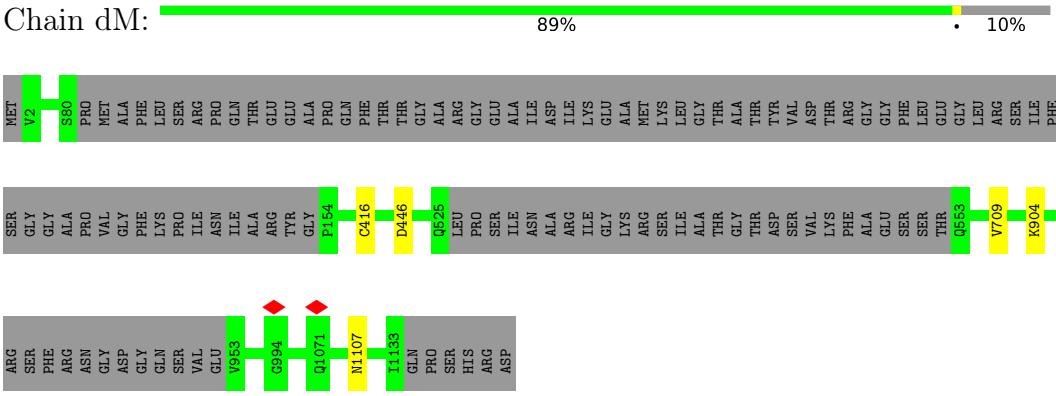
Chain aM:





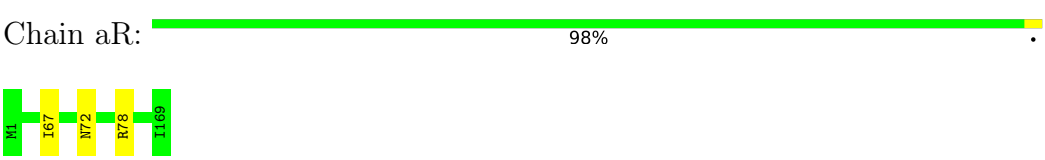
• Molecule 3: Phycobiliprotein ApcE

Chain dM:



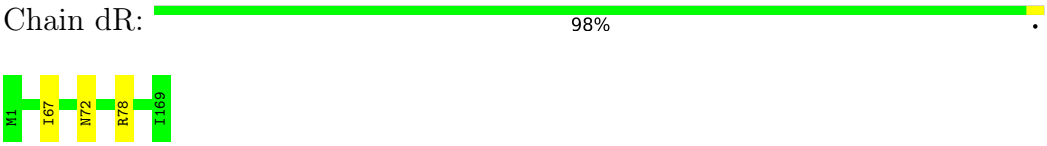
• Molecule 4: Phycobilisome core component

Chain aR:



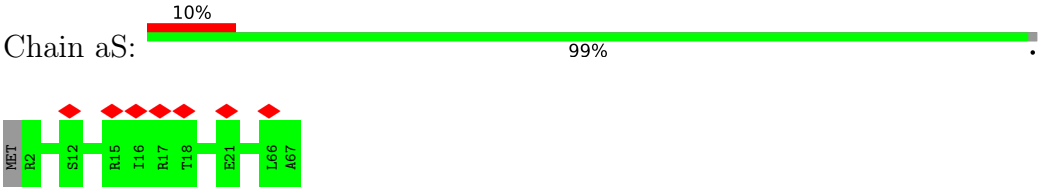
• Molecule 4: Phycobilisome core component

Chain dR:



• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain aS:

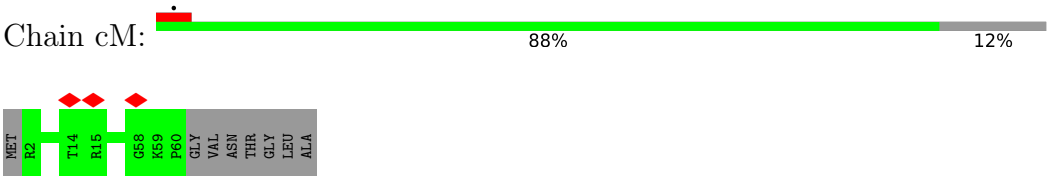


• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain bY:

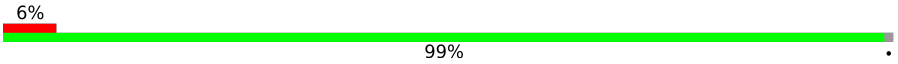
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

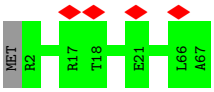
Chain cM:



• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

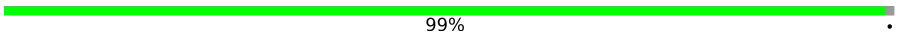
Chain dS:





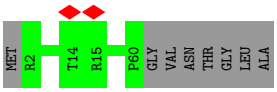
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain eY:



• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain fM:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25532	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	84.1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.241	Depositor
Minimum map value	-0.150	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.00612	Depositor
Map size (Å)	372.0, 372.0, 372.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality

5.1 Standard geometry

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

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	aA	0.27	0/1209	0.49	0/1640
1	aC	0.25	0/992	0.46	0/1359
1	aE	0.25	0/1212	0.49	0/1644
1	aG	0.28	0/1218	0.51	0/1651
1	aI	0.29	0/1233	0.51	0/1669
1	aK	0.28	0/1198	0.49	0/1628
1	aO	0.28	0/1206	0.50	0/1635
1	aQ	0.30	0/1232	0.51	0/1668
1	bM	0.27	0/1236	0.52	0/1673
1	bO	0.29	0/1236	0.51	0/1673
1	bQ	0.27	0/1232	0.49	0/1668
1	bS	0.25	0/1218	0.49	0/1651
1	bU	0.27	0/1228	0.49	0/1663
1	bW	0.26	0/1214	0.51	0/1646
1	cA	0.24	0/811	0.36	0/1124
1	cC	0.24	0/845	0.42	0/1165
1	cE	0.26	0/957	0.45	0/1306
1	cG	0.24	0/785	0.35	0/1089
1	cI	0.24	0/801	0.36	0/1111
1	cK	0.24	0/826	0.39	0/1141
1	dA	0.28	0/1209	0.49	0/1640
1	dC	0.25	0/992	0.46	0/1359
1	dE	0.25	0/1212	0.49	0/1644
1	dG	0.27	0/1218	0.51	0/1651
1	dI	0.29	0/1233	0.51	0/1669
1	dK	0.28	0/1198	0.49	0/1628
1	dO	0.28	0/1206	0.50	0/1635
1	dQ	0.29	0/1232	0.50	0/1668
1	eM	0.27	0/1236	0.52	0/1673
1	eO	0.29	0/1236	0.51	0/1673
1	eQ	0.27	0/1232	0.49	0/1668
1	eS	0.25	0/1218	0.49	0/1651

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	eU	0.27	0/1228	0.49	0/1663
1	eW	0.26	0/1214	0.51	0/1646
1	fA	0.24	0/811	0.36	0/1124
1	fC	0.24	0/845	0.42	0/1165
1	fE	0.25	0/957	0.45	0/1306
1	fG	0.24	0/785	0.35	0/1089
1	fI	0.24	0/801	0.36	0/1111
1	fK	0.24	0/826	0.38	0/1141
2	aB	0.26	0/1180	0.44	0/1603
2	aD	0.25	0/1181	0.46	0/1601
2	aF	0.26	0/1185	0.44	0/1607
2	aH	0.31	0/1222	0.48	0/1653
2	aJ	0.29	0/1214	0.48	0/1643
2	aL	0.29	0/1222	0.47	0/1653
2	aN	0.27	0/1214	0.46	0/1643
2	aP	0.29	0/1222	0.48	0/1653
2	bN	0.31	0/1222	0.50	0/1653
2	bP	0.29	0/1222	0.49	0/1653
2	bR	0.28	0/1212	0.48	0/1641
2	bT	0.25	0/1213	0.46	0/1642
2	bV	0.26	0/1201	0.46	0/1628
2	bX	0.25	0/1203	0.46	0/1629
2	cB	0.24	0/803	0.34	0/1114
2	cD	0.25	0/993	0.43	0/1362
2	cF	0.25	0/988	0.43	0/1351
2	cH	0.24	0/787	0.34	0/1092
2	cJ	0.23	0/803	0.36	0/1114
2	cL	0.23	0/793	0.36	0/1099
2	dB	0.26	0/1180	0.45	0/1603
2	dD	0.25	0/1181	0.46	0/1601
2	dF	0.26	0/1185	0.44	0/1607
2	dH	0.31	0/1222	0.48	0/1653
2	dJ	0.29	0/1214	0.48	0/1643
2	dL	0.29	0/1222	0.47	0/1653
2	dN	0.27	0/1214	0.46	0/1643
2	dP	0.29	0/1222	0.48	0/1653
2	eN	0.31	0/1222	0.50	0/1653
2	eP	0.29	0/1222	0.49	0/1653
2	eR	0.28	0/1212	0.48	0/1641
2	eT	0.26	0/1213	0.46	0/1642
2	eV	0.26	0/1201	0.46	0/1628
2	eX	0.25	0/1203	0.46	0/1629
2	fB	0.24	0/803	0.34	0/1114

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	fD	0.25	0/993	0.43	0/1362
2	fF	0.25	0/988	0.43	0/1351
2	fH	0.24	0/787	0.34	0/1092
2	fJ	0.23	0/803	0.36	0/1114
2	fL	0.23	0/793	0.36	0/1099
3	aM	0.28	0/8018	0.52	0/10878
3	dM	0.28	0/8018	0.52	0/10878
4	aR	0.29	0/1321	0.51	0/1788
4	dR	0.29	0/1321	0.51	0/1788
5	aS	0.24	0/324	0.48	0/449
5	bY	0.26	0/522	0.54	0/703
5	cM	0.24	0/291	0.43	0/404
5	dS	0.24	0/324	0.48	0/449
5	eY	0.26	0/522	0.54	0/703
5	fM	0.23	0/291	0.43	0/404
All	All	0.27	0/108890	0.47	0/148120

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	1193	0	1183	0	0
1	aC	982	0	739	0	0
1	aE	1196	0	1183	0	0
1	aG	1202	0	1192	0	0
1	aI	1217	0	1217	0	0
1	aK	1182	0	1155	0	0
1	aO	1191	0	1187	0	0
1	aQ	1216	0	1215	0	0
1	bM	1220	0	1219	0	0
1	bO	1220	0	1219	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	bQ	1216	0	1215	0	0
1	bS	1202	0	1196	0	0
1	bU	1212	0	1211	0	0
1	bW	1198	0	1190	0	0
1	cA	809	0	408	0	0
1	cC	843	0	484	0	0
1	cE	948	0	647	0	0
1	cG	786	0	378	0	0
1	cI	800	0	392	0	0
1	cK	824	0	431	0	0
1	dA	1193	0	1183	0	0
1	dC	982	0	739	0	0
1	dE	1196	0	1183	0	0
1	dG	1202	0	1192	0	0
1	dI	1217	0	1217	0	0
1	dK	1182	0	1155	0	0
1	dO	1191	0	1187	0	0
1	dQ	1216	0	1215	0	0
1	eM	1220	0	1219	0	0
1	eO	1220	0	1219	0	0
1	eQ	1216	0	1215	0	0
1	eS	1202	0	1196	0	0
1	eU	1212	0	1211	0	0
1	eW	1198	0	1190	0	0
1	fA	809	0	408	0	0
1	fC	843	0	484	0	0
1	fE	948	0	647	0	0
1	fG	786	0	378	0	0
1	fI	800	0	392	0	0
1	fK	824	0	431	0	0
2	aB	1174	0	1144	0	0
2	aD	1176	0	1161	0	0
2	aF	1179	0	1159	0	0
2	aH	1216	0	1228	0	0
2	aJ	1208	0	1220	0	0
2	aL	1216	0	1228	0	0
2	aN	1208	0	1220	0	0
2	aP	1216	0	1228	0	0
2	bN	1216	0	1228	0	0
2	bP	1216	0	1228	0	0
2	bR	1206	0	1213	0	0
2	bT	1207	0	1210	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	bV	1195	0	1183	0	0
2	bX	1198	0	1204	0	0
2	cB	808	0	423	0	0
2	cD	985	0	748	0	0
2	cF	983	0	742	0	0
2	cH	794	0	409	0	0
2	cJ	808	0	423	0	0
2	cL	800	0	420	0	0
2	dB	1174	0	1144	0	0
2	dD	1176	0	1161	0	0
2	dF	1179	0	1159	0	0
2	dH	1216	0	1228	0	0
2	dJ	1208	0	1220	0	0
2	dL	1216	0	1228	0	0
2	dN	1208	0	1220	0	0
2	dP	1216	0	1228	0	0
2	eN	1216	0	1228	0	0
2	eP	1216	0	1228	0	0
2	eR	1206	0	1213	0	0
2	eT	1207	0	1210	0	0
2	eV	1195	0	1183	0	0
2	eX	1198	0	1204	0	0
2	fB	808	0	423	0	0
2	fD	985	0	748	0	0
2	fF	983	0	742	0	0
2	fH	794	0	409	0	0
2	fJ	808	0	423	0	0
2	fL	800	0	420	0	0
3	aM	7856	0	7714	0	0
3	dM	7856	0	7714	0	0
4	aR	1313	0	1310	0	0
4	dR	1313	0	1310	0	0
5	aS	325	0	139	0	0
5	bY	513	0	516	0	0
5	cM	292	0	120	0	0
5	dS	325	0	139	0	0
5	eY	513	0	516	0	0
5	fM	292	0	120	0	0
6	aA	43	0	37	0	0
6	aB	43	0	37	0	0
6	aC	43	0	37	0	0
6	aD	43	0	37	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	aE	43	0	37	0	0
6	aF	43	0	37	0	0
6	aG	43	0	37	0	0
6	aH	43	0	37	0	0
6	aI	43	0	37	0	0
6	aJ	43	0	37	0	0
6	aK	43	0	37	0	0
6	aL	43	0	37	0	0
6	aM	172	0	147	0	0
6	aN	43	0	37	0	0
6	aO	43	0	37	0	0
6	aP	43	0	37	0	0
6	aQ	43	0	37	0	0
6	bM	43	0	37	0	0
6	bN	43	0	37	0	0
6	bO	43	0	37	0	0
6	bP	43	0	37	0	0
6	bQ	43	0	37	0	0
6	bR	43	0	37	0	0
6	bS	43	0	37	0	0
6	bT	43	0	37	0	0
6	bU	43	0	37	0	0
6	bV	43	0	37	0	0
6	bW	43	0	37	0	0
6	bX	43	0	37	0	0
6	cB	43	0	38	0	0
6	cD	86	0	76	0	0
6	cF	86	0	76	0	0
6	cG	43	0	38	0	0
6	cI	43	0	38	0	0
6	cJ	43	0	38	0	0
6	cL	43	0	38	0	0
6	cM	43	0	38	0	0
6	dA	43	0	37	0	0
6	dB	43	0	37	0	0
6	dC	43	0	37	0	0
6	dD	43	0	37	0	0
6	dE	43	0	37	0	0
6	dF	43	0	37	0	0
6	dG	43	0	37	0	0
6	dH	43	0	37	0	0
6	dI	43	0	37	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	dJ	43	0	37	0	0
6	dK	43	0	37	0	0
6	dL	43	0	37	0	0
6	dM	129	0	112	0	0
6	dN	43	0	37	0	0
6	dO	43	0	37	0	0
6	dP	43	0	37	0	0
6	dQ	43	0	37	0	0
6	dR	43	0	35	0	0
6	eM	43	0	37	0	0
6	eN	43	0	37	0	0
6	eO	43	0	37	0	0
6	eP	43	0	37	0	0
6	eQ	43	0	37	0	0
6	eR	43	0	37	0	0
6	eS	43	0	37	0	0
6	eT	43	0	37	0	0
6	eU	43	0	37	0	0
6	eV	43	0	37	0	0
6	eW	43	0	37	0	0
6	eX	43	0	37	0	0
6	fB	43	0	38	0	0
6	fD	86	0	76	0	0
6	fF	86	0	76	0	0
6	fG	43	0	38	0	0
6	fI	43	0	38	0	0
6	fJ	43	0	38	0	0
6	fL	43	0	38	0	0
6	fM	43	0	38	0	0
All	All	111542	0	100884	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	aC	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
1	aE	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	aG	158/161 (98%)	158 (100%)	0	0	100	100
1	aI	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	aK	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	aO	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	aQ	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	bM	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	bO	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	bQ	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	bS	158/161 (98%)	158 (100%)	0	0	100	100
1	bU	158/161 (98%)	158 (100%)	0	0	100	100
1	bW	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	cA	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	cC	158/161 (98%)	158 (100%)	0	0	100	100
1	cE	158/161 (98%)	158 (100%)	0	0	100	100
1	cG	158/161 (98%)	158 (100%)	0	0	100	100
1	cI	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	cK	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	dA	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	dC	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
1	dE	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	dG	158/161 (98%)	158 (100%)	0	0	100	100
1	dI	158/161 (98%)	157 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	dK	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	dO	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	dQ	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	eM	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	eO	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	eQ	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	eS	158/161 (98%)	158 (100%)	0	0	100	100
1	eU	158/161 (98%)	158 (100%)	0	0	100	100
1	eW	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	fA	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	fC	158/161 (98%)	158 (100%)	0	0	100	100
1	fE	158/161 (98%)	158 (100%)	0	0	100	100
1	fG	158/161 (98%)	158 (100%)	0	0	100	100
1	fI	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	fK	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	aB	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	aD	157/161 (98%)	157 (100%)	0	0	100	100
2	aF	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
2	aH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	aJ	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	aL	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	aN	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	aP	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	bN	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	25	62
2	bP	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	bR	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	bT	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	bV	158/161 (98%)	157 (99%)	0	1 (1%)	25	62
2	bX	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	cB	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	cD	158/161 (98%)	158 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	cF	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	cH	158/161 (98%)	158 (100%)	0	0	100	100
2	cJ	158/161 (98%)	158 (100%)	0	0	100	100
2	cL	158/161 (98%)	158 (100%)	0	0	100	100
2	dB	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	dD	157/161 (98%)	157 (100%)	0	0	100	100
2	dF	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
2	dH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	dJ	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	dL	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	dN	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	dP	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	eN	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	25	62
2	eP	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	eR	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	eT	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	eV	158/161 (98%)	157 (99%)	0	1 (1%)	25	62
2	eX	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	fB	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	fD	158/161 (98%)	158 (100%)	0	0	100	100
2	fF	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	fH	158/161 (98%)	158 (100%)	0	0	100	100
2	fJ	158/161 (98%)	158 (100%)	0	0	100	100
2	fL	158/161 (98%)	158 (100%)	0	0	100	100
3	aM	1012/1139 (89%)	962 (95%)	50 (5%)	0	100	100
3	dM	1012/1139 (89%)	962 (95%)	50 (5%)	0	100	100
4	aR	166/169 (98%)	164 (99%)	2 (1%)	0	100	100
4	dR	166/169 (98%)	164 (99%)	2 (1%)	0	100	100
5	aS	64/67 (96%)	61 (95%)	3 (5%)	0	100	100
5	bY	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
5	cM	57/67 (85%)	57 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	dS	64/67 (96%)	61 (95%)	3 (5%)	0	100	100
5	eY	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
5	fM	57/67 (85%)	57 (100%)	0	0	100	100
All	All	15360/15898 (97%)	15120 (98%)	236 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	bV	77	THR
2	eV	77	THR
2	bN	77	THR
2	eN	77	THR

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	aA	123/130 (95%)	122 (99%)	1 (1%)	81	89
1	aC	56/130 (43%)	56 (100%)	0	100	100
1	aE	124/130 (95%)	123 (99%)	1 (1%)	81	89
1	aG	124/130 (95%)	124 (100%)	0	100	100
1	aI	128/130 (98%)	128 (100%)	0	100	100
1	aK	121/130 (93%)	120 (99%)	1 (1%)	81	89
1	aO	122/130 (94%)	121 (99%)	1 (1%)	81	89
1	aQ	128/130 (98%)	127 (99%)	1 (1%)	81	89
1	bM	129/130 (99%)	129 (100%)	0	100	100
1	bO	129/130 (99%)	126 (98%)	3 (2%)	50	71
1	bQ	128/130 (98%)	126 (98%)	2 (2%)	62	80
1	bS	125/130 (96%)	125 (100%)	0	100	100
1	bU	127/130 (98%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	bW	124/130 (95%)	123 (99%)	1 (1%)	81 89
1	cA	4/130 (3%)	4 (100%)	0	100 100
1	cC	12/130 (9%)	12 (100%)	0	100 100
1	cE	33/130 (25%)	33 (100%)	0	100 100
1	cI	2/130 (2%)	2 (100%)	0	100 100
1	cK	7/130 (5%)	7 (100%)	0	100 100
1	dA	123/130 (95%)	122 (99%)	1 (1%)	81 89
1	dC	56/130 (43%)	56 (100%)	0	100 100
1	dE	124/130 (95%)	123 (99%)	1 (1%)	81 89
1	dG	124/130 (95%)	124 (100%)	0	100 100
1	dI	128/130 (98%)	128 (100%)	0	100 100
1	dK	121/130 (93%)	120 (99%)	1 (1%)	81 89
1	dO	122/130 (94%)	121 (99%)	1 (1%)	81 89
1	dQ	128/130 (98%)	127 (99%)	1 (1%)	81 89
1	eM	129/130 (99%)	129 (100%)	0	100 100
1	eO	129/130 (99%)	126 (98%)	3 (2%)	50 71
1	eQ	128/130 (98%)	126 (98%)	2 (2%)	62 80
1	eS	125/130 (96%)	125 (100%)	0	100 100
1	eU	127/130 (98%)	127 (100%)	0	100 100
1	eW	124/130 (95%)	123 (99%)	1 (1%)	81 89
1	fA	4/130 (3%)	4 (100%)	0	100 100
1	fC	12/130 (9%)	12 (100%)	0	100 100
1	fE	33/130 (25%)	33 (100%)	0	100 100
1	fI	2/130 (2%)	2 (100%)	0	100 100
1	fK	7/130 (5%)	7 (100%)	0	100 100
2	aB	112/123 (91%)	112 (100%)	0	100 100
2	aD	115/123 (94%)	115 (100%)	0	100 100
2	aF	114/123 (93%)	114 (100%)	0	100 100
2	aH	123/123 (100%)	121 (98%)	2 (2%)	62 80
2	aJ	121/123 (98%)	120 (99%)	1 (1%)	81 89
2	aL	123/123 (100%)	122 (99%)	1 (1%)	81 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	aN	121/123 (98%)	121 (100%)	0	100	100
2	aP	123/123 (100%)	121 (98%)	2 (2%)	62	80
2	bN	123/123 (100%)	123 (100%)	0	100	100
2	bP	123/123 (100%)	122 (99%)	1 (1%)	81	89
2	bR	121/123 (98%)	120 (99%)	1 (1%)	81	89
2	bT	120/123 (98%)	118 (98%)	2 (2%)	60	79
2	bV	117/123 (95%)	116 (99%)	1 (1%)	78	88
2	bX	119/123 (97%)	119 (100%)	0	100	100
2	cB	2/123 (2%)	2 (100%)	0	100	100
2	cD	46/123 (37%)	45 (98%)	1 (2%)	52	72
2	cF	43/123 (35%)	43 (100%)	0	100	100
2	cJ	2/123 (2%)	2 (100%)	0	100	100
2	cL	1/123 (1%)	1 (100%)	0	100	100
2	dB	112/123 (91%)	112 (100%)	0	100	100
2	dD	115/123 (94%)	115 (100%)	0	100	100
2	dF	114/123 (93%)	114 (100%)	0	100	100
2	dH	123/123 (100%)	121 (98%)	2 (2%)	62	80
2	dJ	121/123 (98%)	120 (99%)	1 (1%)	81	89
2	dL	123/123 (100%)	122 (99%)	1 (1%)	81	89
2	dN	121/123 (98%)	121 (100%)	0	100	100
2	dP	123/123 (100%)	121 (98%)	2 (2%)	62	80
2	eN	123/123 (100%)	123 (100%)	0	100	100
2	eP	123/123 (100%)	122 (99%)	1 (1%)	81	89
2	eR	121/123 (98%)	120 (99%)	1 (1%)	81	89
2	eT	120/123 (98%)	118 (98%)	2 (2%)	60	79
2	eV	117/123 (95%)	116 (99%)	1 (1%)	78	88
2	eX	119/123 (97%)	119 (100%)	0	100	100
2	fB	2/123 (2%)	2 (100%)	0	100	100
2	fD	46/123 (37%)	45 (98%)	1 (2%)	52	72
2	fF	43/123 (35%)	43 (100%)	0	100	100
2	fJ	2/123 (2%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	fL	1/123 (1%)	1 (100%)	0	100 100
3	aM	791/956 (83%)	785 (99%)	6 (1%)	81 89
3	dM	791/956 (83%)	785 (99%)	6 (1%)	81 89
4	aR	134/135 (99%)	132 (98%)	2 (2%)	65 81
4	dR	134/135 (99%)	132 (98%)	2 (2%)	65 81
5	bY	51/60 (85%)	51 (100%)	0	100 100
5	eY	51/60 (85%)	51 (100%)	0	100 100
All	All	8982/11916 (75%)	8920 (99%)	62 (1%)	84 91

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	aA	119	TYR
1	aE	105	THR
2	aH	10	ASN
2	aH	86	ARG
2	aJ	115	LEU
1	aK	72	ASN
2	aL	90	TYR
3	aM	416	CYS
3	aM	446	ASP
3	aM	709	VAL
3	aM	904	LYS
3	aM	937	ILE
3	aM	1107	ASN
1	aO	119	TYR
2	aP	89	ASP
2	aP	90	TYR
1	aQ	27	ILE
4	aR	67	ILE
4	aR	78	ARG
1	bO	25	ASP
1	bO	72	ASN
1	bO	104	VAL
2	bP	65	ILE
1	bQ	66	VAL
1	bQ	72	ASN
2	bR	108	ASP
2	bT	126	ILE
2	bT	166	PHE

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Mol	Chain	Res	Type
2	bV	134	GLN
1	bW	66	VAL
2	cD	87	ASP
1	dA	119	TYR
1	dE	105	THR
2	dH	10	ASN
2	dH	86	ARG
2	dJ	115	LEU
1	dK	72	ASN
2	dL	90	TYR
3	dM	416	CYS
3	dM	446	ASP
3	dM	709	VAL
3	dM	904	LYS
3	dM	937	ILE
3	dM	1107	ASN
1	dO	119	TYR
2	dP	89	ASP
2	dP	90	TYR
1	dQ	27	ILE
4	dR	67	ILE
4	dR	78	ARG
1	eO	25	ASP
1	eO	72	ASN
1	eO	104	VAL
2	eP	65	ILE
1	eQ	66	VAL
1	eQ	72	ASN
2	eR	108	ASP
2	eT	126	ILE
2	eT	166	PHE
2	eV	134	GLN
1	eW	66	VAL
2	fD	87	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	aH	10	ASN
2	dH	10	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MEN	dR	72	4	7,8,9	1.15	1 (14%)	6,9,11	1.10	0
2	MEN	bN	71	2	7,8,9	1.09	1 (14%)	6,9,11	1.14	1 (16%)
2	MEN	cF	71	2	3,4,9	0.53	0	2,4,11	1.04	0
2	MEN	bP	71	2	7,8,9	1.13	1 (14%)	6,9,11	1.12	1 (16%)
2	MEN	dB	71	2	7,8,9	1.15	1 (14%)	6,9,11	0.90	0
2	MEN	aH	71	2	7,8,9	1.12	1 (14%)	6,9,11	1.26	1 (16%)
2	MEN	dF	71	2	7,8,9	1.17	1 (14%)	6,9,11	1.13	1 (16%)
2	MEN	cH	71	2	3,4,9	0.54	0	2,4,11	0.93	0
2	MEN	fL	71	2	3,4,9	0.53	0	2,4,11	0.99	0
2	MEN	aB	71	2	7,8,9	1.15	1 (14%)	6,9,11	0.90	0
2	MEN	dH	71	2	7,8,9	1.12	1 (14%)	6,9,11	1.26	1 (16%)
2	MEN	aD	71	2	7,8,9	1.15	1 (14%)	6,9,11	0.89	0
2	MEN	aN	71	2	7,8,9	1.12	1 (14%)	6,9,11	1.51	1 (16%)
2	MEN	bT	71	2	7,8,9	1.16	1 (14%)	6,9,11	1.12	1 (16%)
2	MEN	fJ	71	2	3,4,9	0.53	0	2,4,11	0.99	0
2	MEN	dP	71	2	7,8,9	1.14	1 (14%)	6,9,11	1.19	1 (16%)
2	MEN	aJ	71	2	7,8,9	1.18	1 (14%)	6,9,11	1.10	0
2	MEN	eV	71	2	7,8,9	1.17	1 (14%)	6,9,11	0.93	0
2	MEN	eT	71	2	7,8,9	1.16	1 (14%)	6,9,11	1.11	1 (16%)
2	MEN	fB	71	2	3,4,9	0.55	0	2,4,11	1.03	0
2	MEN	aF	71	2	7,8,9	1.17	1 (14%)	6,9,11	1.13	1 (16%)
2	MEN	aL	71	2	7,8,9	1.11	1 (14%)	6,9,11	1.37	1 (16%)
2	MEN	cL	71	2	3,4,9	0.54	0	2,4,11	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	dL	71	2	7,8,9	1.11	1 (14%)	6,9,11	1.37	1 (16%)
2	MEN	fF	71	2	3,4,9	0.52	0	2,4,11	1.04	0
2	MEN	bR	71	2	7,8,9	1.14	1 (14%)	6,9,11	1.27	1 (16%)
2	MEN	aP	71	2	7,8,9	1.14	1 (14%)	6,9,11	1.18	1 (16%)
2	MEN	dJ	71	2	7,8,9	1.18	1 (14%)	6,9,11	1.10	0
2	MEN	eR	71	2	7,8,9	1.14	1 (14%)	6,9,11	1.26	1 (16%)
2	MEN	fD	71	2	3,4,9	0.54	0	2,4,11	1.04	0
2	MEN	bX	71	2	7,8,9	1.15	1 (14%)	6,9,11	1.08	1 (16%)
4	MEN	aR	72	4	7,8,9	1.15	1 (14%)	6,9,11	1.10	0
2	MEN	bV	71	2	7,8,9	1.17	1 (14%)	6,9,11	0.93	0
2	MEN	eN	71	2	7,8,9	1.09	1 (14%)	6,9,11	1.14	1 (16%)
2	MEN	cD	71	2	3,4,9	0.54	0	2,4,11	1.04	0
2	MEN	cJ	71	2	3,4,9	0.53	0	2,4,11	0.99	0
2	MEN	dD	71	2	7,8,9	1.15	1 (14%)	6,9,11	0.89	0
2	MEN	dN	71	2	7,8,9	1.12	1 (14%)	6,9,11	1.51	1 (16%)
2	MEN	cB	71	2	3,4,9	0.54	0	2,4,11	1.03	0
2	MEN	eX	71	2	7,8,9	1.15	1 (14%)	6,9,11	1.08	1 (16%)
2	MEN	eP	71	2	7,8,9	1.13	1 (14%)	6,9,11	1.12	1 (16%)
2	MEN	fH	71	2	3,4,9	0.54	0	2,4,11	0.93	0

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
4	MEN	dR	72	4	-	4/7/8/10	-
2	MEN	bN	71	2	-	1/7/8/10	-
2	MEN	cF	71	2	-	0/0/2/10	-
2	MEN	bP	71	2	-	2/7/8/10	-
2	MEN	dB	71	2	-	4/7/8/10	-
2	MEN	aH	71	2	-	4/7/8/10	-
2	MEN	dF	71	2	-	0/7/8/10	-
2	MEN	cH	71	2	-	0/0/2/10	-
2	MEN	fL	71	2	-	0/0/2/10	-
2	MEN	aB	71	2	-	4/7/8/10	-
2	MEN	dH	71	2	-	4/7/8/10	-
2	MEN	aD	71	2	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	aN	71	2	-	5/7/8/10	-
2	MEN	bT	71	2	-	1/7/8/10	-
2	MEN	fJ	71	2	-	0/0/2/10	-
2	MEN	dP	71	2	-	2/7/8/10	-
2	MEN	aJ	71	2	-	4/7/8/10	-
2	MEN	eV	71	2	-	2/7/8/10	-
2	MEN	eT	71	2	-	1/7/8/10	-
2	MEN	fB	71	2	-	0/0/2/10	-
2	MEN	aF	71	2	-	0/7/8/10	-
2	MEN	aL	71	2	-	5/7/8/10	-
2	MEN	cL	71	2	-	0/0/2/10	-
2	MEN	dL	71	2	-	5/7/8/10	-
2	MEN	fF	71	2	-	0/0/2/10	-
2	MEN	bR	71	2	-	3/7/8/10	-
2	MEN	aP	71	2	-	2/7/8/10	-
2	MEN	dJ	71	2	-	4/7/8/10	-
2	MEN	eR	71	2	-	3/7/8/10	-
2	MEN	fD	71	2	-	0/0/2/10	-
2	MEN	bX	71	2	-	1/7/8/10	-
4	MEN	aR	72	4	-	4/7/8/10	-
2	MEN	bV	71	2	-	2/7/8/10	-
2	MEN	eN	71	2	-	1/7/8/10	-
2	MEN	cD	71	2	-	0/0/2/10	-
2	MEN	cJ	71	2	-	0/0/2/10	-
2	MEN	dD	71	2	-	2/7/8/10	-
2	MEN	dN	71	2	-	5/7/8/10	-
2	MEN	cB	71	2	-	0/0/2/10	-
2	MEN	eX	71	2	-	1/7/8/10	-
2	MEN	eP	71	2	-	2/7/8/10	-
2	MEN	fH	71	2	-	0/0/2/10	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	aF	71	MEN	CE2-ND2	2.96	1.50	1.45
2	dF	71	MEN	CE2-ND2	2.96	1.50	1.45
2	bV	71	MEN	CE2-ND2	2.96	1.50	1.45
2	eV	71	MEN	CE2-ND2	2.96	1.50	1.45
2	eT	71	MEN	CE2-ND2	2.93	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	bX	71	MEN	CE2-ND2	2.93	1.50	1.45
2	eX	71	MEN	CE2-ND2	2.92	1.50	1.45
2	bT	71	MEN	CE2-ND2	2.92	1.50	1.45
2	dD	71	MEN	CE2-ND2	2.92	1.50	1.45
2	aD	71	MEN	CE2-ND2	2.92	1.50	1.45
2	eR	71	MEN	CE2-ND2	2.91	1.50	1.45
2	bR	71	MEN	CE2-ND2	2.91	1.50	1.45
2	dP	71	MEN	CE2-ND2	2.90	1.50	1.45
2	aP	71	MEN	CE2-ND2	2.90	1.50	1.45
2	dJ	71	MEN	CE2-ND2	2.89	1.50	1.45
2	aJ	71	MEN	CE2-ND2	2.89	1.50	1.45
2	bP	71	MEN	CE2-ND2	2.88	1.50	1.45
2	dB	71	MEN	CE2-ND2	2.87	1.50	1.45
2	aB	71	MEN	CE2-ND2	2.87	1.50	1.45
2	eP	71	MEN	CE2-ND2	2.87	1.50	1.45
2	dH	71	MEN	CE2-ND2	2.86	1.50	1.45
2	aH	71	MEN	CE2-ND2	2.86	1.50	1.45
2	aN	71	MEN	CE2-ND2	2.84	1.50	1.45
2	dN	71	MEN	CE2-ND2	2.84	1.50	1.45
4	aR	72	MEN	CE2-ND2	2.82	1.50	1.45
4	dR	72	MEN	CE2-ND2	2.82	1.50	1.45
2	aL	71	MEN	CE2-ND2	2.81	1.50	1.45
2	dL	71	MEN	CE2-ND2	2.81	1.50	1.45
2	bN	71	MEN	CE2-ND2	2.77	1.50	1.45
2	eN	71	MEN	CE2-ND2	2.77	1.50	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	aL	71	MEN	CB-CA-C	-2.96	105.92	111.47
2	dL	71	MEN	CB-CA-C	-2.96	105.92	111.47
2	aN	71	MEN	CB-CA-C	-2.95	105.94	111.47
2	dN	71	MEN	CB-CA-C	-2.95	105.94	111.47
2	bR	71	MEN	CB-CA-C	-2.78	106.25	111.47
2	eR	71	MEN	CB-CA-C	-2.77	106.27	111.47
2	aH	71	MEN	CB-CA-C	-2.71	106.39	111.47
2	dH	71	MEN	CB-CA-C	-2.71	106.39	111.47
2	dP	71	MEN	CB-CA-C	-2.55	106.68	111.47
2	aP	71	MEN	CB-CA-C	-2.55	106.69	111.47
2	eP	71	MEN	CB-CA-C	-2.42	106.94	111.47
2	bP	71	MEN	CB-CA-C	-2.41	106.94	111.47
2	aF	71	MEN	CB-CA-C	-2.40	106.97	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	dF	71	MEN	CB-CA-C	-2.40	106.97	111.47
2	bN	71	MEN	CB-CA-C	-2.39	106.99	111.47
2	eN	71	MEN	CB-CA-C	-2.39	106.99	111.47
2	eT	71	MEN	CB-CA-C	-2.32	107.12	111.47
2	bT	71	MEN	CB-CA-C	-2.32	107.12	111.47
2	bX	71	MEN	CB-CA-C	-2.17	107.41	111.47
2	eX	71	MEN	CB-CA-C	-2.16	107.42	111.47

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	aB	71	MEN	C-CA-CB-CG
2	aJ	71	MEN	C-CA-CB-CG
2	aL	71	MEN	O-C-CA-CB
2	aL	71	MEN	C-CA-CB-CG
2	aN	71	MEN	O-C-CA-CB
2	aN	71	MEN	C-CA-CB-CG
2	dB	71	MEN	C-CA-CB-CG
2	dJ	71	MEN	C-CA-CB-CG
2	dL	71	MEN	O-C-CA-CB
2	dL	71	MEN	C-CA-CB-CG
2	dN	71	MEN	O-C-CA-CB
2	dN	71	MEN	N-CA-CB-CG
2	dN	71	MEN	C-CA-CB-CG
2	aB	71	MEN	N-CA-CB-CG
2	aH	71	MEN	N-CA-CB-CG
2	aJ	71	MEN	N-CA-CB-CG
2	aL	71	MEN	N-CA-CB-CG
2	aN	71	MEN	N-CA-CB-CG
4	aR	72	MEN	N-CA-CB-CG
2	dB	71	MEN	N-CA-CB-CG
2	dH	71	MEN	N-CA-CB-CG
2	dJ	71	MEN	N-CA-CB-CG
2	dL	71	MEN	N-CA-CB-CG
4	dR	72	MEN	N-CA-CB-CG
2	aJ	71	MEN	CA-CB-CG-OD1
2	aN	71	MEN	CA-CB-CG-OD1
2	aP	71	MEN	CA-CB-CG-OD1
2	dJ	71	MEN	CA-CB-CG-OD1
2	dN	71	MEN	CA-CB-CG-OD1
2	dP	71	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	aJ	71	MEN	CA-CB-CG-ND2
2	aL	71	MEN	CA-CB-CG-ND2
2	bR	71	MEN	CA-CB-CG-ND2
2	dJ	71	MEN	CA-CB-CG-ND2
2	dL	71	MEN	CA-CB-CG-ND2
2	eR	71	MEN	CA-CB-CG-ND2
2	aH	71	MEN	CA-CB-CG-OD1
2	aL	71	MEN	CA-CB-CG-OD1
4	aR	72	MEN	CA-CB-CG-OD1
2	bP	71	MEN	CA-CB-CG-OD1
2	bR	71	MEN	CA-CB-CG-OD1
2	dH	71	MEN	CA-CB-CG-OD1
2	dL	71	MEN	CA-CB-CG-OD1
4	dR	72	MEN	CA-CB-CG-OD1
2	eP	71	MEN	CA-CB-CG-OD1
2	eR	71	MEN	CA-CB-CG-OD1
2	aN	71	MEN	CA-CB-CG-ND2
4	aR	72	MEN	CA-CB-CG-ND2
2	dN	71	MEN	CA-CB-CG-ND2
4	dR	72	MEN	CA-CB-CG-ND2
2	aH	71	MEN	C-CA-CB-CG
4	aR	72	MEN	C-CA-CB-CG
2	dH	71	MEN	C-CA-CB-CG
4	dR	72	MEN	C-CA-CB-CG
2	aD	71	MEN	CA-CB-CG-OD1
2	dD	71	MEN	CA-CB-CG-OD1
2	aD	71	MEN	CA-CB-CG-ND2
2	aH	71	MEN	CA-CB-CG-ND2
2	aP	71	MEN	CA-CB-CG-ND2
2	bP	71	MEN	CA-CB-CG-ND2
2	dD	71	MEN	CA-CB-CG-ND2
2	dH	71	MEN	CA-CB-CG-ND2
2	dP	71	MEN	CA-CB-CG-ND2
2	eP	71	MEN	CA-CB-CG-ND2
2	bR	71	MEN	N-CA-CB-CG
2	eR	71	MEN	N-CA-CB-CG
2	bV	71	MEN	CA-CB-CG-OD1
2	eV	71	MEN	CA-CB-CG-OD1
2	bX	71	MEN	CA-CB-CG-OD1
2	eX	71	MEN	CA-CB-CG-OD1
2	aB	71	MEN	CA-CB-CG-OD1
2	bN	71	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	bT	71	MEN	CA-CB-CG-OD1
2	dB	71	MEN	CA-CB-CG-OD1
2	eN	71	MEN	CA-CB-CG-OD1
2	eT	71	MEN	CA-CB-CG-OD1
2	aB	71	MEN	CA-CB-CG-ND2
2	bV	71	MEN	CA-CB-CG-ND2
2	dB	71	MEN	CA-CB-CG-ND2
2	eV	71	MEN	CA-CB-CG-ND2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

84 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	aN	201	2	42,46,46	2.14	12 (28%)	50,67,67	3.36	21 (42%)
6	CYC	cB	201	-	42,46,46	2.16	13 (30%)	50,67,67	3.30	23 (46%)
6	CYC	fL	201	-	42,46,46	2.15	13 (30%)	50,67,67	3.27	23 (46%)
6	CYC	aC	201	1	42,46,46	2.13	12 (28%)	50,67,67	3.39	23 (46%)
6	CYC	bX	201	2	42,46,46	2.13	13 (30%)	50,67,67	3.32	20 (40%)
6	CYC	fI	201	-	42,46,46	2.16	12 (28%)	50,67,67	3.31	22 (44%)
6	CYC	aQ	201	1	42,46,46	2.16	12 (28%)	50,67,67	3.44	21 (42%)
6	CYC	dH	201	2	42,46,46	2.15	13 (30%)	50,67,67	3.34	24 (48%)
6	CYC	bN	201	2	42,46,46	2.14	12 (28%)	50,67,67	3.44	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CYC	aM	1202	-	42,46,46	2.15	13 (30%)	50,67,67	3.27	23 (46%)
6	CYC	eO	201	1	42,46,46	2.16	12 (28%)	50,67,67	3.39	22 (44%)
6	CYC	bM	201	1	42,46,46	2.15	12 (28%)	50,67,67	3.34	22 (44%)
6	CYC	fG	201	-	42,46,46	2.16	13 (30%)	50,67,67	3.30	23 (46%)
6	CYC	bR	201	2	42,46,46	2.13	12 (28%)	50,67,67	3.38	22 (44%)
6	CYC	cF	202	-	42,46,46	2.13	13 (30%)	50,67,67	3.33	21 (42%)
6	CYC	aD	201	2	42,46,46	2.12	12 (28%)	50,67,67	3.32	17 (34%)
6	CYC	aO	201	1	42,46,46	2.19	14 (33%)	50,67,67	3.31	22 (44%)
6	CYC	eV	201	2	42,46,46	2.14	12 (28%)	50,67,67	3.35	20 (40%)
6	CYC	dQ	201	1	42,46,46	2.16	12 (28%)	50,67,67	3.44	21 (42%)
6	CYC	cD	202	-	42,46,46	2.14	12 (28%)	50,67,67	3.33	24 (48%)
6	CYC	aA	201	1	42,46,46	2.13	12 (28%)	50,67,67	3.37	21 (42%)
6	CYC	dG	201	1	42,46,46	2.14	12 (28%)	50,67,67	3.37	20 (40%)
6	CYC	eT	201	2	42,46,46	2.15	14 (33%)	50,67,67	3.42	22 (44%)
6	CYC	dD	201	2	42,46,46	2.12	12 (28%)	50,67,67	3.32	17 (34%)
6	CYC	dM	1203	-	42,46,46	2.12	13 (30%)	50,67,67	3.29	21 (42%)
6	CYC	aK	201	1	42,46,46	2.14	13 (30%)	50,67,67	3.43	22 (44%)
6	CYC	bV	201	2	42,46,46	2.14	12 (28%)	50,67,67	3.35	20 (40%)
6	CYC	eN	201	2	42,46,46	2.13	12 (28%)	50,67,67	3.44	21 (42%)
6	CYC	eM	201	1	42,46,46	2.15	12 (28%)	50,67,67	3.33	22 (44%)
6	CYC	cG	201	-	42,46,46	2.16	13 (30%)	50,67,67	3.30	23 (46%)
6	CYC	bT	201	2	42,46,46	2.15	14 (33%)	50,67,67	3.42	22 (44%)
6	CYC	eX	201	2	42,46,46	2.13	13 (30%)	50,67,67	3.32	20 (40%)
6	CYC	dO	201	1	42,46,46	2.19	14 (33%)	50,67,67	3.31	22 (44%)
6	CYC	dA	201	1	42,46,46	2.12	12 (28%)	50,67,67	3.37	21 (42%)
6	CYC	dE	201	1	42,46,46	2.17	12 (28%)	50,67,67	3.41	24 (48%)
6	CYC	aL	201	2	42,46,46	2.15	12 (28%)	50,67,67	3.47	22 (44%)
6	CYC	fD	202	-	42,46,46	2.14	12 (28%)	50,67,67	3.33	24 (48%)
6	CYC	dM	1202	-	42,46,46	2.15	13 (30%)	50,67,67	3.27	23 (46%)
6	CYC	bP	201	2	42,46,46	2.13	12 (28%)	50,67,67	3.33	19 (38%)
6	CYC	fJ	201	-	42,46,46	2.16	13 (30%)	50,67,67	3.34	22 (44%)
6	CYC	dN	201	2	42,46,46	2.14	12 (28%)	50,67,67	3.36	21 (42%)
6	CYC	bU	201	1	42,46,46	2.16	12 (28%)	50,67,67	3.41	23 (46%)
6	CYC	dI	201	1	42,46,46	2.15	12 (28%)	50,67,67	3.49	23 (46%)
6	CYC	cL	201	-	42,46,46	2.15	13 (30%)	50,67,67	3.28	23 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CYC	aJ	201	2	42,46,46	2.14	13 (30%)	50,67,67	3.62	23 (46%)
6	CYC	fB	201	-	42,46,46	2.16	13 (30%)	50,67,67	3.30	23 (46%)
6	CYC	eQ	201	1	42,46,46	2.15	13 (30%)	50,67,67	3.29	21 (42%)
6	CYC	cJ	201	-	42,46,46	2.16	13 (30%)	50,67,67	3.34	22 (44%)
6	CYC	fM	101	-	42,46,46	2.14	13 (30%)	50,67,67	3.22	22 (44%)
6	CYC	aM	1203	-	42,46,46	2.12	13 (30%)	50,67,67	3.30	21 (42%)
6	CYC	dL	201	2	42,46,46	2.15	12 (28%)	50,67,67	3.47	22 (44%)
6	CYC	eW	201	1	42,46,46	2.16	13 (30%)	50,67,67	3.29	22 (44%)
6	CYC	cD	201	-	42,46,46	2.14	13 (30%)	50,67,67	3.23	21 (42%)
6	CYC	dJ	201	2	42,46,46	2.14	13 (30%)	50,67,67	3.62	23 (46%)
6	CYC	aH	201	2	42,46,46	2.15	13 (30%)	50,67,67	3.34	24 (48%)
6	CYC	eR	201	2	42,46,46	2.13	12 (28%)	50,67,67	3.38	22 (44%)
6	CYC	dC	201	1	42,46,46	2.13	12 (28%)	50,67,67	3.39	23 (46%)
6	CYC	cF	201	-	42,46,46	2.15	13 (30%)	50,67,67	3.34	22 (44%)
6	CYC	aB	201	2	42,46,46	2.14	13 (30%)	50,67,67	3.31	21 (42%)
6	CYC	aM	1201	3	42,46,46	2.17	13 (30%)	50,67,67	3.44	24 (48%)
6	CYC	bS	201	1	42,46,46	2.15	12 (28%)	50,67,67	3.42	22 (44%)
6	CYC	eP	201	2	42,46,46	2.13	12 (28%)	50,67,67	3.33	19 (38%)
6	CYC	aF	201	2	42,46,46	2.13	12 (28%)	50,67,67	3.31	18 (36%)
6	CYC	aG	201	1	42,46,46	2.14	12 (28%)	50,67,67	3.37	20 (40%)
6	CYC	aI	201	1	42,46,46	2.15	12 (28%)	50,67,67	3.49	23 (46%)
6	CYC	dK	201	1	42,46,46	2.14	13 (30%)	50,67,67	3.43	22 (44%)
6	CYC	fF	201	-	42,46,46	2.15	13 (30%)	50,67,67	3.34	22 (44%)
6	CYC	dM	1201	3	42,46,46	2.17	12 (28%)	50,67,67	3.44	24 (48%)
6	CYC	eS	201	1	42,46,46	2.15	12 (28%)	50,67,67	3.42	22 (44%)
6	CYC	dF	201	2	42,46,46	2.13	12 (28%)	50,67,67	3.32	18 (36%)
6	CYC	aP	201	2	42,46,46	2.18	11 (26%)	50,67,67	3.44	23 (46%)
6	CYC	bO	201	1	42,46,46	2.16	12 (28%)	50,67,67	3.39	22 (44%)
6	CYC	aE	201	1	42,46,46	2.17	12 (28%)	50,67,67	3.42	24 (48%)
6	CYC	bQ	201	1	42,46,46	2.15	13 (30%)	50,67,67	3.29	21 (42%)
6	CYC	cI	201	-	42,46,46	2.16	12 (28%)	50,67,67	3.30	22 (44%)
6	CYC	dB	201	2	42,46,46	2.14	13 (30%)	50,67,67	3.32	21 (42%)
6	CYC	aM	1204	4,3	42,46,46	2.24	13 (30%)	50,67,67	3.35	22 (44%)
6	CYC	fF	202	-	42,46,46	2.13	13 (30%)	50,67,67	3.32	21 (42%)
6	CYC	cM	101	-	42,46,46	2.14	13 (30%)	50,67,67	3.22	22 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CYC	fD	201	-	42,46,46	2.14	13 (30%)	50,67,67	3.23	21 (42%)
6	CYC	eU	201	1	42,46,46	2.16	12 (28%)	50,67,67	3.41	23 (46%)
6	CYC	dR	201	4	42,46,46	2.24	13 (30%)	50,67,67	3.35	22 (44%)
6	CYC	dP	201	2	42,46,46	2.18	11 (26%)	50,67,67	3.44	23 (46%)
6	CYC	bW	201	1	42,46,46	2.16	13 (30%)	50,67,67	3.29	22 (44%)

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	aN	201	2	-	10/25/74/74	0/4/4/4
6	CYC	cB	201	-	-	10/25/74/74	0/4/4/4
6	CYC	fL	201	-	-	11/25/74/74	0/4/4/4
6	CYC	aC	201	1	-	9/25/74/74	0/4/4/4
6	CYC	bX	201	2	-	8/25/74/74	0/4/4/4
6	CYC	fI	201	-	-	12/25/74/74	0/4/4/4
6	CYC	aQ	201	1	-	9/25/74/74	0/4/4/4
6	CYC	dH	201	2	-	10/25/74/74	0/4/4/4
6	CYC	bN	201	2	-	9/25/74/74	0/4/4/4
6	CYC	aM	1202	-	-	10/25/74/74	0/4/4/4
6	CYC	eO	201	1	-	8/25/74/74	0/4/4/4
6	CYC	bM	201	1	-	11/25/74/74	0/4/4/4
6	CYC	fG	201	-	-	9/25/74/74	0/4/4/4
6	CYC	bR	201	2	-	10/25/74/74	0/4/4/4
6	CYC	cF	202	-	-	10/25/74/74	0/4/4/4
6	CYC	aD	201	2	-	9/25/74/74	0/4/4/4
6	CYC	aO	201	1	-	9/25/74/74	0/4/4/4
6	CYC	eV	201	2	-	8/25/74/74	0/4/4/4
6	CYC	dQ	201	1	-	9/25/74/74	0/4/4/4
6	CYC	cD	202	-	-	10/25/74/74	0/4/4/4
6	CYC	aA	201	1	-	9/25/74/74	0/4/4/4
6	CYC	dG	201	1	-	13/25/74/74	0/4/4/4
6	CYC	eT	201	2	-	11/25/74/74	0/4/4/4
6	CYC	dD	201	2	-	9/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	dM	1203	-	-	9/25/74/74	0/4/4/4
6	CYC	aK	201	1	-	10/25/74/74	0/4/4/4
6	CYC	bV	201	2	-	8/25/74/74	0/4/4/4
6	CYC	eN	201	2	-	9/25/74/74	0/4/4/4
6	CYC	eM	201	1	-	11/25/74/74	0/4/4/4
6	CYC	cG	201	-	-	9/25/74/74	0/4/4/4
6	CYC	bT	201	2	-	11/25/74/74	0/4/4/4
6	CYC	eX	201	2	-	8/25/74/74	0/4/4/4
6	CYC	dO	201	1	-	9/25/74/74	0/4/4/4
6	CYC	dA	201	1	-	9/25/74/74	0/4/4/4
6	CYC	dE	201	1	-	11/25/74/74	0/4/4/4
6	CYC	aL	201	2	-	7/25/74/74	0/4/4/4
6	CYC	fD	202	-	-	10/25/74/74	0/4/4/4
6	CYC	dM	1202	-	-	10/25/74/74	0/4/4/4
6	CYC	bP	201	2	-	9/25/74/74	0/4/4/4
6	CYC	fJ	201	-	-	9/25/74/74	0/4/4/4
6	CYC	dN	201	2	-	10/25/74/74	0/4/4/4
6	CYC	bU	201	1	-	9/25/74/74	0/4/4/4
6	CYC	dI	201	1	-	9/25/74/74	0/4/4/4
6	CYC	cL	201	-	-	11/25/74/74	0/4/4/4
6	CYC	aJ	201	2	-	14/25/74/74	0/4/4/4
6	CYC	fB	201	-	-	10/25/74/74	0/4/4/4
6	CYC	eQ	201	1	-	10/25/74/74	0/4/4/4
6	CYC	cJ	201	-	-	9/25/74/74	0/4/4/4
6	CYC	fM	101	-	-	12/25/74/74	0/4/4/4
6	CYC	aM	1203	-	-	9/25/74/74	0/4/4/4
6	CYC	dL	201	2	-	7/25/74/74	0/4/4/4
6	CYC	eW	201	1	-	10/25/74/74	0/4/4/4
6	CYC	cD	201	-	-	10/25/74/74	0/4/4/4
6	CYC	dJ	201	2	-	14/25/74/74	0/4/4/4
6	CYC	aH	201	2	-	10/25/74/74	0/4/4/4
6	CYC	eR	201	2	-	10/25/74/74	0/4/4/4
6	CYC	dC	201	1	-	9/25/74/74	0/4/4/4
6	CYC	cF	201	-	-	12/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	aB	201	2	-	10/25/74/74	0/4/4/4
6	CYC	aM	1201	3	-	12/25/74/74	0/4/4/4
6	CYC	bS	201	1	-	14/25/74/74	0/4/4/4
6	CYC	eP	201	2	-	9/25/74/74	0/4/4/4
6	CYC	aF	201	2	-	12/25/74/74	0/4/4/4
6	CYC	aG	201	1	-	13/25/74/74	0/4/4/4
6	CYC	aI	201	1	-	9/25/74/74	0/4/4/4
6	CYC	dK	201	1	-	10/25/74/74	0/4/4/4
6	CYC	fF	201	-	-	12/25/74/74	0/4/4/4
6	CYC	dM	1201	3	-	12/25/74/74	0/4/4/4
6	CYC	eS	201	1	-	14/25/74/74	0/4/4/4
6	CYC	dF	201	2	-	12/25/74/74	0/4/4/4
6	CYC	aP	201	2	-	11/25/74/74	0/4/4/4
6	CYC	bO	201	1	-	8/25/74/74	0/4/4/4
6	CYC	aE	201	1	-	11/25/74/74	0/4/4/4
6	CYC	bQ	201	1	-	10/25/74/74	0/4/4/4
6	CYC	cI	201	-	-	12/25/74/74	0/4/4/4
6	CYC	dB	201	2	-	10/25/74/74	0/4/4/4
6	CYC	aM	1204	4,3	-	11/25/74/74	0/4/4/4
6	CYC	fF	202	-	-	10/25/74/74	0/4/4/4
6	CYC	cM	101	-	-	12/25/74/74	0/4/4/4
6	CYC	fD	201	-	-	10/25/74/74	0/4/4/4
6	CYC	eU	201	1	-	9/25/74/74	0/4/4/4
6	CYC	dR	201	4	-	11/25/74/74	0/4/4/4
6	CYC	dP	201	2	-	10/25/74/74	0/4/4/4
6	CYC	bW	201	1	-	10/25/74/74	0/4/4/4

All (1051) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	dE	201	CYC	OB-C4B	7.05	1.37	1.23
6	aE	201	CYC	OB-C4B	7.04	1.37	1.23
6	fB	201	CYC	OB-C4B	7.04	1.37	1.23
6	cB	201	CYC	OB-C4B	7.04	1.37	1.23
6	cI	201	CYC	OB-C4B	7.04	1.37	1.23
6	fI	201	CYC	OB-C4B	7.04	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	dC	201	CYC	OB-C4B	7.03	1.37	1.23
6	aC	201	CYC	OB-C4B	7.03	1.37	1.23
6	eW	201	CYC	OB-C4B	7.02	1.36	1.23
6	cG	201	CYC	OB-C4B	7.01	1.36	1.23
6	fG	201	CYC	OB-C4B	7.01	1.36	1.23
6	bW	201	CYC	OB-C4B	7.00	1.36	1.23
6	fD	202	CYC	OB-C4B	6.99	1.36	1.23
6	cD	202	CYC	OB-C4B	6.98	1.36	1.23
6	aD	201	CYC	OB-C4B	6.98	1.36	1.23
6	dD	201	CYC	OB-C4B	6.98	1.36	1.23
6	fJ	201	CYC	OB-C4B	6.98	1.36	1.23
6	bS	201	CYC	OB-C4B	6.98	1.36	1.23
6	eS	201	CYC	OB-C4B	6.98	1.36	1.23
6	eN	201	CYC	OB-C4B	6.97	1.36	1.23
6	cJ	201	CYC	OB-C4B	6.97	1.36	1.23
6	aM	1202	CYC	OB-C4B	6.97	1.36	1.23
6	bN	201	CYC	OB-C4B	6.97	1.36	1.23
6	dM	1202	CYC	OB-C4B	6.97	1.36	1.23
6	dB	201	CYC	OB-C4B	6.96	1.36	1.23
6	fM	101	CYC	OB-C4B	6.96	1.36	1.23
6	eU	201	CYC	OB-C4B	6.96	1.36	1.23
6	aB	201	CYC	OB-C4B	6.96	1.36	1.23
6	bU	201	CYC	OB-C4B	6.96	1.36	1.23
6	aM	1203	CYC	OB-C4B	6.95	1.36	1.23
6	dM	1203	CYC	OB-C4B	6.95	1.36	1.23
6	cM	101	CYC	OB-C4B	6.95	1.36	1.23
6	fD	201	CYC	OB-C4B	6.94	1.36	1.23
6	cD	201	CYC	OB-C4B	6.94	1.36	1.23
6	aA	201	CYC	OB-C4B	6.93	1.36	1.23
6	dK	201	CYC	OB-C4B	6.93	1.36	1.23
6	aK	201	CYC	OB-C4B	6.93	1.36	1.23
6	dA	201	CYC	OB-C4B	6.93	1.36	1.23
6	cF	202	CYC	OB-C4B	6.93	1.36	1.23
6	fF	202	CYC	OB-C4B	6.92	1.36	1.23
6	cL	201	CYC	OB-C4B	6.92	1.36	1.23
6	fL	201	CYC	OB-C4B	6.92	1.36	1.23
6	aF	201	CYC	OB-C4B	6.91	1.36	1.23
6	dF	201	CYC	OB-C4B	6.91	1.36	1.23
6	bQ	201	CYC	OB-C4B	6.90	1.36	1.23
6	eQ	201	CYC	OB-C4B	6.89	1.36	1.23
6	eO	201	CYC	OB-C4B	6.89	1.36	1.23
6	bO	201	CYC	OB-C4B	6.89	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	bM	201	CYC	OB-C4B	6.88	1.36	1.23
6	eM	201	CYC	OB-C4B	6.88	1.36	1.23
6	eT	201	CYC	OB-C4B	6.87	1.36	1.23
6	bT	201	CYC	OB-C4B	6.86	1.36	1.23
6	eV	201	CYC	OB-C4B	6.86	1.36	1.23
6	dQ	201	CYC	OB-C4B	6.85	1.36	1.23
6	bV	201	CYC	OB-C4B	6.85	1.36	1.23
6	aQ	201	CYC	OB-C4B	6.85	1.36	1.23
6	eP	201	CYC	OB-C4B	6.85	1.36	1.23
6	bX	201	CYC	OB-C4B	6.85	1.36	1.23
6	dG	201	CYC	OB-C4B	6.85	1.36	1.23
6	eX	201	CYC	OB-C4B	6.85	1.36	1.23
6	aG	201	CYC	OB-C4B	6.85	1.36	1.23
6	bP	201	CYC	OB-C4B	6.85	1.36	1.23
6	aO	201	CYC	OB-C4B	6.81	1.36	1.23
6	dO	201	CYC	OB-C4B	6.81	1.36	1.23
6	aP	201	CYC	OB-C4B	6.80	1.36	1.23
6	dP	201	CYC	OB-C4B	6.80	1.36	1.23
6	aN	201	CYC	OB-C4B	6.79	1.36	1.23
6	dN	201	CYC	OB-C4B	6.78	1.36	1.23
6	aI	201	CYC	OB-C4B	6.78	1.36	1.23
6	dI	201	CYC	OB-C4B	6.78	1.36	1.23
6	dH	201	CYC	OB-C4B	6.75	1.36	1.23
6	aH	201	CYC	OB-C4B	6.74	1.36	1.23
6	eR	201	CYC	OB-C4B	6.68	1.36	1.23
6	bR	201	CYC	OB-C4B	6.67	1.36	1.23
6	cF	201	CYC	OB-C4B	6.63	1.36	1.23
6	fF	201	CYC	OB-C4B	6.62	1.36	1.23
6	aJ	201	CYC	OB-C4B	6.61	1.36	1.23
6	dJ	201	CYC	OB-C4B	6.61	1.36	1.23
6	aM	1204	CYC	OB-C4B	6.60	1.36	1.23
6	dR	201	CYC	OB-C4B	6.60	1.36	1.23
6	dL	201	CYC	OB-C4B	6.55	1.36	1.23
6	aL	201	CYC	OB-C4B	6.54	1.36	1.23
6	dM	1201	CYC	OB-C4B	6.49	1.35	1.23
6	aM	1201	CYC	OB-C4B	6.48	1.35	1.23
6	aO	201	CYC	C1C-NC	-6.29	1.29	1.37
6	dO	201	CYC	C1C-NC	-6.29	1.29	1.37
6	aM	1204	CYC	C1C-NC	-6.09	1.29	1.37
6	dR	201	CYC	C1C-NC	-6.08	1.29	1.37
6	aJ	201	CYC	C1C-NC	-5.99	1.29	1.37
6	dJ	201	CYC	C1C-NC	-5.98	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	aP	201	CYC	C1C-NC	-5.85	1.30	1.37
6	dP	201	CYC	C1C-NC	-5.84	1.30	1.37
6	bO	201	CYC	C1C-NC	-5.80	1.30	1.37
6	eO	201	CYC	C1C-NC	-5.79	1.30	1.37
6	aL	201	CYC	C1C-NC	-5.79	1.30	1.37
6	dL	201	CYC	C1C-NC	-5.79	1.30	1.37
6	dQ	201	CYC	C1C-NC	-5.72	1.30	1.37
6	aQ	201	CYC	C1C-NC	-5.72	1.30	1.37
6	bQ	201	CYC	C1C-NC	-5.66	1.30	1.37
6	eQ	201	CYC	C1C-NC	-5.66	1.30	1.37
6	aH	201	CYC	C1C-NC	-5.65	1.30	1.37
6	dH	201	CYC	C1C-NC	-5.65	1.30	1.37
6	dI	201	CYC	C1C-NC	-5.64	1.30	1.37
6	aI	201	CYC	C1C-NC	-5.64	1.30	1.37
6	dM	1201	CYC	C1C-NC	-5.61	1.30	1.37
6	aM	1201	CYC	C1C-NC	-5.60	1.30	1.37
6	aE	201	CYC	C1C-NC	-5.56	1.30	1.37
6	dE	201	CYC	C1C-NC	-5.56	1.30	1.37
6	aN	201	CYC	C1C-NC	-5.53	1.30	1.37
6	dN	201	CYC	C1C-NC	-5.53	1.30	1.37
6	cD	202	CYC	C1C-NC	-5.52	1.30	1.37
6	fD	202	CYC	C1C-NC	-5.52	1.30	1.37
6	cJ	201	CYC	C1C-NC	-5.50	1.30	1.37
6	fJ	201	CYC	C1C-NC	-5.48	1.30	1.37
6	bN	201	CYC	C1C-NC	-5.46	1.30	1.37
6	fF	201	CYC	C1C-NC	-5.46	1.30	1.37
6	fI	201	CYC	C1C-NC	-5.45	1.30	1.37
6	cI	201	CYC	C1C-NC	-5.45	1.30	1.37
6	cF	201	CYC	C1C-NC	-5.44	1.30	1.37
6	eN	201	CYC	C1C-NC	-5.44	1.30	1.37
6	bU	201	CYC	C1C-NC	-5.44	1.30	1.37
6	eU	201	CYC	C1C-NC	-5.44	1.30	1.37
6	bW	201	CYC	C1C-NC	-5.42	1.30	1.37
6	eW	201	CYC	C1C-NC	-5.42	1.30	1.37
6	eM	201	CYC	C1C-NC	-5.41	1.30	1.37
6	bM	201	CYC	C1C-NC	-5.41	1.30	1.37
6	cD	201	CYC	C1C-NC	-5.34	1.30	1.37
6	fD	201	CYC	C1C-NC	-5.34	1.30	1.37
6	bP	201	CYC	C1C-NC	-5.28	1.30	1.37
6	cG	201	CYC	C1C-NC	-5.28	1.30	1.37
6	fG	201	CYC	C1C-NC	-5.28	1.30	1.37
6	eP	201	CYC	C1C-NC	-5.28	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	cB	201	CYC	C1C-NC	-5.28	1.30	1.37
6	fB	201	CYC	C1C-NC	-5.27	1.30	1.37
6	eR	201	CYC	C1C-NC	-5.24	1.30	1.37
6	bR	201	CYC	C1C-NC	-5.23	1.30	1.37
6	eT	201	CYC	C1C-NC	-5.23	1.30	1.37
6	bT	201	CYC	C1C-NC	-5.22	1.30	1.37
6	aK	201	CYC	C1C-NC	-5.22	1.30	1.37
6	dK	201	CYC	C1C-NC	-5.21	1.30	1.37
6	dD	201	CYC	C1C-NC	-5.18	1.30	1.37
6	aD	201	CYC	C1C-NC	-5.18	1.30	1.37
6	fF	202	CYC	C1C-NC	-5.14	1.30	1.37
6	cF	202	CYC	C1C-NC	-5.13	1.31	1.37
6	bS	201	CYC	C1C-NC	-5.08	1.31	1.37
6	eS	201	CYC	C1C-NC	-5.07	1.31	1.37
6	dG	201	CYC	C1C-NC	-5.06	1.31	1.37
6	aG	201	CYC	C1C-NC	-5.05	1.31	1.37
6	eV	201	CYC	C1C-NC	-5.03	1.31	1.37
6	bV	201	CYC	C1C-NC	-5.02	1.31	1.37
6	dF	201	CYC	C1C-NC	-5.01	1.31	1.37
6	aF	201	CYC	C1C-NC	-5.01	1.31	1.37
6	fL	201	CYC	C1C-NC	-5.01	1.31	1.37
6	cL	201	CYC	C1C-NC	-5.01	1.31	1.37
6	aB	201	CYC	C1C-NC	-5.00	1.31	1.37
6	dB	201	CYC	C1C-NC	-5.00	1.31	1.37
6	eX	201	CYC	C1C-NC	-4.99	1.31	1.37
6	bX	201	CYC	C1C-NC	-4.99	1.31	1.37
6	aA	201	CYC	C1C-NC	-4.97	1.31	1.37
6	aC	201	CYC	C1C-NC	-4.97	1.31	1.37
6	dA	201	CYC	C1C-NC	-4.97	1.31	1.37
6	dM	1202	CYC	C1C-NC	-4.97	1.31	1.37
6	dC	201	CYC	C1C-NC	-4.96	1.31	1.37
6	aM	1202	CYC	C1C-NC	-4.96	1.31	1.37
6	cM	101	CYC	C1C-NC	-4.93	1.31	1.37
6	fM	101	CYC	C1C-NC	-4.92	1.31	1.37
6	aM	1203	CYC	C1C-NC	-4.79	1.31	1.37
6	dM	1203	CYC	C1C-NC	-4.79	1.31	1.37
6	cG	201	CYC	OC-C1C	4.72	1.32	1.23
6	fG	201	CYC	OC-C1C	4.72	1.32	1.23
6	cB	201	CYC	OC-C1C	4.72	1.32	1.23
6	fB	201	CYC	OC-C1C	4.71	1.32	1.23
6	aM	1203	CYC	OC-C1C	4.70	1.32	1.23
6	dM	1203	CYC	OC-C1C	4.69	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	dM	1202	CYC	OC-C1C	4.68	1.32	1.23
6	aM	1202	CYC	OC-C1C	4.68	1.32	1.23
6	fL	201	CYC	OC-C1C	4.66	1.32	1.23
6	cL	201	CYC	OC-C1C	4.66	1.32	1.23
6	cM	101	CYC	OC-C1C	4.66	1.32	1.23
6	fM	101	CYC	OC-C1C	4.65	1.32	1.23
6	eX	201	CYC	OC-C1C	4.64	1.32	1.23
6	fI	201	CYC	OC-C1C	4.64	1.32	1.23
6	cI	201	CYC	OC-C1C	4.64	1.32	1.23
6	bX	201	CYC	OC-C1C	4.64	1.32	1.23
6	fF	202	CYC	OC-C1C	4.64	1.32	1.23
6	cF	202	CYC	OC-C1C	4.63	1.32	1.23
6	fF	201	CYC	OC-C1C	4.60	1.32	1.23
6	cF	201	CYC	OC-C1C	4.60	1.32	1.23
6	bM	201	CYC	OC-C1C	4.59	1.32	1.23
6	eM	201	CYC	OC-C1C	4.59	1.32	1.23
6	fJ	201	CYC	OC-C1C	4.58	1.32	1.23
6	cJ	201	CYC	OC-C1C	4.58	1.32	1.23
6	bV	201	CYC	OC-C1C	4.57	1.32	1.23
6	eV	201	CYC	OC-C1C	4.57	1.32	1.23
6	dD	201	CYC	OC-C1C	4.55	1.32	1.23
6	aD	201	CYC	OC-C1C	4.55	1.32	1.23
6	aB	201	CYC	OC-C1C	4.54	1.32	1.23
6	dB	201	CYC	OC-C1C	4.54	1.32	1.23
6	eT	201	CYC	OC-C1C	4.52	1.32	1.23
6	cD	201	CYC	OC-C1C	4.52	1.32	1.23
6	fD	201	CYC	OC-C1C	4.52	1.32	1.23
6	bT	201	CYC	OC-C1C	4.52	1.32	1.23
6	aF	201	CYC	OC-C1C	4.51	1.32	1.23
6	dF	201	CYC	OC-C1C	4.51	1.32	1.23
6	cD	202	CYC	OC-C1C	4.49	1.32	1.23
6	fD	202	CYC	OC-C1C	4.49	1.32	1.23
6	aG	201	CYC	OC-C1C	4.48	1.32	1.23
6	eP	201	CYC	OC-C1C	4.48	1.32	1.23
6	dG	201	CYC	OC-C1C	4.48	1.32	1.23
6	bR	201	CYC	OC-C1C	4.47	1.32	1.23
6	bP	201	CYC	OC-C1C	4.47	1.32	1.23
6	eR	201	CYC	OC-C1C	4.47	1.32	1.23
6	dK	201	CYC	OC-C1C	4.44	1.32	1.23
6	aK	201	CYC	OC-C1C	4.44	1.32	1.23
6	dA	201	CYC	OC-C1C	4.44	1.32	1.23
6	aA	201	CYC	OC-C1C	4.44	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	bU	201	CYC	OC-C1C	4.43	1.32	1.23
6	eU	201	CYC	OC-C1C	4.43	1.32	1.23
6	dC	201	CYC	OC-C1C	4.42	1.32	1.23
6	aC	201	CYC	OC-C1C	4.42	1.32	1.23
6	aI	201	CYC	OC-C1C	4.39	1.32	1.23
6	dI	201	CYC	OC-C1C	4.39	1.32	1.23
6	eW	201	CYC	OC-C1C	4.37	1.32	1.23
6	bQ	201	CYC	OC-C1C	4.37	1.32	1.23
6	bW	201	CYC	OC-C1C	4.36	1.32	1.23
6	eQ	201	CYC	OC-C1C	4.36	1.32	1.23
6	aM	1204	CYC	OC-C1C	4.36	1.32	1.23
6	dE	201	CYC	OC-C1C	4.36	1.32	1.23
6	aE	201	CYC	OC-C1C	4.35	1.32	1.23
6	dR	201	CYC	OC-C1C	4.35	1.32	1.23
6	dQ	201	CYC	OC-C1C	4.35	1.32	1.23
6	bS	201	CYC	OC-C1C	4.34	1.32	1.23
6	aQ	201	CYC	OC-C1C	4.34	1.32	1.23
6	eS	201	CYC	OC-C1C	4.34	1.32	1.23
6	eN	201	CYC	OC-C1C	4.34	1.32	1.23
6	bN	201	CYC	OC-C1C	4.33	1.32	1.23
6	dN	201	CYC	OC-C1C	4.33	1.32	1.23
6	aN	201	CYC	OC-C1C	4.33	1.32	1.23
6	aP	201	CYC	OC-C1C	4.29	1.31	1.23
6	dP	201	CYC	OC-C1C	4.29	1.31	1.23
6	aM	1201	CYC	OC-C1C	4.27	1.31	1.23
6	dH	201	CYC	OC-C1C	4.27	1.31	1.23
6	dM	1201	CYC	OC-C1C	4.27	1.31	1.23
6	aH	201	CYC	OC-C1C	4.26	1.31	1.23
6	dL	201	CYC	OC-C1C	4.24	1.31	1.23
6	aL	201	CYC	OC-C1C	4.24	1.31	1.23
6	aJ	201	CYC	OC-C1C	4.21	1.31	1.23
6	dJ	201	CYC	OC-C1C	4.20	1.31	1.23
6	bO	201	CYC	OC-C1C	4.20	1.31	1.23
6	eO	201	CYC	OC-C1C	4.20	1.31	1.23
6	dR	201	CYC	C4B-C3B	-4.12	1.40	1.48
6	aM	1204	CYC	C4B-C3B	-4.12	1.40	1.48
6	aO	201	CYC	OC-C1C	3.95	1.31	1.23
6	dO	201	CYC	OC-C1C	3.95	1.31	1.23
6	aM	1204	CYC	C4B-NB	-3.57	1.30	1.38
6	dR	201	CYC	C4B-NB	-3.57	1.30	1.38
6	eS	201	CYC	C2A-C3A	3.50	1.44	1.36
6	bS	201	CYC	C2A-C3A	3.50	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	eS	201	CYC	CHB-C4A	3.41	1.48	1.40
6	bS	201	CYC	CHB-C4A	3.41	1.48	1.40
6	dM	1201	CYC	C4B-NB	-3.40	1.30	1.38
6	dB	201	CYC	CHB-C4A	3.40	1.48	1.40
6	aM	1201	CYC	C4B-NB	-3.40	1.30	1.38
6	aB	201	CYC	CHB-C4A	3.39	1.48	1.40
6	cG	201	CYC	CHB-C4A	3.39	1.48	1.40
6	cI	201	CYC	CHB-C4A	3.39	1.48	1.40
6	fI	201	CYC	CHB-C4A	3.39	1.48	1.40
6	aG	201	CYC	C2A-C3A	3.39	1.43	1.36
6	dG	201	CYC	C2A-C3A	3.39	1.43	1.36
6	fG	201	CYC	CHB-C4A	3.39	1.48	1.40
6	aC	201	CYC	CHB-C4A	3.37	1.48	1.40
6	cJ	201	CYC	CHB-C4A	3.37	1.48	1.40
6	dC	201	CYC	CHB-C4A	3.37	1.48	1.40
6	aM	1201	CYC	CHB-C4A	3.37	1.48	1.40
6	fJ	201	CYC	CHB-C4A	3.37	1.48	1.40
6	fF	201	CYC	CHB-C4A	3.37	1.48	1.40
6	dM	1201	CYC	CHB-C4A	3.37	1.48	1.40
6	cF	201	CYC	CHB-C4A	3.36	1.48	1.40
6	cD	202	CYC	CHB-C4A	3.36	1.48	1.40
6	bW	201	CYC	CHB-C4A	3.36	1.48	1.40
6	fD	202	CYC	CHB-C4A	3.36	1.48	1.40
6	eW	201	CYC	CHB-C4A	3.36	1.48	1.40
6	aK	201	CYC	CHB-C4A	3.34	1.48	1.40
6	dK	201	CYC	CHB-C4A	3.33	1.48	1.40
6	fB	201	CYC	CHB-C4A	3.32	1.48	1.40
6	cB	201	CYC	CHB-C4A	3.31	1.48	1.40
6	dM	1202	CYC	CHB-C4A	3.30	1.48	1.40
6	aM	1202	CYC	CHB-C4A	3.30	1.48	1.40
6	dA	201	CYC	CHB-C4A	3.30	1.48	1.40
6	cM	101	CYC	CHB-C4A	3.30	1.48	1.40
6	fM	101	CYC	CHB-C4A	3.30	1.48	1.40
6	aA	201	CYC	CHB-C4A	3.29	1.48	1.40
6	aC	201	CYC	C2C-C3C	-3.29	1.45	1.54
6	dI	201	CYC	C2C-C3C	-3.29	1.45	1.54
6	dC	201	CYC	C2C-C3C	-3.29	1.45	1.54
6	aI	201	CYC	C2C-C3C	-3.28	1.45	1.54
6	eR	201	CYC	CHB-C4A	3.28	1.48	1.40
6	bR	201	CYC	CHB-C4A	3.28	1.48	1.40
6	bQ	201	CYC	CHB-C4A	3.28	1.48	1.40
6	eQ	201	CYC	CHB-C4A	3.28	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	dE	201	CYC	CHB-C4A	3.27	1.48	1.40
6	aE	201	CYC	CHB-C4A	3.27	1.48	1.40
6	eM	201	CYC	CHB-C4A	3.26	1.48	1.40
6	eU	201	CYC	CHB-C4A	3.26	1.48	1.40
6	bM	201	CYC	CHB-C4A	3.26	1.48	1.40
6	bU	201	CYC	CHB-C4A	3.26	1.48	1.40
6	dH	201	CYC	CHB-C4A	3.23	1.48	1.40
6	aH	201	CYC	CHB-C4A	3.23	1.48	1.40
6	dN	201	CYC	CHB-C4A	3.23	1.48	1.40
6	fB	201	CYC	C2A-C3A	3.22	1.43	1.36
6	cB	201	CYC	C2A-C3A	3.22	1.43	1.36
6	aN	201	CYC	CHB-C4A	3.22	1.48	1.40
6	fL	201	CYC	CHB-C4A	3.22	1.48	1.40
6	cL	201	CYC	CHB-C4A	3.22	1.48	1.40
6	eO	201	CYC	CHB-C4A	3.21	1.47	1.40
6	bO	201	CYC	CHB-C4A	3.21	1.47	1.40
6	bN	201	CYC	CHB-C4A	3.21	1.47	1.40
6	aM	1201	CYC	C3D-C2D	3.21	1.47	1.37
6	dM	1201	CYC	C3D-C2D	3.21	1.47	1.37
6	cD	201	CYC	CHB-C4A	3.21	1.47	1.40
6	cI	201	CYC	C2A-C3A	3.21	1.43	1.36
6	eV	201	CYC	CHB-C4A	3.20	1.47	1.40
6	fD	201	CYC	CHB-C4A	3.20	1.47	1.40
6	aF	201	CYC	C3D-C2D	3.20	1.47	1.37
6	dF	201	CYC	C3D-C2D	3.20	1.47	1.37
6	bV	201	CYC	CHB-C4A	3.20	1.47	1.40
6	dE	201	CYC	C2A-C3A	3.20	1.43	1.36
6	eN	201	CYC	CHB-C4A	3.20	1.47	1.40
6	aE	201	CYC	C2A-C3A	3.19	1.43	1.36
6	aB	201	CYC	C3D-C2D	3.19	1.47	1.37
6	dB	201	CYC	C3D-C2D	3.19	1.47	1.37
6	dF	201	CYC	CHB-C4A	3.19	1.47	1.40
6	fI	201	CYC	C2A-C3A	3.19	1.43	1.36
6	aF	201	CYC	CHB-C4A	3.18	1.47	1.40
6	dD	201	CYC	C3D-C2D	3.18	1.47	1.37
6	aD	201	CYC	C3D-C2D	3.18	1.47	1.37
6	aO	201	CYC	CHB-C4A	3.18	1.47	1.40
6	dC	201	CYC	C2A-C3A	3.18	1.43	1.36
6	dO	201	CYC	CHB-C4A	3.18	1.47	1.40
6	aC	201	CYC	C2A-C3A	3.18	1.43	1.36
6	dM	1203	CYC	C2A-C3A	3.16	1.43	1.36
6	fG	201	CYC	C2A-C3A	3.16	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	cG	201	CYC	C2A-C3A	3.16	1.43	1.36
6	dM	1203	CYC	CHB-C4A	3.16	1.47	1.40
6	aC	201	CYC	C3D-C2D	3.16	1.47	1.37
6	dC	201	CYC	C3D-C2D	3.16	1.47	1.37
6	aM	1203	CYC	C2A-C3A	3.15	1.43	1.36
6	eU	201	CYC	C2A-C3A	3.15	1.43	1.36
6	bU	201	CYC	C2A-C3A	3.15	1.43	1.36
6	eO	201	CYC	C2C-C3C	-3.15	1.45	1.54
6	aM	1203	CYC	CHB-C4A	3.15	1.47	1.40
6	bV	201	CYC	C3D-C2D	3.15	1.47	1.37
6	eV	201	CYC	C3D-C2D	3.14	1.47	1.37
6	bO	201	CYC	C2C-C3C	-3.14	1.45	1.54
6	eX	201	CYC	CHB-C4A	3.14	1.47	1.40
6	bX	201	CYC	CHB-C4A	3.14	1.47	1.40
6	aQ	201	CYC	C2C-C3C	-3.13	1.45	1.54
6	cM	101	CYC	C3D-C2D	3.13	1.47	1.37
6	dQ	201	CYC	C2C-C3C	-3.13	1.45	1.54
6	fM	101	CYC	C3D-C2D	3.13	1.46	1.37
6	eW	201	CYC	C2A-C3A	3.13	1.43	1.36
6	cF	202	CYC	C2A-C3A	3.13	1.43	1.36
6	bP	201	CYC	CHB-C4A	3.13	1.47	1.40
6	eP	201	CYC	CHB-C4A	3.13	1.47	1.40
6	fJ	201	CYC	C2A-C3A	3.13	1.43	1.36
6	aM	1204	CYC	C2C-C3C	-3.13	1.45	1.54
6	aP	201	CYC	C2C-C3C	-3.13	1.45	1.54
6	cJ	201	CYC	C2A-C3A	3.13	1.43	1.36
6	fF	202	CYC	C2A-C3A	3.13	1.43	1.36
6	dP	201	CYC	C2C-C3C	-3.13	1.45	1.54
6	dR	201	CYC	C2C-C3C	-3.12	1.45	1.54
6	bW	201	CYC	C2A-C3A	3.12	1.43	1.36
6	bV	201	CYC	C2A-C3A	3.12	1.43	1.36
6	dH	201	CYC	C4B-C3B	-3.12	1.42	1.48
6	dN	201	CYC	C2A-C3A	3.12	1.43	1.36
6	eV	201	CYC	C2A-C3A	3.12	1.43	1.36
6	aN	201	CYC	C2A-C3A	3.12	1.43	1.36
6	dP	201	CYC	CHB-C4A	3.12	1.47	1.40
6	aK	201	CYC	C2C-C3C	-3.11	1.45	1.54
6	aP	201	CYC	CHB-C4A	3.11	1.47	1.40
6	aG	201	CYC	C2C-C3C	-3.11	1.45	1.54
6	dK	201	CYC	C2C-C3C	-3.11	1.45	1.54
6	dG	201	CYC	C2C-C3C	-3.11	1.45	1.54
6	aH	201	CYC	C4B-C3B	-3.11	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	dM	1203	CYC	C3D-C2D	3.11	1.46	1.37
6	aM	1203	CYC	C3D-C2D	3.10	1.46	1.37
6	aG	201	CYC	CHB-C4A	3.10	1.47	1.40
6	eT	201	CYC	C3D-C2D	3.09	1.46	1.37
6	cL	201	CYC	C2A-C3A	3.09	1.43	1.36
6	bT	201	CYC	C3D-C2D	3.09	1.46	1.37
6	dG	201	CYC	CHB-C4A	3.09	1.47	1.40
6	aE	201	CYC	C2C-C3C	-3.09	1.45	1.54
6	dE	201	CYC	C2C-C3C	-3.09	1.45	1.54
6	eN	201	CYC	C2C-C3C	-3.09	1.45	1.54
6	fL	201	CYC	C2A-C3A	3.09	1.43	1.36
6	bN	201	CYC	C2C-C3C	-3.09	1.45	1.54
6	aA	201	CYC	C2C-C3C	-3.09	1.45	1.54
6	dA	201	CYC	C2C-C3C	-3.09	1.45	1.54
6	aL	201	CYC	C4B-C3B	-3.08	1.42	1.48
6	aL	201	CYC	CHB-C4A	3.08	1.47	1.40
6	aD	201	CYC	C2A-C3A	3.08	1.43	1.36
6	dD	201	CYC	C2A-C3A	3.08	1.43	1.36
6	eX	201	CYC	C2A-C3A	3.07	1.43	1.36
6	dL	201	CYC	C4B-C3B	-3.07	1.42	1.48
6	dL	201	CYC	CHB-C4A	3.07	1.47	1.40
6	bX	201	CYC	C2A-C3A	3.07	1.43	1.36
6	eX	201	CYC	C3D-C2D	3.07	1.46	1.37
6	bR	201	CYC	C3D-C2D	3.07	1.46	1.37
6	bX	201	CYC	C3D-C2D	3.07	1.46	1.37
6	dF	201	CYC	C2A-C3A	3.06	1.43	1.36
6	eR	201	CYC	C3D-C2D	3.06	1.46	1.37
6	aF	201	CYC	C2A-C3A	3.06	1.43	1.36
6	cF	201	CYC	C2A-C3A	3.05	1.43	1.36
6	bO	201	CYC	C4B-C3B	-3.05	1.42	1.48
6	aM	1202	CYC	C3D-C2D	3.05	1.46	1.37
6	eO	201	CYC	C4B-C3B	-3.05	1.42	1.48
6	fF	201	CYC	C2A-C3A	3.05	1.43	1.36
6	dM	1202	CYC	C3D-C2D	3.05	1.46	1.37
6	aH	201	CYC	C4B-NB	-3.05	1.31	1.38
6	dH	201	CYC	C4B-NB	-3.04	1.31	1.38
6	bU	201	CYC	C2C-C3C	-3.04	1.46	1.54
6	aM	1201	CYC	C1B-NB	-3.04	1.32	1.37
6	aM	1202	CYC	C2A-C3A	3.04	1.43	1.36
6	fF	202	CYC	CHB-C4A	3.04	1.47	1.40
6	eU	201	CYC	C2C-C3C	-3.04	1.46	1.54
6	fM	101	CYC	C2A-C3A	3.04	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	dM	1202	CYC	C2A-C3A	3.04	1.43	1.36
6	cM	101	CYC	C2A-C3A	3.03	1.43	1.36
6	cF	202	CYC	CHB-C4A	3.03	1.47	1.40
6	dM	1201	CYC	C1B-NB	-3.03	1.32	1.37
6	aK	201	CYC	C2A-C3A	3.03	1.43	1.36
6	bN	201	CYC	C4B-C3B	-3.03	1.42	1.48
6	eN	201	CYC	C4B-C3B	-3.03	1.42	1.48
6	dK	201	CYC	C2A-C3A	3.03	1.43	1.36
6	fD	201	CYC	C3D-C2D	3.02	1.46	1.37
6	eS	201	CYC	C2C-C3C	-3.02	1.46	1.54
6	cD	201	CYC	C3D-C2D	3.02	1.46	1.37
6	bS	201	CYC	C2C-C3C	-3.02	1.46	1.54
6	cD	201	CYC	C2A-C3A	3.02	1.43	1.36
6	fL	201	CYC	C3D-C2D	3.02	1.46	1.37
6	eR	201	CYC	C2A-C3A	3.02	1.43	1.36
6	bP	201	CYC	C2C-C3C	-3.02	1.46	1.54
6	cL	201	CYC	C3D-C2D	3.01	1.46	1.37
6	fD	201	CYC	C2A-C3A	3.01	1.43	1.36
6	eP	201	CYC	C2C-C3C	-3.01	1.46	1.54
6	bR	201	CYC	C2A-C3A	3.01	1.43	1.36
6	bU	201	CYC	C3D-C2D	3.01	1.46	1.37
6	eU	201	CYC	C3D-C2D	3.01	1.46	1.37
6	aA	201	CYC	C3D-C2D	3.01	1.46	1.37
6	dA	201	CYC	C3D-C2D	3.01	1.46	1.37
6	eP	201	CYC	C3D-C2D	3.01	1.46	1.37
6	aA	201	CYC	C2A-C3A	3.00	1.43	1.36
6	dI	201	CYC	C2A-C3A	3.00	1.43	1.36
6	dG	201	CYC	C3D-C2D	3.00	1.46	1.37
6	aB	201	CYC	C2A-C3A	3.00	1.43	1.36
6	aG	201	CYC	C3D-C2D	3.00	1.46	1.37
6	cJ	201	CYC	C3D-C2D	3.00	1.46	1.37
6	fJ	201	CYC	C3D-C2D	3.00	1.46	1.37
6	eN	201	CYC	C2A-C3A	3.00	1.43	1.36
6	fF	202	CYC	C3D-C2D	3.00	1.46	1.37
6	dB	201	CYC	C2A-C3A	3.00	1.43	1.36
6	bN	201	CYC	C2A-C3A	3.00	1.43	1.36
6	aI	201	CYC	C2A-C3A	3.00	1.43	1.36
6	dA	201	CYC	C2A-C3A	3.00	1.43	1.36
6	bP	201	CYC	C3D-C2D	3.00	1.46	1.37
6	cF	202	CYC	C3D-C2D	3.00	1.46	1.37
6	eM	201	CYC	C2A-C3A	2.99	1.43	1.36
6	bM	201	CYC	C2A-C3A	2.99	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	aO	201	CYC	C4B-C3B	-2.99	1.42	1.48
6	dO	201	CYC	C4B-C3B	-2.99	1.42	1.48
6	bV	201	CYC	C4B-C3B	-2.98	1.42	1.48
6	cB	201	CYC	C3D-C2D	2.98	1.46	1.37
6	fB	201	CYC	C3D-C2D	2.98	1.46	1.37
6	eV	201	CYC	C4B-C3B	-2.98	1.42	1.48
6	aE	201	CYC	C3D-C2D	2.98	1.46	1.37
6	cG	201	CYC	C3D-C2D	2.98	1.46	1.37
6	dE	201	CYC	C3D-C2D	2.98	1.46	1.37
6	dK	201	CYC	C3D-C2D	2.98	1.46	1.37
6	fG	201	CYC	C3D-C2D	2.98	1.46	1.37
6	aK	201	CYC	C3D-C2D	2.98	1.46	1.37
6	eW	201	CYC	C3D-C2D	2.98	1.46	1.37
6	bW	201	CYC	C3D-C2D	2.97	1.46	1.37
6	aQ	201	CYC	C2A-C3A	2.97	1.43	1.36
6	dQ	201	CYC	C2A-C3A	2.97	1.43	1.36
6	dJ	201	CYC	C2C-C3C	-2.97	1.46	1.54
6	aJ	201	CYC	C2C-C3C	-2.97	1.46	1.54
6	cF	202	CYC	C4B-C3B	-2.96	1.42	1.48
6	fF	202	CYC	C4B-C3B	-2.96	1.42	1.48
6	aN	201	CYC	C3D-C2D	2.95	1.46	1.37
6	dQ	201	CYC	CHB-C4A	2.95	1.47	1.40
6	dL	201	CYC	C3D-C2D	2.95	1.46	1.37
6	aQ	201	CYC	CHB-C4A	2.95	1.47	1.40
6	aL	201	CYC	C3D-C2D	2.95	1.46	1.37
6	bU	201	CYC	C4B-C3B	-2.95	1.42	1.48
6	cD	202	CYC	C2A-C3A	2.95	1.43	1.36
6	dN	201	CYC	C3D-C2D	2.95	1.46	1.37
6	bN	201	CYC	C3D-C2D	2.95	1.46	1.37
6	eQ	201	CYC	C2A-C3A	2.95	1.43	1.36
6	bQ	201	CYC	C2A-C3A	2.95	1.43	1.36
6	fD	202	CYC	C2A-C3A	2.94	1.43	1.36
6	eN	201	CYC	C3D-C2D	2.94	1.46	1.37
6	eU	201	CYC	C4B-C3B	-2.94	1.42	1.48
6	dO	201	CYC	C2C-C3C	-2.94	1.46	1.54
6	eS	201	CYC	C3D-C2D	2.94	1.46	1.37
6	aO	201	CYC	C2C-C3C	-2.94	1.46	1.54
6	bR	201	CYC	C2C-C3C	-2.94	1.46	1.54
6	eO	201	CYC	C2A-C3A	2.94	1.43	1.36
6	aJ	201	CYC	C2A-C3A	2.94	1.43	1.36
6	aO	201	CYC	C2A-C3A	2.94	1.43	1.36
6	dO	201	CYC	C2A-C3A	2.94	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	bS	201	CYC	C3D-C2D	2.94	1.46	1.37
6	bW	201	CYC	C4B-C3B	-2.94	1.42	1.48
6	eR	201	CYC	C2C-C3C	-2.94	1.46	1.54
6	eW	201	CYC	C4B-C3B	-2.94	1.42	1.48
6	bO	201	CYC	C2A-C3A	2.94	1.43	1.36
6	dJ	201	CYC	C2A-C3A	2.94	1.43	1.36
6	dH	201	CYC	C2C-C3C	-2.93	1.46	1.54
6	aH	201	CYC	C2C-C3C	-2.93	1.46	1.54
6	dI	201	CYC	C4B-C3B	-2.93	1.42	1.48
6	aI	201	CYC	C4B-C3B	-2.92	1.42	1.48
6	bX	201	CYC	C4B-C3B	-2.92	1.42	1.48
6	dN	201	CYC	C4B-C3B	-2.92	1.42	1.48
6	eX	201	CYC	C4B-C3B	-2.92	1.42	1.48
6	aN	201	CYC	C4B-C3B	-2.92	1.42	1.48
6	bR	201	CYC	C4B-C3B	-2.91	1.42	1.48
6	aD	201	CYC	CHB-C4A	2.91	1.47	1.40
6	dD	201	CYC	CHB-C4A	2.91	1.47	1.40
6	eR	201	CYC	C4B-C3B	-2.91	1.42	1.48
6	dP	201	CYC	C4B-C3B	-2.91	1.42	1.48
6	aP	201	CYC	C4B-C3B	-2.91	1.42	1.48
6	dK	201	CYC	C4B-C3B	-2.90	1.42	1.48
6	aL	201	CYC	C2C-C3C	-2.90	1.46	1.54
6	dL	201	CYC	C2C-C3C	-2.90	1.46	1.54
6	aK	201	CYC	C4B-C3B	-2.90	1.42	1.48
6	dP	201	CYC	C3D-C2D	2.90	1.46	1.37
6	eR	201	CYC	C4B-NB	-2.90	1.31	1.38
6	bR	201	CYC	C4B-NB	-2.90	1.31	1.38
6	aP	201	CYC	C3D-C2D	2.90	1.46	1.37
6	dM	1202	CYC	C4B-C3B	-2.90	1.42	1.48
6	bM	201	CYC	C4B-C3B	-2.90	1.42	1.48
6	cL	201	CYC	C4B-C3B	-2.89	1.42	1.48
6	eM	201	CYC	C4B-C3B	-2.89	1.42	1.48
6	cJ	201	CYC	C4B-C3B	-2.89	1.42	1.48
6	fD	202	CYC	C4B-C3B	-2.89	1.42	1.48
6	cD	202	CYC	C4B-C3B	-2.89	1.42	1.48
6	bP	201	CYC	C2A-C3A	2.89	1.42	1.36
6	aJ	201	CYC	C4B-C3B	-2.89	1.42	1.48
6	fJ	201	CYC	C4B-C3B	-2.89	1.42	1.48
6	fL	201	CYC	C4B-C3B	-2.89	1.42	1.48
6	eV	201	CYC	C2C-C3C	-2.89	1.46	1.54
6	aM	1202	CYC	C4B-C3B	-2.88	1.42	1.48
6	dP	201	CYC	C2A-C3A	2.88	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	fM	101	CYC	C4B-C3B	-2.88	1.42	1.48
6	eP	201	CYC	C2A-C3A	2.88	1.42	1.36
6	bV	201	CYC	C2C-C3C	-2.88	1.46	1.54
6	dJ	201	CYC	C4B-C3B	-2.88	1.42	1.48
6	cM	101	CYC	C4B-C3B	-2.88	1.42	1.48
6	bT	201	CYC	CHB-C4A	2.88	1.47	1.40
6	aP	201	CYC	C2A-C3A	2.88	1.42	1.36
6	eQ	201	CYC	C4B-C3B	-2.88	1.42	1.48
6	dL	201	CYC	C4B-NB	-2.88	1.31	1.38
6	eT	201	CYC	CHB-C4A	2.88	1.47	1.40
6	dH	201	CYC	C3D-C2D	2.88	1.46	1.37
6	aL	201	CYC	C4B-NB	-2.87	1.31	1.38
6	aH	201	CYC	C3D-C2D	2.87	1.46	1.37
6	aP	201	CYC	C4B-NB	-2.87	1.31	1.38
6	bQ	201	CYC	C4B-C3B	-2.87	1.42	1.48
6	dM	1201	CYC	C2A-C3A	2.87	1.42	1.36
6	bT	201	CYC	C4B-C3B	-2.87	1.42	1.48
6	eT	201	CYC	C4B-C3B	-2.87	1.42	1.48
6	fI	201	CYC	C3D-C2D	2.87	1.46	1.37
6	dL	201	CYC	C2A-C3A	2.87	1.42	1.36
6	aL	201	CYC	C2A-C3A	2.87	1.42	1.36
6	dP	201	CYC	C4B-NB	-2.87	1.31	1.38
6	aM	1201	CYC	C2A-C3A	2.87	1.42	1.36
6	cI	201	CYC	C3D-C2D	2.87	1.46	1.37
6	eP	201	CYC	C4B-C3B	-2.86	1.42	1.48
6	aA	201	CYC	C4B-C3B	-2.86	1.42	1.48
6	bP	201	CYC	C4B-C3B	-2.86	1.42	1.48
6	cF	201	CYC	C4B-NB	-2.86	1.31	1.38
6	dA	201	CYC	C4B-C3B	-2.86	1.42	1.48
6	eM	201	CYC	C3D-C2D	2.86	1.46	1.37
6	fF	201	CYC	C4B-NB	-2.86	1.31	1.38
6	aB	201	CYC	C4B-C3B	-2.86	1.42	1.48
6	bM	201	CYC	C3D-C2D	2.85	1.46	1.37
6	cD	202	CYC	C3D-C2D	2.85	1.46	1.37
6	dB	201	CYC	C4B-C3B	-2.85	1.42	1.48
6	bO	201	CYC	C3D-C2D	2.85	1.46	1.37
6	eO	201	CYC	C3D-C2D	2.85	1.46	1.37
6	fD	202	CYC	C3D-C2D	2.85	1.46	1.37
6	aI	201	CYC	CHB-C4A	2.85	1.47	1.40
6	dI	201	CYC	CHB-C4A	2.84	1.47	1.40
6	aM	1204	CYC	C2A-C3A	2.84	1.42	1.36
6	aM	1201	CYC	C4B-C3B	-2.84	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	aN	201	CYC	C2C-C3C	-2.84	1.46	1.54
6	dN	201	CYC	C2C-C3C	-2.84	1.46	1.54
6	fF	201	CYC	C4B-C3B	-2.84	1.42	1.48
6	dR	201	CYC	C2A-C3A	2.84	1.42	1.36
6	dQ	201	CYC	C4B-C3B	-2.84	1.42	1.48
6	cF	201	CYC	C4B-C3B	-2.84	1.42	1.48
6	dM	1201	CYC	C4B-C3B	-2.84	1.42	1.48
6	aQ	201	CYC	C4B-C3B	-2.84	1.42	1.48
6	fF	201	CYC	C3D-C2D	2.84	1.46	1.37
6	fI	201	CYC	C4B-C3B	-2.84	1.42	1.48
6	cF	201	CYC	C3D-C2D	2.83	1.46	1.37
6	cI	201	CYC	C4B-C3B	-2.83	1.42	1.48
6	aO	201	CYC	C3D-C2D	2.83	1.46	1.37
6	dO	201	CYC	C3D-C2D	2.83	1.46	1.37
6	bQ	201	CYC	C3D-C2D	2.82	1.46	1.37
6	eQ	201	CYC	C3D-C2D	2.82	1.46	1.37
6	eT	201	CYC	C2A-C3A	2.81	1.42	1.36
6	bT	201	CYC	C2A-C3A	2.80	1.42	1.36
6	dD	201	CYC	C4B-C3B	-2.80	1.42	1.48
6	aM	1203	CYC	C4B-C3B	-2.80	1.42	1.48
6	aD	201	CYC	C4B-C3B	-2.80	1.42	1.48
6	dM	1203	CYC	C4B-C3B	-2.80	1.42	1.48
6	fM	101	CYC	C4B-NB	-2.80	1.32	1.38
6	cM	101	CYC	C4B-NB	-2.79	1.32	1.38
6	cG	201	CYC	C4B-C3B	-2.79	1.42	1.48
6	aB	201	CYC	C2C-C3C	-2.79	1.46	1.54
6	cB	201	CYC	C4B-C3B	-2.79	1.42	1.48
6	fG	201	CYC	C4B-C3B	-2.79	1.42	1.48
6	fB	201	CYC	C4B-C3B	-2.79	1.42	1.48
6	dB	201	CYC	C2C-C3C	-2.79	1.46	1.54
6	cL	201	CYC	C4B-NB	-2.78	1.32	1.38
6	bP	201	CYC	C4B-NB	-2.78	1.32	1.38
6	fL	201	CYC	C4B-NB	-2.78	1.32	1.38
6	aM	1201	CYC	C2C-C3C	-2.78	1.46	1.54
6	fD	201	CYC	C4B-C3B	-2.78	1.43	1.48
6	dM	1201	CYC	C2C-C3C	-2.78	1.46	1.54
6	eP	201	CYC	C4B-NB	-2.78	1.32	1.38
6	bV	201	CYC	C4B-NB	-2.77	1.32	1.38
6	eV	201	CYC	C4B-NB	-2.77	1.32	1.38
6	cD	201	CYC	C4B-C3B	-2.77	1.43	1.48
6	aH	201	CYC	C2A-C3A	2.77	1.42	1.36
6	dH	201	CYC	C2A-C3A	2.77	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	dJ	201	CYC	C3D-C2D	2.76	1.45	1.37
6	aJ	201	CYC	C3D-C2D	2.76	1.45	1.37
6	aN	201	CYC	C4B-NB	-2.76	1.32	1.38
6	dN	201	CYC	C4B-NB	-2.75	1.32	1.38
6	aM	1202	CYC	C4B-NB	-2.75	1.32	1.38
6	dM	1202	CYC	C4B-NB	-2.75	1.32	1.38
6	aQ	201	CYC	CAD-C3D	-2.75	1.48	1.52
6	bX	201	CYC	C4B-NB	-2.75	1.32	1.38
6	dQ	201	CYC	CAD-C3D	-2.75	1.48	1.52
6	eQ	201	CYC	C4B-NB	-2.74	1.32	1.38
6	eX	201	CYC	C4B-NB	-2.74	1.32	1.38
6	aG	201	CYC	C4B-C3B	-2.74	1.43	1.48
6	bQ	201	CYC	C4B-NB	-2.74	1.32	1.38
6	eT	201	CYC	C4B-NB	-2.74	1.32	1.38
6	aF	201	CYC	C2C-C3C	-2.74	1.46	1.54
6	bT	201	CYC	C4B-NB	-2.74	1.32	1.38
6	dG	201	CYC	C4B-C3B	-2.73	1.43	1.48
6	dF	201	CYC	C2C-C3C	-2.73	1.46	1.54
6	aC	201	CYC	C4B-C3B	-2.73	1.43	1.48
6	dC	201	CYC	C4B-C3B	-2.73	1.43	1.48
6	dF	201	CYC	C4B-NB	-2.72	1.32	1.38
6	aP	201	CYC	C1B-NB	-2.72	1.33	1.37
6	dP	201	CYC	C1B-NB	-2.72	1.33	1.37
6	aF	201	CYC	C4B-NB	-2.72	1.32	1.38
6	fD	201	CYC	C4B-NB	-2.72	1.32	1.38
6	cD	201	CYC	C4B-NB	-2.72	1.32	1.38
6	dR	201	CYC	C3D-C2D	2.71	1.45	1.37
6	aM	1204	CYC	C3D-C2D	2.71	1.45	1.37
6	dJ	201	CYC	CHB-C4A	2.71	1.46	1.40
6	dB	201	CYC	C4B-NB	-2.71	1.32	1.38
6	aB	201	CYC	C4B-NB	-2.70	1.32	1.38
6	aJ	201	CYC	CHB-C4A	2.70	1.46	1.40
6	dI	201	CYC	CAD-C3D	-2.70	1.48	1.52
6	dI	201	CYC	C3D-C2D	2.70	1.45	1.37
6	aI	201	CYC	C3D-C2D	2.69	1.45	1.37
6	aI	201	CYC	CAD-C3D	-2.69	1.48	1.52
6	eM	201	CYC	C4B-NB	-2.69	1.32	1.38
6	dE	201	CYC	C4B-C3B	-2.68	1.43	1.48
6	bM	201	CYC	C4B-NB	-2.68	1.32	1.38
6	aE	201	CYC	C4B-C3B	-2.68	1.43	1.48
6	eS	201	CYC	C4B-C3B	-2.68	1.43	1.48
6	cF	202	CYC	C4B-NB	-2.68	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	bS	201	CYC	C4B-C3B	-2.67	1.43	1.48
6	fD	202	CYC	C4B-NB	-2.67	1.32	1.38
6	aJ	201	CYC	CMB-C2B	-2.67	1.45	1.50
6	dJ	201	CYC	CMB-C2B	-2.67	1.45	1.50
6	aO	201	CYC	C4B-NB	-2.67	1.32	1.38
6	cD	202	CYC	C4B-NB	-2.67	1.32	1.38
6	fF	202	CYC	C4B-NB	-2.67	1.32	1.38
6	dO	201	CYC	C4B-NB	-2.66	1.32	1.38
6	bT	201	CYC	C2C-C3C	-2.66	1.47	1.54
6	dQ	201	CYC	C4B-NB	-2.66	1.32	1.38
6	eT	201	CYC	C2C-C3C	-2.66	1.47	1.54
6	aQ	201	CYC	C4B-NB	-2.65	1.32	1.38
6	eO	201	CYC	C4B-NB	-2.65	1.32	1.38
6	bO	201	CYC	C4B-NB	-2.65	1.32	1.38
6	aH	201	CYC	C1B-NB	-2.63	1.33	1.37
6	dH	201	CYC	C1B-NB	-2.63	1.33	1.37
6	dM	1203	CYC	C4B-NB	-2.62	1.32	1.38
6	aM	1203	CYC	C4B-NB	-2.62	1.32	1.38
6	aF	201	CYC	C4B-C3B	-2.62	1.43	1.48
6	dF	201	CYC	C4B-C3B	-2.62	1.43	1.48
6	bR	201	CYC	C1B-NB	-2.61	1.33	1.37
6	eR	201	CYC	C1B-NB	-2.61	1.33	1.37
6	bN	201	CYC	C4B-NB	-2.61	1.32	1.38
6	eN	201	CYC	C4B-NB	-2.61	1.32	1.38
6	cJ	201	CYC	C4B-NB	-2.61	1.32	1.38
6	aI	201	CYC	CMB-C2B	-2.60	1.45	1.50
6	fJ	201	CYC	C4B-NB	-2.60	1.32	1.38
6	dK	201	CYC	C4B-NB	-2.60	1.32	1.38
6	dI	201	CYC	CMB-C2B	-2.60	1.45	1.50
6	eW	201	CYC	C2C-C1C	2.59	1.54	1.52
6	aK	201	CYC	C4B-NB	-2.59	1.32	1.38
6	fG	201	CYC	C4B-NB	-2.59	1.32	1.38
6	cG	201	CYC	C4B-NB	-2.59	1.32	1.38
6	bW	201	CYC	C2C-C1C	2.59	1.54	1.52
6	aG	201	CYC	CMB-C2B	-2.58	1.45	1.50
6	dM	1202	CYC	C2C-C1C	2.58	1.54	1.52
6	bX	201	CYC	C2C-C3C	-2.58	1.47	1.54
6	eX	201	CYC	C2C-C3C	-2.58	1.47	1.54
6	dG	201	CYC	CMB-C2B	-2.57	1.45	1.50
6	bS	201	CYC	C4B-NB	-2.57	1.32	1.38
6	aQ	201	CYC	C3D-C2D	2.57	1.45	1.37
6	dQ	201	CYC	C3D-C2D	2.57	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	aM	1202	CYC	C2C-C1C	2.57	1.54	1.52
6	eS	201	CYC	C4B-NB	-2.57	1.32	1.38
6	aQ	201	CYC	C1B-NB	-2.57	1.33	1.37
6	dQ	201	CYC	CMB-C2B	-2.56	1.45	1.50
6	aQ	201	CYC	CMB-C2B	-2.56	1.45	1.50
6	dQ	201	CYC	C1B-NB	-2.56	1.33	1.37
6	aM	1201	CYC	CMB-C2B	-2.56	1.45	1.50
6	dM	1201	CYC	CMB-C2B	-2.55	1.45	1.50
6	cI	201	CYC	C4B-NB	-2.55	1.32	1.38
6	fI	201	CYC	C4B-NB	-2.55	1.32	1.38
6	dD	201	CYC	C4B-NB	-2.55	1.32	1.38
6	aD	201	CYC	C4B-NB	-2.55	1.32	1.38
6	aG	201	CYC	C4B-NB	-2.54	1.32	1.38
6	aL	201	CYC	C1B-NB	-2.54	1.33	1.37
6	dG	201	CYC	C4B-NB	-2.54	1.32	1.38
6	dL	201	CYC	C1B-NB	-2.54	1.33	1.37
6	fJ	201	CYC	C2C-C3C	-2.53	1.47	1.54
6	aD	201	CYC	C2C-C3C	-2.53	1.47	1.54
6	cJ	201	CYC	C2C-C3C	-2.53	1.47	1.54
6	fD	202	CYC	C2C-C3C	-2.53	1.47	1.54
6	dD	201	CYC	C2C-C3C	-2.52	1.47	1.54
6	fM	101	CYC	C2C-C1C	2.52	1.54	1.52
6	bW	201	CYC	C4B-NB	-2.52	1.32	1.38
6	aA	201	CYC	C4B-NB	-2.52	1.32	1.38
6	eW	201	CYC	C4B-NB	-2.52	1.32	1.38
6	dA	201	CYC	C4B-NB	-2.52	1.32	1.38
6	cD	202	CYC	C2C-C3C	-2.52	1.47	1.54
6	aO	201	CYC	CMB-C2B	-2.52	1.45	1.50
6	eU	201	CYC	C4B-NB	-2.51	1.32	1.38
6	bU	201	CYC	C4B-NB	-2.51	1.32	1.38
6	cM	101	CYC	C2C-C1C	2.51	1.54	1.52
6	dO	201	CYC	CMB-C2B	-2.51	1.45	1.50
6	cF	201	CYC	C1B-NB	-2.51	1.33	1.37
6	fF	201	CYC	C1B-NB	-2.51	1.33	1.37
6	eO	201	CYC	CMB-C2B	-2.50	1.45	1.50
6	cB	201	CYC	C4B-NB	-2.50	1.32	1.38
6	fB	201	CYC	C4B-NB	-2.50	1.32	1.38
6	bO	201	CYC	CMB-C2B	-2.50	1.45	1.50
6	bQ	201	CYC	C2C-C3C	-2.50	1.47	1.54
6	dN	201	CYC	C1B-NB	-2.50	1.33	1.37
6	dO	201	CYC	C1B-NB	-2.49	1.33	1.37
6	aO	201	CYC	C1B-NB	-2.49	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	eM	201	CYC	C2C-C3C	-2.49	1.47	1.54
6	aN	201	CYC	C1B-NB	-2.49	1.33	1.37
6	eQ	201	CYC	C2C-C3C	-2.49	1.47	1.54
6	fF	201	CYC	C2C-C3C	-2.49	1.47	1.54
6	cL	201	CYC	C2C-C1C	2.49	1.54	1.52
6	aM	1203	CYC	C2C-C1C	2.49	1.54	1.52
6	bM	201	CYC	C2C-C3C	-2.49	1.47	1.54
6	cF	201	CYC	C2C-C3C	-2.49	1.47	1.54
6	dM	1203	CYC	C2C-C1C	2.48	1.54	1.52
6	fL	201	CYC	C2C-C1C	2.48	1.54	1.52
6	fM	101	CYC	C2C-C3C	-2.48	1.47	1.54
6	dI	201	CYC	C4B-NB	-2.48	1.32	1.38
6	dF	201	CYC	C3B-C2B	2.48	1.42	1.36
6	aF	201	CYC	C3B-C2B	2.47	1.42	1.36
6	cM	101	CYC	C2C-C3C	-2.47	1.47	1.54
6	fI	201	CYC	C2C-C3C	-2.47	1.47	1.54
6	bU	201	CYC	CMB-C2B	-2.47	1.45	1.50
6	aI	201	CYC	C4B-NB	-2.47	1.32	1.38
6	cI	201	CYC	C2C-C3C	-2.47	1.47	1.54
6	eU	201	CYC	CMB-C2B	-2.47	1.45	1.50
6	aE	201	CYC	C4B-NB	-2.47	1.32	1.38
6	eT	201	CYC	C3B-C2B	2.46	1.41	1.36
6	dE	201	CYC	C4B-NB	-2.46	1.32	1.38
6	bT	201	CYC	C3B-C2B	2.46	1.41	1.36
6	dC	201	CYC	C4B-NB	-2.46	1.32	1.38
6	aB	201	CYC	C3B-C2B	2.45	1.41	1.36
6	dB	201	CYC	C3B-C2B	2.45	1.41	1.36
6	bP	201	CYC	C1B-NB	-2.44	1.33	1.37
6	cM	101	CYC	C3B-C2B	2.44	1.41	1.36
6	eP	201	CYC	C1B-NB	-2.44	1.33	1.37
6	fM	101	CYC	C3B-C2B	2.44	1.41	1.36
6	fF	202	CYC	C2C-C3C	-2.44	1.47	1.54
6	fD	201	CYC	C2C-C3C	-2.44	1.47	1.54
6	aC	201	CYC	C4B-NB	-2.43	1.32	1.38
6	cD	201	CYC	C2C-C3C	-2.43	1.47	1.54
6	cF	202	CYC	C2C-C3C	-2.43	1.47	1.54
6	bM	201	CYC	CMB-C2B	-2.43	1.45	1.50
6	eM	201	CYC	CMB-C2B	-2.43	1.45	1.50
6	aM	1202	CYC	C3B-C2B	2.42	1.41	1.36
6	dM	1202	CYC	C3B-C2B	2.42	1.41	1.36
6	aF	201	CYC	C1B-NB	-2.41	1.33	1.37
6	dF	201	CYC	C1B-NB	-2.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	aM	1202	CYC	C2C-C3C	-2.41	1.47	1.54
6	dM	1202	CYC	C2C-C3C	-2.41	1.47	1.54
6	eV	201	CYC	C1B-NB	-2.41	1.33	1.37
6	bV	201	CYC	C1B-NB	-2.40	1.33	1.37
6	dL	201	CYC	CMB-C2B	-2.40	1.45	1.50
6	bM	201	CYC	C1B-NB	-2.40	1.33	1.37
6	eM	201	CYC	C1B-NB	-2.40	1.33	1.37
6	dJ	201	CYC	C1B-NB	-2.40	1.33	1.37
6	aJ	201	CYC	C1B-NB	-2.40	1.33	1.37
6	cL	201	CYC	C3B-C2B	2.40	1.41	1.36
6	fL	201	CYC	C3B-C2B	2.40	1.41	1.36
6	aL	201	CYC	CMB-C2B	-2.40	1.45	1.50
6	dM	1203	CYC	C2C-C3C	-2.39	1.47	1.54
6	aM	1203	CYC	C2C-C3C	-2.39	1.47	1.54
6	dM	1201	CYC	C3B-C2B	2.39	1.41	1.36
6	aM	1201	CYC	C3B-C2B	2.38	1.41	1.36
6	cB	201	CYC	C2C-C1C	2.38	1.54	1.52
6	bO	201	CYC	C1B-NB	-2.38	1.33	1.37
6	cG	201	CYC	C2C-C3C	-2.38	1.47	1.54
6	fG	201	CYC	C2C-C3C	-2.38	1.47	1.54
6	fJ	201	CYC	C1B-NB	-2.38	1.33	1.37
6	eO	201	CYC	C1B-NB	-2.38	1.33	1.37
6	aM	1204	CYC	C1B-NB	-2.38	1.33	1.37
6	aP	201	CYC	CMB-C2B	-2.38	1.45	1.50
6	cB	201	CYC	C2C-C3C	-2.38	1.47	1.54
6	fB	201	CYC	C2C-C3C	-2.38	1.47	1.54
6	dR	201	CYC	C1B-NB	-2.38	1.33	1.37
6	dP	201	CYC	CMB-C2B	-2.37	1.45	1.50
6	dO	201	CYC	C2C-C1C	2.37	1.54	1.52
6	eQ	201	CYC	C1B-NB	-2.37	1.33	1.37
6	aN	201	CYC	CMB-C2B	-2.37	1.45	1.50
6	dN	201	CYC	CMB-C2B	-2.37	1.45	1.50
6	cJ	201	CYC	C1B-NB	-2.37	1.33	1.37
6	fB	201	CYC	C2C-C1C	2.37	1.54	1.52
6	aO	201	CYC	C2C-C1C	2.37	1.54	1.52
6	aJ	201	CYC	C4B-NB	-2.37	1.33	1.38
6	bQ	201	CYC	C1B-NB	-2.36	1.33	1.37
6	dJ	201	CYC	C4B-NB	-2.36	1.33	1.38
6	cM	101	CYC	C1B-NB	-2.36	1.33	1.37
6	dK	201	CYC	C1B-NB	-2.35	1.33	1.37
6	dM	1203	CYC	C3B-C2B	2.35	1.41	1.36
6	aK	201	CYC	C1B-NB	-2.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	aA	201	CYC	CMB-C2B	-2.35	1.45	1.50
6	fM	101	CYC	C1B-NB	-2.35	1.33	1.37
6	dA	201	CYC	CMB-C2B	-2.35	1.45	1.50
6	aM	1203	CYC	C3B-C2B	2.35	1.41	1.36
6	aH	201	CYC	CMB-C2B	-2.35	1.45	1.50
6	cL	201	CYC	C2C-C3C	-2.34	1.47	1.54
6	fL	201	CYC	C2C-C3C	-2.34	1.47	1.54
6	bN	201	CYC	C1B-NB	-2.34	1.33	1.37
6	bT	201	CYC	C1B-NB	-2.34	1.33	1.37
6	dH	201	CYC	CMB-C2B	-2.34	1.45	1.50
6	dM	1202	CYC	C1B-NB	-2.34	1.33	1.37
6	eT	201	CYC	C1B-NB	-2.34	1.33	1.37
6	dI	201	CYC	C1B-NB	-2.33	1.33	1.37
6	bV	201	CYC	C3B-C2B	2.33	1.41	1.36
6	fG	201	CYC	C3B-C2B	2.33	1.41	1.36
6	cD	202	CYC	C1B-NB	-2.33	1.33	1.37
6	aG	201	CYC	C1B-NB	-2.33	1.33	1.37
6	dG	201	CYC	C1B-NB	-2.33	1.33	1.37
6	aI	201	CYC	C1B-NB	-2.33	1.33	1.37
6	aM	1202	CYC	C1B-NB	-2.33	1.33	1.37
6	eV	201	CYC	C3B-C2B	2.33	1.41	1.36
6	fD	202	CYC	C1B-NB	-2.33	1.33	1.37
6	bX	201	CYC	C3B-C2B	2.33	1.41	1.36
6	cG	201	CYC	C3B-C2B	2.33	1.41	1.36
6	eN	201	CYC	C1B-NB	-2.32	1.33	1.37
6	cI	201	CYC	C3B-C2B	2.32	1.41	1.36
6	bX	201	CYC	C1B-NB	-2.32	1.33	1.37
6	fI	201	CYC	C3B-C2B	2.32	1.41	1.36
6	eQ	201	CYC	CMB-C2B	-2.32	1.45	1.50
6	cL	201	CYC	C1B-NB	-2.32	1.33	1.37
6	bQ	201	CYC	CMB-C2B	-2.32	1.45	1.50
6	bR	201	CYC	CMB-C2B	-2.32	1.45	1.50
6	eX	201	CYC	C3B-C2B	2.32	1.41	1.36
6	fL	201	CYC	C1B-NB	-2.31	1.33	1.37
6	eX	201	CYC	C1B-NB	-2.31	1.33	1.37
6	eR	201	CYC	CMB-C2B	-2.31	1.45	1.50
6	eW	201	CYC	C2C-C3C	-2.31	1.48	1.54
6	bW	201	CYC	C2C-C3C	-2.31	1.48	1.54
6	fG	201	CYC	C2C-C1C	2.30	1.54	1.52
6	eN	201	CYC	CMB-C2B	-2.30	1.45	1.50
6	bW	201	CYC	CMB-C2B	-2.30	1.45	1.50
6	eW	201	CYC	CMB-C2B	-2.30	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	fD	201	CYC	C1B-NB	-2.30	1.34	1.37
6	aK	201	CYC	CMB-C2B	-2.30	1.45	1.50
6	dK	201	CYC	CMB-C2B	-2.30	1.45	1.50
6	cG	201	CYC	C2C-C1C	2.29	1.54	1.52
6	cD	201	CYC	C1B-NB	-2.29	1.34	1.37
6	bN	201	CYC	CMB-C2B	-2.29	1.45	1.50
6	fD	202	CYC	CMB-C2B	-2.29	1.46	1.50
6	cD	202	CYC	CMB-C2B	-2.28	1.46	1.50
6	fD	201	CYC	C3B-C2B	2.28	1.41	1.36
6	eR	201	CYC	C3B-C2B	2.28	1.41	1.36
6	cD	201	CYC	C3B-C2B	2.28	1.41	1.36
6	bR	201	CYC	C3B-C2B	2.27	1.41	1.36
6	bU	201	CYC	C1B-NB	-2.27	1.34	1.37
6	eU	201	CYC	C1B-NB	-2.27	1.34	1.37
6	bP	201	CYC	CMB-C2B	-2.27	1.46	1.50
6	eP	201	CYC	CMB-C2B	-2.27	1.46	1.50
6	fG	201	CYC	C1B-NB	-2.26	1.34	1.37
6	cG	201	CYC	C1B-NB	-2.26	1.34	1.37
6	cF	201	CYC	CMB-C2B	-2.26	1.46	1.50
6	fJ	201	CYC	CMB-C2B	-2.26	1.46	1.50
6	fI	201	CYC	C1B-NB	-2.25	1.34	1.37
6	cB	201	CYC	C3B-C2B	2.25	1.41	1.36
6	cI	201	CYC	C1B-NB	-2.25	1.34	1.37
6	aF	201	CYC	CMB-C2B	-2.25	1.46	1.50
6	dF	201	CYC	CMB-C2B	-2.25	1.46	1.50
6	fB	201	CYC	C3B-C2B	2.25	1.41	1.36
6	fF	201	CYC	CMB-C2B	-2.25	1.46	1.50
6	dC	201	CYC	C3B-C2B	2.25	1.41	1.36
6	cJ	201	CYC	CMB-C2B	-2.25	1.46	1.50
6	aC	201	CYC	C3B-C2B	2.25	1.41	1.36
6	eS	201	CYC	C1B-NB	-2.25	1.34	1.37
6	cF	202	CYC	C1B-NB	-2.25	1.34	1.37
6	aA	201	CYC	C1B-NB	-2.24	1.34	1.37
6	bS	201	CYC	C1B-NB	-2.24	1.34	1.37
6	fD	202	CYC	C3B-C2B	2.24	1.41	1.36
6	fF	202	CYC	C1B-NB	-2.24	1.34	1.37
6	dA	201	CYC	C1B-NB	-2.24	1.34	1.37
6	eM	201	CYC	C2C-C1C	2.23	1.54	1.52
6	fF	202	CYC	C2C-C1C	2.23	1.54	1.52
6	cD	202	CYC	C3B-C2B	2.23	1.41	1.36
6	eX	201	CYC	CMB-C2B	-2.23	1.46	1.50
6	dH	201	CYC	C3B-C2B	2.23	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	aH	201	CYC	C3B-C2B	2.23	1.41	1.36
6	bX	201	CYC	CMB-C2B	-2.23	1.46	1.50
6	eP	201	CYC	C3B-C2B	2.23	1.41	1.36
6	dD	201	CYC	CMB-C2B	-2.23	1.46	1.50
6	aB	201	CYC	CMB-C2B	-2.23	1.46	1.50
6	aD	201	CYC	CMB-C2B	-2.23	1.46	1.50
6	eW	201	CYC	C1B-NB	-2.22	1.34	1.37
6	bP	201	CYC	C3B-C2B	2.22	1.41	1.36
6	bW	201	CYC	C1B-NB	-2.22	1.34	1.37
6	bM	201	CYC	C2C-C1C	2.22	1.54	1.52
6	dB	201	CYC	CMB-C2B	-2.22	1.46	1.50
6	eV	201	CYC	CMB-C2B	-2.22	1.46	1.50
6	cB	201	CYC	C1B-NB	-2.22	1.34	1.37
6	eS	201	CYC	C3B-C2B	2.22	1.41	1.36
6	bS	201	CYC	C3B-C2B	2.22	1.41	1.36
6	fF	202	CYC	CMB-C2B	-2.22	1.46	1.50
6	aM	1204	CYC	CHB-C4A	2.21	1.45	1.40
6	bV	201	CYC	CMB-C2B	-2.21	1.46	1.50
6	dR	201	CYC	CHB-C4A	2.21	1.45	1.40
6	fL	201	CYC	CMB-C2B	-2.21	1.46	1.50
6	fM	101	CYC	CMB-C2B	-2.21	1.46	1.50
6	fB	201	CYC	C1B-NB	-2.21	1.34	1.37
6	aN	201	CYC	C3B-C2B	2.21	1.41	1.36
6	dN	201	CYC	C3B-C2B	2.21	1.41	1.36
6	cM	101	CYC	CMB-C2B	-2.21	1.46	1.50
6	aM	1203	CYC	C1B-NB	-2.21	1.34	1.37
6	cF	202	CYC	CMB-C2B	-2.21	1.46	1.50
6	aB	201	CYC	C1B-NB	-2.21	1.34	1.37
6	aE	201	CYC	CMB-C2B	-2.20	1.46	1.50
6	cD	201	CYC	CMB-C2B	-2.20	1.46	1.50
6	dB	201	CYC	C1B-NB	-2.20	1.34	1.37
6	dM	1203	CYC	C1B-NB	-2.20	1.34	1.37
6	dE	201	CYC	CMB-C2B	-2.20	1.46	1.50
6	fD	201	CYC	CMB-C2B	-2.20	1.46	1.50
6	cL	201	CYC	CMB-C2B	-2.20	1.46	1.50
6	bW	201	CYC	C3B-C2B	2.20	1.41	1.36
6	eW	201	CYC	C3B-C2B	2.20	1.41	1.36
6	eQ	201	CYC	C2C-C1C	2.20	1.54	1.52
6	cF	201	CYC	C3B-C2B	2.20	1.41	1.36
6	eS	201	CYC	CMB-C2B	-2.20	1.46	1.50
6	bS	201	CYC	CMB-C2B	-2.19	1.46	1.50
6	cD	201	CYC	C2C-C1C	2.19	1.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	cF	202	CYC	C2C-C1C	2.19	1.54	1.52
6	fF	201	CYC	C3B-C2B	2.19	1.41	1.36
6	fD	201	CYC	C2C-C1C	2.19	1.54	1.52
6	bQ	201	CYC	C2C-C1C	2.19	1.54	1.52
6	fI	201	CYC	CMB-C2B	-2.19	1.46	1.50
6	cI	201	CYC	CMB-C2B	-2.19	1.46	1.50
6	aE	201	CYC	C3B-C2B	2.18	1.41	1.36
6	dD	201	CYC	C3B-C2B	2.18	1.41	1.36
6	dE	201	CYC	C3B-C2B	2.18	1.41	1.36
6	fB	201	CYC	CMB-C2B	-2.18	1.46	1.50
6	bT	201	CYC	CMB-C2B	-2.18	1.46	1.50
6	aD	201	CYC	C3B-C2B	2.18	1.41	1.36
6	cB	201	CYC	CMB-C2B	-2.18	1.46	1.50
6	aM	1204	CYC	CMB-C2B	-2.17	1.46	1.50
6	eT	201	CYC	CMB-C2B	-2.17	1.46	1.50
6	aC	201	CYC	CMB-C2B	-2.17	1.46	1.50
6	dC	201	CYC	CMB-C2B	-2.17	1.46	1.50
6	dR	201	CYC	CMB-C2B	-2.17	1.46	1.50
6	eT	201	CYC	C3C-C4C	2.17	1.54	1.50
6	dO	201	CYC	CAD-C3D	-2.17	1.48	1.52
6	aM	1202	CYC	CMB-C2B	-2.17	1.46	1.50
6	bT	201	CYC	C3C-C4C	2.16	1.54	1.50
6	dM	1202	CYC	CMB-C2B	-2.16	1.46	1.50
6	aO	201	CYC	CAD-C3D	-2.16	1.48	1.52
6	aM	1204	CYC	C1B-C2B	-2.16	1.41	1.45
6	dR	201	CYC	C1B-C2B	-2.16	1.41	1.45
6	dM	1203	CYC	CMB-C2B	-2.16	1.46	1.50
6	fF	201	CYC	C2C-C1C	2.16	1.54	1.52
6	aM	1203	CYC	CMB-C2B	-2.16	1.46	1.50
6	aA	201	CYC	C3B-C2B	2.15	1.41	1.36
6	cF	201	CYC	C2C-C1C	2.15	1.54	1.52
6	dA	201	CYC	C3B-C2B	2.15	1.41	1.36
6	dD	201	CYC	C1B-NB	-2.15	1.34	1.37
6	aD	201	CYC	C1B-NB	-2.15	1.34	1.37
6	eO	201	CYC	CAD-C3D	-2.14	1.48	1.52
6	bO	201	CYC	CAD-C3D	-2.13	1.48	1.52
6	cG	201	CYC	CMB-C2B	-2.13	1.46	1.50
6	fG	201	CYC	CMB-C2B	-2.13	1.46	1.50
6	bQ	201	CYC	C3B-C2B	2.12	1.41	1.36
6	fJ	201	CYC	C2C-C1C	2.12	1.54	1.52
6	cJ	201	CYC	C2C-C1C	2.12	1.54	1.52
6	eQ	201	CYC	C3B-C2B	2.12	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	dE	201	CYC	C1B-NB	-2.12	1.34	1.37
6	aE	201	CYC	C1B-NB	-2.12	1.34	1.37
6	fJ	201	CYC	C3B-C2B	2.11	1.41	1.36
6	aM	1204	CYC	CAD-C3D	-2.11	1.48	1.52
6	dR	201	CYC	CAD-C3D	-2.11	1.48	1.52
6	aK	201	CYC	CAD-C3D	-2.11	1.48	1.52
6	dK	201	CYC	CAD-C3D	-2.11	1.48	1.52
6	cJ	201	CYC	C3B-C2B	2.10	1.41	1.36
6	cF	202	CYC	C3B-C2B	2.10	1.41	1.36
6	dG	201	CYC	C3B-C2B	2.10	1.41	1.36
6	aB	201	CYC	C2C-C1C	2.10	1.54	1.52
6	fF	202	CYC	C3B-C2B	2.10	1.41	1.36
6	aG	201	CYC	C3B-C2B	2.09	1.41	1.36
6	aC	201	CYC	C1B-NB	-2.09	1.34	1.37
6	dB	201	CYC	C2C-C1C	2.08	1.53	1.52
6	dC	201	CYC	C1B-NB	-2.08	1.34	1.37
6	aK	201	CYC	C3B-C2B	2.08	1.41	1.36
6	dK	201	CYC	C3B-C2B	2.08	1.41	1.36
6	eX	201	CYC	C2C-C1C	2.08	1.53	1.52
6	bX	201	CYC	C2C-C1C	2.07	1.53	1.52
6	dJ	201	CYC	CAD-C3D	-2.06	1.49	1.52
6	aJ	201	CYC	CAD-C3D	-2.06	1.49	1.52
6	aH	201	CYC	CAD-C3D	-2.05	1.49	1.52
6	eN	201	CYC	C3B-C2B	2.05	1.41	1.36
6	bN	201	CYC	C3B-C2B	2.05	1.41	1.36
6	dO	201	CYC	C3B-C2B	2.05	1.41	1.36
6	dH	201	CYC	CAD-C3D	-2.04	1.49	1.52
6	aO	201	CYC	C3B-C2B	2.04	1.41	1.36
6	eT	201	CYC	C1D-CHD	2.04	1.49	1.41
6	bT	201	CYC	C1D-CHD	2.04	1.49	1.41
6	aJ	201	CYC	C1D-CHD	2.03	1.49	1.41
6	dJ	201	CYC	C1D-CHD	2.03	1.49	1.41
6	aL	201	CYC	C3B-C2B	2.03	1.41	1.36
6	dL	201	CYC	C3B-C2B	2.01	1.41	1.36
6	eU	201	CYC	C3B-C2B	2.00	1.41	1.36
6	bU	201	CYC	C3B-C2B	2.00	1.41	1.36
6	aM	1201	CYC	CBA-CAA	-2.00	1.45	1.52

All (1828) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	aJ	201	CYC	C3B-C4B-NB	13.05	117.32	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	dJ	201	CYC	C3B-C4B-NB	13.05	117.32	106.78
6	eR	201	CYC	C3B-C4B-NB	12.71	117.05	106.78
6	bR	201	CYC	C3B-C4B-NB	12.70	117.04	106.78
6	fF	201	CYC	C3B-C4B-NB	12.63	116.98	106.78
6	cF	201	CYC	C3B-C4B-NB	12.62	116.98	106.78
6	aN	201	CYC	C3B-C4B-NB	12.61	116.97	106.78
6	dN	201	CYC	C3B-C4B-NB	12.61	116.97	106.78
6	aI	201	CYC	C3B-C4B-NB	12.61	116.96	106.78
6	dL	201	CYC	C3B-C4B-NB	12.60	116.96	106.78
6	aL	201	CYC	C3B-C4B-NB	12.60	116.95	106.78
6	dI	201	CYC	C3B-C4B-NB	12.59	116.95	106.78
6	dO	201	CYC	C3B-C4B-NB	12.52	116.89	106.78
6	aO	201	CYC	C3B-C4B-NB	12.51	116.89	106.78
6	dM	1201	CYC	C3B-C4B-NB	12.51	116.88	106.78
6	aM	1201	CYC	C3B-C4B-NB	12.50	116.88	106.78
6	bX	201	CYC	C3B-C4B-NB	12.42	116.81	106.78
6	eX	201	CYC	C3B-C4B-NB	12.42	116.81	106.78
6	eT	201	CYC	C3B-C4B-NB	12.41	116.81	106.78
6	bT	201	CYC	C3B-C4B-NB	12.40	116.80	106.78
6	aQ	201	CYC	C3B-C4B-NB	12.39	116.79	106.78
6	dQ	201	CYC	C3B-C4B-NB	12.38	116.78	106.78
6	aH	201	CYC	C3B-C4B-NB	12.38	116.78	106.78
6	dH	201	CYC	C3B-C4B-NB	12.38	116.78	106.78
6	bV	201	CYC	C3B-C4B-NB	12.38	116.78	106.78
6	eV	201	CYC	C3B-C4B-NB	12.37	116.77	106.78
6	bM	201	CYC	C3B-C4B-NB	12.36	116.77	106.78
6	eM	201	CYC	C3B-C4B-NB	12.36	116.76	106.78
6	eP	201	CYC	C3B-C4B-NB	12.35	116.76	106.78
6	bP	201	CYC	C3B-C4B-NB	12.35	116.75	106.78
6	dF	201	CYC	C3B-C4B-NB	12.32	116.73	106.78
6	aF	201	CYC	C3B-C4B-NB	12.30	116.72	106.78
6	aM	1203	CYC	C3B-C4B-NB	12.29	116.70	106.78
6	aG	201	CYC	C3B-C4B-NB	12.28	116.70	106.78
6	dM	1203	CYC	C3B-C4B-NB	12.28	116.70	106.78
6	dG	201	CYC	C3B-C4B-NB	12.27	116.69	106.78
6	fJ	201	CYC	C3B-C4B-NB	12.27	116.69	106.78
6	cJ	201	CYC	C3B-C4B-NB	12.26	116.68	106.78
6	dA	201	CYC	C3B-C4B-NB	12.25	116.68	106.78
6	aA	201	CYC	C3B-C4B-NB	12.24	116.67	106.78
6	dP	201	CYC	C3B-C4B-NB	12.21	116.64	106.78
6	bN	201	CYC	C3B-C4B-NB	12.20	116.64	106.78
6	aC	201	CYC	C3B-C4B-NB	12.20	116.63	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	dC	201	CYC	C3B-C4B-NB	12.20	116.63	106.78
6	aP	201	CYC	C3B-C4B-NB	12.19	116.63	106.78
6	dD	201	CYC	C3B-C4B-NB	12.19	116.63	106.78
6	aD	201	CYC	C3B-C4B-NB	12.19	116.63	106.78
6	eN	201	CYC	C3B-C4B-NB	12.18	116.62	106.78
6	cL	201	CYC	C3B-C4B-NB	12.18	116.62	106.78
6	fL	201	CYC	C3B-C4B-NB	12.16	116.60	106.78
6	eU	201	CYC	C3B-C4B-NB	12.15	116.59	106.78
6	bU	201	CYC	C3B-C4B-NB	12.14	116.59	106.78
6	bO	201	CYC	C3B-C4B-NB	12.14	116.58	106.78
6	eO	201	CYC	C3B-C4B-NB	12.13	116.58	106.78
6	fI	201	CYC	C3B-C4B-NB	12.11	116.56	106.78
6	dK	201	CYC	C3B-C4B-NB	12.10	116.56	106.78
6	aK	201	CYC	C3B-C4B-NB	12.10	116.55	106.78
6	bW	201	CYC	C3B-C4B-NB	12.09	116.55	106.78
6	cI	201	CYC	C3B-C4B-NB	12.09	116.55	106.78
6	eW	201	CYC	C3B-C4B-NB	12.07	116.53	106.78
6	cF	202	CYC	C3B-C4B-NB	12.07	116.53	106.78
6	cB	201	CYC	C3B-C4B-NB	12.07	116.53	106.78
6	eQ	201	CYC	C3B-C4B-NB	12.06	116.53	106.78
6	dM	1202	CYC	C3B-C4B-NB	12.06	116.52	106.78
6	bQ	201	CYC	C3B-C4B-NB	12.06	116.52	106.78
6	fB	201	CYC	C3B-C4B-NB	12.06	116.52	106.78
6	fG	201	CYC	C3B-C4B-NB	12.06	116.52	106.78
6	cG	201	CYC	C3B-C4B-NB	12.06	116.52	106.78
6	aM	1202	CYC	C3B-C4B-NB	12.05	116.51	106.78
6	dB	201	CYC	C3B-C4B-NB	12.04	116.51	106.78
6	fF	202	CYC	C3B-C4B-NB	12.04	116.51	106.78
6	eS	201	CYC	C3B-C4B-NB	12.04	116.50	106.78
6	bS	201	CYC	C3B-C4B-NB	12.03	116.50	106.78
6	aB	201	CYC	C3B-C4B-NB	12.03	116.50	106.78
6	aE	201	CYC	C3B-C4B-NB	11.95	116.44	106.78
6	cM	101	CYC	C3B-C4B-NB	11.95	116.43	106.78
6	dE	201	CYC	C3B-C4B-NB	11.95	116.43	106.78
6	fM	101	CYC	C3B-C4B-NB	11.94	116.42	106.78
6	fD	202	CYC	C3B-C4B-NB	11.93	116.42	106.78
6	cD	202	CYC	C3B-C4B-NB	11.93	116.41	106.78
6	cD	201	CYC	C3B-C4B-NB	11.89	116.39	106.78
6	fD	201	CYC	C3B-C4B-NB	11.89	116.39	106.78
6	aC	201	CYC	OC-C1C-C2C	-11.14	117.31	126.17
6	dC	201	CYC	OC-C1C-C2C	-11.13	117.32	126.17
6	bN	201	CYC	OC-C1C-C2C	-11.08	117.36	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	eN	201	CYC	OC-C1C-C2C	-11.07	117.37	126.17
6	dF	201	CYC	OC-C1C-C2C	-10.82	117.57	126.17
6	aF	201	CYC	OC-C1C-C2C	-10.81	117.57	126.17
6	eR	201	CYC	OC-C1C-C2C	-10.73	117.64	126.17
6	eV	201	CYC	OC-C1C-C2C	-10.73	117.64	126.17
6	bV	201	CYC	OC-C1C-C2C	-10.72	117.65	126.17
6	bR	201	CYC	OC-C1C-C2C	-10.71	117.66	126.17
6	aA	201	CYC	OC-C1C-C2C	-10.70	117.67	126.17
6	dA	201	CYC	OC-C1C-C2C	-10.67	117.69	126.17
6	eT	201	CYC	OC-C1C-C2C	-10.67	117.69	126.17
6	aK	201	CYC	OC-C1C-C2C	-10.67	117.69	126.17
6	bT	201	CYC	OC-C1C-C2C	-10.65	117.70	126.17
6	dK	201	CYC	OC-C1C-C2C	-10.65	117.70	126.17
6	bP	201	CYC	OC-C1C-C2C	-10.63	117.72	126.17
6	eP	201	CYC	OC-C1C-C2C	-10.63	117.72	126.17
6	eS	201	CYC	OC-C1C-C2C	-10.62	117.73	126.17
6	bS	201	CYC	OC-C1C-C2C	-10.61	117.74	126.17
6	dB	201	CYC	OC-C1C-C2C	-10.58	117.76	126.17
6	aB	201	CYC	OC-C1C-C2C	-10.57	117.77	126.17
6	aM	1204	CYC	C3B-C4B-NB	10.44	115.21	106.78
6	dG	201	CYC	OC-C1C-C2C	-10.44	117.87	126.17
6	dR	201	CYC	C3B-C4B-NB	10.44	115.21	106.78
6	aG	201	CYC	OC-C1C-C2C	-10.43	117.88	126.17
6	bU	201	CYC	OC-C1C-C2C	-10.27	118.01	126.17
6	eU	201	CYC	OC-C1C-C2C	-10.26	118.01	126.17
6	aD	201	CYC	OC-C1C-C2C	-10.25	118.03	126.17
6	dD	201	CYC	OC-C1C-C2C	-10.24	118.03	126.17
6	dI	201	CYC	OC-C1C-C2C	-10.23	118.04	126.17
6	aI	201	CYC	OC-C1C-C2C	-10.23	118.04	126.17
6	bX	201	CYC	OC-C1C-C2C	-10.19	118.07	126.17
6	eX	201	CYC	OC-C1C-C2C	-10.18	118.08	126.17
6	aE	201	CYC	OC-C1C-C2C	-10.15	118.11	126.17
6	dE	201	CYC	OC-C1C-C2C	-10.14	118.11	126.17
6	aQ	201	CYC	OC-C1C-C2C	-10.09	118.15	126.17
6	dQ	201	CYC	OC-C1C-C2C	-10.09	118.15	126.17
6	aM	1203	CYC	OC-C1C-C2C	-10.05	118.19	126.17
6	dM	1203	CYC	OC-C1C-C2C	-10.04	118.19	126.17
6	dJ	201	CYC	OC-C1C-C2C	-10.00	118.22	126.17
6	aJ	201	CYC	OC-C1C-C2C	-9.98	118.24	126.17
6	eO	201	CYC	OC-C1C-C2C	-9.97	118.25	126.17
6	dP	201	CYC	OC-C1C-C2C	-9.96	118.26	126.17
6	aP	201	CYC	OC-C1C-C2C	-9.94	118.27	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	bO	201	CYC	OC-C1C-C2C	-9.94	118.27	126.17
6	aN	201	CYC	OC-C1C-C2C	-9.93	118.28	126.17
6	dN	201	CYC	OC-C1C-C2C	-9.93	118.28	126.17
6	cF	202	CYC	OC-C1C-C2C	-9.78	118.39	126.17
6	fM	101	CYC	OC-C1C-C2C	-9.76	118.41	126.17
6	cL	201	CYC	OC-C1C-C2C	-9.76	118.41	126.17
6	cM	101	CYC	OC-C1C-C2C	-9.76	118.41	126.17
6	fL	201	CYC	OC-C1C-C2C	-9.74	118.43	126.17
6	dL	201	CYC	OC-C1C-C2C	-9.73	118.43	126.17
6	fF	202	CYC	OC-C1C-C2C	-9.73	118.43	126.17
6	aL	201	CYC	OC-C1C-C2C	-9.73	118.44	126.17
6	dM	1201	CYC	OC-C1C-C2C	-9.72	118.44	126.17
6	aM	1201	CYC	OC-C1C-C2C	-9.71	118.45	126.17
6	aH	201	CYC	OC-C1C-C2C	-9.67	118.49	126.17
6	cD	202	CYC	OC-C1C-C2C	-9.66	118.50	126.17
6	fD	202	CYC	OC-C1C-C2C	-9.66	118.50	126.17
6	dH	201	CYC	OC-C1C-C2C	-9.64	118.50	126.17
6	aM	1202	CYC	OC-C1C-C2C	-9.59	118.55	126.17
6	dM	1202	CYC	OC-C1C-C2C	-9.59	118.55	126.17
6	cD	201	CYC	OC-C1C-C2C	-9.39	118.70	126.17
6	fD	201	CYC	OC-C1C-C2C	-9.39	118.71	126.17
6	fI	201	CYC	OC-C1C-C2C	-9.33	118.76	126.17
6	cI	201	CYC	OC-C1C-C2C	-9.33	118.76	126.17
6	bM	201	CYC	OC-C1C-C2C	-9.28	118.79	126.17
6	eM	201	CYC	OC-C1C-C2C	-9.27	118.81	126.17
6	cJ	201	CYC	OC-C1C-C2C	-9.17	118.89	126.17
6	fJ	201	CYC	OC-C1C-C2C	-9.16	118.89	126.17
6	cG	201	CYC	OC-C1C-C2C	-9.15	118.90	126.17
6	fG	201	CYC	OC-C1C-C2C	-9.14	118.91	126.17
6	cB	201	CYC	OC-C1C-C2C	-9.05	118.98	126.17
6	fB	201	CYC	OC-C1C-C2C	-9.04	118.99	126.17
6	cF	201	CYC	OC-C1C-C2C	-9.01	119.01	126.17
6	fF	201	CYC	OC-C1C-C2C	-9.01	119.01	126.17
6	aM	1204	CYC	OB-C4B-C3B	-8.98	118.29	128.04
6	dR	201	CYC	OB-C4B-C3B	-8.97	118.30	128.04
6	bQ	201	CYC	OC-C1C-C2C	-8.94	119.06	126.17
6	eQ	201	CYC	OC-C1C-C2C	-8.94	119.06	126.17
6	eW	201	CYC	OC-C1C-C2C	-8.81	119.17	126.17
6	bW	201	CYC	OC-C1C-C2C	-8.80	119.18	126.17
6	aH	201	CYC	C2C-C1C-NC	8.69	115.76	108.27
6	dH	201	CYC	C2C-C1C-NC	8.68	115.76	108.27
6	aM	1204	CYC	OC-C1C-C2C	-8.67	119.28	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	dJ	201	CYC	C2C-C1C-NC	8.67	115.74	108.27
6	aM	1201	CYC	C2C-C1C-NC	8.66	115.74	108.27
6	dM	1201	CYC	C2C-C1C-NC	8.66	115.74	108.27
6	dR	201	CYC	OC-C1C-C2C	-8.65	119.29	126.17
6	aJ	201	CYC	C2C-C1C-NC	8.65	115.73	108.27
6	aP	201	CYC	C2C-C1C-NC	8.61	115.69	108.27
6	dP	201	CYC	C2C-C1C-NC	8.60	115.69	108.27
6	dL	201	CYC	C2C-C1C-NC	8.60	115.69	108.27
6	aL	201	CYC	C2C-C1C-NC	8.59	115.68	108.27
6	aF	201	CYC	C2C-C1C-NC	8.59	115.67	108.27
6	dF	201	CYC	C2C-C1C-NC	8.58	115.67	108.27
6	aK	201	CYC	C2C-C1C-NC	8.53	115.62	108.27
6	dK	201	CYC	C2C-C1C-NC	8.52	115.62	108.27
6	aN	201	CYC	C2C-C1C-NC	8.52	115.61	108.27
6	dN	201	CYC	C2C-C1C-NC	8.51	115.61	108.27
6	eR	201	CYC	C2C-C1C-NC	8.49	115.60	108.27
6	bR	201	CYC	C2C-C1C-NC	8.48	115.59	108.27
6	bN	201	CYC	C2C-C1C-NC	8.47	115.57	108.27
6	eN	201	CYC	C2C-C1C-NC	8.47	115.57	108.27
6	dG	201	CYC	C2C-C1C-NC	8.44	115.55	108.27
6	aG	201	CYC	C2C-C1C-NC	8.44	115.55	108.27
6	eS	201	CYC	C2C-C1C-NC	8.43	115.54	108.27
6	bS	201	CYC	C2C-C1C-NC	8.42	115.53	108.27
6	dB	201	CYC	C2C-C1C-NC	8.42	115.53	108.27
6	aB	201	CYC	C2C-C1C-NC	8.42	115.53	108.27
6	aD	201	CYC	C2C-C1C-NC	8.42	115.53	108.27
6	dD	201	CYC	C2C-C1C-NC	8.41	115.53	108.27
6	eT	201	CYC	C2C-C1C-NC	8.39	115.51	108.27
6	eV	201	CYC	C2C-C1C-NC	8.39	115.50	108.27
6	bV	201	CYC	C2C-C1C-NC	8.38	115.50	108.27
6	bT	201	CYC	C2C-C1C-NC	8.38	115.49	108.27
6	cM	101	CYC	C2C-C1C-NC	8.37	115.49	108.27
6	fM	101	CYC	C2C-C1C-NC	8.36	115.48	108.27
6	bO	201	CYC	C2C-C1C-NC	8.35	115.47	108.27
6	eO	201	CYC	C2C-C1C-NC	8.35	115.47	108.27
6	cD	202	CYC	C2C-C1C-NC	8.33	115.46	108.27
6	eP	201	CYC	C2C-C1C-NC	8.33	115.46	108.27
6	fD	202	CYC	C2C-C1C-NC	8.33	115.45	108.27
6	aM	1203	CYC	C2C-C1C-NC	8.33	115.45	108.27
6	bP	201	CYC	C2C-C1C-NC	8.33	115.45	108.27
6	cF	202	CYC	C2C-C1C-NC	8.33	115.45	108.27
6	bU	201	CYC	C2C-C1C-NC	8.32	115.45	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	dM	1203	CYC	C2C-C1C-NC	8.31	115.44	108.27
6	eU	201	CYC	C2C-C1C-NC	8.31	115.44	108.27
6	aO	201	CYC	C2C-C1C-NC	8.29	115.42	108.27
6	fD	201	CYC	C2C-C1C-NC	8.29	115.42	108.27
6	fF	202	CYC	C2C-C1C-NC	8.29	115.42	108.27
6	dO	201	CYC	C2C-C1C-NC	8.28	115.41	108.27
6	dE	201	CYC	C2C-C1C-NC	8.28	115.41	108.27
6	aE	201	CYC	C2C-C1C-NC	8.28	115.41	108.27
6	cD	201	CYC	C2C-C1C-NC	8.27	115.40	108.27
6	cL	201	CYC	C2C-C1C-NC	8.23	115.37	108.27
6	fL	201	CYC	C2C-C1C-NC	8.23	115.37	108.27
6	dJ	201	CYC	OB-C4B-C3B	-8.19	119.16	128.04
6	aJ	201	CYC	OB-C4B-C3B	-8.18	119.16	128.04
6	bX	201	CYC	C2C-C1C-NC	8.15	115.30	108.27
6	eX	201	CYC	C2C-C1C-NC	8.14	115.29	108.27
6	aM	1202	CYC	C2C-C1C-NC	8.12	115.28	108.27
6	dM	1202	CYC	C2C-C1C-NC	8.12	115.28	108.27
6	fJ	201	CYC	C2C-C1C-NC	8.10	115.26	108.27
6	cJ	201	CYC	C2C-C1C-NC	8.10	115.25	108.27
6	dI	201	CYC	OB-C4B-C3B	-7.98	119.38	128.04
6	aI	201	CYC	OB-C4B-C3B	-7.96	119.40	128.04
6	dQ	201	CYC	C2C-C1C-NC	7.96	115.13	108.27
6	aQ	201	CYC	C2C-C1C-NC	7.96	115.13	108.27
6	cF	201	CYC	C2C-C1C-NC	7.93	115.11	108.27
6	fF	201	CYC	C2C-C1C-NC	7.91	115.09	108.27
6	aA	201	CYC	C2C-C1C-NC	7.90	115.08	108.27
6	aI	201	CYC	C2C-C1C-NC	7.89	115.08	108.27
6	dI	201	CYC	C2C-C1C-NC	7.89	115.08	108.27
6	dA	201	CYC	C2C-C1C-NC	7.89	115.08	108.27
6	fB	201	CYC	C2C-C1C-NC	7.87	115.06	108.27
6	bQ	201	CYC	C2C-C1C-NC	7.86	115.05	108.27
6	cB	201	CYC	C2C-C1C-NC	7.86	115.05	108.27
6	eQ	201	CYC	C2C-C1C-NC	7.86	115.05	108.27
6	eW	201	CYC	C2C-C1C-NC	7.85	115.04	108.27
6	bW	201	CYC	C2C-C1C-NC	7.84	115.03	108.27
6	cG	201	CYC	C2C-C1C-NC	7.79	114.99	108.27
6	fG	201	CYC	C2C-C1C-NC	7.79	114.98	108.27
6	aM	1204	CYC	C2C-C1C-NC	7.78	114.98	108.27
6	fI	201	CYC	C2C-C1C-NC	7.77	114.97	108.27
6	cI	201	CYC	C2C-C1C-NC	7.76	114.97	108.27
6	dR	201	CYC	C2C-C1C-NC	7.76	114.96	108.27
6	dD	201	CYC	OB-C4B-C3B	-7.67	119.72	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	cF	202	CYC	OB-C4B-C3B	-7.67	119.72	128.04
6	fF	202	CYC	OB-C4B-C3B	-7.67	119.72	128.04
6	aO	201	CYC	OB-C4B-C3B	-7.66	119.73	128.04
6	aD	201	CYC	OB-C4B-C3B	-7.66	119.73	128.04
6	dO	201	CYC	OB-C4B-C3B	-7.65	119.74	128.04
6	eN	201	CYC	OB-C4B-C3B	-7.61	119.78	128.04
6	bN	201	CYC	OB-C4B-C3B	-7.61	119.78	128.04
6	bW	201	CYC	OB-C4B-C3B	-7.60	119.79	128.04
6	eW	201	CYC	OB-C4B-C3B	-7.59	119.80	128.04
6	bM	201	CYC	C2C-C1C-NC	7.57	114.80	108.27
6	eM	201	CYC	C2C-C1C-NC	7.57	114.80	108.27
6	eU	201	CYC	OB-C4B-C3B	-7.56	119.83	128.04
6	bU	201	CYC	OB-C4B-C3B	-7.56	119.83	128.04
6	aC	201	CYC	OB-C4B-C3B	-7.53	119.87	128.04
6	dC	201	CYC	OB-C4B-C3B	-7.52	119.88	128.04
6	fI	201	CYC	OB-C4B-C3B	-7.52	119.88	128.04
6	dA	201	CYC	OB-C4B-C3B	-7.51	119.89	128.04
6	bO	201	CYC	OB-C4B-C3B	-7.51	119.89	128.04
6	aA	201	CYC	OB-C4B-C3B	-7.50	119.90	128.04
6	eO	201	CYC	OB-C4B-C3B	-7.50	119.90	128.04
6	cI	201	CYC	OB-C4B-C3B	-7.49	119.91	128.04
6	cJ	201	CYC	OB-C4B-C3B	-7.47	119.94	128.04
6	fJ	201	CYC	OB-C4B-C3B	-7.45	119.95	128.04
6	eT	201	CYC	OB-C4B-C3B	-7.45	119.96	128.04
6	bT	201	CYC	OB-C4B-C3B	-7.44	119.96	128.04
6	bV	201	CYC	OB-C4B-C3B	-7.41	120.00	128.04
6	eV	201	CYC	OB-C4B-C3B	-7.41	120.00	128.04
6	bX	201	CYC	OB-C4B-C3B	-7.41	120.00	128.04
6	eX	201	CYC	OB-C4B-C3B	-7.40	120.00	128.04
6	fB	201	CYC	OB-C4B-C3B	-7.40	120.01	128.04
6	cB	201	CYC	OB-C4B-C3B	-7.39	120.02	128.04
6	bM	201	CYC	OB-C4B-C3B	-7.38	120.04	128.04
6	dM	1203	CYC	OB-C4B-C3B	-7.37	120.04	128.04
6	aM	1203	CYC	OB-C4B-C3B	-7.36	120.05	128.04
6	eM	201	CYC	OB-C4B-C3B	-7.35	120.06	128.04
6	fG	201	CYC	OB-C4B-C3B	-7.32	120.09	128.04
6	cG	201	CYC	OB-C4B-C3B	-7.32	120.09	128.04
6	dK	201	CYC	OB-C4B-C3B	-7.29	120.13	128.04
6	aK	201	CYC	OB-C4B-C3B	-7.29	120.13	128.04
6	aE	201	CYC	OB-C4B-C3B	-7.29	120.13	128.04
6	aQ	201	CYC	OB-C4B-C3B	-7.27	120.14	128.04
6	dE	201	CYC	OB-C4B-C3B	-7.27	120.15	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	dQ	201	CYC	OB-C4B-C3B	-7.27	120.15	128.04
6	aL	201	CYC	OB-C4B-C3B	-7.23	120.19	128.04
6	dL	201	CYC	OB-C4B-C3B	-7.22	120.21	128.04
6	aN	201	CYC	OB-C4B-C3B	-7.17	120.26	128.04
6	dN	201	CYC	OB-C4B-C3B	-7.17	120.26	128.04
6	cD	202	CYC	OB-C4B-C3B	-7.17	120.26	128.04
6	fD	202	CYC	OB-C4B-C3B	-7.16	120.27	128.04
6	eQ	201	CYC	OB-C4B-C3B	-7.15	120.28	128.04
6	bQ	201	CYC	OB-C4B-C3B	-7.14	120.29	128.04
6	aB	201	CYC	OB-C4B-C3B	-7.13	120.31	128.04
6	dB	201	CYC	OB-C4B-C3B	-7.13	120.31	128.04
6	dM	1202	CYC	OB-C4B-C3B	-7.12	120.31	128.04
6	aM	1202	CYC	OB-C4B-C3B	-7.11	120.32	128.04
6	cL	201	CYC	OB-C4B-C3B	-7.10	120.34	128.04
6	fL	201	CYC	OB-C4B-C3B	-7.08	120.36	128.04
6	aH	201	CYC	OB-C4B-C3B	-7.03	120.41	128.04
6	dH	201	CYC	OB-C4B-C3B	-7.02	120.42	128.04
6	bP	201	CYC	OB-C4B-C3B	-6.93	120.52	128.04
6	eP	201	CYC	OB-C4B-C3B	-6.93	120.52	128.04
6	fD	201	CYC	OB-C4B-C3B	-6.91	120.54	128.04
6	eR	201	CYC	OB-C4B-C3B	-6.91	120.54	128.04
6	bR	201	CYC	OB-C4B-C3B	-6.91	120.54	128.04
6	cD	201	CYC	OB-C4B-C3B	-6.90	120.56	128.04
6	aG	201	CYC	OB-C4B-C3B	-6.88	120.58	128.04
6	dG	201	CYC	OB-C4B-C3B	-6.87	120.58	128.04
6	cM	101	CYC	OB-C4B-C3B	-6.87	120.59	128.04
6	fM	101	CYC	OB-C4B-C3B	-6.86	120.60	128.04
6	aO	201	CYC	OC-C1C-C2C	-6.84	120.73	126.17
6	dO	201	CYC	OC-C1C-C2C	-6.84	120.74	126.17
6	bS	201	CYC	OB-C4B-C3B	-6.81	120.65	128.04
6	eS	201	CYC	OB-C4B-C3B	-6.81	120.65	128.04
6	aC	201	CYC	C2C-C1C-NC	6.75	114.09	108.27
6	dC	201	CYC	C2C-C1C-NC	6.75	114.09	108.27
6	cF	201	CYC	OB-C4B-C3B	-6.73	120.74	128.04
6	fF	201	CYC	OB-C4B-C3B	-6.73	120.74	128.04
6	aJ	201	CYC	CAB-C3B-C4B	6.66	131.90	121.38
6	dJ	201	CYC	CAB-C3B-C4B	6.66	131.89	121.38
6	dP	201	CYC	OB-C4B-C3B	-6.56	120.93	128.04
6	aP	201	CYC	OB-C4B-C3B	-6.54	120.94	128.04
6	dF	201	CYC	OB-C4B-C3B	-6.18	121.33	128.04
6	aG	201	CYC	CAB-C3B-C4B	6.18	131.14	121.38
6	dG	201	CYC	CAB-C3B-C4B	6.17	131.13	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	aF	201	CYC	OB-C4B-C3B	-6.17	121.34	128.04
6	aI	201	CYC	CAB-C3B-C4B	5.98	130.83	121.38
6	dI	201	CYC	CAB-C3B-C4B	5.95	130.78	121.38
6	bS	201	CYC	CAB-C3B-C4B	5.92	130.72	121.38
6	eS	201	CYC	CAB-C3B-C4B	5.91	130.72	121.38
6	aQ	201	CYC	CAB-C3B-C4B	5.90	130.69	121.38
6	dQ	201	CYC	CAB-C3B-C4B	5.89	130.68	121.38
6	dP	201	CYC	CAB-C3B-C4B	5.85	130.61	121.38
6	dM	1201	CYC	CAB-C3B-C4B	5.84	130.61	121.38
6	aP	201	CYC	CAB-C3B-C4B	5.84	130.60	121.38
6	aM	1201	CYC	CAB-C3B-C4B	5.83	130.59	121.38
6	dJ	201	CYC	C1B-NB-C4B	-5.64	103.49	110.67
6	aJ	201	CYC	C1B-NB-C4B	-5.63	103.50	110.67
6	eM	201	CYC	CAB-C3B-C4B	5.61	130.24	121.38
6	bM	201	CYC	CAB-C3B-C4B	5.60	130.23	121.38
6	bU	201	CYC	CAB-C3B-C4B	5.56	130.16	121.38
6	eU	201	CYC	CAB-C3B-C4B	5.55	130.15	121.38
6	dF	201	CYC	CAB-C3B-C4B	5.53	130.11	121.38
6	aF	201	CYC	CAB-C3B-C4B	5.52	130.10	121.38
6	dK	201	CYC	CAB-C3B-C4B	5.52	130.09	121.38
6	aK	201	CYC	CAB-C3B-C4B	5.51	130.09	121.38
6	bO	201	CYC	CAB-C3B-C4B	5.48	130.04	121.38
6	eO	201	CYC	CAB-C3B-C4B	5.48	130.04	121.38
6	aA	201	CYC	CAB-C3B-C4B	5.48	130.03	121.38
6	dA	201	CYC	CAB-C3B-C4B	5.48	130.03	121.38
6	aE	201	CYC	CAB-C3B-C4B	5.47	130.01	121.38
6	dE	201	CYC	CAB-C3B-C4B	5.46	130.00	121.38
6	cF	201	CYC	CAB-C3B-C4B	5.40	129.91	121.38
6	fF	201	CYC	CAB-C3B-C4B	5.40	129.90	121.38
6	aO	201	CYC	CAB-C3B-C4B	5.39	129.90	121.38
6	dO	201	CYC	CAB-C3B-C4B	5.39	129.90	121.38
6	aL	201	CYC	CAB-C3B-C4B	5.33	129.80	121.38
6	dL	201	CYC	CAB-C3B-C4B	5.32	129.77	121.38
6	cJ	201	CYC	CAB-C3B-C4B	5.31	129.77	121.38
6	eQ	201	CYC	CAB-C3B-C4B	5.31	129.76	121.38
6	bQ	201	CYC	CAB-C3B-C4B	5.30	129.76	121.38
6	fJ	201	CYC	CAB-C3B-C4B	5.30	129.75	121.38
6	dC	201	CYC	CAB-C3B-C4B	5.27	129.70	121.38
6	aC	201	CYC	CAB-C3B-C4B	5.26	129.69	121.38
6	fD	201	CYC	CAB-C3B-C4B	5.24	129.66	121.38
6	dR	201	CYC	C1B-NB-C4B	-5.24	104.00	110.67
6	aM	1204	CYC	C1B-NB-C4B	-5.24	104.00	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	cD	201	CYC	CAB-C3B-C4B	5.23	129.64	121.38
6	eN	201	CYC	CAB-C3B-C4B	5.18	129.56	121.38
6	bN	201	CYC	CAB-C3B-C4B	5.18	129.56	121.38
6	bW	201	CYC	CAB-C3B-C4B	5.17	129.55	121.38
6	dD	201	CYC	CAB-C3B-C4B	5.17	129.55	121.38
6	cD	202	CYC	CAB-C3B-C4B	5.17	129.55	121.38
6	eW	201	CYC	CAB-C3B-C4B	5.17	129.54	121.38
6	cB	201	CYC	CAB-C3B-C4B	5.17	129.54	121.38
6	fB	201	CYC	CAB-C3B-C4B	5.17	129.54	121.38
6	aD	201	CYC	CAB-C3B-C4B	5.17	129.54	121.38
6	fD	202	CYC	CAB-C3B-C4B	5.16	129.53	121.38
6	aI	201	CYC	C1B-NB-C4B	-5.15	104.11	110.67
6	dI	201	CYC	C1B-NB-C4B	-5.14	104.12	110.67
6	eP	201	CYC	CAB-C3B-C4B	5.08	129.41	121.38
6	bP	201	CYC	CAB-C3B-C4B	5.08	129.40	121.38
6	cG	201	CYC	CAB-C3B-C4B	5.08	129.40	121.38
6	fG	201	CYC	CAB-C3B-C4B	5.08	129.40	121.38
6	eR	201	CYC	CAB-C3B-C4B	5.06	129.38	121.38
6	bR	201	CYC	CAB-C3B-C4B	5.06	129.37	121.38
6	dN	201	CYC	CAB-C3B-C4B	5.02	129.30	121.38
6	aN	201	CYC	CAB-C3B-C4B	5.01	129.30	121.38
6	fI	201	CYC	CAB-C3B-C4B	5.01	129.29	121.38
6	cI	201	CYC	CAB-C3B-C4B	5.00	129.28	121.38
6	aQ	201	CYC	C1B-NB-C4B	-4.99	104.32	110.67
6	dQ	201	CYC	C1B-NB-C4B	-4.98	104.32	110.67
6	dM	1201	CYC	OB-C4B-C3B	-4.93	122.69	128.04
6	aM	1201	CYC	OB-C4B-C3B	-4.93	122.69	128.04
6	dD	201	CYC	C1B-NB-C4B	-4.90	104.43	110.67
6	aD	201	CYC	C1B-NB-C4B	-4.90	104.43	110.67
6	cF	202	CYC	C1B-NB-C4B	-4.89	104.44	110.67
6	fF	202	CYC	C1B-NB-C4B	-4.88	104.45	110.67
6	aM	1203	CYC	CAB-C3B-C4B	4.86	129.06	121.38
6	eT	201	CYC	C1B-NB-C4B	-4.86	104.48	110.67
6	bT	201	CYC	C1B-NB-C4B	-4.86	104.48	110.67
6	dM	1203	CYC	CAB-C3B-C4B	4.85	129.04	121.38
6	dL	201	CYC	C1B-NB-C4B	-4.85	104.50	110.67
6	aL	201	CYC	C1B-NB-C4B	-4.83	104.51	110.67
6	cF	202	CYC	CAB-C3B-C4B	4.81	128.97	121.38
6	fF	202	CYC	CAB-C3B-C4B	4.80	128.97	121.38
6	eX	201	CYC	CAB-C3B-C4B	4.76	128.89	121.38
6	bX	201	CYC	CAB-C3B-C4B	4.75	128.89	121.38
6	dO	201	CYC	C1B-NB-C4B	-4.74	104.63	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	aO	201	CYC	C1B-NB-C4B	-4.74	104.64	110.67
6	cM	101	CYC	CAB-C3B-C4B	4.72	128.84	121.38
6	fM	101	CYC	CAB-C3B-C4B	4.72	128.83	121.38
6	bX	201	CYC	C1B-NB-C4B	-4.68	104.71	110.67
6	eX	201	CYC	C1B-NB-C4B	-4.68	104.71	110.67
6	fL	201	CYC	CAB-C3B-C4B	4.67	128.76	121.38
6	dP	201	CYC	C1B-NB-C4B	-4.67	104.72	110.67
6	cL	201	CYC	CAB-C3B-C4B	4.67	128.75	121.38
6	bM	201	CYC	C1B-NB-C4B	-4.66	104.73	110.67
6	aP	201	CYC	C1B-NB-C4B	-4.66	104.74	110.67
6	aN	201	CYC	C1B-NB-C4B	-4.66	104.74	110.67
6	eM	201	CYC	C1B-NB-C4B	-4.66	104.74	110.67
6	dN	201	CYC	C1B-NB-C4B	-4.66	104.74	110.67
6	aC	201	CYC	C1B-NB-C4B	-4.65	104.75	110.67
6	aB	201	CYC	CAB-C3B-C4B	4.65	128.72	121.38
6	dB	201	CYC	CAB-C3B-C4B	4.65	128.72	121.38
6	dE	201	CYC	C1B-NB-C4B	-4.64	104.76	110.67
6	aE	201	CYC	C1B-NB-C4B	-4.64	104.76	110.67
6	dJ	201	CYC	CHD-C4C-NC	-4.64	119.69	125.20
6	eP	201	CYC	C1B-NB-C4B	-4.64	104.77	110.67
6	bP	201	CYC	C1B-NB-C4B	-4.63	104.77	110.67
6	aJ	201	CYC	CHD-C4C-NC	-4.63	119.70	125.20
6	dC	201	CYC	C1B-NB-C4B	-4.63	104.77	110.67
6	aM	1203	CYC	C1B-NB-C4B	-4.63	104.78	110.67
6	dO	201	CYC	CHD-C4C-NC	-4.63	119.70	125.20
6	aM	1202	CYC	CAB-C3B-C4B	4.62	128.68	121.38
6	aO	201	CYC	CHD-C4C-NC	-4.62	119.71	125.20
6	dM	1203	CYC	C1B-NB-C4B	-4.62	104.79	110.67
6	dM	1202	CYC	CAB-C3B-C4B	4.62	128.67	121.38
6	fF	201	CYC	C1B-NB-C4B	-4.60	104.81	110.67
6	bR	201	CYC	C1B-NB-C4B	-4.60	104.82	110.67
6	cF	201	CYC	C1B-NB-C4B	-4.60	104.82	110.67
6	aG	201	CYC	C1B-NB-C4B	-4.59	104.82	110.67
6	eR	201	CYC	C1B-NB-C4B	-4.59	104.82	110.67
6	dG	201	CYC	C1B-NB-C4B	-4.59	104.83	110.67
6	bV	201	CYC	C1B-NB-C4B	-4.58	104.84	110.67
6	bU	201	CYC	C1B-NB-C4B	-4.58	104.84	110.67
6	eV	201	CYC	C1B-NB-C4B	-4.57	104.85	110.67
6	dA	201	CYC	C1B-NB-C4B	-4.57	104.85	110.67
6	eU	201	CYC	C1B-NB-C4B	-4.57	104.85	110.67
6	aA	201	CYC	C1B-NB-C4B	-4.57	104.86	110.67
6	bN	201	CYC	C1B-NB-C4B	-4.56	104.86	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	eN	201	CYC	C1B-NB-C4B	-4.55	104.88	110.67
6	fJ	201	CYC	C1B-NB-C4B	-4.54	104.88	110.67
6	cJ	201	CYC	C1B-NB-C4B	-4.54	104.89	110.67
6	eQ	201	CYC	C1B-NB-C4B	-4.53	104.90	110.67
6	bQ	201	CYC	C1B-NB-C4B	-4.53	104.90	110.67
6	cB	201	CYC	C1B-NB-C4B	-4.52	104.91	110.67
6	fB	201	CYC	C1B-NB-C4B	-4.52	104.92	110.67
6	eV	201	CYC	CAB-C3B-C4B	4.51	128.51	121.38
6	bV	201	CYC	CAB-C3B-C4B	4.51	128.51	121.38
6	eO	201	CYC	C1B-NB-C4B	-4.51	104.93	110.67
6	bO	201	CYC	C1B-NB-C4B	-4.51	104.93	110.67
6	aK	201	CYC	C1B-NB-C4B	-4.48	104.96	110.67
6	dK	201	CYC	C1B-NB-C4B	-4.48	104.96	110.67
6	fI	201	CYC	C1B-NB-C4B	-4.46	104.99	110.67
6	aH	201	CYC	C1B-NB-C4B	-4.46	105.00	110.67
6	dH	201	CYC	C1B-NB-C4B	-4.46	105.00	110.67
6	cL	201	CYC	C1B-NB-C4B	-4.45	105.00	110.67
6	cI	201	CYC	C1B-NB-C4B	-4.45	105.01	110.67
6	fL	201	CYC	C1B-NB-C4B	-4.45	105.01	110.67
6	cG	201	CYC	C1B-NB-C4B	-4.44	105.02	110.67
6	aF	201	CYC	C1B-NB-C4B	-4.43	105.02	110.67
6	fG	201	CYC	C1B-NB-C4B	-4.43	105.03	110.67
6	dF	201	CYC	C1B-NB-C4B	-4.43	105.03	110.67
6	bW	201	CYC	C1B-NB-C4B	-4.41	105.05	110.67
6	dH	201	CYC	CAB-C3B-C4B	4.41	128.34	121.38
6	aH	201	CYC	CAB-C3B-C4B	4.40	128.34	121.38
6	eW	201	CYC	C1B-NB-C4B	-4.40	105.07	110.67
6	eS	201	CYC	C1B-NB-C4B	-4.37	105.11	110.67
6	bS	201	CYC	C1B-NB-C4B	-4.36	105.12	110.67
6	cD	201	CYC	C1B-NB-C4B	-4.32	105.17	110.67
6	fD	201	CYC	C1B-NB-C4B	-4.32	105.17	110.67
6	dM	1202	CYC	C1B-NB-C4B	-4.29	105.21	110.67
6	eT	201	CYC	CAB-C3B-C4B	4.28	128.14	121.38
6	aM	1202	CYC	C1B-NB-C4B	-4.28	105.22	110.67
6	bT	201	CYC	CAB-C3B-C4B	4.28	128.13	121.38
6	cD	202	CYC	C1B-NB-C4B	-4.27	105.23	110.67
6	fD	202	CYC	C1B-NB-C4B	-4.27	105.23	110.67
6	cM	101	CYC	C1B-NB-C4B	-4.20	105.32	110.67
6	fM	101	CYC	C1B-NB-C4B	-4.20	105.32	110.67
6	dB	201	CYC	C1B-NB-C4B	-4.19	105.33	110.67
6	aB	201	CYC	C1B-NB-C4B	-4.19	105.33	110.67
6	dM	1201	CYC	CHD-C4C-NC	-4.16	120.25	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	aM	1201	CYC	CHB-C1B-NB	-4.16	117.12	126.06
6	dM	1201	CYC	CHB-C1B-NB	-4.16	117.12	126.06
6	aM	1201	CYC	CHD-C4C-NC	-4.16	120.26	125.20
6	dP	201	CYC	CHD-C4C-NC	-4.13	120.29	125.20
6	cF	201	CYC	CHB-C4A-C3A	4.12	135.50	124.90
6	fF	201	CYC	CHB-C4A-C3A	4.12	135.50	124.90
6	aP	201	CYC	CHD-C4C-NC	-4.11	120.32	125.20
6	fB	201	CYC	CHB-C4A-C3A	4.10	135.44	124.90
6	cB	201	CYC	CHB-C4A-C3A	4.09	135.42	124.90
6	aQ	201	CYC	CHB-C4A-C3A	4.09	135.41	124.90
6	dE	201	CYC	CHD-C4C-NC	-4.08	120.35	125.20
6	aE	201	CYC	CHD-C4C-NC	-4.08	120.35	125.20
6	dQ	201	CYC	CHB-C4A-C3A	4.08	135.40	124.90
6	dL	201	CYC	CAA-CBA-CGA	-4.07	104.84	113.60
6	aL	201	CYC	CAA-CBA-CGA	-4.06	104.86	113.60
6	eM	201	CYC	CHB-C4A-C3A	4.03	135.26	124.90
6	bM	201	CYC	CHB-C4A-C3A	4.03	135.26	124.90
6	aE	201	CYC	CHB-C4A-C3A	4.01	135.21	124.90
6	aC	201	CYC	CHB-C4A-C3A	4.01	135.20	124.90
6	dC	201	CYC	CHB-C4A-C3A	4.00	135.20	124.90
6	aM	1204	CYC	CHB-C4A-C3A	4.00	135.20	124.90
6	dE	201	CYC	CHB-C4A-C3A	4.00	135.20	124.90
6	dR	201	CYC	CHB-C4A-C3A	4.00	135.19	124.90
6	eQ	201	CYC	CHB-C4A-C3A	3.97	135.10	124.90
6	bQ	201	CYC	CHB-C4A-C3A	3.96	135.09	124.90
6	fJ	201	CYC	CHB-C4A-C3A	3.95	135.05	124.90
6	cJ	201	CYC	CHB-C4A-C3A	3.95	135.05	124.90
6	cG	201	CYC	CHB-C4A-C3A	3.94	135.03	124.90
6	aL	201	CYC	CHD-C4C-NC	-3.94	120.53	125.20
6	dL	201	CYC	CHD-C4C-NC	-3.94	120.53	125.20
6	fI	201	CYC	CHB-C4A-C3A	3.93	135.01	124.90
6	fG	201	CYC	CHB-C4A-C3A	3.93	135.01	124.90
6	cI	201	CYC	CHB-C4A-C3A	3.93	135.01	124.90
6	aP	201	CYC	CHB-C4A-C3A	3.92	134.97	124.90
6	dP	201	CYC	CHB-C4A-C3A	3.91	134.96	124.90
6	dK	201	CYC	CHB-C4A-C3A	3.90	134.93	124.90
6	aK	201	CYC	CHB-C4A-C3A	3.90	134.92	124.90
6	eW	201	CYC	CHB-C4A-C3A	3.88	134.88	124.90
6	bW	201	CYC	CHB-C4A-C3A	3.88	134.88	124.90
6	aI	201	CYC	C1A-C2A-C3A	-3.88	102.49	106.78
6	aI	201	CYC	CBD-CAD-C3D	-3.88	106.00	112.62
6	eU	201	CYC	CHB-C4A-C3A	3.88	134.87	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	bU	201	CYC	CHB-C4A-C3A	3.88	134.87	124.90
6	dI	201	CYC	C1A-C2A-C3A	-3.87	102.49	106.78
6	dI	201	CYC	CBD-CAD-C3D	-3.87	106.01	112.62
6	aO	201	CYC	CHB-C4A-C3A	3.86	134.84	124.90
6	dO	201	CYC	CHB-C4A-C3A	3.86	134.84	124.90
6	aM	1204	CYC	CHD-C4C-NC	-3.86	120.62	125.20
6	bS	201	CYC	CHB-C4A-C3A	3.85	134.79	124.90
6	eS	201	CYC	CHB-C4A-C3A	3.84	134.79	124.90
6	dR	201	CYC	CHD-C4C-NC	-3.84	120.64	125.20
6	dR	201	CYC	C2B-C1B-NB	3.84	112.61	106.99
6	aM	1204	CYC	C2B-C1B-NB	3.83	112.60	106.99
6	dR	201	CYC	CHB-C4A-NA	-3.80	116.99	124.93
6	aM	1204	CYC	CHB-C4A-NA	-3.80	116.99	124.93
6	eO	201	CYC	CHB-C4A-C3A	3.77	134.59	124.90
6	bO	201	CYC	CHB-C4A-C3A	3.77	134.59	124.90
6	dM	1201	CYC	C1B-NB-C4B	-3.76	105.88	110.67
6	aM	1201	CYC	CAA-CBA-CGA	-3.76	105.51	113.60
6	aM	1201	CYC	C1B-NB-C4B	-3.76	105.88	110.67
6	dM	1201	CYC	CAA-CBA-CGA	-3.76	105.52	113.60
6	dQ	201	CYC	CBD-CAD-C3D	-3.72	106.28	112.62
6	aQ	201	CYC	CBD-CAD-C3D	-3.71	106.30	112.62
6	cD	202	CYC	CHB-C4A-C3A	3.70	134.42	124.90
6	fD	202	CYC	CHB-C4A-C3A	3.70	134.41	124.90
6	dR	201	CYC	CMA-C3A-C4A	3.68	130.73	125.06
6	aM	1204	CYC	CMA-C3A-C4A	3.68	130.73	125.06
6	aJ	201	CYC	C1A-C2A-C3A	-3.65	102.74	106.78
6	dJ	201	CYC	C1A-C2A-C3A	-3.65	102.74	106.78
6	aL	201	CYC	CHB-C4A-C3A	3.64	134.26	124.90
6	dL	201	CYC	CHB-C4A-C3A	3.64	134.26	124.90
6	aP	201	CYC	C1A-C2A-C3A	-3.57	102.83	106.78
6	dP	201	CYC	C1A-C2A-C3A	-3.57	102.83	106.78
6	bO	201	CYC	CHD-C4C-NC	-3.57	120.97	125.20
6	aA	201	CYC	CHB-C4A-C3A	3.56	134.05	124.90
6	dA	201	CYC	CHB-C4A-C3A	3.56	134.05	124.90
6	eO	201	CYC	CHD-C4C-NC	-3.56	120.98	125.20
6	bN	201	CYC	CBD-CAD-C3D	3.56	118.69	112.62
6	eN	201	CYC	CBD-CAD-C3D	3.56	118.69	112.62
6	aN	201	CYC	CAA-CBA-CGA	-3.54	105.98	113.60
6	dN	201	CYC	CAA-CBA-CGA	-3.54	105.98	113.60
6	bT	201	CYC	CAA-CBA-CGA	-3.50	106.06	113.60
6	eT	201	CYC	CAA-CBA-CGA	-3.50	106.06	113.60
6	cF	201	CYC	CMA-C3A-C4A	3.47	130.41	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	fF	201	CYC	CMA-C3A-C4A	3.47	130.41	125.06
6	dI	201	CYC	CHB-C4A-C3A	3.45	133.78	124.90
6	aI	201	CYC	CHB-C4A-C3A	3.45	133.78	124.90
6	eS	201	CYC	C1A-C2A-C3A	-3.45	102.97	106.78
6	bS	201	CYC	C1A-C2A-C3A	-3.44	102.97	106.78
6	dH	201	CYC	C1A-C2A-C3A	-3.44	102.97	106.78
6	cF	202	CYC	CHB-C4A-C3A	3.44	133.75	124.90
6	aH	201	CYC	C1A-C2A-C3A	-3.44	102.98	106.78
6	fF	202	CYC	CHB-C4A-C3A	3.44	133.73	124.90
6	aJ	201	CYC	CHB-C4A-C3A	3.43	133.72	124.90
6	dJ	201	CYC	CHB-C4A-C3A	3.43	133.71	124.90
6	cF	202	CYC	C1A-C2A-C3A	-3.40	103.02	106.78
6	fF	202	CYC	C1A-C2A-C3A	-3.39	103.03	106.78
6	aM	1204	CYC	C1A-C2A-C3A	-3.37	103.05	106.78
6	dR	201	CYC	C1A-C2A-C3A	-3.37	103.05	106.78
6	bS	201	CYC	C2C-C3C-C4C	3.36	106.37	101.34
6	eS	201	CYC	C2C-C3C-C4C	3.36	106.37	101.34
6	eT	201	CYC	CHD-C4C-NC	-3.34	121.23	125.20
6	dL	201	CYC	C1A-C2A-C3A	-3.34	103.09	106.78
6	bT	201	CYC	CHD-C4C-NC	-3.34	121.24	125.20
6	aL	201	CYC	C1A-C2A-C3A	-3.33	103.10	106.78
6	cB	201	CYC	C1A-C2A-C3A	-3.33	103.10	106.78
6	fB	201	CYC	C1A-C2A-C3A	-3.33	103.10	106.78
6	fD	201	CYC	CHB-C4A-C3A	3.32	133.44	124.90
6	cD	201	CYC	CHB-C4A-C3A	3.32	133.44	124.90
6	dG	201	CYC	C1A-C2A-C3A	-3.32	103.11	106.78
6	aG	201	CYC	C1A-C2A-C3A	-3.31	103.12	106.78
6	fM	101	CYC	C1A-C2A-C3A	-3.31	103.12	106.78
6	cM	101	CYC	C1A-C2A-C3A	-3.31	103.12	106.78
6	bU	201	CYC	CHD-C4C-NC	-3.28	121.30	125.20
6	eU	201	CYC	CHD-C4C-NC	-3.28	121.30	125.20
6	eO	201	CYC	C1A-C2A-C3A	-3.28	103.15	106.78
6	cD	202	CYC	CMA-C3A-C4A	3.27	130.11	125.06
6	dG	201	CYC	CHB-C4A-C3A	3.27	133.32	124.90
6	cJ	201	CYC	C1A-C2A-C3A	-3.27	103.16	106.78
6	fD	202	CYC	C1A-C2A-C3A	-3.27	103.16	106.78
6	fD	202	CYC	CMA-C3A-C4A	3.27	130.10	125.06
6	aG	201	CYC	CHB-C4A-C3A	3.27	133.31	124.90
6	cD	202	CYC	C1A-C2A-C3A	-3.27	103.16	106.78
6	fJ	201	CYC	C1A-C2A-C3A	-3.27	103.16	106.78
6	cG	201	CYC	C1A-C2A-C3A	-3.27	103.17	106.78
6	eX	201	CYC	C1A-C2A-C3A	-3.27	103.17	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	fG	201	CYC	C1A-C2A-C3A	-3.27	103.17	106.78
6	bX	201	CYC	C1A-C2A-C3A	-3.27	103.17	106.78
6	fI	201	CYC	C1A-C2A-C3A	-3.27	103.17	106.78
6	bO	201	CYC	C1A-C2A-C3A	-3.26	103.17	106.78
6	eQ	201	CYC	CMA-C3A-C4A	3.26	130.09	125.06
6	bQ	201	CYC	CMA-C3A-C4A	3.26	130.09	125.06
6	cI	201	CYC	C1A-C2A-C3A	-3.26	103.18	106.78
6	dR	201	CYC	C2C-C3C-C4C	3.25	106.20	101.34
6	aM	1204	CYC	C2C-C3C-C4C	3.24	106.20	101.34
6	eN	201	CYC	C1A-C2A-C3A	-3.23	103.21	106.78
6	bN	201	CYC	C1A-C2A-C3A	-3.23	103.21	106.78
6	aM	1201	CYC	CHB-C1B-C2B	3.22	133.32	126.95
6	dM	1201	CYC	CHB-C1B-C2B	3.22	133.32	126.95
6	eS	201	CYC	CBA-CAA-C2A	3.21	121.56	112.63
6	bS	201	CYC	CBA-CAA-C2A	3.21	121.55	112.63
6	cF	201	CYC	C1A-C2A-C3A	-3.21	103.23	106.78
6	dE	201	CYC	C1A-C2A-C3A	-3.21	103.23	106.78
6	dM	1201	CYC	O2D-CGD-O1D	-3.21	115.31	123.30
6	fF	201	CYC	C1A-C2A-C3A	-3.20	103.24	106.78
6	aM	1201	CYC	O2D-CGD-O1D	-3.20	115.32	123.30
6	aE	201	CYC	C1A-C2A-C3A	-3.20	103.24	106.78
6	dM	1202	CYC	C1A-C2A-C3A	-3.20	103.25	106.78
6	aM	1202	CYC	C1A-C2A-C3A	-3.19	103.25	106.78
6	eU	201	CYC	C1A-C2A-C3A	-3.19	103.25	106.78
6	aQ	201	CYC	CHB-C4A-NA	-3.19	118.26	124.93
6	dQ	201	CYC	CHB-C4A-NA	-3.19	118.27	124.93
6	bN	201	CYC	CHD-C4C-NC	-3.18	121.42	125.20
6	bU	201	CYC	C1A-C2A-C3A	-3.18	103.26	106.78
6	aM	1204	CYC	CAC-C3C-C2C	-3.18	106.31	114.26
6	eN	201	CYC	CHD-C4C-NC	-3.18	121.42	125.20
6	dR	201	CYC	CAC-C3C-C2C	-3.18	106.32	114.26
6	eV	201	CYC	C1A-C2A-C3A	-3.18	103.27	106.78
6	bP	201	CYC	C1A-C2A-C3A	-3.17	103.27	106.78
6	bV	201	CYC	C1A-C2A-C3A	-3.17	103.27	106.78
6	aB	201	CYC	C1A-C2A-C3A	-3.17	103.28	106.78
6	eP	201	CYC	C1A-C2A-C3A	-3.17	103.28	106.78
6	dB	201	CYC	C1A-C2A-C3A	-3.16	103.28	106.78
6	aG	201	CYC	C2C-C3C-C4C	3.16	106.08	101.34
6	dM	1203	CYC	C1A-C2A-C3A	-3.16	103.28	106.78
6	dG	201	CYC	C2C-C3C-C4C	3.16	106.07	101.34
6	aM	1203	CYC	C1A-C2A-C3A	-3.16	103.29	106.78
6	dD	201	CYC	C1A-C2A-C3A	-3.16	103.29	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	dR	201	CYC	O2D-CGD-CBD	3.16	124.17	114.03
6	aM	1204	CYC	O2D-CGD-CBD	3.16	124.17	114.03
6	dC	201	CYC	C1A-C2A-C3A	-3.15	103.30	106.78
6	aC	201	CYC	C1A-C2A-C3A	-3.15	103.30	106.78
6	aD	201	CYC	C1A-C2A-C3A	-3.15	103.30	106.78
6	cI	201	CYC	CHD-C4C-NC	-3.14	121.47	125.20
6	fI	201	CYC	CHD-C4C-NC	-3.14	121.47	125.20
6	aM	1201	CYC	C1B-CHB-C4A	-3.14	120.42	128.08
6	dM	1201	CYC	C1B-CHB-C4A	-3.14	120.42	128.08
6	dM	1201	CYC	C1A-C2A-C3A	-3.14	103.31	106.78
6	aQ	201	CYC	C1A-C2A-C3A	-3.13	103.31	106.78
6	eR	201	CYC	C1A-C2A-C3A	-3.13	103.32	106.78
6	aM	1201	CYC	C1A-C2A-C3A	-3.13	103.32	106.78
6	bR	201	CYC	C1A-C2A-C3A	-3.13	103.32	106.78
6	dQ	201	CYC	C1A-C2A-C3A	-3.13	103.32	106.78
6	aP	201	CYC	CAA-CBA-CGA	-3.12	106.88	113.60
6	dP	201	CYC	CAA-CBA-CGA	-3.12	106.89	113.60
6	cG	201	CYC	CMA-C3A-C4A	3.10	129.84	125.06
6	eQ	201	CYC	C1A-C2A-C3A	-3.10	103.35	106.78
6	aF	201	CYC	C1A-C2A-C3A	-3.10	103.36	106.78
6	aJ	201	CYC	CAA-CBA-CGA	-3.10	106.94	113.60
6	dJ	201	CYC	CAA-CBA-CGA	-3.09	106.94	113.60
6	bQ	201	CYC	C1A-C2A-C3A	-3.09	103.36	106.78
6	fG	201	CYC	CMA-C3A-C4A	3.09	129.83	125.06
6	bT	201	CYC	C1A-C2A-C3A	-3.09	103.36	106.78
6	dF	201	CYC	C1A-C2A-C3A	-3.09	103.36	106.78
6	eT	201	CYC	C1A-C2A-C3A	-3.09	103.36	106.78
6	bM	201	CYC	C1A-C2A-C3A	-3.08	103.38	106.78
6	eM	201	CYC	C1A-C2A-C3A	-3.08	103.38	106.78
6	dN	201	CYC	C1A-C2A-C3A	-3.08	103.38	106.78
6	bS	201	CYC	C1A-NA-C4A	3.07	112.30	106.51
6	cG	201	CYC	CHD-C4C-NC	-3.07	121.55	125.20
6	aF	201	CYC	O2D-CGD-O1D	-3.07	115.64	123.30
6	cL	201	CYC	C1A-C2A-C3A	-3.07	103.38	106.78
6	fL	201	CYC	C1A-C2A-C3A	-3.07	103.38	106.78
6	dF	201	CYC	O2D-CGD-O1D	-3.07	115.64	123.30
6	eS	201	CYC	C1A-NA-C4A	3.07	112.30	106.51
6	fG	201	CYC	CHD-C4C-NC	-3.07	121.56	125.20
6	aN	201	CYC	C1A-C2A-C3A	-3.07	103.39	106.78
6	eQ	201	CYC	O1A-CGA-CBA	-3.06	113.25	123.08
6	bQ	201	CYC	O1A-CGA-CBA	-3.06	113.25	123.08
6	eW	201	CYC	C1A-C2A-C3A	-3.04	103.41	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	bW	201	CYC	C1A-C2A-C3A	-3.04	103.42	106.78
6	dM	1201	CYC	O2D-CGD-CBD	3.04	123.80	114.03
6	eM	201	CYC	CMA-C3A-C4A	3.04	129.74	125.06
6	bM	201	CYC	CMA-C3A-C4A	3.04	129.74	125.06
6	aM	1201	CYC	O2D-CGD-CBD	3.03	123.78	114.03
6	fL	201	CYC	C4D-CHA-C1A	3.03	132.43	128.81
6	cL	201	CYC	C4D-CHA-C1A	3.03	132.43	128.81
6	aG	201	CYC	CBA-CAA-C2A	3.03	121.04	112.63
6	dG	201	CYC	CBA-CAA-C2A	3.03	121.03	112.63
6	eS	201	CYC	O2D-CGD-CBD	3.02	123.75	114.03
6	eS	201	CYC	O2D-CGD-O1D	-3.02	115.77	123.30
6	bS	201	CYC	O2D-CGD-CBD	3.02	123.73	114.03
6	bM	201	CYC	O1A-CGA-CBA	-3.02	113.38	123.08
6	eW	201	CYC	C1A-NA-C4A	3.02	112.20	106.51
6	eM	201	CYC	O1A-CGA-CBA	-3.02	113.39	123.08
6	bW	201	CYC	C1A-NA-C4A	3.01	112.19	106.51
6	bS	201	CYC	O2D-CGD-O1D	-3.01	115.78	123.30
6	dN	201	CYC	O1A-CGA-CBA	-3.01	113.40	123.08
6	cJ	201	CYC	O2D-CGD-CBD	3.01	123.71	114.03
6	aN	201	CYC	O1A-CGA-CBA	-3.01	113.40	123.08
6	fF	201	CYC	O1A-CGA-CBA	-3.01	113.42	123.08
6	dK	201	CYC	C1A-NA-C4A	3.01	112.18	106.51
6	cF	201	CYC	O1A-CGA-CBA	-3.01	113.42	123.08
6	aK	201	CYC	C1A-NA-C4A	3.01	112.17	106.51
6	cF	201	CYC	CHB-C4A-NA	-3.01	118.65	124.93
6	fF	201	CYC	CHB-C4A-NA	-3.00	118.65	124.93
6	fJ	201	CYC	O2D-CGD-CBD	3.00	123.67	114.03
6	aM	1202	CYC	O2D-CGD-O1D	-3.00	115.83	123.30
6	dM	1202	CYC	O2D-CGD-O1D	-3.00	115.83	123.30
6	aA	201	CYC	O1A-CGA-CBA	-2.99	113.48	123.08
6	bN	201	CYC	O2D-CGD-CBD	2.99	123.63	114.03
6	dA	201	CYC	O1A-CGA-CBA	-2.99	113.49	123.08
6	eW	201	CYC	CHD-C4C-NC	-2.99	121.66	125.20
6	eN	201	CYC	O2D-CGD-CBD	2.98	123.62	114.03
6	bQ	201	CYC	CAA-CBA-CGA	-2.98	107.18	113.60
6	aE	201	CYC	CHB-C4A-NA	-2.98	118.69	124.93
6	aH	201	CYC	CHB-C4A-C3A	2.98	132.57	124.90
6	eQ	201	CYC	CAA-CBA-CGA	-2.98	107.18	113.60
6	dE	201	CYC	CHB-C4A-NA	-2.98	118.69	124.93
6	dH	201	CYC	CHB-C4A-C3A	2.98	132.56	124.90
6	fB	201	CYC	CHB-C4A-NA	-2.98	118.70	124.93
6	eR	201	CYC	O2D-CGD-O1D	-2.98	115.88	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	bW	201	CYC	CHD-C4C-NC	-2.98	121.67	125.20
6	bR	201	CYC	O2D-CGD-O1D	-2.97	115.89	123.30
6	bX	201	CYC	O2D-CGD-O1D	-2.97	115.89	123.30
6	cB	201	CYC	CHB-C4A-NA	-2.97	118.72	124.93
6	dN	201	CYC	O2D-CGD-O1D	-2.97	115.90	123.30
6	eX	201	CYC	O2D-CGD-O1D	-2.97	115.90	123.30
6	cD	202	CYC	O2D-CGD-CBD	2.97	123.57	114.03
6	fD	202	CYC	O2D-CGD-CBD	2.97	123.56	114.03
6	eP	201	CYC	O2D-CGD-O1D	-2.97	115.90	123.30
6	fI	201	CYC	O2D-CGD-CBD	2.97	123.56	114.03
6	bP	201	CYC	O2D-CGD-O1D	-2.97	115.91	123.30
6	cI	201	CYC	O2D-CGD-CBD	2.96	123.56	114.03
6	cD	202	CYC	O2D-CGD-O1D	-2.96	115.92	123.30
6	aN	201	CYC	O2D-CGD-O1D	-2.96	115.92	123.30
6	cJ	201	CYC	O2D-CGD-O1D	-2.96	115.92	123.30
6	bU	201	CYC	O2D-CGD-CBD	2.96	123.54	114.03
6	eU	201	CYC	O2D-CGD-CBD	2.96	123.53	114.03
6	fJ	201	CYC	O2D-CGD-O1D	-2.96	115.93	123.30
6	aC	201	CYC	OC-C1C-NC	2.96	128.52	124.94
6	fD	202	CYC	O2D-CGD-O1D	-2.96	115.93	123.30
6	bX	201	CYC	O2D-CGD-CBD	2.96	123.53	114.03
6	aK	201	CYC	C1A-C2A-C3A	-2.96	103.51	106.78
6	fI	201	CYC	O2D-CGD-O1D	-2.95	115.93	123.30
6	dO	201	CYC	CMA-C3A-C4A	2.95	129.61	125.06
6	aC	201	CYC	O2D-CGD-O1D	-2.95	115.94	123.30
6	eX	201	CYC	O2D-CGD-CBD	2.95	123.52	114.03
6	aC	201	CYC	C1A-NA-C4A	2.95	112.07	106.51
6	dC	201	CYC	C1A-NA-C4A	2.95	112.07	106.51
6	dK	201	CYC	C1A-C2A-C3A	-2.95	103.52	106.78
6	dC	201	CYC	OC-C1C-NC	2.95	128.51	124.94
6	dM	1202	CYC	O2D-CGD-CBD	2.95	123.51	114.03
6	aM	1202	CYC	O2D-CGD-CBD	2.95	123.51	114.03
6	dC	201	CYC	O2D-CGD-O1D	-2.95	115.95	123.30
6	aA	201	CYC	O2D-CGD-O1D	-2.95	115.96	123.30
6	fB	201	CYC	O2D-CGD-O1D	-2.94	115.96	123.30
6	dA	201	CYC	O2D-CGD-O1D	-2.94	115.96	123.30
6	aO	201	CYC	C1A-C2A-C3A	-2.94	103.52	106.78
6	aO	201	CYC	CMA-C3A-C4A	2.94	129.60	125.06
6	cB	201	CYC	O2D-CGD-O1D	-2.94	115.97	123.30
6	dO	201	CYC	C1A-C2A-C3A	-2.94	103.53	106.78
6	fB	201	CYC	C1A-NA-C4A	2.94	112.04	106.51
6	cB	201	CYC	C1A-NA-C4A	2.94	112.04	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	fL	201	CYC	O2D-CGD-O1D	-2.93	115.98	123.30
6	dH	201	CYC	CHD-C4C-NC	-2.93	121.72	125.20
6	cL	201	CYC	O2D-CGD-O1D	-2.93	115.98	123.30
6	cD	201	CYC	C1A-C2A-C3A	-2.93	103.53	106.78
6	eV	201	CYC	O2D-CGD-O1D	-2.93	115.99	123.30
6	bV	201	CYC	O2D-CGD-O1D	-2.93	115.99	123.30
6	aM	1203	CYC	O2D-CGD-O1D	-2.93	115.99	123.30
6	cI	201	CYC	O2D-CGD-O1D	-2.93	116.00	123.30
6	eW	201	CYC	O1A-CGA-CBA	-2.93	113.67	123.08
6	bO	201	CYC	CMA-C3A-C4A	2.93	129.57	125.06
6	cJ	201	CYC	CMA-C3A-C4A	2.93	129.57	125.06
6	dG	201	CYC	O1A-CGA-CBA	-2.93	113.67	123.08
6	dM	1203	CYC	O2D-CGD-O1D	-2.93	116.00	123.30
6	bW	201	CYC	O1A-CGA-CBA	-2.93	113.67	123.08
6	cD	202	CYC	CAA-CBA-CGA	-2.93	107.30	113.60
6	fJ	201	CYC	CMA-C3A-C4A	2.93	129.57	125.06
6	eM	201	CYC	C1A-NA-C4A	2.93	112.03	106.51
6	aM	1202	CYC	CHB-C4A-C3A	2.93	132.43	124.90
6	aH	201	CYC	CHD-C4C-NC	-2.93	121.72	125.20
6	fD	202	CYC	CAA-CBA-CGA	-2.93	107.31	113.60
6	dD	201	CYC	O2D-CGD-CBD	2.93	123.43	114.03
6	aG	201	CYC	O1A-CGA-CBA	-2.93	113.68	123.08
6	aD	201	CYC	O2D-CGD-CBD	2.92	123.43	114.03
6	fB	201	CYC	O2D-CGD-CBD	2.92	123.43	114.03
6	dM	1202	CYC	CHB-C4A-C3A	2.92	132.42	124.90
6	bM	201	CYC	C1A-NA-C4A	2.92	112.02	106.51
6	eN	201	CYC	O2D-CGD-O1D	-2.92	116.02	123.30
6	fI	201	CYC	CMA-C3A-C4A	2.92	129.56	125.06
6	fD	201	CYC	C1A-C2A-C3A	-2.92	103.55	106.78
6	eU	201	CYC	C1A-NA-C4A	2.92	112.01	106.51
6	cB	201	CYC	O2D-CGD-CBD	2.92	123.41	114.03
6	cF	201	CYC	O2D-CGD-O1D	-2.92	116.03	123.30
6	eQ	201	CYC	O2D-CGD-O1D	-2.92	116.03	123.30
6	bV	201	CYC	O2D-CGD-CBD	2.92	123.40	114.03
6	bU	201	CYC	C1A-NA-C4A	2.92	112.00	106.51
6	bP	201	CYC	CHB-C4A-C3A	2.92	132.40	124.90
6	eV	201	CYC	O2D-CGD-CBD	2.91	123.39	114.03
6	aL	201	CYC	O1A-CGA-CBA	-2.91	113.72	123.08
6	dL	201	CYC	O1A-CGA-CBA	-2.91	113.72	123.08
6	eP	201	CYC	CHB-C4A-C3A	2.91	132.39	124.90
6	aK	201	CYC	C2C-C3C-C4C	2.91	105.70	101.34
6	bN	201	CYC	O2D-CGD-O1D	-2.91	116.04	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	dO	201	CYC	O2D-CGD-O1D	-2.91	116.04	123.30
6	dN	201	CYC	O2D-CGD-CBD	2.91	123.38	114.03
6	dP	201	CYC	CMA-C3A-C4A	2.91	129.55	125.06
6	cI	201	CYC	CMA-C3A-C4A	2.91	129.54	125.06
6	fF	201	CYC	O2D-CGD-O1D	-2.91	116.05	123.30
6	dK	201	CYC	C2C-C3C-C4C	2.91	105.70	101.34
6	dN	201	CYC	CHB-C4A-C3A	2.91	132.38	124.90
6	aN	201	CYC	O2D-CGD-CBD	2.91	123.38	114.03
6	aP	201	CYC	CMA-C3A-C4A	2.91	129.54	125.06
6	eQ	201	CYC	O2D-CGD-CBD	2.91	123.37	114.03
6	aN	201	CYC	CHB-C4A-C3A	2.91	132.38	124.90
6	bQ	201	CYC	O2D-CGD-CBD	2.91	123.37	114.03
6	bQ	201	CYC	O2D-CGD-O1D	-2.91	116.05	123.30
6	fL	201	CYC	O2D-CGD-CBD	2.91	123.37	114.03
6	cL	201	CYC	O2D-CGD-CBD	2.91	123.36	114.03
6	eR	201	CYC	O2D-CGD-CBD	2.90	123.36	114.03
6	aO	201	CYC	O2D-CGD-O1D	-2.90	116.06	123.30
6	bR	201	CYC	O2D-CGD-CBD	2.90	123.36	114.03
6	cJ	201	CYC	O1A-CGA-CBA	-2.90	113.76	123.08
6	dD	201	CYC	O2D-CGD-O1D	-2.90	116.07	123.30
6	cM	101	CYC	O2D-CGD-O1D	-2.90	116.07	123.30
6	fJ	201	CYC	O1A-CGA-CBA	-2.90	113.76	123.08
6	dR	201	CYC	C1B-C2B-C3B	-2.90	104.84	107.87
6	dM	1201	CYC	O1A-CGA-CBA	-2.90	113.77	123.08
6	eO	201	CYC	CMA-C3A-C4A	2.90	129.53	125.06
6	aD	201	CYC	O2D-CGD-O1D	-2.90	116.07	123.30
6	fM	101	CYC	O2D-CGD-O1D	-2.90	116.07	123.30
6	aM	1201	CYC	O1A-CGA-CBA	-2.90	113.77	123.08
6	cJ	201	CYC	CHD-C4C-NC	-2.90	121.76	125.20
6	dB	201	CYC	CHB-C4A-C3A	2.90	132.35	124.90
6	fG	201	CYC	O2D-CGD-CBD	2.90	123.34	114.03
6	fJ	201	CYC	CHD-C4C-NC	-2.90	121.76	125.20
6	cF	201	CYC	O2D-CGD-CBD	2.90	123.33	114.03
6	eT	201	CYC	O2D-CGD-O1D	-2.90	116.08	123.30
6	aB	201	CYC	CHB-C4A-C3A	2.90	132.34	124.90
6	cG	201	CYC	O2D-CGD-CBD	2.89	123.33	114.03
6	aC	201	CYC	O2D-CGD-CBD	2.89	123.33	114.03
6	dA	201	CYC	O2D-CGD-CBD	2.89	123.33	114.03
6	eN	201	CYC	CHB-C4A-C3A	2.89	132.34	124.90
6	dO	201	CYC	O2D-CGD-CBD	2.89	123.32	114.03
6	dH	201	CYC	CAA-CBA-CGA	-2.89	107.38	113.60
6	dC	201	CYC	O2D-CGD-CBD	2.89	123.32	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	aH	201	CYC	CAA-CBA-CGA	-2.89	107.38	113.60
6	bT	201	CYC	O2D-CGD-O1D	-2.89	116.09	123.30
6	aA	201	CYC	O2D-CGD-CBD	2.89	123.31	114.03
6	fF	201	CYC	O2D-CGD-CBD	2.89	123.31	114.03
6	aM	1204	CYC	C1B-C2B-C3B	-2.89	104.86	107.87
6	eU	201	CYC	O2D-CGD-O1D	-2.89	116.10	123.30
6	cD	202	CYC	O1A-CGA-CBA	-2.89	113.80	123.08
6	eQ	201	CYC	CHB-C4A-NA	-2.89	118.89	124.93
6	aO	201	CYC	O2D-CGD-CBD	2.89	123.31	114.03
6	bN	201	CYC	CHB-C4A-C3A	2.89	132.33	124.90
6	fD	202	CYC	O1A-CGA-CBA	-2.89	113.81	123.08
6	bQ	201	CYC	CHB-C4A-NA	-2.89	118.90	124.93
6	fD	201	CYC	O2D-CGD-O1D	-2.89	116.11	123.30
6	bU	201	CYC	O2D-CGD-O1D	-2.88	116.11	123.30
6	cD	201	CYC	O2D-CGD-O1D	-2.88	116.11	123.30
6	dJ	201	CYC	O2D-CGD-O1D	-2.88	116.11	123.30
6	fD	201	CYC	O2D-CGD-CBD	2.88	123.29	114.03
6	cD	201	CYC	O2D-CGD-CBD	2.88	123.28	114.03
6	aL	201	CYC	C1A-NA-C4A	2.88	111.94	106.51
6	dK	201	CYC	CMA-C3A-C4A	2.88	129.50	125.06
6	aH	201	CYC	CMA-C3A-C4A	2.88	129.50	125.06
6	dG	201	CYC	O2D-CGD-O1D	-2.88	116.12	123.30
6	aJ	201	CYC	O2D-CGD-O1D	-2.88	116.13	123.30
6	aG	201	CYC	O2D-CGD-O1D	-2.88	116.13	123.30
6	aK	201	CYC	CMA-C3A-C4A	2.88	129.49	125.06
6	dL	201	CYC	C1A-NA-C4A	2.88	111.93	106.51
6	aK	201	CYC	CAA-CBA-CGA	-2.88	107.42	113.60
6	dH	201	CYC	CMA-C3A-C4A	2.87	129.49	125.06
6	bM	201	CYC	CHB-C4A-NA	-2.87	118.92	124.93
6	fG	201	CYC	O2D-CGD-O1D	-2.87	116.14	123.30
6	eM	201	CYC	CHB-C4A-NA	-2.87	118.92	124.93
6	eO	201	CYC	C1A-NA-C4A	2.87	111.92	106.51
6	bM	201	CYC	O2D-CGD-CBD	2.87	123.26	114.03
6	dK	201	CYC	CAA-CBA-CGA	-2.87	107.42	113.60
6	eM	201	CYC	O2D-CGD-CBD	2.87	123.25	114.03
6	aN	201	CYC	C1A-NA-C4A	2.87	111.91	106.51
6	bO	201	CYC	C1A-NA-C4A	2.87	111.91	106.51
6	cF	202	CYC	O2D-CGD-CBD	2.87	123.24	114.03
6	cG	201	CYC	O2D-CGD-O1D	-2.87	116.16	123.30
6	eP	201	CYC	O2D-CGD-CBD	2.87	123.24	114.03
6	fF	202	CYC	O2D-CGD-CBD	2.87	123.24	114.03
6	bW	201	CYC	CMA-C3A-C4A	2.87	129.48	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	fF	202	CYC	O2D-CGD-O1D	-2.87	116.16	123.30
6	bP	201	CYC	O2D-CGD-CBD	2.86	123.23	114.03
6	dN	201	CYC	C1A-NA-C4A	2.86	111.91	106.51
6	eN	201	CYC	C2C-C3C-C4C	2.86	105.63	101.34
6	eW	201	CYC	CMA-C3A-C4A	2.86	129.47	125.06
6	aG	201	CYC	O2D-CGD-CBD	2.86	123.22	114.03
6	dG	201	CYC	O2D-CGD-CBD	2.86	123.22	114.03
6	cF	202	CYC	O2D-CGD-O1D	-2.86	116.17	123.30
6	dE	201	CYC	O2D-CGD-O1D	-2.86	116.17	123.30
6	bN	201	CYC	C2C-C3C-C4C	2.86	105.62	101.34
6	aC	201	CYC	CHB-C4A-NA	-2.85	118.96	124.93
6	fD	201	CYC	CAA-CBA-CGA	-2.85	107.47	113.60
6	dC	201	CYC	CHB-C4A-NA	-2.85	118.97	124.93
6	dH	201	CYC	O1A-CGA-CBA	-2.85	113.92	123.08
6	aF	201	CYC	O2D-CGD-CBD	2.85	123.19	114.03
6	bO	201	CYC	O2D-CGD-CBD	2.85	123.19	114.03
6	cD	201	CYC	CAA-CBA-CGA	-2.85	107.47	113.60
6	eR	201	CYC	CHB-C4A-C3A	2.85	132.22	124.90
6	aA	201	CYC	C2C-C3C-C4C	2.85	105.61	101.34
6	aH	201	CYC	O1A-CGA-CBA	-2.85	113.93	123.08
6	dF	201	CYC	O2D-CGD-CBD	2.85	123.18	114.03
6	eO	201	CYC	O2D-CGD-CBD	2.85	123.18	114.03
6	bR	201	CYC	CHB-C4A-C3A	2.85	132.22	124.90
6	dA	201	CYC	C2C-C3C-C4C	2.85	105.60	101.34
6	dL	201	CYC	CMA-C3A-C4A	2.84	129.44	125.06
6	fI	201	CYC	C1A-NA-C4A	2.84	111.87	106.51
6	bO	201	CYC	O1A-CGA-CBA	-2.84	113.94	123.08
6	dM	1203	CYC	O2D-CGD-CBD	2.84	123.16	114.03
6	cI	201	CYC	C1A-NA-C4A	2.84	111.86	106.51
6	bW	201	CYC	O2D-CGD-O1D	-2.84	116.22	123.30
6	eW	201	CYC	O2D-CGD-O1D	-2.84	116.22	123.30
6	aM	1203	CYC	O2D-CGD-CBD	2.84	123.16	114.03
6	bW	201	CYC	O2D-CGD-CBD	2.84	123.16	114.03
6	eW	201	CYC	O2D-CGD-CBD	2.84	123.15	114.03
6	aE	201	CYC	O2D-CGD-O1D	-2.84	116.22	123.30
6	aL	201	CYC	CMA-C3A-C4A	2.84	129.44	125.06
6	fJ	201	CYC	C1A-NA-C4A	2.84	111.86	106.51
6	cJ	201	CYC	C1A-NA-C4A	2.84	111.86	106.51
6	eO	201	CYC	O1A-CGA-CBA	-2.84	113.97	123.08
6	aA	201	CYC	C1A-NA-C4A	2.84	111.85	106.51
6	dA	201	CYC	C1A-NA-C4A	2.83	111.85	106.51
6	aP	201	CYC	O2D-CGD-O1D	-2.83	116.25	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	eX	201	CYC	CHB-C4A-C3A	2.83	132.17	124.90
6	dQ	201	CYC	CHD-C4C-NC	-2.83	121.85	125.20
6	aQ	201	CYC	CHD-C4C-NC	-2.82	121.85	125.20
6	aB	201	CYC	O2D-CGD-O1D	-2.82	116.26	123.30
6	dB	201	CYC	O2D-CGD-O1D	-2.82	116.26	123.30
6	bX	201	CYC	CHB-C4A-C3A	2.82	132.16	124.90
6	fM	101	CYC	O2D-CGD-CBD	2.82	123.10	114.03
6	dP	201	CYC	O2D-CGD-O1D	-2.82	116.26	123.30
6	cM	101	CYC	O2D-CGD-CBD	2.82	123.10	114.03
6	fF	201	CYC	CAA-CBA-CGA	-2.82	107.54	113.60
6	bO	201	CYC	O2D-CGD-O1D	-2.82	116.28	123.30
6	dC	201	CYC	O1A-CGA-CBA	-2.82	114.03	123.08
6	dA	201	CYC	CAA-CBA-CGA	-2.82	107.54	113.60
6	aC	201	CYC	O1A-CGA-CBA	-2.81	114.04	123.08
6	eT	201	CYC	O2D-CGD-CBD	2.81	123.07	114.03
6	fG	201	CYC	O1A-CGA-CBA	-2.81	114.05	123.08
6	eO	201	CYC	O2D-CGD-O1D	-2.81	116.29	123.30
6	bT	201	CYC	O2D-CGD-CBD	2.81	123.06	114.03
6	aA	201	CYC	CAA-CBA-CGA	-2.81	107.55	113.60
6	cF	201	CYC	CAA-CBA-CGA	-2.81	107.55	113.60
6	cG	201	CYC	O1A-CGA-CBA	-2.81	114.05	123.08
6	bM	201	CYC	O2D-CGD-O1D	-2.81	116.30	123.30
6	eM	201	CYC	O2D-CGD-O1D	-2.81	116.30	123.30
6	dD	201	CYC	O1A-CGA-CBA	-2.81	114.07	123.08
6	aD	201	CYC	O1A-CGA-CBA	-2.81	114.07	123.08
6	dO	201	CYC	C1A-NA-C4A	2.80	111.79	106.51
6	dK	201	CYC	O1A-CGA-CBA	-2.80	114.07	123.08
6	aO	201	CYC	C1A-NA-C4A	2.80	111.79	106.51
6	aK	201	CYC	O1A-CGA-CBA	-2.80	114.08	123.08
6	dQ	201	CYC	CMA-C3A-C4A	2.80	129.38	125.06
6	fF	201	CYC	C1A-NA-C4A	2.80	111.79	106.51
6	aQ	201	CYC	CMA-C3A-C4A	2.80	129.38	125.06
6	dH	201	CYC	O2D-CGD-O1D	-2.80	116.32	123.30
6	cF	201	CYC	C1A-NA-C4A	2.80	111.78	106.51
6	aH	201	CYC	O2D-CGD-O1D	-2.80	116.32	123.30
6	dE	201	CYC	O2D-CGD-CBD	2.80	123.02	114.03
6	aO	201	CYC	C2C-C3C-C4C	2.80	105.53	101.34
6	bQ	201	CYC	CHD-C4C-NC	-2.80	121.88	125.20
6	dO	201	CYC	C2C-C3C-C4C	2.80	105.53	101.34
6	aC	201	CYC	CMA-C3A-C4A	2.79	129.37	125.06
6	aQ	201	CYC	C1A-NA-C4A	2.79	111.77	106.51
6	dQ	201	CYC	C1A-NA-C4A	2.79	111.77	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	cB	201	CYC	CHD-C4C-NC	-2.79	121.89	125.20
6	aA	201	CYC	C1A-C2A-C3A	-2.79	103.69	106.78
6	aE	201	CYC	O2D-CGD-CBD	2.79	123.00	114.03
6	dH	201	CYC	O2D-CGD-CBD	2.79	123.00	114.03
6	dA	201	CYC	CMA-C3A-C4A	2.79	129.36	125.06
6	aM	1201	CYC	CMA-C3A-C4A	2.79	129.36	125.06
6	dJ	201	CYC	O2D-CGD-CBD	2.79	122.99	114.03
6	dC	201	CYC	CMA-C3A-C4A	2.79	129.36	125.06
6	dM	1201	CYC	CMA-C3A-C4A	2.79	129.36	125.06
6	aK	201	CYC	O2D-CGD-O1D	-2.79	116.35	123.30
6	aJ	201	CYC	O2D-CGD-CBD	2.79	122.99	114.03
6	cG	201	CYC	C1A-NA-C4A	2.79	111.76	106.51
6	fD	201	CYC	C1A-NA-C4A	2.79	111.76	106.51
6	aL	201	CYC	O2D-CGD-O1D	-2.79	116.35	123.30
6	fB	201	CYC	CHD-C4C-NC	-2.79	121.89	125.20
6	dK	201	CYC	O2D-CGD-O1D	-2.79	116.35	123.30
6	dE	201	CYC	CMA-C3A-C4A	2.78	129.35	125.06
6	dL	201	CYC	O2D-CGD-O1D	-2.78	116.36	123.30
6	cD	201	CYC	C1A-NA-C4A	2.78	111.75	106.51
6	fG	201	CYC	C1A-NA-C4A	2.78	111.75	106.51
6	eU	201	CYC	O1A-CGA-CBA	-2.78	114.14	123.08
6	bU	201	CYC	O1A-CGA-CBA	-2.78	114.14	123.08
6	dA	201	CYC	C1A-C2A-C3A	-2.78	103.70	106.78
6	aK	201	CYC	O2D-CGD-CBD	2.78	122.97	114.03
6	aH	201	CYC	O2D-CGD-CBD	2.78	122.97	114.03
6	aA	201	CYC	CMA-C3A-C4A	2.78	129.35	125.06
6	aP	201	CYC	CHB-C4A-NA	-2.78	119.11	124.93
6	dP	201	CYC	CHB-C4A-NA	-2.78	119.12	124.93
6	aE	201	CYC	CMA-C3A-C4A	2.78	129.34	125.06
6	eQ	201	CYC	CHD-C4C-NC	-2.78	121.90	125.20
6	dK	201	CYC	O2D-CGD-CBD	2.78	122.96	114.03
6	cI	201	CYC	O1A-CGA-CBA	-2.78	114.16	123.08
6	aE	201	CYC	C1A-NA-C4A	2.78	111.74	106.51
6	aM	1202	CYC	C4D-CHA-C1A	2.78	132.13	128.81
6	dO	201	CYC	O1A-CGA-CBA	-2.78	114.16	123.08
6	fI	201	CYC	O1A-CGA-CBA	-2.78	114.16	123.08
6	cG	201	CYC	CHB-C4A-NA	-2.77	119.13	124.93
6	fG	201	CYC	CHB-C4A-NA	-2.77	119.13	124.93
6	aO	201	CYC	O1A-CGA-CBA	-2.77	114.17	123.08
6	cD	201	CYC	CHD-C4C-NC	-2.77	121.91	125.20
6	dE	201	CYC	C1A-NA-C4A	2.77	111.73	106.51
6	fD	201	CYC	CHD-C4C-NC	-2.77	121.91	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	eP	201	CYC	O1A-CGA-CBA	-2.77	114.19	123.08
6	bP	201	CYC	O1A-CGA-CBA	-2.76	114.20	123.08
6	dI	201	CYC	O1A-CGA-CBA	-2.76	114.20	123.08
6	fB	201	CYC	CMA-C3A-C4A	2.76	129.32	125.06
6	aI	201	CYC	O1A-CGA-CBA	-2.76	114.20	123.08
6	dM	1202	CYC	C4D-CHA-C1A	2.76	132.11	128.81
6	cI	201	CYC	CHB-C4A-NA	-2.76	119.16	124.93
6	fF	202	CYC	O1A-CGA-CBA	-2.76	114.22	123.08
6	cF	202	CYC	O1A-CGA-CBA	-2.75	114.23	123.08
6	aO	201	CYC	CHB-C4A-NA	-2.75	119.17	124.93
6	fI	201	CYC	CHB-C4A-NA	-2.75	119.17	124.93
6	fD	201	CYC	O1A-CGA-CBA	-2.75	114.23	123.08
6	dO	201	CYC	CHB-C4A-NA	-2.75	119.18	124.93
6	cD	201	CYC	O1A-CGA-CBA	-2.75	114.24	123.08
6	aP	201	CYC	O1A-CGA-CBA	-2.75	114.25	123.08
6	dP	201	CYC	O1A-CGA-CBA	-2.75	114.25	123.08
6	fG	201	CYC	CAA-CBA-CGA	-2.75	107.69	113.60
6	eU	201	CYC	C2C-C3C-C4C	2.75	105.45	101.34
6	bU	201	CYC	C2C-C3C-C4C	2.74	105.45	101.34
6	cB	201	CYC	CMA-C3A-C4A	2.74	129.29	125.06
6	cG	201	CYC	CAA-CBA-CGA	-2.74	107.70	113.60
6	eX	201	CYC	O1A-CGA-CBA	-2.74	114.27	123.08
6	bX	201	CYC	O1A-CGA-CBA	-2.74	114.27	123.08
6	eU	201	CYC	CMA-C3A-C4A	2.74	129.29	125.06
6	aG	201	CYC	C1A-NA-C4A	2.74	111.67	106.51
6	dG	201	CYC	C1A-NA-C4A	2.74	111.67	106.51
6	aC	201	CYC	CAA-CBA-CGA	-2.74	107.71	113.60
6	fJ	201	CYC	CHB-C4A-NA	-2.74	119.20	124.93
6	bU	201	CYC	CMA-C3A-C4A	2.74	129.28	125.06
6	cJ	201	CYC	CHB-C4A-NA	-2.74	119.20	124.93
6	dC	201	CYC	CAA-CBA-CGA	-2.74	107.71	113.60
6	aM	1202	CYC	O1A-CGA-CBA	-2.74	114.29	123.08
6	dM	1202	CYC	O1A-CGA-CBA	-2.74	114.29	123.08
6	eT	201	CYC	O1A-CGA-CBA	-2.74	114.29	123.08
6	aP	201	CYC	C1A-NA-C4A	2.74	111.66	106.51
6	bT	201	CYC	O1A-CGA-CBA	-2.73	114.30	123.08
6	dR	201	CYC	CAA-CBA-CGA	-2.73	107.72	113.60
6	bR	201	CYC	O1A-CGA-CBA	-2.73	114.30	123.08
6	dP	201	CYC	C1A-NA-C4A	2.73	111.66	106.51
6	aM	1204	CYC	CAA-CBA-CGA	-2.73	107.73	113.60
6	eR	201	CYC	O1A-CGA-CBA	-2.73	114.31	123.08
6	bS	201	CYC	O1A-CGA-CBA	-2.73	114.31	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	eS	201	CYC	O1A-CGA-CBA	-2.73	114.32	123.08
6	aB	201	CYC	C2C-C3C-C4C	2.72	105.42	101.34
6	fB	201	CYC	O1A-CGA-CBA	-2.72	114.34	123.08
6	bT	201	CYC	CHB-C4A-C3A	2.72	131.90	124.90
6	eT	201	CYC	CHB-C4A-C3A	2.72	131.90	124.90
6	bU	201	CYC	CHB-C4A-NA	-2.72	119.24	124.93
6	cB	201	CYC	O1A-CGA-CBA	-2.72	114.34	123.08
6	fF	202	CYC	CAA-CBA-CGA	-2.72	107.75	113.60
6	dH	201	CYC	C4A-C3A-C2A	2.72	109.63	106.51
6	dB	201	CYC	C2C-C3C-C4C	2.72	105.41	101.34
6	eU	201	CYC	CHB-C4A-NA	-2.72	119.24	124.93
6	aQ	201	CYC	O1A-CGA-CBA	-2.72	114.34	123.08
6	aQ	201	CYC	O2D-CGD-CBD	2.72	122.76	114.03
6	aI	201	CYC	C2C-C3C-C4C	2.72	105.41	101.34
6	aH	201	CYC	C4A-C3A-C2A	2.72	109.63	106.51
6	dQ	201	CYC	O2D-CGD-CBD	2.72	122.76	114.03
6	dQ	201	CYC	O1A-CGA-CBA	-2.72	114.35	123.08
6	cF	202	CYC	CAA-CBA-CGA	-2.72	107.76	113.60
6	eU	201	CYC	CAA-CBA-CGA	-2.72	107.76	113.60
6	bU	201	CYC	CAA-CBA-CGA	-2.72	107.76	113.60
6	aE	201	CYC	O1A-CGA-CBA	-2.71	114.36	123.08
6	dE	201	CYC	O1A-CGA-CBA	-2.71	114.37	123.08
6	bQ	201	CYC	C1A-NA-C4A	2.71	111.62	106.51
6	dI	201	CYC	C2C-C3C-C4C	2.71	105.40	101.34
6	eQ	201	CYC	C1A-NA-C4A	2.71	111.62	106.51
6	aM	1204	CYC	CAB-C3B-C4B	2.71	125.65	121.38
6	bM	201	CYC	CAA-CBA-CGA	-2.71	107.78	113.60
6	eM	201	CYC	CAA-CBA-CGA	-2.70	107.78	113.60
6	eT	201	CYC	CAC-C3C-C4C	2.70	119.62	112.67
6	dR	201	CYC	CAB-C3B-C4B	2.70	125.64	121.38
6	bT	201	CYC	C2B-C1B-NB	2.70	110.94	106.99
6	dR	201	CYC	O2D-CGD-O1D	-2.70	116.57	123.30
6	eT	201	CYC	C2B-C1B-NB	2.70	110.94	106.99
6	aM	1204	CYC	O2D-CGD-O1D	-2.70	116.58	123.30
6	bT	201	CYC	CAC-C3C-C4C	2.70	119.60	112.67
6	aI	201	CYC	CHD-C4C-NC	-2.70	122.00	125.20
6	dI	201	CYC	CHD-C4C-NC	-2.69	122.00	125.20
6	dF	201	CYC	O1A-CGA-CBA	-2.69	114.44	123.08
6	dL	201	CYC	C2C-C3C-C4C	2.69	105.37	101.34
6	aF	201	CYC	O1A-CGA-CBA	-2.69	114.44	123.08
6	aL	201	CYC	C2C-C3C-C4C	2.69	105.36	101.34
6	eS	201	CYC	CHB-C4A-NA	-2.68	119.33	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	bS	201	CYC	CHB-C4A-NA	-2.68	119.33	124.93
6	eO	201	CYC	C2C-C3C-C4C	2.67	105.34	101.34
6	eV	201	CYC	O1A-CGA-CBA	-2.67	114.49	123.08
6	bV	201	CYC	O1A-CGA-CBA	-2.67	114.50	123.08
6	aJ	201	CYC	O1A-CGA-CBA	-2.66	114.53	123.08
6	dJ	201	CYC	O1A-CGA-CBA	-2.66	114.53	123.08
6	bO	201	CYC	C2C-C3C-C4C	2.66	105.33	101.34
6	bV	201	CYC	C2C-C3C-C4C	2.66	105.32	101.34
6	eV	201	CYC	C2C-C3C-C4C	2.66	105.32	101.34
6	cF	202	CYC	C2B-C1B-NB	2.66	110.88	106.99
6	bR	201	CYC	C1A-NA-C4A	2.65	111.51	106.51
6	cD	202	CYC	C1A-NA-C4A	2.65	111.51	106.51
6	eR	201	CYC	C1A-NA-C4A	2.65	111.51	106.51
6	dD	201	CYC	CHB-C4A-C3A	2.65	131.71	124.90
6	fM	101	CYC	O1A-CGA-CBA	-2.65	114.57	123.08
6	fF	202	CYC	C2B-C1B-NB	2.65	110.87	106.99
6	fD	201	CYC	CMA-C3A-C4A	2.65	129.14	125.06
6	aQ	201	CYC	C2C-C3C-C4C	2.65	105.31	101.34
6	fL	201	CYC	O1A-CGA-CBA	-2.65	114.58	123.08
6	cM	101	CYC	O1A-CGA-CBA	-2.65	114.58	123.08
6	aP	201	CYC	O2D-CGD-CBD	2.65	122.53	114.03
6	aB	201	CYC	C1A-NA-C4A	2.64	111.49	106.51
6	aD	201	CYC	CHB-C4A-C3A	2.64	131.70	124.90
6	cD	201	CYC	CMA-C3A-C4A	2.64	129.14	125.06
6	bW	201	CYC	CAA-CBA-CGA	-2.64	107.91	113.60
6	aQ	201	CYC	O2D-CGD-O1D	-2.64	116.71	123.30
6	cL	201	CYC	O1A-CGA-CBA	-2.64	114.59	123.08
6	eW	201	CYC	CAA-CBA-CGA	-2.64	107.92	113.60
6	dQ	201	CYC	O2D-CGD-O1D	-2.64	116.71	123.30
6	dB	201	CYC	C1A-NA-C4A	2.64	111.49	106.51
6	dQ	201	CYC	C2C-C3C-C4C	2.64	105.30	101.34
6	dJ	201	CYC	C2B-C1B-NB	2.64	110.86	106.99
6	fD	202	CYC	C1A-NA-C4A	2.64	111.49	106.51
6	bV	201	CYC	CHB-C4A-C3A	2.64	131.68	124.90
6	eV	201	CYC	CHB-C4A-C3A	2.64	131.68	124.90
6	dP	201	CYC	O2D-CGD-CBD	2.63	122.49	114.03
6	eP	201	CYC	C2C-C3C-C4C	2.63	105.28	101.34
6	bP	201	CYC	C2C-C3C-C4C	2.63	105.28	101.34
6	aJ	201	CYC	C2B-C1B-NB	2.63	110.84	106.99
6	aB	201	CYC	O1A-CGA-CBA	-2.63	114.63	123.08
6	dB	201	CYC	O1A-CGA-CBA	-2.63	114.64	123.08
6	aJ	201	CYC	C2C-C3C-C4C	2.62	105.27	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	dJ	201	CYC	C2C-C3C-C4C	2.62	105.27	101.34
6	aI	201	CYC	C4A-C3A-C2A	2.62	109.52	106.51
6	dI	201	CYC	C4A-C3A-C2A	2.62	109.52	106.51
6	eW	201	CYC	CHB-C4A-NA	-2.62	119.45	124.93
6	eT	201	CYC	CMA-C3A-C4A	2.62	129.10	125.06
6	bW	201	CYC	CHB-C4A-NA	-2.62	119.45	124.93
6	fJ	201	CYC	CAA-CBA-CGA	-2.62	107.97	113.60
6	dF	201	CYC	C2C-C3C-C4C	2.62	105.26	101.34
6	bT	201	CYC	CMA-C3A-C4A	2.62	129.10	125.06
6	aK	201	CYC	CHB-C4A-NA	-2.62	119.46	124.93
6	aF	201	CYC	C2C-C3C-C4C	2.62	105.26	101.34
6	dK	201	CYC	CHB-C4A-NA	-2.62	119.46	124.93
6	dE	201	CYC	CAC-C3C-C2C	-2.62	107.72	114.26
6	fF	201	CYC	CHD-C4C-NC	-2.62	122.09	125.20
6	aE	201	CYC	CAC-C3C-C2C	-2.61	107.73	114.26
6	bN	201	CYC	C1A-NA-C4A	2.61	111.43	106.51
6	cJ	201	CYC	CAA-CBA-CGA	-2.61	107.98	113.60
6	dN	201	CYC	C2C-C3C-C4C	2.61	105.25	101.34
6	aI	201	CYC	O2D-CGD-CBD	2.61	122.42	114.03
6	cF	201	CYC	CHD-C4C-NC	-2.61	122.10	125.20
6	aN	201	CYC	C2C-C3C-C4C	2.61	105.25	101.34
6	dI	201	CYC	O2D-CGD-CBD	2.61	122.41	114.03
6	eN	201	CYC	C1A-NA-C4A	2.61	111.42	106.51
6	eV	201	CYC	C1A-NA-C4A	2.60	111.42	106.51
6	dI	201	CYC	O2D-CGD-O1D	-2.60	116.81	123.30
6	aI	201	CYC	O2D-CGD-O1D	-2.60	116.81	123.30
6	bV	201	CYC	C1A-NA-C4A	2.60	111.41	106.51
6	bP	201	CYC	C1A-NA-C4A	2.60	111.41	106.51
6	eP	201	CYC	C1A-NA-C4A	2.60	111.41	106.51
6	dI	201	CYC	C1A-NA-C4A	2.60	111.41	106.51
6	aI	201	CYC	C1A-NA-C4A	2.60	111.40	106.51
6	bT	201	CYC	C1A-NA-C4A	2.60	111.40	106.51
6	aB	201	CYC	C4A-C3A-C2A	2.60	109.49	106.51
6	bR	201	CYC	C2C-C3C-C4C	2.60	105.23	101.34
6	dB	201	CYC	C4A-C3A-C2A	2.60	109.49	106.51
6	aF	201	CYC	C4A-C3A-C2A	2.60	109.49	106.51
6	dJ	201	CYC	CHB-C1B-C2B	-2.60	121.81	126.95
6	dF	201	CYC	C4A-C3A-C2A	2.59	109.49	106.51
6	eT	201	CYC	C1A-NA-C4A	2.59	111.40	106.51
6	eT	201	CYC	CAB-C3B-C2B	2.59	131.97	127.53
6	bT	201	CYC	CAB-C3B-C2B	2.59	131.96	127.53
6	aJ	201	CYC	CHB-C1B-C2B	-2.59	121.81	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	eR	201	CYC	C2C-C3C-C4C	2.59	105.22	101.34
6	cM	101	CYC	CAC-C3C-C2C	2.59	120.73	114.26
6	cM	101	CYC	C4A-C3A-C2A	2.59	109.48	106.51
6	fM	101	CYC	C4A-C3A-C2A	2.59	109.48	106.51
6	bM	201	CYC	CHD-C4C-NC	-2.59	122.13	125.20
6	dF	201	CYC	C1A-NA-C4A	2.59	111.39	106.51
6	eN	201	CYC	O1A-CGA-CBA	-2.59	114.78	123.08
6	aM	1203	CYC	O1A-CGA-CBA	-2.59	114.78	123.08
6	fM	101	CYC	CAC-C3C-C2C	2.58	120.72	114.26
6	bN	201	CYC	O1A-CGA-CBA	-2.58	114.78	123.08
6	aF	201	CYC	C1A-NA-C4A	2.58	111.38	106.51
6	aJ	201	CYC	CHB-C4A-NA	-2.58	119.53	124.93
6	eM	201	CYC	CHD-C4C-NC	-2.58	122.14	125.20
6	dD	201	CYC	C2B-C1B-NB	2.58	110.77	106.99
6	dM	1203	CYC	O1A-CGA-CBA	-2.58	114.79	123.08
6	dC	201	CYC	C2C-C3C-C4C	2.58	105.20	101.34
6	dL	201	CYC	O2D-CGD-CBD	2.58	122.32	114.03
6	dJ	201	CYC	CHB-C4A-NA	-2.58	119.54	124.93
6	aL	201	CYC	O2D-CGD-CBD	2.58	122.31	114.03
6	eO	201	CYC	C4A-C3A-C2A	2.58	109.47	106.51
6	aC	201	CYC	C2C-C3C-C4C	2.58	105.20	101.34
6	eX	201	CYC	C2C-C3C-C4C	2.58	105.20	101.34
6	aD	201	CYC	C2B-C1B-NB	2.57	110.76	106.99
6	bX	201	CYC	C2C-C3C-C4C	2.57	105.19	101.34
6	dB	201	CYC	O2D-CGD-CBD	2.57	122.30	114.03
6	dJ	201	CYC	CAC-C3C-C4C	2.57	119.28	112.67
6	aM	1202	CYC	CMA-C3A-C4A	2.57	129.03	125.06
6	dB	201	CYC	CMA-C3A-C4A	2.57	129.03	125.06
6	aB	201	CYC	O2D-CGD-CBD	2.57	122.30	114.03
6	aJ	201	CYC	CAC-C3C-C4C	2.57	119.28	112.67
6	aB	201	CYC	CMA-C3A-C4A	2.57	129.03	125.06
6	dF	201	CYC	CAA-CBA-CGA	-2.57	108.07	113.60
6	dM	1202	CYC	CMA-C3A-C4A	2.57	129.02	125.06
6	aF	201	CYC	CAA-CBA-CGA	-2.57	108.08	113.60
6	aM	1202	CYC	C1A-NA-C4A	2.56	111.34	106.51
6	cF	202	CYC	C1A-NA-C4A	2.56	111.34	106.51
6	dM	1202	CYC	C1A-NA-C4A	2.56	111.34	106.51
6	bT	201	CYC	CAA-C2A-C1A	2.56	129.54	125.01
6	aM	1201	CYC	C1A-NA-C4A	2.56	111.33	106.51
6	eT	201	CYC	CAA-C2A-C1A	2.56	129.53	125.01
6	bO	201	CYC	C4A-C3A-C2A	2.55	109.44	106.51
6	dM	1201	CYC	C1A-NA-C4A	2.55	111.32	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	bX	201	CYC	CAA-CBA-CGA	-2.55	108.11	113.60
6	fF	202	CYC	C1A-NA-C4A	2.55	111.32	106.51
6	eX	201	CYC	CAA-CBA-CGA	-2.55	108.11	113.60
6	dB	201	CYC	CHD-C4C-NC	-2.55	122.17	125.20
6	bO	201	CYC	CHB-C4A-NA	-2.55	119.60	124.93
6	cF	202	CYC	CHD-C4C-NC	-2.55	122.18	125.20
6	fF	202	CYC	CHD-C4C-NC	-2.55	122.18	125.20
6	bT	201	CYC	C2C-C3C-C4C	2.54	105.15	101.34
6	eO	201	CYC	CHB-C4A-NA	-2.54	119.62	124.93
6	aP	201	CYC	C4A-C3A-C2A	2.54	109.43	106.51
6	cD	202	CYC	C4A-C3A-C2A	2.54	109.43	106.51
6	eT	201	CYC	C2C-C3C-C4C	2.54	105.14	101.34
6	aB	201	CYC	CHD-C4C-NC	-2.54	122.19	125.20
6	bP	201	CYC	CAA-CBA-CGA	-2.54	108.14	113.60
6	dH	201	CYC	C1A-NA-C4A	2.53	111.29	106.51
6	aE	201	CYC	CAC-C3C-C4C	2.53	119.18	112.67
6	dE	201	CYC	CAC-C3C-C4C	2.53	119.18	112.67
6	dR	201	CYC	O1A-CGA-CBA	-2.53	114.94	123.08
6	dM	1201	CYC	CAC-C3C-C4C	2.53	119.18	112.67
6	dP	201	CYC	C4A-C3A-C2A	2.53	109.42	106.51
6	aM	1201	CYC	CAC-C3C-C4C	2.53	119.18	112.67
6	aH	201	CYC	C1A-NA-C4A	2.53	111.28	106.51
6	aM	1204	CYC	O1A-CGA-CBA	-2.53	114.95	123.08
6	fD	202	CYC	C4A-C3A-C2A	2.53	109.41	106.51
6	eP	201	CYC	CAA-CBA-CGA	-2.53	108.16	113.60
6	aB	201	CYC	CBD-CAD-C3D	2.53	116.93	112.62
6	dB	201	CYC	CBD-CAD-C3D	2.53	116.93	112.62
6	dM	1201	CYC	C4A-C3A-C2A	2.53	109.41	106.51
6	aM	1201	CYC	C4A-C3A-C2A	2.52	109.41	106.51
6	dK	201	CYC	CBD-CAD-C3D	-2.52	108.32	112.62
6	dO	201	CYC	CAA-CBA-CGA	-2.52	108.18	113.60
6	aK	201	CYC	CBD-CAD-C3D	-2.52	108.32	112.62
6	aQ	201	CYC	CAA-CBA-CGA	-2.52	108.18	113.60
6	aE	201	CYC	CAA-CBA-CGA	-2.52	108.19	113.60
6	aO	201	CYC	CAA-CBA-CGA	-2.52	108.19	113.60
6	dQ	201	CYC	CAA-CBA-CGA	-2.52	108.19	113.60
6	aQ	201	CYC	C2B-C1B-NB	2.51	110.67	106.99
6	dQ	201	CYC	C2B-C1B-NB	2.51	110.67	106.99
6	dE	201	CYC	CAA-CBA-CGA	-2.51	108.21	113.60
6	bN	201	CYC	C4A-C3A-C2A	2.50	109.38	106.51
6	dJ	201	CYC	C1A-NA-C4A	2.50	111.22	106.51
6	aF	201	CYC	CHB-C1B-NB	-2.50	120.69	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	aD	201	CYC	CAA-CBA-CGA	-2.50	108.23	113.60
6	cF	202	CYC	CHB-C4A-NA	-2.50	119.71	124.93
6	fF	202	CYC	CHB-C4A-NA	-2.50	119.71	124.93
6	dF	201	CYC	CHB-C1B-NB	-2.50	120.70	126.06
6	aJ	201	CYC	C1A-NA-C4A	2.50	111.21	106.51
6	dD	201	CYC	CAA-CBA-CGA	-2.49	108.23	113.60
6	eX	201	CYC	C1A-NA-C4A	2.49	111.21	106.51
6	fJ	201	CYC	C4A-C3A-C2A	2.49	109.37	106.51
6	cJ	201	CYC	C4A-C3A-C2A	2.49	109.37	106.51
6	cM	101	CYC	C1A-NA-C4A	2.49	111.20	106.51
6	eN	201	CYC	C4A-C3A-C2A	2.49	109.36	106.51
6	bX	201	CYC	C1A-NA-C4A	2.49	111.20	106.51
6	cL	201	CYC	C1A-NA-C4A	2.49	111.20	106.51
6	fL	201	CYC	C1A-NA-C4A	2.49	111.19	106.51
6	fM	101	CYC	C1A-NA-C4A	2.49	111.19	106.51
6	aM	1203	CYC	C1A-NA-C4A	2.48	111.18	106.51
6	dM	1203	CYC	C1A-NA-C4A	2.48	111.18	106.51
6	aL	201	CYC	CHB-C4A-NA	-2.48	119.75	124.93
6	bS	201	CYC	CAC-C3C-C2C	-2.48	108.07	114.26
6	eS	201	CYC	CAC-C3C-C2C	-2.48	108.07	114.26
6	aN	201	CYC	CHD-C4C-NC	-2.47	122.26	125.20
6	dL	201	CYC	CHB-C4A-NA	-2.47	119.76	124.93
6	dL	201	CYC	C4A-C3A-C2A	2.47	109.34	106.51
6	bR	201	CYC	CAA-CBA-CGA	-2.47	108.29	113.60
6	dG	201	CYC	O2A-CGA-CBA	2.46	121.95	114.03
6	cF	202	CYC	C2C-C3C-C4C	2.46	105.03	101.34
6	eR	201	CYC	CAA-CBA-CGA	-2.46	108.30	113.60
6	aG	201	CYC	O2A-CGA-CBA	2.46	121.94	114.03
6	aL	201	CYC	C4A-C3A-C2A	2.46	109.34	106.51
6	fD	202	CYC	CHB-C4A-NA	-2.46	119.78	124.93
6	aM	1202	CYC	CAC-C3C-C2C	2.46	120.41	114.26
6	dJ	201	CYC	C1B-CHB-C4A	2.46	134.09	128.08
6	aJ	201	CYC	C1B-CHB-C4A	2.46	134.09	128.08
6	eS	201	CYC	C4A-C3A-C2A	2.46	109.33	106.51
6	cD	202	CYC	CHB-C4A-NA	-2.46	119.79	124.93
6	dN	201	CYC	CHD-C4C-NC	-2.46	122.28	125.20
6	bS	201	CYC	C4A-C3A-C2A	2.46	109.33	106.51
6	dI	201	CYC	C1B-CHB-C4A	2.46	134.09	128.08
6	dM	1202	CYC	CAC-C3C-C2C	2.46	120.39	114.26
6	aI	201	CYC	C1B-CHB-C4A	2.45	134.08	128.08
6	cF	202	CYC	CMA-C3A-C4A	2.44	128.82	125.06
6	aI	201	CYC	CHB-C4A-NA	-2.44	119.83	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	fF	202	CYC	CMA-C3A-C4A	2.44	128.82	125.06
6	fF	202	CYC	C2C-C3C-C4C	2.44	104.99	101.34
6	dI	201	CYC	CHB-C4A-NA	-2.44	119.83	124.93
6	cM	101	CYC	CHB-C4A-C3A	2.44	131.17	124.90
6	fM	101	CYC	CHB-C4A-C3A	2.44	131.17	124.90
6	aM	1203	CYC	C2C-C3C-C4C	2.44	104.99	101.34
6	dM	1203	CYC	C2C-C3C-C4C	2.43	104.98	101.34
6	aH	201	CYC	CAB-C3B-C2B	2.42	131.67	127.53
6	dL	201	CYC	C2B-C1B-NB	2.42	110.53	106.99
6	aD	201	CYC	C2C-C3C-C4C	2.42	104.96	101.34
6	dC	201	CYC	C1B-CHB-C4A	2.42	133.99	128.08
6	dK	201	CYC	C4A-C3A-C2A	2.42	109.28	106.51
6	fI	201	CYC	CAA-CBA-CGA	-2.42	108.40	113.60
6	aK	201	CYC	C4A-C3A-C2A	2.42	109.28	106.51
6	bV	201	CYC	CHD-C4C-NC	-2.42	122.33	125.20
6	dH	201	CYC	CAB-C3B-C2B	2.41	131.66	127.53
6	aC	201	CYC	C1B-CHB-C4A	2.41	133.98	128.08
6	eV	201	CYC	C4A-C3A-C2A	2.41	109.28	106.51
6	eV	201	CYC	CHD-C4C-NC	-2.41	122.34	125.20
6	cB	201	CYC	C4A-C3A-C2A	2.41	109.28	106.51
6	dD	201	CYC	C2C-C3C-C4C	2.41	104.95	101.34
6	aL	201	CYC	C2B-C1B-NB	2.41	110.52	106.99
6	cI	201	CYC	CAA-CBA-CGA	-2.41	108.42	113.60
6	dN	201	CYC	C4A-C3A-C2A	2.41	109.27	106.51
6	aN	201	CYC	C4A-C3A-C2A	2.41	109.27	106.51
6	fB	201	CYC	C4A-C3A-C2A	2.41	109.27	106.51
6	fI	201	CYC	C4A-C3A-C2A	2.41	109.27	106.51
6	bR	201	CYC	C4A-C3A-C2A	2.41	109.27	106.51
6	dM	1202	CYC	C4A-C3A-C2A	2.40	109.27	106.51
6	eS	201	CYC	C1B-CHB-C4A	2.40	133.95	128.08
6	bV	201	CYC	C4A-C3A-C2A	2.40	109.27	106.51
6	bX	201	CYC	C2B-C1B-NB	2.40	110.50	106.99
6	bS	201	CYC	C1B-CHB-C4A	2.40	133.95	128.08
6	eR	201	CYC	C4A-C3A-C2A	2.40	109.27	106.51
6	aM	1202	CYC	C4A-C3A-C2A	2.40	109.27	106.51
6	cG	201	CYC	C4A-C3A-C2A	2.40	109.26	106.51
6	fG	201	CYC	C4A-C3A-C2A	2.40	109.26	106.51
6	dP	201	CYC	C2B-C1B-NB	2.40	110.50	106.99
6	eX	201	CYC	C2B-C1B-NB	2.39	110.49	106.99
6	aP	201	CYC	C2B-C1B-NB	2.39	110.49	106.99
6	eR	201	CYC	CMA-C3A-C4A	2.39	128.75	125.06
6	fD	202	CYC	CHD-C4C-NC	-2.39	122.37	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	dA	201	CYC	CHB-C4A-NA	-2.39	119.94	124.93
6	cD	202	CYC	CHD-C4C-NC	-2.39	122.37	125.20
6	bO	201	CYC	O2A-CGA-CBA	2.39	121.70	114.03
6	aP	201	CYC	C2C-C3C-C4C	2.39	104.91	101.34
6	cL	201	CYC	CHB-C4A-C3A	2.38	131.03	124.90
6	aD	201	CYC	C1A-NA-C4A	2.38	111.00	106.51
6	aA	201	CYC	CHB-C4A-NA	-2.38	119.94	124.93
6	eU	201	CYC	C4A-C3A-C2A	2.38	109.25	106.51
6	fL	201	CYC	CHB-C4A-C3A	2.38	131.03	124.90
6	bU	201	CYC	C1B-CHB-C4A	2.38	133.90	128.08
6	eU	201	CYC	C1B-CHB-C4A	2.38	133.90	128.08
6	dD	201	CYC	C1A-NA-C4A	2.38	111.00	106.51
6	bR	201	CYC	CMA-C3A-C4A	2.38	128.73	125.06
6	eO	201	CYC	O2A-CGA-CBA	2.38	121.68	114.03
6	dI	201	CYC	C2B-C1B-NB	2.38	110.47	106.99
6	cI	201	CYC	C4A-C3A-C2A	2.38	109.24	106.51
6	dP	201	CYC	C2C-C3C-C4C	2.38	104.90	101.34
6	aI	201	CYC	C2B-C1B-NB	2.38	110.47	106.99
6	bW	201	CYC	C4A-C3A-C2A	2.38	109.24	106.51
6	eW	201	CYC	C4A-C3A-C2A	2.38	109.24	106.51
6	dM	1201	CYC	CMB-C2B-C1B	2.38	127.14	124.17
6	bU	201	CYC	C4A-C3A-C2A	2.38	109.24	106.51
6	bX	201	CYC	CHD-C4C-NC	-2.37	122.38	125.20
6	eX	201	CYC	CHD-C4C-NC	-2.37	122.38	125.20
6	aD	201	CYC	CHD-C4C-NC	-2.37	122.39	125.20
6	dD	201	CYC	CHD-C4C-NC	-2.37	122.39	125.20
6	bP	201	CYC	C4A-C3A-C2A	2.37	109.23	106.51
6	aM	1201	CYC	CMB-C2B-C1B	2.37	127.12	124.17
6	aE	201	CYC	C2C-C3C-C4C	2.37	104.88	101.34
6	eP	201	CYC	C4A-C3A-C2A	2.37	109.22	106.51
6	dE	201	CYC	C2C-C3C-C4C	2.37	104.88	101.34
6	bP	201	CYC	C2B-C1B-NB	2.37	110.45	106.99
6	eP	201	CYC	C2B-C1B-NB	2.37	110.45	106.99
6	cL	201	CYC	C2C-C3C-C4C	2.36	104.88	101.34
6	aH	201	CYC	C2C-C3C-C4C	2.36	104.88	101.34
6	dH	201	CYC	C2C-C3C-C4C	2.36	104.88	101.34
6	eV	201	CYC	CAB-C3B-C2B	2.36	131.57	127.53
6	bV	201	CYC	CAB-C3B-C2B	2.36	131.57	127.53
6	fL	201	CYC	C2C-C3C-C4C	2.36	104.87	101.34
6	dM	1203	CYC	CAC-C3C-C2C	2.36	120.14	114.26
6	dC	201	CYC	C4A-C3A-C2A	2.35	109.21	106.51
6	aM	1203	CYC	CAC-C3C-C2C	2.35	120.14	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	aC	201	CYC	C4A-C3A-C2A	2.35	109.21	106.51
6	fL	201	CYC	CAC-C3C-C2C	2.35	120.13	114.26
6	eW	201	CYC	O2A-CGA-CBA	2.35	121.58	114.03
6	dM	1203	CYC	C2B-C1B-NB	2.35	110.42	106.99
6	bW	201	CYC	O2A-CGA-CBA	2.35	121.57	114.03
6	cL	201	CYC	CAC-C3C-C2C	2.35	120.12	114.26
6	fD	201	CYC	C2C-C3C-C4C	2.35	104.85	101.34
6	aM	1203	CYC	C2B-C1B-NB	2.35	110.42	106.99
6	cB	201	CYC	C1B-CHB-C4A	2.34	133.81	128.08
6	dE	201	CYC	C1B-CHB-C4A	2.34	133.81	128.08
6	aE	201	CYC	C1B-CHB-C4A	2.34	133.80	128.08
6	aM	1203	CYC	CBD-CAD-C3D	2.34	116.61	112.62
6	cD	201	CYC	C2C-C3C-C4C	2.34	104.84	101.34
6	fB	201	CYC	C1B-CHB-C4A	2.33	133.78	128.08
6	aM	1203	CYC	CHB-C4A-C3A	2.33	130.90	124.90
6	bV	201	CYC	C2B-C1B-NB	2.33	110.40	106.99
6	dM	1203	CYC	CHB-C4A-C3A	2.33	130.90	124.90
6	dM	1203	CYC	CBD-CAD-C3D	2.33	116.60	112.62
6	bM	201	CYC	O2A-CGA-CBA	2.33	121.52	114.03
6	eV	201	CYC	C2B-C1B-NB	2.33	110.40	106.99
6	eM	201	CYC	O2A-CGA-CBA	2.33	121.51	114.03
6	aA	201	CYC	O2A-CGA-CBA	2.32	121.50	114.03
6	fF	201	CYC	C4A-C3A-C2A	2.32	109.17	106.51
6	dA	201	CYC	O2A-CGA-CBA	2.32	121.48	114.03
6	eV	201	CYC	CAA-CBA-CGA	-2.32	108.61	113.60
6	cF	201	CYC	C4A-C3A-C2A	2.32	109.17	106.51
6	aM	1202	CYC	CAA-CBA-CGA	-2.32	108.62	113.60
6	dM	1202	CYC	CAA-CBA-CGA	-2.32	108.62	113.60
6	cL	201	CYC	CAA-CBA-CGA	-2.32	108.62	113.60
6	bV	201	CYC	CAA-CBA-CGA	-2.31	108.62	113.60
6	aM	1201	CYC	CHB-C4A-C3A	2.31	130.85	124.90
6	dM	1201	CYC	CHB-C4A-C3A	2.31	130.85	124.90
6	aM	1203	CYC	C4A-C3A-C2A	2.31	109.16	106.51
6	fL	201	CYC	CAA-CBA-CGA	-2.31	108.63	113.60
6	eP	201	CYC	CMA-C3A-C4A	2.31	128.62	125.06
6	dM	1203	CYC	C4A-C3A-C2A	2.31	109.16	106.51
6	eP	201	CYC	CHD-C4C-NC	-2.31	122.46	125.20
6	dH	201	CYC	CHA-C1A-C2A	-2.31	119.99	125.32
6	cB	201	CYC	CAA-CBA-CGA	-2.31	108.64	113.60
6	bQ	201	CYC	O2A-CGA-CBA	2.31	121.44	114.03
6	dE	201	CYC	C2B-C1B-NB	2.31	110.36	106.99
6	eQ	201	CYC	O2A-CGA-CBA	2.31	121.44	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	aH	201	CYC	CHA-C1A-C2A	-2.30	120.00	125.32
6	bP	201	CYC	CMA-C3A-C4A	2.30	128.61	125.06
6	fJ	201	CYC	O2A-CGA-CBA	2.30	121.43	114.03
6	aE	201	CYC	C2B-C1B-NB	2.30	110.36	106.99
6	cJ	201	CYC	O2A-CGA-CBA	2.30	121.43	114.03
6	cD	202	CYC	CAC-C3C-C2C	2.30	120.01	114.26
6	fD	202	CYC	CAC-C3C-C2C	2.30	120.01	114.26
6	cF	201	CYC	O2A-CGA-CBA	2.30	121.42	114.03
6	dJ	201	CYC	C4A-C3A-C2A	2.30	109.15	106.51
6	eQ	201	CYC	CAC-C3C-C2C	2.30	120.00	114.26
6	fF	201	CYC	O2A-CGA-CBA	2.30	121.42	114.03
6	dK	201	CYC	C3A-C4A-NA	-2.30	105.61	110.53
6	aH	201	CYC	C2B-C1B-NB	2.30	110.35	106.99
6	fB	201	CYC	CAA-CBA-CGA	-2.30	108.66	113.60
6	bQ	201	CYC	CAC-C3C-C2C	2.30	120.00	114.26
6	dH	201	CYC	C2B-C1B-NB	2.30	110.35	106.99
6	aK	201	CYC	C3A-C4A-NA	-2.30	105.62	110.53
6	aJ	201	CYC	C4A-C3A-C2A	2.29	109.14	106.51
6	bP	201	CYC	CHD-C4C-NC	-2.29	122.48	125.20
6	fB	201	CYC	C2C-C3C-C4C	2.29	104.77	101.34
6	cL	201	CYC	C2B-C1B-NB	2.29	110.34	106.99
6	aK	201	CYC	C1B-CHB-C4A	2.29	133.68	128.08
6	fL	201	CYC	C2B-C1B-NB	2.29	110.34	106.99
6	dK	201	CYC	C1B-CHB-C4A	2.29	133.67	128.08
6	dB	201	CYC	CAA-CBA-CGA	-2.29	108.68	113.60
6	aM	1202	CYC	C2C-C3C-C4C	2.29	104.77	101.34
6	aB	201	CYC	CAA-CBA-CGA	-2.29	108.68	113.60
6	bR	201	CYC	C2B-C1B-NB	2.29	110.33	106.99
6	dM	1202	CYC	C2C-C3C-C4C	2.29	104.76	101.34
6	aI	201	CYC	CHB-C1B-C2B	-2.28	122.42	126.95
6	cB	201	CYC	C2C-C3C-C4C	2.28	104.76	101.34
6	eX	201	CYC	C4A-C3A-C2A	2.28	109.13	106.51
6	dI	201	CYC	CHB-C1B-C2B	-2.28	122.43	126.95
6	aF	201	CYC	C2B-C1B-NB	2.28	110.33	106.99
6	eM	201	CYC	C4A-C3A-C2A	2.28	109.13	106.51
6	bX	201	CYC	C4A-C3A-C2A	2.28	109.12	106.51
6	eR	201	CYC	C2B-C1B-NB	2.28	110.32	106.99
6	bM	201	CYC	C4A-C3A-C2A	2.28	109.12	106.51
6	eS	201	CYC	CHD-C4C-NC	-2.28	122.50	125.20
6	bW	201	CYC	C3A-C4A-NA	-2.27	105.67	110.53
6	eW	201	CYC	C3A-C4A-NA	-2.27	105.67	110.53
6	dF	201	CYC	C2B-C1B-NB	2.27	110.32	106.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	bS	201	CYC	CHD-C4C-NC	-2.27	122.51	125.20
6	cL	201	CYC	C4A-C3A-C2A	2.27	109.11	106.51
6	aN	201	CYC	C2B-C1B-NB	2.27	110.30	106.99
6	fL	201	CYC	C4A-C3A-C2A	2.27	109.11	106.51
6	cM	101	CYC	CAA-CBA-CGA	-2.26	108.73	113.60
6	aL	201	CYC	O2A-CGA-CBA	2.26	121.30	114.03
6	dN	201	CYC	C2B-C1B-NB	2.26	110.30	106.99
6	bS	201	CYC	O2A-CGA-CBA	2.26	121.30	114.03
6	dL	201	CYC	O2A-CGA-CBA	2.26	121.29	114.03
6	eS	201	CYC	O2A-CGA-CBA	2.26	121.29	114.03
6	dB	201	CYC	CAB-C3B-C2B	2.26	131.39	127.53
6	dI	201	CYC	O2A-CGA-CBA	2.26	121.28	114.03
6	fM	101	CYC	C2C-C3C-C4C	2.26	104.72	101.34
6	eN	201	CYC	CAC-C3C-C2C	-2.25	108.63	114.26
6	eQ	201	CYC	C2B-C1B-NB	2.25	110.29	106.99
6	aI	201	CYC	O2A-CGA-CBA	2.25	121.27	114.03
6	bN	201	CYC	CAC-C3C-C2C	-2.25	108.63	114.26
6	fM	101	CYC	CAA-CBA-CGA	-2.25	108.75	113.60
6	bQ	201	CYC	C2B-C1B-NB	2.25	110.28	106.99
6	dH	201	CYC	O2A-CGA-CBA	2.25	121.26	114.03
6	aB	201	CYC	CAB-C3B-C2B	2.25	131.38	127.53
6	cM	101	CYC	C2C-C3C-C4C	2.25	104.71	101.34
6	dN	201	CYC	O2A-CGA-CBA	2.25	121.25	114.03
6	aH	201	CYC	O2A-CGA-CBA	2.25	121.25	114.03
6	aN	201	CYC	O2A-CGA-CBA	2.25	121.25	114.03
6	aM	1204	CYC	CBA-CAA-C2A	2.25	118.87	112.63
6	eX	201	CYC	O2A-CGA-CBA	2.24	121.24	114.03
6	dR	201	CYC	CBA-CAA-C2A	2.24	118.86	112.63
6	aH	201	CYC	CHB-C1B-NB	-2.24	121.25	126.06
6	bX	201	CYC	O2A-CGA-CBA	2.24	121.23	114.03
6	cI	201	CYC	C2C-C3C-C4C	2.24	104.70	101.34
6	fI	201	CYC	C2C-C3C-C4C	2.24	104.70	101.34
6	aG	201	CYC	CHB-C4A-NA	-2.24	120.25	124.93
6	dG	201	CYC	CHB-C4A-NA	-2.24	120.25	124.93
6	dH	201	CYC	CHB-C1B-NB	-2.24	121.25	126.06
6	fJ	201	CYC	C3A-C4A-NA	-2.24	105.74	110.53
6	cJ	201	CYC	C3A-C4A-NA	-2.24	105.75	110.53
6	cF	201	CYC	C2C-C3C-C4C	2.23	104.69	101.34
6	fB	201	CYC	O2A-CGA-CBA	2.23	121.21	114.03
6	cF	201	CYC	C2B-C1B-NB	2.23	110.26	106.99
6	cD	201	CYC	C4A-C3A-C2A	2.23	109.07	106.51
6	dP	201	CYC	C4D-CHA-C1A	-2.23	126.14	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	fD	202	CYC	O2A-CGA-CBA	2.23	121.20	114.03
6	dM	1202	CYC	CAB-C3B-C2B	2.23	131.35	127.53
6	cD	202	CYC	O2A-CGA-CBA	2.23	121.20	114.03
6	eW	201	CYC	CAC-C3C-C2C	2.23	119.83	114.26
6	fF	201	CYC	C2B-C1B-NB	2.23	110.25	106.99
6	bW	201	CYC	CAC-C3C-C2C	2.23	119.83	114.26
6	aP	201	CYC	C4D-CHA-C1A	-2.23	126.15	128.81
6	cB	201	CYC	O2A-CGA-CBA	2.23	121.19	114.03
6	aM	1202	CYC	CAB-C3B-C2B	2.23	131.34	127.53
6	fF	201	CYC	C2C-C3C-C4C	2.22	104.67	101.34
6	fD	201	CYC	C4A-C3A-C2A	2.22	109.06	106.51
6	dO	201	CYC	C2B-C1B-NB	2.22	110.24	106.99
6	aC	201	CYC	CAC-C3C-C2C	-2.22	108.71	114.26
6	aC	201	CYC	C2B-C1B-NB	2.22	110.23	106.99
6	cD	202	CYC	C3A-C4A-NA	-2.22	105.79	110.53
6	eO	201	CYC	C3A-C4A-NA	-2.22	105.79	110.53
6	aO	201	CYC	C2B-C1B-NB	2.22	110.23	106.99
6	dM	1202	CYC	CHA-C1A-C2A	-2.22	120.20	125.32
6	cI	201	CYC	O2A-CGA-CBA	2.22	121.15	114.03
6	dC	201	CYC	CAC-C3C-C2C	-2.22	108.72	114.26
6	aA	201	CYC	C4A-C3A-C2A	2.22	109.05	106.51
6	aM	1202	CYC	CHA-C1A-C2A	-2.22	120.20	125.32
6	bX	201	CYC	CMA-C3A-C4A	2.21	128.47	125.06
6	bT	201	CYC	C4A-C3A-C2A	2.21	109.05	106.51
6	dK	201	CYC	O2A-CGA-CBA	2.21	121.14	114.03
6	fD	202	CYC	C3A-C4A-NA	-2.21	105.80	110.53
6	aP	201	CYC	CAC-C3C-C4C	2.21	118.35	112.67
6	fI	201	CYC	O2A-CGA-CBA	2.21	121.13	114.03
6	eX	201	CYC	CMA-C3A-C4A	2.21	128.47	125.06
6	bO	201	CYC	C3A-C4A-NA	-2.21	105.81	110.53
6	aK	201	CYC	O2A-CGA-CBA	2.21	121.13	114.03
6	fI	201	CYC	C3A-C4A-NA	-2.21	105.81	110.53
6	eM	201	CYC	C3A-C4A-NA	-2.21	105.81	110.53
6	dD	201	CYC	O2A-CGA-CBA	2.21	121.12	114.03
6	aD	201	CYC	O2A-CGA-CBA	2.21	121.12	114.03
6	dC	201	CYC	C2B-C1B-NB	2.21	110.22	106.99
6	dA	201	CYC	C4A-C3A-C2A	2.21	109.04	106.51
6	bM	201	CYC	C3A-C4A-NA	-2.20	105.82	110.53
6	eQ	201	CYC	C4A-C3A-C2A	2.20	109.04	106.51
6	eT	201	CYC	C4A-C3A-C2A	2.20	109.04	106.51
6	fL	201	CYC	CHA-C1A-C2A	-2.20	120.24	125.32
6	aC	201	CYC	C3A-C4A-NA	-2.20	105.83	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	cB	201	CYC	C2B-C1B-NB	2.20	110.20	106.99
6	bQ	201	CYC	C4A-C3A-C2A	2.20	109.03	106.51
6	dC	201	CYC	C3A-C4A-NA	-2.20	105.83	110.53
6	eU	201	CYC	CAC-C3C-C2C	-2.20	108.77	114.26
6	cI	201	CYC	C3A-C4A-NA	-2.20	105.83	110.53
6	dP	201	CYC	CAC-C3C-C4C	2.20	118.31	112.67
6	aC	201	CYC	O2A-CGA-CBA	2.19	121.08	114.03
6	cL	201	CYC	CHA-C1A-C2A	-2.19	120.25	125.32
6	fB	201	CYC	C2B-C1B-NB	2.19	110.20	106.99
6	dC	201	CYC	O2A-CGA-CBA	2.19	121.08	114.03
6	fG	201	CYC	O2A-CGA-CBA	2.19	121.07	114.03
6	fG	201	CYC	C2B-C1B-NB	2.19	110.20	106.99
6	cG	201	CYC	C3A-C4A-NA	-2.19	105.84	110.53
6	cG	201	CYC	O2A-CGA-CBA	2.19	121.07	114.03
6	fF	202	CYC	O2A-CGA-CBA	2.19	121.07	114.03
6	bU	201	CYC	CAC-C3C-C2C	-2.19	108.79	114.26
6	fF	201	CYC	C3A-C4A-NA	-2.19	105.85	110.53
6	cG	201	CYC	C2B-C1B-NB	2.19	110.19	106.99
6	cJ	201	CYC	C1B-CHB-C4A	2.19	133.43	128.08
6	fJ	201	CYC	C1B-CHB-C4A	2.19	133.43	128.08
6	cG	201	CYC	C2C-C3C-C4C	2.19	104.62	101.34
6	cF	202	CYC	O2A-CGA-CBA	2.19	121.06	114.03
6	cF	201	CYC	C3A-C4A-NA	-2.19	105.85	110.53
6	aE	201	CYC	C4A-C3A-C2A	2.19	109.02	106.51
6	fG	201	CYC	C2C-C3C-C4C	2.18	104.61	101.34
6	fG	201	CYC	C3A-C4A-NA	-2.18	105.86	110.53
6	fB	201	CYC	C3A-C4A-NA	-2.18	105.86	110.53
6	cB	201	CYC	C3A-C4A-NA	-2.18	105.86	110.53
6	dE	201	CYC	C4A-C3A-C2A	2.18	109.01	106.51
6	aF	201	CYC	CHD-C4C-NC	-2.18	122.61	125.20
6	fD	201	CYC	O2A-CGA-CBA	2.18	121.04	114.03
6	bS	201	CYC	C3A-C4A-NA	-2.18	105.88	110.53
6	cD	201	CYC	O2A-CGA-CBA	2.18	121.02	114.03
6	dI	201	CYC	CAC-C3C-C2C	-2.17	108.83	114.26
6	fD	202	CYC	CHA-C1A-C2A	-2.17	120.30	125.32
6	bR	201	CYC	O2A-CGA-CBA	2.17	121.02	114.03
6	aI	201	CYC	CAC-C3C-C2C	-2.17	108.83	114.26
6	eS	201	CYC	C3A-C4A-NA	-2.17	105.88	110.53
6	dF	201	CYC	CHD-C4C-NC	-2.17	122.62	125.20
6	eU	201	CYC	C3A-C4A-NA	-2.17	105.89	110.53
6	eR	201	CYC	O2A-CGA-CBA	2.17	121.01	114.03
6	aO	201	CYC	O2A-CGA-CBA	2.17	121.00	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	dH	201	CYC	C3A-C4A-NA	-2.17	105.89	110.53
6	aI	201	CYC	CAA-CBA-CGA	-2.17	108.93	113.60
6	cD	202	CYC	CHA-C1A-C2A	-2.17	120.31	125.32
6	aH	201	CYC	C3A-C4A-NA	-2.17	105.89	110.53
6	bU	201	CYC	C3A-C4A-NA	-2.17	105.89	110.53
6	dO	201	CYC	O2A-CGA-CBA	2.17	121.00	114.03
6	aN	201	CYC	C3A-C4A-NA	-2.17	105.89	110.53
6	aF	201	CYC	O2A-CGA-CBA	2.17	121.00	114.03
6	dF	201	CYC	O2A-CGA-CBA	2.17	121.00	114.03
6	dJ	201	CYC	O2A-CGA-CBA	2.17	121.00	114.03
6	cL	201	CYC	CAB-C3B-C2B	2.17	131.24	127.53
6	dI	201	CYC	CAA-CBA-CGA	-2.17	108.94	113.60
6	dB	201	CYC	O2A-CGA-CBA	2.17	120.99	114.03
6	bN	201	CYC	CAA-CBA-CGA	-2.17	108.94	113.60
6	aB	201	CYC	O2A-CGA-CBA	2.17	120.99	114.03
6	dN	201	CYC	C3A-C4A-NA	-2.17	105.90	110.53
6	eN	201	CYC	CAA-CBA-CGA	-2.17	108.94	113.60
6	fL	201	CYC	CAB-C3B-C2B	2.16	131.23	127.53
6	aJ	201	CYC	O2A-CGA-CBA	2.16	120.98	114.03
6	aE	201	CYC	O2A-CGA-CBA	2.16	120.97	114.03
6	dE	201	CYC	O2A-CGA-CBA	2.16	120.97	114.03
6	aP	201	CYC	C3A-C4A-NA	-2.16	105.91	110.53
6	aB	201	CYC	C3A-C4A-NA	-2.16	105.92	110.53
6	bU	201	CYC	O2A-CGA-CBA	2.16	120.96	114.03
6	dB	201	CYC	C3A-C4A-NA	-2.16	105.92	110.53
6	eU	201	CYC	O2A-CGA-CBA	2.16	120.96	114.03
6	aM	1202	CYC	O2A-CGA-CBA	2.15	120.95	114.03
6	bM	201	CYC	C2B-C1B-NB	2.15	110.14	106.99
6	cD	201	CYC	C2B-C1B-NB	2.15	110.14	106.99
6	eM	201	CYC	C2B-C1B-NB	2.15	110.14	106.99
6	dP	201	CYC	C3A-C4A-NA	-2.15	105.92	110.53
6	fI	201	CYC	C2B-C1B-NB	2.15	110.14	106.99
6	fD	201	CYC	C2B-C1B-NB	2.15	110.14	106.99
6	bX	201	CYC	CAB-C3B-C2B	2.15	131.21	127.53
6	dM	1202	CYC	O2A-CGA-CBA	2.15	120.94	114.03
6	bV	201	CYC	CMA-C3A-C4A	2.15	128.38	125.06
6	aQ	201	CYC	O2A-CGA-CBA	2.15	120.94	114.03
6	dQ	201	CYC	O2A-CGA-CBA	2.15	120.94	114.03
6	cI	201	CYC	C2B-C1B-NB	2.15	110.13	106.99
6	bP	201	CYC	O2A-CGA-CBA	2.15	120.93	114.03
6	eV	201	CYC	CMA-C3A-C4A	2.15	128.37	125.06
6	eP	201	CYC	O2A-CGA-CBA	2.15	120.93	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	cM	101	CYC	CHA-C1A-C2A	-2.15	120.36	125.32
6	fM	101	CYC	CHA-C1A-C2A	-2.15	120.36	125.32
6	eX	201	CYC	CAB-C3B-C2B	2.14	131.19	127.53
6	eR	201	CYC	CHD-C4C-NC	-2.14	122.66	125.20
6	dM	1202	CYC	C2B-C1B-NB	2.14	110.12	106.99
6	fG	201	CYC	CAC-C3C-C2C	2.14	119.61	114.26
6	bR	201	CYC	CHD-C4C-NC	-2.14	122.66	125.20
6	eO	201	CYC	CAC-C3C-C2C	-2.14	108.92	114.26
6	aO	201	CYC	C4A-C3A-C2A	2.14	108.96	106.51
6	aM	1202	CYC	C2B-C1B-NB	2.14	110.12	106.99
6	dO	201	CYC	C4A-C3A-C2A	2.14	108.96	106.51
6	eV	201	CYC	O2A-CGA-CBA	2.14	120.89	114.03
6	bV	201	CYC	O2A-CGA-CBA	2.13	120.89	114.03
6	cG	201	CYC	CAC-C3C-C2C	2.13	119.59	114.26
6	fM	101	CYC	O2A-CGA-CBA	2.13	120.88	114.03
6	fD	201	CYC	C3A-C4A-NA	-2.13	105.97	110.53
6	dL	201	CYC	C3A-C4A-NA	-2.13	105.97	110.53
6	cD	201	CYC	C3A-C4A-NA	-2.13	105.98	110.53
6	cM	101	CYC	O2A-CGA-CBA	2.13	120.87	114.03
6	aL	201	CYC	C3A-C4A-NA	-2.13	105.98	110.53
6	aM	1203	CYC	CAA-CBA-CGA	-2.13	109.03	113.60
6	dO	201	CYC	C3A-C4A-NA	-2.13	105.99	110.53
6	cM	101	CYC	CAB-C3B-C2B	2.12	131.16	127.53
6	cF	202	CYC	C4A-C3A-C2A	2.12	108.95	106.51
6	aO	201	CYC	C3A-C4A-NA	-2.12	105.99	110.53
6	fM	101	CYC	CAB-C3B-C2B	2.12	131.16	127.53
6	fM	101	CYC	CMA-C3A-C4A	2.12	128.33	125.06
6	fJ	201	CYC	C2B-C1B-NB	2.12	110.09	106.99
6	cM	101	CYC	C2B-C1B-NB	2.12	110.09	106.99
6	aL	201	CYC	CAA-C2A-C1A	2.12	128.76	125.01
6	cM	101	CYC	CMA-C3A-C4A	2.12	128.33	125.06
6	aH	201	CYC	C4D-CHA-C1A	2.12	131.34	128.81
6	dP	201	CYC	O2A-CGA-CBA	2.12	120.84	114.03
6	aA	201	CYC	C3A-C4A-NA	-2.12	106.00	110.53
6	bW	201	CYC	C2C-C3C-C4C	2.12	104.51	101.34
6	fM	101	CYC	C2B-C1B-NB	2.12	110.09	106.99
6	dM	1203	CYC	CAA-CBA-CGA	-2.12	109.05	113.60
6	aP	201	CYC	O2A-CGA-CBA	2.12	120.83	114.03
6	fF	202	CYC	C4A-C3A-C2A	2.12	108.94	106.51
6	fG	201	CYC	C1B-CHB-C4A	2.12	133.25	128.08
6	fJ	201	CYC	C2C-C3C-C4C	2.12	104.51	101.34
6	dL	201	CYC	CAA-C2A-C1A	2.11	128.75	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	dA	201	CYC	C3A-C4A-NA	-2.11	106.01	110.53
6	eW	201	CYC	C2C-C3C-C4C	2.11	104.50	101.34
6	dH	201	CYC	C4D-CHA-C1A	2.11	131.33	128.81
6	fI	201	CYC	C1B-CHB-C4A	2.11	133.25	128.08
6	eQ	201	CYC	C3A-C4A-NA	-2.11	106.01	110.53
6	bQ	201	CYC	C3A-C4A-NA	-2.11	106.01	110.53
6	eW	201	CYC	C1B-CHB-C4A	2.11	133.24	128.08
6	bN	201	CYC	C2B-C1B-NB	2.11	110.08	106.99
6	bW	201	CYC	C1B-CHB-C4A	2.11	133.24	128.08
6	cJ	201	CYC	C2C-C3C-C4C	2.11	104.50	101.34
6	cJ	201	CYC	C2B-C1B-NB	2.11	110.08	106.99
6	dG	201	CYC	C4A-C3A-C2A	2.11	108.93	106.51
6	bO	201	CYC	CAC-C3C-C2C	-2.11	108.99	114.26
6	cG	201	CYC	C1B-CHB-C4A	2.11	133.23	128.08
6	fL	201	CYC	O2A-CGA-CBA	2.10	120.79	114.03
6	cI	201	CYC	C1B-CHB-C4A	2.10	133.22	128.08
6	aG	201	CYC	C4A-C3A-C2A	2.10	108.92	106.51
6	cL	201	CYC	O2A-CGA-CBA	2.10	120.78	114.03
6	fF	201	CYC	CMA-C3A-C2A	-2.10	120.42	126.12
6	cF	201	CYC	CMA-C3A-C2A	-2.10	120.42	126.12
6	eN	201	CYC	C2B-C1B-NB	2.09	110.05	106.99
6	aM	1201	CYC	O2A-CGA-CBA	2.09	120.76	114.03
6	bM	201	CYC	C2C-C3C-C4C	2.09	104.48	101.34
6	aM	1203	CYC	O2A-CGA-CBA	2.09	120.76	114.03
6	dM	1201	CYC	O2A-CGA-CBA	2.09	120.75	114.03
6	dM	1203	CYC	O2A-CGA-CBA	2.09	120.75	114.03
6	eM	201	CYC	C2C-C3C-C4C	2.09	104.47	101.34
6	aM	1201	CYC	C3A-C4A-NA	-2.09	106.06	110.53
6	dM	1201	CYC	C3A-C4A-NA	-2.09	106.07	110.53
6	bR	201	CYC	C3A-C4A-NA	-2.09	106.07	110.53
6	eR	201	CYC	C3A-C4A-NA	-2.08	106.08	110.53
6	aK	201	CYC	C2B-C1B-NB	2.08	110.03	106.99
6	cL	201	CYC	CHB-C1B-NB	-2.08	121.59	126.06
6	cD	201	CYC	CHB-C4A-NA	-2.08	120.58	124.93
6	cD	202	CYC	CMA-C3A-C2A	-2.08	120.47	126.12
6	eR	201	CYC	CAB-C3B-C2B	2.08	131.09	127.53
6	fD	201	CYC	CHB-C4A-NA	-2.08	120.58	124.93
6	dK	201	CYC	C2B-C1B-NB	2.08	110.03	106.99
6	bM	201	CYC	C1B-CHB-C4A	2.08	133.16	128.08
6	eM	201	CYC	C1B-CHB-C4A	2.08	133.16	128.08
6	dN	201	CYC	CAB-C3B-C2B	2.08	131.08	127.53
6	aN	201	CYC	CAB-C3B-C2B	2.08	131.08	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	bR	201	CYC	CAB-C3B-C2B	2.08	131.08	127.53
6	fL	201	CYC	CHB-C1B-NB	-2.08	121.60	126.06
6	bO	201	CYC	C1B-CHB-C4A	2.08	133.15	128.08
6	dA	201	CYC	C2B-C1B-NB	2.08	110.03	106.99
6	fD	202	CYC	CMA-C3A-C2A	-2.08	120.48	126.12
6	aA	201	CYC	C2B-C1B-NB	2.07	110.03	106.99
6	eO	201	CYC	C1B-CHB-C4A	2.07	133.15	128.08
6	dM	1203	CYC	CHA-C1A-C2A	-2.07	120.53	125.32
6	aE	201	CYC	C3A-C4A-NA	-2.07	106.10	110.53
6	dE	201	CYC	C3A-C4A-NA	-2.07	106.11	110.53
6	aM	1203	CYC	CHA-C1A-C2A	-2.07	120.54	125.32
6	dO	201	CYC	CBD-CAD-C3D	-2.07	109.09	112.62
6	bN	201	CYC	C3A-C4A-NA	-2.06	106.12	110.53
6	dG	201	CYC	CAA-C2A-C3A	2.06	131.72	127.88
6	eN	201	CYC	O2A-CGA-CBA	2.06	120.65	114.03
6	bN	201	CYC	O2A-CGA-CBA	2.06	120.65	114.03
6	cB	201	CYC	CAC-C3C-C2C	2.06	119.40	114.26
6	aG	201	CYC	CAA-C2A-C3A	2.06	131.71	127.88
6	dG	201	CYC	C2B-C1B-NB	2.06	110.00	106.99
6	fB	201	CYC	CAC-C3C-C2C	2.06	119.40	114.26
6	aO	201	CYC	CBD-CAD-C3D	-2.06	109.11	112.62
6	eN	201	CYC	C3A-C4A-NA	-2.05	106.14	110.53
6	aG	201	CYC	C2B-C1B-NB	2.05	110.00	106.99
6	aN	201	CYC	CBA-CAA-C2A	2.05	118.33	112.63
6	cF	202	CYC	CBD-CAD-C3D	2.05	116.12	112.62
6	dN	201	CYC	CBA-CAA-C2A	2.05	118.33	112.63
6	fF	202	CYC	CBD-CAD-C3D	2.05	116.12	112.62
6	eT	201	CYC	O2A-CGA-CBA	2.05	120.60	114.03
6	aM	1202	CYC	C3A-C4A-NA	-2.04	106.16	110.53
6	bT	201	CYC	O2A-CGA-CBA	2.04	120.60	114.03
6	cM	101	CYC	C3A-C4A-NA	-2.04	106.16	110.53
6	aA	201	CYC	C1B-CHB-C4A	2.04	133.07	128.08
6	dM	1202	CYC	C3A-C4A-NA	-2.04	106.16	110.53
6	fM	101	CYC	C3A-C4A-NA	-2.04	106.16	110.53
6	dA	201	CYC	C1B-CHB-C4A	2.04	133.07	128.08
6	bU	201	CYC	C2B-C1B-NB	2.04	109.97	106.99
6	aM	1204	CYC	CAB-C3B-C2B	2.04	131.02	127.53
6	dQ	201	CYC	C1B-CHB-C4A	2.04	133.06	128.08
6	fD	202	CYC	C2C-C3C-C4C	2.04	104.39	101.34
6	cD	202	CYC	C2C-C3C-C4C	2.04	104.39	101.34
6	dR	201	CYC	CAB-C3B-C2B	2.04	131.01	127.53
6	aQ	201	CYC	C1B-CHB-C4A	2.04	133.06	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	eU	201	CYC	C2B-C1B-NB	2.04	109.97	106.99
6	aG	201	CYC	CAC-C3C-C2C	-2.03	109.18	114.26
6	eS	201	CYC	C2B-C1B-NB	2.03	109.96	106.99
6	fL	201	CYC	CMA-C3A-C4A	2.03	128.19	125.06
6	eO	201	CYC	C2B-C1B-NB	2.03	109.96	106.99
6	dG	201	CYC	CAC-C3C-C2C	-2.03	109.19	114.26
6	bO	201	CYC	C2B-C1B-NB	2.03	109.95	106.99
6	fD	202	CYC	C2B-C1B-NB	2.02	109.95	106.99
6	cD	202	CYC	C2B-C1B-NB	2.02	109.95	106.99
6	dJ	201	CYC	CMD-C2D-C3D	-2.02	121.13	124.94
6	bS	201	CYC	C2B-C1B-NB	2.02	109.95	106.99
6	aJ	201	CYC	CMD-C2D-C3D	-2.02	121.14	124.94
6	cL	201	CYC	CMA-C3A-C4A	2.02	128.17	125.06
6	bR	201	CYC	CHA-C1A-C2A	-2.02	120.66	125.32
6	eR	201	CYC	CHA-C1A-C2A	-2.02	120.67	125.32
6	dM	1203	CYC	CAB-C3B-C2B	2.01	130.97	127.53
6	dR	201	CYC	CMB-C2B-C1B	2.01	126.67	124.17
6	aM	1203	CYC	CAB-C3B-C2B	2.00	130.96	127.53
6	aM	1201	CYC	OB-C4B-NB	-2.00	120.43	125.08
6	dM	1201	CYC	OB-C4B-NB	-2.00	120.43	125.08
6	aM	1204	CYC	O2A-CGA-CBA	2.00	120.46	114.03

There are no chirality outliers.

All (851) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	aA	201	CYC	ND-C1D-CHD-C4C
6	aA	201	CYC	C2D-C1D-CHD-C4C
6	aB	201	CYC	NA-C4A-CHB-C1B
6	aB	201	CYC	C3A-C4A-CHB-C1B
6	aB	201	CYC	ND-C1D-CHD-C4C
6	aB	201	CYC	C2D-C1D-CHD-C4C
6	aC	201	CYC	ND-C1D-CHD-C4C
6	aC	201	CYC	C2D-C1D-CHD-C4C
6	aD	201	CYC	NA-C4A-CHB-C1B
6	aD	201	CYC	C3A-C4A-CHB-C1B
6	aD	201	CYC	ND-C1D-CHD-C4C
6	aD	201	CYC	C2D-C1D-CHD-C4C
6	aE	201	CYC	ND-C4D-CHA-C1A
6	aE	201	CYC	C3D-C4D-CHA-C1A
6	aE	201	CYC	C4C-C3C-CAC-CBC
6	aE	201	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
6	aE	201	CYC	C2D-C1D-CHD-C4C
6	aF	201	CYC	NA-C4A-CHB-C1B
6	aF	201	CYC	C3A-C4A-CHB-C1B
6	aF	201	CYC	C4B-C3B-CAB-CBB
6	aF	201	CYC	ND-C1D-CHD-C4C
6	aF	201	CYC	C2D-C1D-CHD-C4C
6	aG	201	CYC	C1A-C2A-CAA-CBA
6	aG	201	CYC	C3A-C2A-CAA-CBA
6	aG	201	CYC	NA-C4A-CHB-C1B
6	aG	201	CYC	C3A-C4A-CHB-C1B
6	aG	201	CYC	C4B-C3B-CAB-CBB
6	aG	201	CYC	ND-C1D-CHD-C4C
6	aG	201	CYC	C2D-C1D-CHD-C4C
6	aH	201	CYC	NA-C4A-CHB-C1B
6	aH	201	CYC	C3A-C4A-CHB-C1B
6	aH	201	CYC	ND-C1D-CHD-C4C
6	aH	201	CYC	C2D-C1D-CHD-C4C
6	aI	201	CYC	NA-C4A-CHB-C1B
6	aI	201	CYC	ND-C1D-CHD-C4C
6	aI	201	CYC	C2D-C1D-CHD-C4C
6	aJ	201	CYC	NA-C4A-CHB-C1B
6	aJ	201	CYC	C3A-C4A-CHB-C1B
6	aJ	201	CYC	ND-C1D-CHD-C4C
6	aJ	201	CYC	C2D-C1D-CHD-C4C
6	aK	201	CYC	ND-C1D-CHD-C4C
6	aK	201	CYC	C2D-C1D-CHD-C4C
6	aL	201	CYC	NA-C4A-CHB-C1B
6	aL	201	CYC	C3A-C4A-CHB-C1B
6	aL	201	CYC	ND-C1D-CHD-C4C
6	aL	201	CYC	C2D-C1D-CHD-C4C
6	aM	1201	CYC	ND-C4D-CHA-C1A
6	aM	1201	CYC	C3D-C4D-CHA-C1A
6	aM	1201	CYC	NA-C4A-CHB-C1B
6	aM	1201	CYC	C3A-C4A-CHB-C1B
6	aM	1201	CYC	C4B-C3B-CAB-CBB
6	aM	1201	CYC	C4C-C3C-CAC-CBC
6	aM	1201	CYC	NC-C4C-CHD-C1D
6	aM	1201	CYC	ND-C1D-CHD-C4C
6	aM	1201	CYC	C2D-C1D-CHD-C4C
6	aM	1202	CYC	NA-C4A-CHB-C1B
6	aM	1202	CYC	C3A-C4A-CHB-C1B
6	aM	1202	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
6	aM	1202	CYC	C2D-C1D-CHD-C4C
6	aM	1203	CYC	NA-C4A-CHB-C1B
6	aM	1203	CYC	C3A-C4A-CHB-C1B
6	aM	1203	CYC	ND-C1D-CHD-C4C
6	aM	1203	CYC	C2D-C1D-CHD-C4C
6	aM	1204	CYC	NA-C4A-CHB-C1B
6	aM	1204	CYC	ND-C1D-CHD-C4C
6	aM	1204	CYC	C2D-C1D-CHD-C4C
6	aN	201	CYC	NA-C4A-CHB-C1B
6	aN	201	CYC	C3A-C4A-CHB-C1B
6	aN	201	CYC	ND-C1D-CHD-C4C
6	aN	201	CYC	C2D-C1D-CHD-C4C
6	aO	201	CYC	ND-C1D-CHD-C4C
6	aO	201	CYC	C2D-C1D-CHD-C4C
6	aP	201	CYC	NA-C4A-CHB-C1B
6	aP	201	CYC	ND-C1D-CHD-C4C
6	aP	201	CYC	C2D-C1D-CHD-C4C
6	aQ	201	CYC	ND-C1D-CHD-C4C
6	aQ	201	CYC	C2D-C1D-CHD-C4C
6	bM	201	CYC	C2C-C3C-CAC-CBC
6	bM	201	CYC	ND-C1D-CHD-C4C
6	bM	201	CYC	C2D-C1D-CHD-C4C
6	bN	201	CYC	NA-C4A-CHB-C1B
6	bN	201	CYC	C3A-C4A-CHB-C1B
6	bN	201	CYC	ND-C1D-CHD-C4C
6	bN	201	CYC	C2D-C1D-CHD-C4C
6	bO	201	CYC	ND-C1D-CHD-C4C
6	bO	201	CYC	C2D-C1D-CHD-C4C
6	bP	201	CYC	NA-C4A-CHB-C1B
6	bP	201	CYC	C3A-C4A-CHB-C1B
6	bP	201	CYC	ND-C1D-CHD-C4C
6	bP	201	CYC	C2D-C1D-CHD-C4C
6	bQ	201	CYC	C2C-C3C-CAC-CBC
6	bQ	201	CYC	ND-C1D-CHD-C4C
6	bQ	201	CYC	C2D-C1D-CHD-C4C
6	bR	201	CYC	NA-C4A-CHB-C1B
6	bR	201	CYC	C3A-C4A-CHB-C1B
6	bR	201	CYC	ND-C1D-CHD-C4C
6	bR	201	CYC	C2D-C1D-CHD-C4C
6	bS	201	CYC	ND-C1D-CHD-C4C
6	bS	201	CYC	C2D-C1D-CHD-C4C
6	bT	201	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
6	bT	201	CYC	C3A-C4A-CHB-C1B
6	bT	201	CYC	C4B-C3B-CAB-CBB
6	bT	201	CYC	C4C-C3C-CAC-CBC
6	bT	201	CYC	ND-C1D-CHD-C4C
6	bT	201	CYC	C2D-C1D-CHD-C4C
6	bU	201	CYC	ND-C1D-CHD-C4C
6	bU	201	CYC	C2D-C1D-CHD-C4C
6	bV	201	CYC	NA-C4A-CHB-C1B
6	bV	201	CYC	C3A-C4A-CHB-C1B
6	bV	201	CYC	ND-C1D-CHD-C4C
6	bV	201	CYC	C2D-C1D-CHD-C4C
6	bW	201	CYC	C2C-C3C-CAC-CBC
6	bW	201	CYC	ND-C1D-CHD-C4C
6	bW	201	CYC	C2D-C1D-CHD-C4C
6	bX	201	CYC	NA-C4A-CHB-C1B
6	bX	201	CYC	C3A-C4A-CHB-C1B
6	bX	201	CYC	ND-C1D-CHD-C4C
6	bX	201	CYC	C2D-C1D-CHD-C4C
6	cB	201	CYC	C2C-C3C-CAC-CBC
6	cB	201	CYC	ND-C1D-CHD-C4C
6	cB	201	CYC	C2D-C1D-CHD-C4C
6	cD	201	CYC	NA-C4A-CHB-C1B
6	cD	201	CYC	C3A-C4A-CHB-C1B
6	cD	201	CYC	C2C-C3C-CAC-CBC
6	cD	201	CYC	C4C-C3C-CAC-CBC
6	cD	201	CYC	ND-C1D-CHD-C4C
6	cD	201	CYC	C2D-C1D-CHD-C4C
6	cD	202	CYC	C2C-C3C-CAC-CBC
6	cD	202	CYC	C4C-C3C-CAC-CBC
6	cD	202	CYC	ND-C1D-CHD-C4C
6	cD	202	CYC	C2D-C1D-CHD-C4C
6	cF	201	CYC	C3A-C4A-CHB-C1B
6	cF	201	CYC	C2C-C3C-CAC-CBC
6	cF	201	CYC	C4C-C3C-CAC-CBC
6	cF	201	CYC	ND-C1D-CHD-C4C
6	cF	201	CYC	C2D-C1D-CHD-C4C
6	cF	202	CYC	NA-C4A-CHB-C1B
6	cF	202	CYC	C3A-C4A-CHB-C1B
6	cF	202	CYC	C2C-C3C-CAC-CBC
6	cF	202	CYC	C4C-C3C-CAC-CBC
6	cF	202	CYC	NC-C4C-CHD-C1D
6	cF	202	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
6	cG	201	CYC	C2C-C3C-CAC-CBC
6	cG	201	CYC	ND-C1D-CHD-C4C
6	cG	201	CYC	C2D-C1D-CHD-C4C
6	cI	201	CYC	C2C-C3C-CAC-CBC
6	cI	201	CYC	C4C-C3C-CAC-CBC
6	cI	201	CYC	ND-C1D-CHD-C4C
6	cI	201	CYC	C2D-C1D-CHD-C4C
6	cJ	201	CYC	C2C-C3C-CAC-CBC
6	cJ	201	CYC	C4C-C3C-CAC-CBC
6	cJ	201	CYC	ND-C1D-CHD-C4C
6	cJ	201	CYC	C2D-C1D-CHD-C4C
6	cL	201	CYC	NA-C4A-CHB-C1B
6	cL	201	CYC	C3A-C4A-CHB-C1B
6	cL	201	CYC	ND-C1D-CHD-C4C
6	cL	201	CYC	C2D-C1D-CHD-C4C
6	cM	101	CYC	NA-C4A-CHB-C1B
6	cM	101	CYC	C3A-C4A-CHB-C1B
6	cM	101	CYC	ND-C1D-CHD-C4C
6	cM	101	CYC	C2D-C1D-CHD-C4C
6	dA	201	CYC	ND-C1D-CHD-C4C
6	dA	201	CYC	C2D-C1D-CHD-C4C
6	dB	201	CYC	NA-C4A-CHB-C1B
6	dB	201	CYC	C3A-C4A-CHB-C1B
6	dB	201	CYC	ND-C1D-CHD-C4C
6	dB	201	CYC	C2D-C1D-CHD-C4C
6	dC	201	CYC	ND-C1D-CHD-C4C
6	dC	201	CYC	C2D-C1D-CHD-C4C
6	dD	201	CYC	NA-C4A-CHB-C1B
6	dD	201	CYC	C3A-C4A-CHB-C1B
6	dD	201	CYC	ND-C1D-CHD-C4C
6	dD	201	CYC	C2D-C1D-CHD-C4C
6	dE	201	CYC	ND-C4D-CHA-C1A
6	dE	201	CYC	C3D-C4D-CHA-C1A
6	dE	201	CYC	C4C-C3C-CAC-CBC
6	dE	201	CYC	ND-C1D-CHD-C4C
6	dE	201	CYC	C2D-C1D-CHD-C4C
6	dF	201	CYC	NA-C4A-CHB-C1B
6	dF	201	CYC	C3A-C4A-CHB-C1B
6	dF	201	CYC	C4B-C3B-CAB-CBB
6	dF	201	CYC	ND-C1D-CHD-C4C
6	dF	201	CYC	C2D-C1D-CHD-C4C
6	dG	201	CYC	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
6	dG	201	CYC	C3A-C2A-CAA-CBA
6	dG	201	CYC	NA-C4A-CHB-C1B
6	dG	201	CYC	C3A-C4A-CHB-C1B
6	dG	201	CYC	C4B-C3B-CAB-CBB
6	dG	201	CYC	ND-C1D-CHD-C4C
6	dG	201	CYC	C2D-C1D-CHD-C4C
6	dH	201	CYC	NA-C4A-CHB-C1B
6	dH	201	CYC	C3A-C4A-CHB-C1B
6	dH	201	CYC	ND-C1D-CHD-C4C
6	dH	201	CYC	C2D-C1D-CHD-C4C
6	dI	201	CYC	NA-C4A-CHB-C1B
6	dI	201	CYC	ND-C1D-CHD-C4C
6	dI	201	CYC	C2D-C1D-CHD-C4C
6	dJ	201	CYC	NA-C4A-CHB-C1B
6	dJ	201	CYC	C3A-C4A-CHB-C1B
6	dJ	201	CYC	ND-C1D-CHD-C4C
6	dJ	201	CYC	C2D-C1D-CHD-C4C
6	dK	201	CYC	ND-C1D-CHD-C4C
6	dK	201	CYC	C2D-C1D-CHD-C4C
6	dL	201	CYC	NA-C4A-CHB-C1B
6	dL	201	CYC	C3A-C4A-CHB-C1B
6	dL	201	CYC	ND-C1D-CHD-C4C
6	dL	201	CYC	C2D-C1D-CHD-C4C
6	dM	1201	CYC	ND-C4D-CHA-C1A
6	dM	1201	CYC	C3D-C4D-CHA-C1A
6	dM	1201	CYC	NA-C4A-CHB-C1B
6	dM	1201	CYC	C3A-C4A-CHB-C1B
6	dM	1201	CYC	C4B-C3B-CAB-CBB
6	dM	1201	CYC	C4C-C3C-CAC-CBC
6	dM	1201	CYC	NC-C4C-CHD-C1D
6	dM	1201	CYC	ND-C1D-CHD-C4C
6	dM	1201	CYC	C2D-C1D-CHD-C4C
6	dM	1202	CYC	NA-C4A-CHB-C1B
6	dM	1202	CYC	C3A-C4A-CHB-C1B
6	dM	1202	CYC	ND-C1D-CHD-C4C
6	dM	1202	CYC	C2D-C1D-CHD-C4C
6	dM	1203	CYC	NA-C4A-CHB-C1B
6	dM	1203	CYC	C3A-C4A-CHB-C1B
6	dM	1203	CYC	ND-C1D-CHD-C4C
6	dM	1203	CYC	C2D-C1D-CHD-C4C
6	dN	201	CYC	NA-C4A-CHB-C1B
6	dN	201	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
6	dN	201	CYC	ND-C1D-CHD-C4C
6	dN	201	CYC	C2D-C1D-CHD-C4C
6	dO	201	CYC	ND-C1D-CHD-C4C
6	dO	201	CYC	C2D-C1D-CHD-C4C
6	dP	201	CYC	NA-C4A-CHB-C1B
6	dP	201	CYC	ND-C1D-CHD-C4C
6	dP	201	CYC	C2D-C1D-CHD-C4C
6	dQ	201	CYC	ND-C1D-CHD-C4C
6	dQ	201	CYC	C2D-C1D-CHD-C4C
6	dR	201	CYC	NA-C4A-CHB-C1B
6	dR	201	CYC	ND-C1D-CHD-C4C
6	dR	201	CYC	C2D-C1D-CHD-C4C
6	eM	201	CYC	C2C-C3C-CAC-CBC
6	eM	201	CYC	ND-C1D-CHD-C4C
6	eM	201	CYC	C2D-C1D-CHD-C4C
6	eN	201	CYC	NA-C4A-CHB-C1B
6	eN	201	CYC	C3A-C4A-CHB-C1B
6	eN	201	CYC	ND-C1D-CHD-C4C
6	eN	201	CYC	C2D-C1D-CHD-C4C
6	eO	201	CYC	ND-C1D-CHD-C4C
6	eO	201	CYC	C2D-C1D-CHD-C4C
6	eP	201	CYC	NA-C4A-CHB-C1B
6	eP	201	CYC	C3A-C4A-CHB-C1B
6	eP	201	CYC	ND-C1D-CHD-C4C
6	eP	201	CYC	C2D-C1D-CHD-C4C
6	eQ	201	CYC	C2C-C3C-CAC-CBC
6	eQ	201	CYC	ND-C1D-CHD-C4C
6	eQ	201	CYC	C2D-C1D-CHD-C4C
6	eR	201	CYC	NA-C4A-CHB-C1B
6	eR	201	CYC	C3A-C4A-CHB-C1B
6	eR	201	CYC	ND-C1D-CHD-C4C
6	eR	201	CYC	C2D-C1D-CHD-C4C
6	eS	201	CYC	ND-C1D-CHD-C4C
6	eS	201	CYC	C2D-C1D-CHD-C4C
6	eT	201	CYC	NA-C4A-CHB-C1B
6	eT	201	CYC	C3A-C4A-CHB-C1B
6	eT	201	CYC	C4B-C3B-CAB-CBB
6	eT	201	CYC	C4C-C3C-CAC-CBC
6	eT	201	CYC	ND-C1D-CHD-C4C
6	eT	201	CYC	C2D-C1D-CHD-C4C
6	eU	201	CYC	ND-C1D-CHD-C4C
6	eU	201	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
6	eV	201	CYC	NA-C4A-CHB-C1B
6	eV	201	CYC	C3A-C4A-CHB-C1B
6	eV	201	CYC	ND-C1D-CHD-C4C
6	eV	201	CYC	C2D-C1D-CHD-C4C
6	eW	201	CYC	C2C-C3C-CAC-CBC
6	eW	201	CYC	ND-C1D-CHD-C4C
6	eW	201	CYC	C2D-C1D-CHD-C4C
6	eX	201	CYC	NA-C4A-CHB-C1B
6	eX	201	CYC	C3A-C4A-CHB-C1B
6	eX	201	CYC	ND-C1D-CHD-C4C
6	eX	201	CYC	C2D-C1D-CHD-C4C
6	fB	201	CYC	C2C-C3C-CAC-CBC
6	fB	201	CYC	ND-C1D-CHD-C4C
6	fB	201	CYC	C2D-C1D-CHD-C4C
6	fD	201	CYC	NA-C4A-CHB-C1B
6	fD	201	CYC	C3A-C4A-CHB-C1B
6	fD	201	CYC	C2C-C3C-CAC-CBC
6	fD	201	CYC	C4C-C3C-CAC-CBC
6	fD	201	CYC	ND-C1D-CHD-C4C
6	fD	201	CYC	C2D-C1D-CHD-C4C
6	fD	202	CYC	C2C-C3C-CAC-CBC
6	fD	202	CYC	C4C-C3C-CAC-CBC
6	fD	202	CYC	ND-C1D-CHD-C4C
6	fD	202	CYC	C2D-C1D-CHD-C4C
6	fF	201	CYC	C3A-C4A-CHB-C1B
6	fF	201	CYC	C2C-C3C-CAC-CBC
6	fF	201	CYC	C4C-C3C-CAC-CBC
6	fF	201	CYC	ND-C1D-CHD-C4C
6	fF	201	CYC	C2D-C1D-CHD-C4C
6	fF	202	CYC	NA-C4A-CHB-C1B
6	fF	202	CYC	C3A-C4A-CHB-C1B
6	fF	202	CYC	C2C-C3C-CAC-CBC
6	fF	202	CYC	C4C-C3C-CAC-CBC
6	fF	202	CYC	NC-C4C-CHD-C1D
6	fF	202	CYC	ND-C1D-CHD-C4C
6	fG	201	CYC	C2C-C3C-CAC-CBC
6	fG	201	CYC	ND-C1D-CHD-C4C
6	fG	201	CYC	C2D-C1D-CHD-C4C
6	fI	201	CYC	C2C-C3C-CAC-CBC
6	fI	201	CYC	C4C-C3C-CAC-CBC
6	fI	201	CYC	ND-C1D-CHD-C4C
6	fI	201	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
6	fJ	201	CYC	C2C-C3C-CAC-CBC
6	fJ	201	CYC	C4C-C3C-CAC-CBC
6	fJ	201	CYC	ND-C1D-CHD-C4C
6	fJ	201	CYC	C2D-C1D-CHD-C4C
6	fL	201	CYC	NA-C4A-CHB-C1B
6	fL	201	CYC	C3A-C4A-CHB-C1B
6	fL	201	CYC	ND-C1D-CHD-C4C
6	fL	201	CYC	C2D-C1D-CHD-C4C
6	fM	101	CYC	NA-C4A-CHB-C1B
6	fM	101	CYC	C3A-C4A-CHB-C1B
6	fM	101	CYC	ND-C1D-CHD-C4C
6	fM	101	CYC	C2D-C1D-CHD-C4C
6	aF	201	CYC	C2B-C3B-CAB-CBB
6	aM	1201	CYC	C2B-C3B-CAB-CBB
6	dF	201	CYC	C2B-C3B-CAB-CBB
6	dM	1201	CYC	C2B-C3B-CAB-CBB
6	aG	201	CYC	C2B-C3B-CAB-CBB
6	dG	201	CYC	C2B-C3B-CAB-CBB
6	bS	201	CYC	C2B-C3B-CAB-CBB
6	bS	201	CYC	C3A-C2A-CAA-CBA
6	eS	201	CYC	C3A-C2A-CAA-CBA
6	eS	201	CYC	C2B-C3B-CAB-CBB
6	aL	201	CYC	C2A-CAA-CBA-CGA
6	aM	1204	CYC	C2A-CAA-CBA-CGA
6	bS	201	CYC	C2A-CAA-CBA-CGA
6	dL	201	CYC	C2A-CAA-CBA-CGA
6	dR	201	CYC	C2A-CAA-CBA-CGA
6	eS	201	CYC	C2A-CAA-CBA-CGA
6	eR	201	CYC	C2B-C3B-CAB-CBB
6	bS	201	CYC	C1A-C2A-CAA-CBA
6	eS	201	CYC	C1A-C2A-CAA-CBA
6	bR	201	CYC	C2B-C3B-CAB-CBB
6	bT	201	CYC	C2B-C3B-CAB-CBB
6	eT	201	CYC	C2B-C3B-CAB-CBB
6	aJ	201	CYC	C2B-C3B-CAB-CBB
6	aF	201	CYC	C3D-CAD-CBD-CGD
6	bS	201	CYC	C3D-CAD-CBD-CGD
6	dF	201	CYC	C3D-CAD-CBD-CGD
6	eS	201	CYC	C3D-CAD-CBD-CGD
6	dJ	201	CYC	C2B-C3B-CAB-CBB
6	aD	201	CYC	NA-C1A-CHA-C4D
6	aJ	201	CYC	NA-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
6	aP	201	CYC	NA-C1A-CHA-C4D
6	bT	201	CYC	NA-C1A-CHA-C4D
6	dD	201	CYC	NA-C1A-CHA-C4D
6	dJ	201	CYC	NA-C1A-CHA-C4D
6	dP	201	CYC	NA-C1A-CHA-C4D
6	eT	201	CYC	NA-C1A-CHA-C4D
6	aB	201	CYC	NB-C1B-CHB-C4A
6	cL	201	CYC	NB-C1B-CHB-C4A
6	dB	201	CYC	NB-C1B-CHB-C4A
6	fL	201	CYC	NB-C1B-CHB-C4A
6	aE	201	CYC	C3A-C4A-CHB-C1B
6	bQ	201	CYC	C3A-C4A-CHB-C1B
6	bU	201	CYC	C3A-C4A-CHB-C1B
6	cJ	201	CYC	C3A-C4A-CHB-C1B
6	dE	201	CYC	C3A-C4A-CHB-C1B
6	eQ	201	CYC	C3A-C4A-CHB-C1B
6	eU	201	CYC	C3A-C4A-CHB-C1B
6	fJ	201	CYC	C3A-C4A-CHB-C1B
6	bP	201	CYC	C2B-C3B-CAB-CBB
6	eP	201	CYC	C2B-C3B-CAB-CBB
6	aB	201	CYC	C2B-C1B-CHB-C4A
6	dB	201	CYC	C2B-C1B-CHB-C4A
6	aK	201	CYC	C2B-C3B-CAB-CBB
6	aN	201	CYC	C2B-C3B-CAB-CBB
6	dK	201	CYC	C2B-C3B-CAB-CBB
6	dN	201	CYC	C2B-C3B-CAB-CBB
6	aA	201	CYC	NA-C4A-CHB-C1B
6	aC	201	CYC	NA-C4A-CHB-C1B
6	aE	201	CYC	NA-C4A-CHB-C1B
6	aK	201	CYC	NA-C4A-CHB-C1B
6	aO	201	CYC	NA-C4A-CHB-C1B
6	aQ	201	CYC	NA-C4A-CHB-C1B
6	bM	201	CYC	NA-C4A-CHB-C1B
6	bO	201	CYC	NA-C4A-CHB-C1B
6	bQ	201	CYC	NA-C4A-CHB-C1B
6	bS	201	CYC	NA-C4A-CHB-C1B
6	bU	201	CYC	NA-C4A-CHB-C1B
6	bW	201	CYC	NA-C4A-CHB-C1B
6	cB	201	CYC	NA-C4A-CHB-C1B
6	cD	202	CYC	NA-C4A-CHB-C1B
6	cF	201	CYC	NA-C4A-CHB-C1B
6	cG	201	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
6	cI	201	CYC	NA-C4A-CHB-C1B
6	cJ	201	CYC	NA-C4A-CHB-C1B
6	dA	201	CYC	NA-C4A-CHB-C1B
6	dC	201	CYC	NA-C4A-CHB-C1B
6	dE	201	CYC	NA-C4A-CHB-C1B
6	dK	201	CYC	NA-C4A-CHB-C1B
6	dO	201	CYC	NA-C4A-CHB-C1B
6	dQ	201	CYC	NA-C4A-CHB-C1B
6	eM	201	CYC	NA-C4A-CHB-C1B
6	eO	201	CYC	NA-C4A-CHB-C1B
6	eQ	201	CYC	NA-C4A-CHB-C1B
6	eS	201	CYC	NA-C4A-CHB-C1B
6	eU	201	CYC	NA-C4A-CHB-C1B
6	eW	201	CYC	NA-C4A-CHB-C1B
6	fB	201	CYC	NA-C4A-CHB-C1B
6	fD	202	CYC	NA-C4A-CHB-C1B
6	fF	201	CYC	NA-C4A-CHB-C1B
6	fG	201	CYC	NA-C4A-CHB-C1B
6	fI	201	CYC	NA-C4A-CHB-C1B
6	fJ	201	CYC	NA-C4A-CHB-C1B
6	eN	201	CYC	NB-C1B-CHB-C4A
6	aA	201	CYC	C3A-C4A-CHB-C1B
6	aC	201	CYC	C3A-C4A-CHB-C1B
6	aI	201	CYC	C3A-C4A-CHB-C1B
6	aK	201	CYC	C3A-C4A-CHB-C1B
6	aM	1204	CYC	C3A-C4A-CHB-C1B
6	aO	201	CYC	C3A-C4A-CHB-C1B
6	aP	201	CYC	C3A-C4A-CHB-C1B
6	aQ	201	CYC	C3A-C4A-CHB-C1B
6	bM	201	CYC	C3A-C4A-CHB-C1B
6	bO	201	CYC	C3A-C4A-CHB-C1B
6	bS	201	CYC	C3A-C4A-CHB-C1B
6	bW	201	CYC	C3A-C4A-CHB-C1B
6	cB	201	CYC	C3A-C4A-CHB-C1B
6	cD	202	CYC	C3A-C4A-CHB-C1B
6	cG	201	CYC	C3A-C4A-CHB-C1B
6	cI	201	CYC	C3A-C4A-CHB-C1B
6	dA	201	CYC	C3A-C4A-CHB-C1B
6	dC	201	CYC	C3A-C4A-CHB-C1B
6	dI	201	CYC	C3A-C4A-CHB-C1B
6	dK	201	CYC	C3A-C4A-CHB-C1B
6	dO	201	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
6	dP	201	CYC	C3A-C4A-CHB-C1B
6	dQ	201	CYC	C3A-C4A-CHB-C1B
6	dR	201	CYC	C3A-C4A-CHB-C1B
6	eM	201	CYC	C3A-C4A-CHB-C1B
6	eO	201	CYC	C3A-C4A-CHB-C1B
6	eS	201	CYC	C3A-C4A-CHB-C1B
6	eW	201	CYC	C3A-C4A-CHB-C1B
6	fB	201	CYC	C3A-C4A-CHB-C1B
6	fD	202	CYC	C3A-C4A-CHB-C1B
6	fG	201	CYC	C3A-C4A-CHB-C1B
6	fI	201	CYC	C3A-C4A-CHB-C1B
6	cL	201	CYC	C2B-C1B-CHB-C4A
6	fL	201	CYC	C2B-C1B-CHB-C4A
6	aC	201	CYC	C3D-CAD-CBD-CGD
6	dC	201	CYC	C3D-CAD-CBD-CGD
6	aB	201	CYC	NA-C1A-CHA-C4D
6	dB	201	CYC	NA-C1A-CHA-C4D
6	bN	201	CYC	C2B-C3B-CAB-CBB
6	eN	201	CYC	C2B-C3B-CAB-CBB
6	bN	201	CYC	NB-C1B-CHB-C4A
6	aD	201	CYC	C2A-CAA-CBA-CGA
6	dD	201	CYC	C2A-CAA-CBA-CGA
6	aI	201	CYC	C2B-C3B-CAB-CBB
6	dI	201	CYC	C2B-C3B-CAB-CBB
6	aP	201	CYC	C2A-C1A-CHA-C4D
6	dP	201	CYC	C2A-C1A-CHA-C4D
6	cB	201	CYC	C2B-C3B-CAB-CBB
6	fB	201	CYC	C2B-C3B-CAB-CBB
6	cF	201	CYC	C2B-C3B-CAB-CBB
6	fF	201	CYC	C2B-C3B-CAB-CBB
6	aM	1204	CYC	NA-C1A-CHA-C4D
6	dR	201	CYC	NA-C1A-CHA-C4D
6	aQ	201	CYC	C2B-C3B-CAB-CBB
6	dQ	201	CYC	C2B-C3B-CAB-CBB
6	bS	201	CYC	C4B-C3B-CAB-CBB
6	eS	201	CYC	C4B-C3B-CAB-CBB
6	aO	201	CYC	C2B-C3B-CAB-CBB
6	dO	201	CYC	C2B-C3B-CAB-CBB
6	aJ	201	CYC	NB-C1B-CHB-C4A
6	dJ	201	CYC	NB-C1B-CHB-C4A
6	aJ	201	CYC	C2A-C1A-CHA-C4D
6	bT	201	CYC	C2A-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
6	dJ	201	CYC	C2A-C1A-CHA-C4D
6	eT	201	CYC	C2A-C1A-CHA-C4D
6	aF	201	CYC	NA-C1A-CHA-C4D
6	aM	1203	CYC	NA-C1A-CHA-C4D
6	dF	201	CYC	NA-C1A-CHA-C4D
6	dM	1203	CYC	NA-C1A-CHA-C4D
6	cM	101	CYC	C2B-C3B-CAB-CBB
6	bN	201	CYC	C2B-C1B-CHB-C4A
6	eN	201	CYC	C2B-C1B-CHB-C4A
6	fM	101	CYC	C2B-C3B-CAB-CBB
6	fJ	201	CYC	C2B-C3B-CAB-CBB
6	cJ	201	CYC	C2B-C3B-CAB-CBB
6	aK	201	CYC	C4C-C3C-CAC-CBC
6	dK	201	CYC	C4C-C3C-CAC-CBC
6	bW	201	CYC	C2B-C3B-CAB-CBB
6	eW	201	CYC	C2B-C3B-CAB-CBB
6	cI	201	CYC	C3D-CAD-CBD-CGD
6	fI	201	CYC	C3D-CAD-CBD-CGD
6	bQ	201	CYC	C2B-C3B-CAB-CBB
6	eQ	201	CYC	C2B-C3B-CAB-CBB
6	aN	201	CYC	NA-C1A-CHA-C4D
6	cF	201	CYC	NA-C1A-CHA-C4D
6	dN	201	CYC	NA-C1A-CHA-C4D
6	fF	201	CYC	NA-C1A-CHA-C4D
6	bR	201	CYC	C4B-C3B-CAB-CBB
6	eR	201	CYC	C4B-C3B-CAB-CBB
6	aA	201	CYC	C2B-C3B-CAB-CBB
6	dA	201	CYC	C2B-C3B-CAB-CBB
6	fI	201	CYC	C2B-C3B-CAB-CBB
6	cI	201	CYC	C2B-C3B-CAB-CBB
6	cL	201	CYC	C3D-CAD-CBD-CGD
6	fL	201	CYC	C3D-CAD-CBD-CGD
6	aH	201	CYC	NB-C1B-CHB-C4A
6	dH	201	CYC	NB-C1B-CHB-C4A
6	cM	101	CYC	NA-C1A-CHA-C4D
6	fM	101	CYC	NA-C1A-CHA-C4D
6	aD	201	CYC	C2A-C1A-CHA-C4D
6	dD	201	CYC	C2A-C1A-CHA-C4D
6	cM	101	CYC	NB-C1B-CHB-C4A
6	fM	101	CYC	NB-C1B-CHB-C4A
6	aM	1204	CYC	C3A-C2A-CAA-CBA
6	dR	201	CYC	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
6	aM	1202	CYC	C3D-CAD-CBD-CGD
6	dM	1202	CYC	C3D-CAD-CBD-CGD
6	aJ	201	CYC	C4B-C3B-CAB-CBB
6	dJ	201	CYC	C4B-C3B-CAB-CBB
6	bU	201	CYC	C2B-C3B-CAB-CBB
6	eU	201	CYC	C2B-C3B-CAB-CBB
6	cG	201	CYC	CAA-CBA-CGA-O2A
6	fG	201	CYC	CAA-CBA-CGA-O2A
6	bS	201	CYC	CAD-CBD-CGD-O2D
6	cD	201	CYC	CAD-CBD-CGD-O1D
6	fD	201	CYC	CAD-CBD-CGD-O1D
6	aM	1202	CYC	C2B-C3B-CAB-CBB
6	aM	1202	CYC	CAD-CBD-CGD-O2D
6	bR	201	CYC	CAD-CBD-CGD-O1D
6	dM	1202	CYC	CAD-CBD-CGD-O2D
6	eR	201	CYC	CAD-CBD-CGD-O1D
6	eS	201	CYC	CAD-CBD-CGD-O2D
6	dM	1202	CYC	C2B-C3B-CAB-CBB
6	aJ	201	CYC	CAA-CBA-CGA-O1A
6	aK	201	CYC	CAA-CBA-CGA-O1A
6	aM	1202	CYC	CAD-CBD-CGD-O1D
6	aQ	201	CYC	CAA-CBA-CGA-O1A
6	bM	201	CYC	CAA-CBA-CGA-O1A
6	bT	201	CYC	CAA-CBA-CGA-O2A
6	bU	201	CYC	CAA-CBA-CGA-O1A
6	bW	201	CYC	CAA-CBA-CGA-O1A
6	cB	201	CYC	CAA-CBA-CGA-O1A
6	cF	201	CYC	CAA-CBA-CGA-O1A
6	cJ	201	CYC	CAA-CBA-CGA-O1A
6	cM	101	CYC	CAA-CBA-CGA-O2A
6	dJ	201	CYC	CAA-CBA-CGA-O1A
6	dK	201	CYC	CAA-CBA-CGA-O1A
6	dM	1202	CYC	CAD-CBD-CGD-O1D
6	dQ	201	CYC	CAA-CBA-CGA-O1A
6	eT	201	CYC	CAA-CBA-CGA-O2A
6	eU	201	CYC	CAA-CBA-CGA-O1A
6	eW	201	CYC	CAA-CBA-CGA-O1A
6	fB	201	CYC	CAA-CBA-CGA-O1A
6	fF	201	CYC	CAA-CBA-CGA-O1A
6	fJ	201	CYC	CAA-CBA-CGA-O1A
6	fM	101	CYC	CAA-CBA-CGA-O2A
6	bM	201	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
6	eM	201	CYC	C2B-C3B-CAB-CBB
6	aF	201	CYC	CAA-CBA-CGA-O2A
6	bO	201	CYC	CAA-CBA-CGA-O1A
6	bP	201	CYC	CAD-CBD-CGD-O1D
6	cF	202	CYC	CAA-CBA-CGA-O2A
6	dF	201	CYC	CAA-CBA-CGA-O2A
6	eM	201	CYC	CAA-CBA-CGA-O1A
6	eO	201	CYC	CAA-CBA-CGA-O1A
6	eP	201	CYC	CAD-CBD-CGD-O1D
6	fF	202	CYC	CAA-CBA-CGA-O2A
6	aA	201	CYC	CAA-CBA-CGA-O2A
6	aG	201	CYC	CAA-CBA-CGA-O1A
6	aI	201	CYC	CAA-CBA-CGA-O1A
6	aP	201	CYC	CAA-CBA-CGA-O2A
6	bQ	201	CYC	CAA-CBA-CGA-O2A
6	bS	201	CYC	CAA-CBA-CGA-O1A
6	cD	202	CYC	CAA-CBA-CGA-O2A
6	cJ	201	CYC	CAA-CBA-CGA-O2A
6	dA	201	CYC	CAA-CBA-CGA-O2A
6	dG	201	CYC	CAA-CBA-CGA-O1A
6	dI	201	CYC	CAA-CBA-CGA-O1A
6	dP	201	CYC	CAA-CBA-CGA-O2A
6	eQ	201	CYC	CAA-CBA-CGA-O2A
6	eS	201	CYC	CAA-CBA-CGA-O1A
6	fD	202	CYC	CAA-CBA-CGA-O2A
6	fJ	201	CYC	CAA-CBA-CGA-O2A
6	aD	201	CYC	CAA-CBA-CGA-O1A
6	bU	201	CYC	CAA-CBA-CGA-O2A
6	bW	201	CYC	CAA-CBA-CGA-O2A
6	bX	201	CYC	CAA-CBA-CGA-O2A
6	dD	201	CYC	CAA-CBA-CGA-O1A
6	eU	201	CYC	CAA-CBA-CGA-O2A
6	eW	201	CYC	CAA-CBA-CGA-O2A
6	eX	201	CYC	CAA-CBA-CGA-O2A
6	aC	201	CYC	CAA-CBA-CGA-O1A
6	cF	201	CYC	CAD-CBD-CGD-O1D
6	dC	201	CYC	CAA-CBA-CGA-O1A
6	aG	201	CYC	NA-C1A-CHA-C4D
6	dG	201	CYC	NA-C1A-CHA-C4D
6	aP	201	CYC	C2B-C3B-CAB-CBB
6	dP	201	CYC	C2B-C3B-CAB-CBB
6	aO	201	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
6	bP	201	CYC	CAD-CBD-CGD-O2D
6	cD	201	CYC	CAA-CBA-CGA-O2A
6	dO	201	CYC	CAA-CBA-CGA-O1A
6	eP	201	CYC	CAD-CBD-CGD-O2D
6	fD	201	CYC	CAA-CBA-CGA-O2A
6	fF	201	CYC	CAD-CBD-CGD-O1D
6	aB	201	CYC	CAA-CBA-CGA-O1A
6	aJ	201	CYC	CAA-CBA-CGA-O2A
6	aK	201	CYC	CAD-CBD-CGD-O1D
6	aP	201	CYC	CAA-CBA-CGA-O1A
6	bN	201	CYC	CAA-CBA-CGA-O1A
6	bR	201	CYC	CAD-CBD-CGD-O2D
6	bT	201	CYC	CAA-CBA-CGA-O1A
6	bV	201	CYC	CAD-CBD-CGD-O2D
6	bX	201	CYC	CAA-CBA-CGA-O1A
6	dB	201	CYC	CAA-CBA-CGA-O1A
6	dJ	201	CYC	CAA-CBA-CGA-O2A
6	dK	201	CYC	CAD-CBD-CGD-O1D
6	dP	201	CYC	CAA-CBA-CGA-O1A
6	eN	201	CYC	CAA-CBA-CGA-O1A
6	eR	201	CYC	CAD-CBD-CGD-O2D
6	eT	201	CYC	CAA-CBA-CGA-O1A
6	eV	201	CYC	CAD-CBD-CGD-O2D
6	eX	201	CYC	CAA-CBA-CGA-O1A
6	aF	201	CYC	CAA-CBA-CGA-O1A
6	aN	201	CYC	CAA-CBA-CGA-O1A
6	aQ	201	CYC	CAD-CBD-CGD-O1D
6	bP	201	CYC	CAA-CBA-CGA-O2A
6	bQ	201	CYC	CAA-CBA-CGA-O1A
6	cL	201	CYC	CAD-CBD-CGD-O2D
6	dF	201	CYC	CAA-CBA-CGA-O1A
6	dN	201	CYC	CAA-CBA-CGA-O1A
6	dQ	201	CYC	CAD-CBD-CGD-O1D
6	eP	201	CYC	CAA-CBA-CGA-O2A
6	eQ	201	CYC	CAA-CBA-CGA-O1A
6	fL	201	CYC	CAD-CBD-CGD-O2D
6	aD	201	CYC	CAA-CBA-CGA-O2A
6	aI	201	CYC	CAA-CBA-CGA-O2A
6	bM	201	CYC	CAA-CBA-CGA-O2A
6	bM	201	CYC	CAD-CBD-CGD-O1D
6	dD	201	CYC	CAA-CBA-CGA-O2A
6	dI	201	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
6	dQ	201	CYC	CAA-CBA-CGA-O2A
6	eM	201	CYC	CAA-CBA-CGA-O2A
6	eM	201	CYC	CAD-CBD-CGD-O1D
6	aB	201	CYC	CAA-CBA-CGA-O2A
6	aE	201	CYC	CAA-CBA-CGA-O1A
6	aL	201	CYC	CAA-CBA-CGA-O1A
6	aO	201	CYC	CAA-CBA-CGA-O2A
6	aQ	201	CYC	CAA-CBA-CGA-O2A
6	bO	201	CYC	CAD-CBD-CGD-O1D
6	bO	201	CYC	CAD-CBD-CGD-O2D
6	bS	201	CYC	CAD-CBD-CGD-O1D
6	cB	201	CYC	CAA-CBA-CGA-O2A
6	cF	201	CYC	CAA-CBA-CGA-O2A
6	cI	201	CYC	CAA-CBA-CGA-O2A
6	dB	201	CYC	CAA-CBA-CGA-O2A
6	dE	201	CYC	CAA-CBA-CGA-O1A
6	dO	201	CYC	CAA-CBA-CGA-O2A
6	eO	201	CYC	CAD-CBD-CGD-O1D
6	eO	201	CYC	CAD-CBD-CGD-O2D
6	fB	201	CYC	CAA-CBA-CGA-O2A
6	fI	201	CYC	CAA-CBA-CGA-O1A
6	fI	201	CYC	CAA-CBA-CGA-O2A
6	aK	201	CYC	CAA-CBA-CGA-O2A
6	aN	201	CYC	CAA-CBA-CGA-O2A
6	bO	201	CYC	CAA-CBA-CGA-O2A
6	bP	201	CYC	CAA-CBA-CGA-O1A
6	bR	201	CYC	CAA-CBA-CGA-O2A
6	cD	202	CYC	CAA-CBA-CGA-O1A
6	cI	201	CYC	CAA-CBA-CGA-O1A
6	dC	201	CYC	CAA-CBA-CGA-O2A
6	dK	201	CYC	CAA-CBA-CGA-O2A
6	dL	201	CYC	CAA-CBA-CGA-O1A
6	dN	201	CYC	CAA-CBA-CGA-O2A
6	eO	201	CYC	CAA-CBA-CGA-O2A
6	eP	201	CYC	CAA-CBA-CGA-O1A
6	eR	201	CYC	CAA-CBA-CGA-O2A
6	eS	201	CYC	CAD-CBD-CGD-O1D
6	fD	202	CYC	CAA-CBA-CGA-O1A
6	aA	201	CYC	CAA-CBA-CGA-O1A
6	aC	201	CYC	CAA-CBA-CGA-O2A
6	aC	201	CYC	CAD-CBD-CGD-O1D
6	aC	201	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
6	aG	201	CYC	CAA-CBA-CGA-O2A
6	bV	201	CYC	CAA-CBA-CGA-O2A
6	cD	201	CYC	CAA-CBA-CGA-O1A
6	cF	202	CYC	CAD-CBD-CGD-O2D
6	dA	201	CYC	CAA-CBA-CGA-O1A
6	dC	201	CYC	CAD-CBD-CGD-O2D
6	dG	201	CYC	CAA-CBA-CGA-O2A
6	eV	201	CYC	CAA-CBA-CGA-O2A
6	fD	201	CYC	CAA-CBA-CGA-O1A
6	fF	201	CYC	CAA-CBA-CGA-O2A
6	fF	202	CYC	CAD-CBD-CGD-O2D
6	aE	201	CYC	CAA-CBA-CGA-O2A
6	aJ	201	CYC	CAD-CBD-CGD-O2D
6	cD	201	CYC	CAD-CBD-CGD-O2D
6	cF	202	CYC	CAA-CBA-CGA-O1A
6	cL	201	CYC	CAD-CBD-CGD-O1D
6	cM	101	CYC	CAD-CBD-CGD-O2D
6	dC	201	CYC	CAD-CBD-CGD-O1D
6	dE	201	CYC	CAA-CBA-CGA-O2A
6	dJ	201	CYC	CAD-CBD-CGD-O2D
6	fD	201	CYC	CAD-CBD-CGD-O2D
6	fF	202	CYC	CAA-CBA-CGA-O1A
6	fL	201	CYC	CAD-CBD-CGD-O1D
6	aE	201	CYC	CAD-CBD-CGD-O1D
6	bQ	201	CYC	CAD-CBD-CGD-O1D
6	bQ	201	CYC	CAD-CBD-CGD-O2D
6	dE	201	CYC	CAD-CBD-CGD-O1D
6	dH	201	CYC	CAA-CBA-CGA-O2A
6	eQ	201	CYC	CAD-CBD-CGD-O1D
6	fM	101	CYC	CAD-CBD-CGD-O2D
6	aH	201	CYC	CAA-CBA-CGA-O2A
6	cF	202	CYC	CAD-CBD-CGD-O1D
6	eQ	201	CYC	CAD-CBD-CGD-O2D
6	fF	201	CYC	CAD-CBD-CGD-O2D
6	fF	202	CYC	CAD-CBD-CGD-O1D
6	aK	201	CYC	CAD-CBD-CGD-O2D
6	aL	201	CYC	CAA-CBA-CGA-O2A
6	aM	1202	CYC	CAA-CBA-CGA-O2A
6	bN	201	CYC	CAA-CBA-CGA-O2A
6	bS	201	CYC	CAA-CBA-CGA-O2A
6	cL	201	CYC	CAA-CBA-CGA-O2A
6	dK	201	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
6	dL	201	CYC	CAA-CBA-CGA-O2A
6	dM	1202	CYC	CAA-CBA-CGA-O2A
6	eS	201	CYC	CAA-CBA-CGA-O2A
6	fL	201	CYC	CAA-CBA-CGA-O2A
6	aM	1204	CYC	C1A-C2A-CAA-CBA
6	dR	201	CYC	C1A-C2A-CAA-CBA
6	aJ	201	CYC	C2B-C1B-CHB-C4A
6	dJ	201	CYC	C2B-C1B-CHB-C4A
6	aM	1203	CYC	CAD-CBD-CGD-O2D
6	aQ	201	CYC	CAD-CBD-CGD-O2D
6	bR	201	CYC	CAA-CBA-CGA-O1A
6	bV	201	CYC	CAA-CBA-CGA-O1A
6	bV	201	CYC	CAD-CBD-CGD-O1D
6	cF	201	CYC	CAD-CBD-CGD-O2D
6	cG	201	CYC	CAA-CBA-CGA-O1A
6	cM	101	CYC	CAA-CBA-CGA-O1A
6	dM	1203	CYC	CAD-CBD-CGD-O2D
6	dQ	201	CYC	CAD-CBD-CGD-O2D
6	eR	201	CYC	CAA-CBA-CGA-O1A
6	eV	201	CYC	CAA-CBA-CGA-O1A
6	eV	201	CYC	CAD-CBD-CGD-O1D
6	fG	201	CYC	CAA-CBA-CGA-O1A
6	fM	101	CYC	CAA-CBA-CGA-O1A
6	cM	101	CYC	CAD-CBD-CGD-O1D
6	eN	201	CYC	CAA-CBA-CGA-O2A
6	fM	101	CYC	CAD-CBD-CGD-O1D
6	eM	201	CYC	CAD-CBD-CGD-O2D
6	bM	201	CYC	C4C-C3C-CAC-CBC
6	eM	201	CYC	C4C-C3C-CAC-CBC
6	aJ	201	CYC	CAD-CBD-CGD-O1D
6	aM	1202	CYC	CAA-CBA-CGA-O1A
6	bM	201	CYC	CAD-CBD-CGD-O2D
6	dJ	201	CYC	CAD-CBD-CGD-O1D
6	dM	1202	CYC	CAA-CBA-CGA-O1A
6	aE	201	CYC	CAD-CBD-CGD-O2D
6	bW	201	CYC	CAD-CBD-CGD-O2D
6	cI	201	CYC	CAD-CBD-CGD-O2D
6	dE	201	CYC	CAD-CBD-CGD-O2D
6	eW	201	CYC	CAD-CBD-CGD-O2D
6	fI	201	CYC	CAD-CBD-CGD-O2D
6	aH	201	CYC	C2B-C1B-CHB-C4A
6	dH	201	CYC	C2B-C1B-CHB-C4A

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Mol	Chain	Res	Type	Atoms
6	bW	201	CYC	CAD-CBD-CGD-O1D
6	cG	201	CYC	CAD-CBD-CGD-O1D
6	cG	201	CYC	CAD-CBD-CGD-O2D
6	eW	201	CYC	CAD-CBD-CGD-O1D
6	fG	201	CYC	CAD-CBD-CGD-O1D
6	fG	201	CYC	CAD-CBD-CGD-O2D
6	aH	201	CYC	CAA-CBA-CGA-O1A
6	aM	1203	CYC	CAA-CBA-CGA-O1A
6	dH	201	CYC	CAA-CBA-CGA-O1A
6	dM	1203	CYC	CAA-CBA-CGA-O1A
6	cI	201	CYC	CAD-CBD-CGD-O1D
6	cL	201	CYC	CAA-CBA-CGA-O1A
6	fI	201	CYC	CAD-CBD-CGD-O1D
6	fL	201	CYC	CAA-CBA-CGA-O1A
6	aM	1203	CYC	CAA-CBA-CGA-O2A
6	dM	1203	CYC	CAA-CBA-CGA-O2A
6	cM	101	CYC	C2B-C1B-CHB-C4A
6	fM	101	CYC	C2B-C1B-CHB-C4A
6	cB	201	CYC	CAD-CBD-CGD-O2D
6	fB	201	CYC	CAD-CBD-CGD-O2D
6	bX	201	CYC	C2A-CAA-CBA-CGA
6	eX	201	CYC	C2A-CAA-CBA-CGA
6	aM	1201	CYC	CAA-CBA-CGA-O2A
6	dM	1201	CYC	CAA-CBA-CGA-O2A
6	aG	201	CYC	CAD-CBD-CGD-O2D
6	aM	1203	CYC	CAD-CBD-CGD-O1D
6	dG	201	CYC	CAD-CBD-CGD-O2D
6	dM	1203	CYC	CAD-CBD-CGD-O1D
6	bU	201	CYC	CAD-CBD-CGD-O2D
6	aF	201	CYC	CAD-CBD-CGD-O2D
6	cD	202	CYC	CAD-CBD-CGD-O2D
6	dF	201	CYC	CAD-CBD-CGD-O2D
6	eU	201	CYC	CAD-CBD-CGD-O2D
6	fD	202	CYC	CAD-CBD-CGD-O2D
6	aA	201	CYC	CAD-CBD-CGD-O2D
6	aO	201	CYC	CAD-CBD-CGD-O1D
6	dN	201	CYC	CAD-CBD-CGD-O2D
6	dO	201	CYC	CAD-CBD-CGD-O1D
6	aB	201	CYC	C2A-C1A-CHA-C4D
6	aM	1204	CYC	C2A-C1A-CHA-C4D
6	dB	201	CYC	C2A-C1A-CHA-C4D
6	dR	201	CYC	C2A-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
6	aN	201	CYC	CAD-CBD-CGD-O2D
6	aO	201	CYC	CAD-CBD-CGD-O2D
6	cD	202	CYC	CAD-CBD-CGD-O1D
6	dA	201	CYC	CAD-CBD-CGD-O2D
6	dO	201	CYC	CAD-CBD-CGD-O2D
6	fD	202	CYC	CAD-CBD-CGD-O1D
6	aF	201	CYC	CAD-CBD-CGD-O1D
6	dF	201	CYC	CAD-CBD-CGD-O1D
6	eU	201	CYC	CAD-CBD-CGD-O1D
6	aG	201	CYC	CAD-CBD-CGD-O1D
6	bU	201	CYC	CAD-CBD-CGD-O1D
6	cB	201	CYC	CAD-CBD-CGD-O1D
6	dG	201	CYC	CAD-CBD-CGD-O1D
6	fB	201	CYC	CAD-CBD-CGD-O1D
6	dN	201	CYC	CAD-CBD-CGD-O1D
6	aA	201	CYC	CAD-CBD-CGD-O1D
6	aI	201	CYC	CAD-CBD-CGD-O2D
6	aN	201	CYC	CAD-CBD-CGD-O1D
6	dA	201	CYC	CAD-CBD-CGD-O1D
6	dI	201	CYC	CAD-CBD-CGD-O2D
6	aH	201	CYC	CAD-CBD-CGD-O1D
6	dH	201	CYC	CAD-CBD-CGD-O1D
6	aM	1201	CYC	CAA-CBA-CGA-O1A
6	dM	1201	CYC	CAA-CBA-CGA-O1A
6	aM	1204	CYC	CAA-CBA-CGA-O2A
6	dR	201	CYC	CAA-CBA-CGA-O2A
6	aP	201	CYC	CAD-CBD-CGD-O2D
6	dP	201	CYC	CAD-CBD-CGD-O2D
6	dI	201	CYC	CAD-CBD-CGD-O1D
6	aI	201	CYC	CAD-CBD-CGD-O1D
6	bX	201	CYC	NB-C1B-CHB-C4A
6	eX	201	CYC	NB-C1B-CHB-C4A
6	aM	1204	CYC	CAA-CBA-CGA-O1A
6	dR	201	CYC	CAA-CBA-CGA-O1A
6	aH	201	CYC	CAD-CBD-CGD-O2D
6	dH	201	CYC	CAD-CBD-CGD-O2D
6	aP	201	CYC	CAD-CBD-CGD-O1D

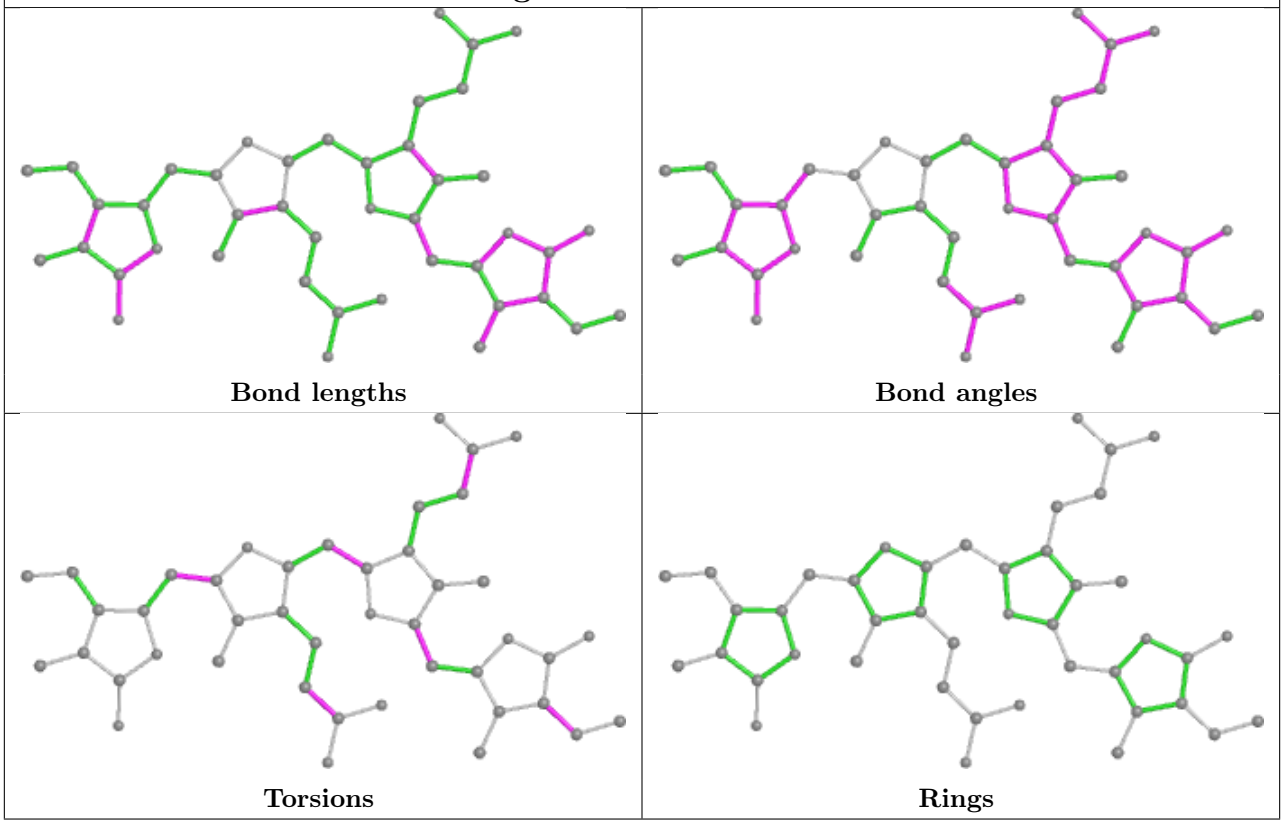
There are no ring outliers.

No monomer is involved in short contacts.

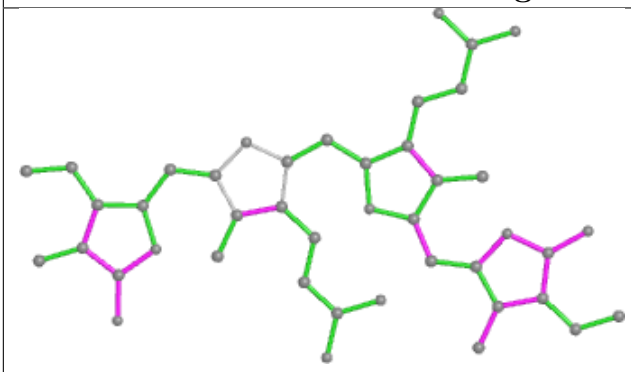
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

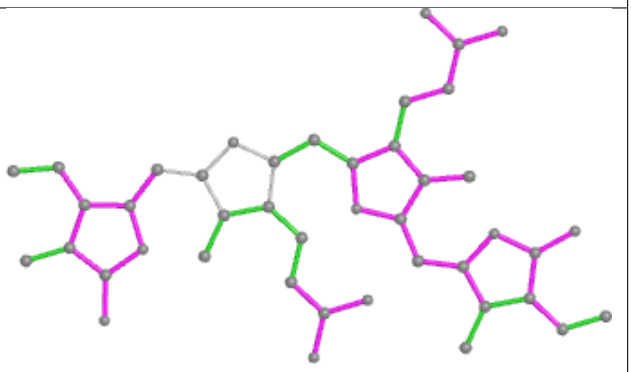
Ligand CYC aN 201



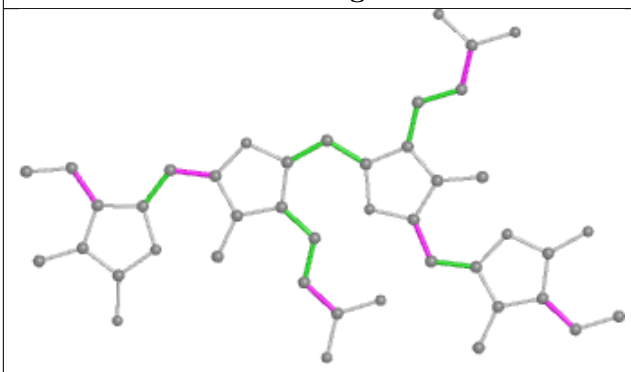
Ligand CYC cB 201



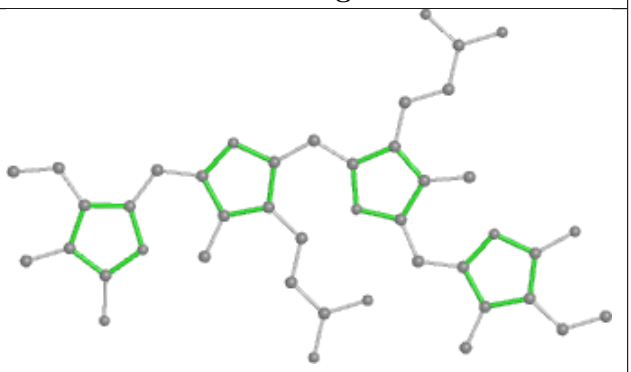
Bond lengths



Bond angles

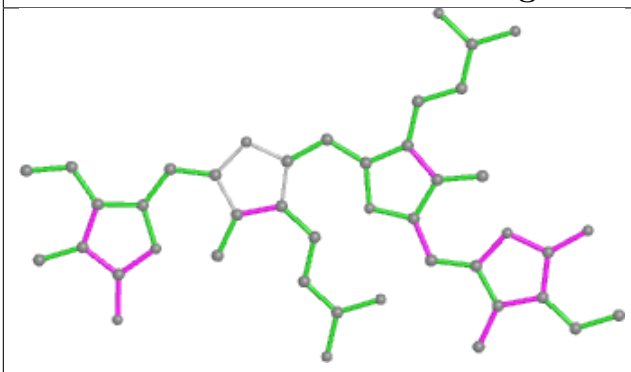


Torsions

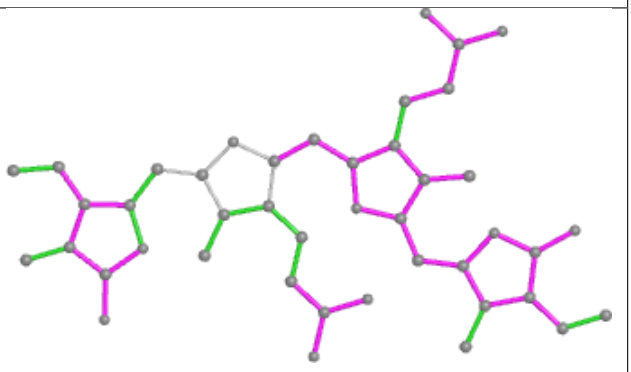


Rings

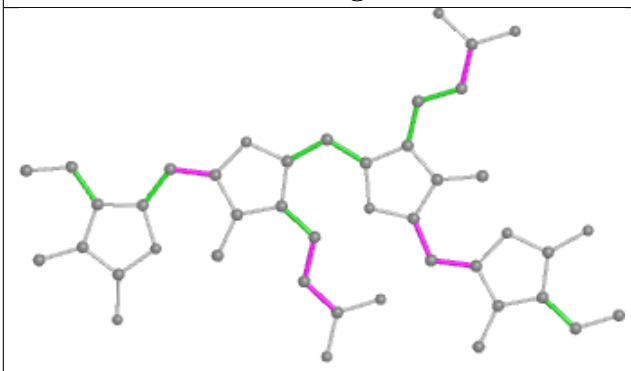
Ligand CYC fL 201



Bond lengths



Bond angles



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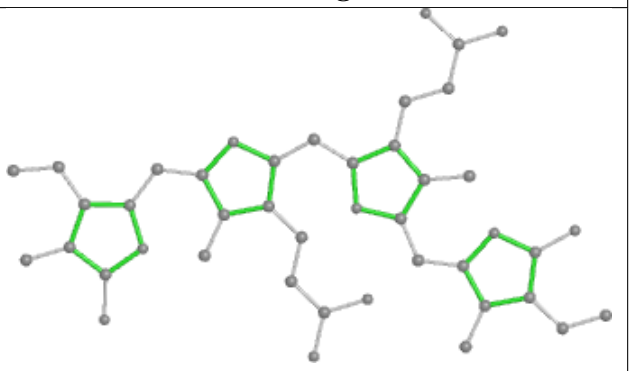
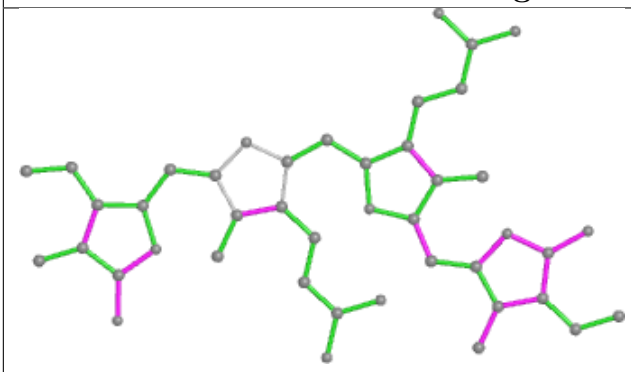
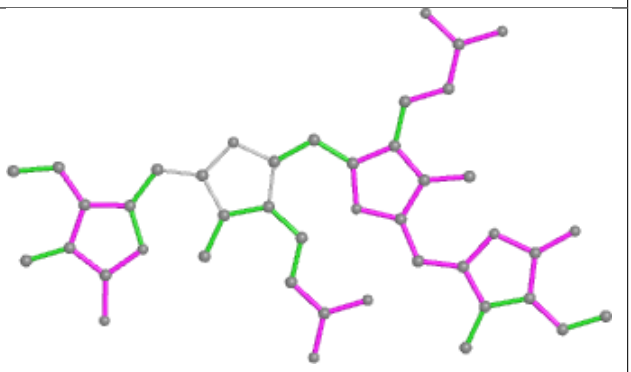


Rings

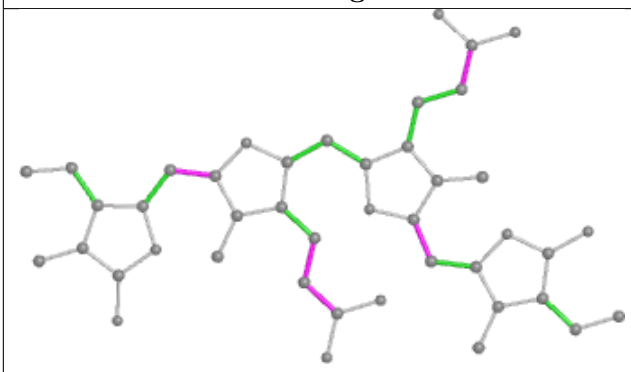
Ligand CYC aC 201



Bond lengths



Bond angles



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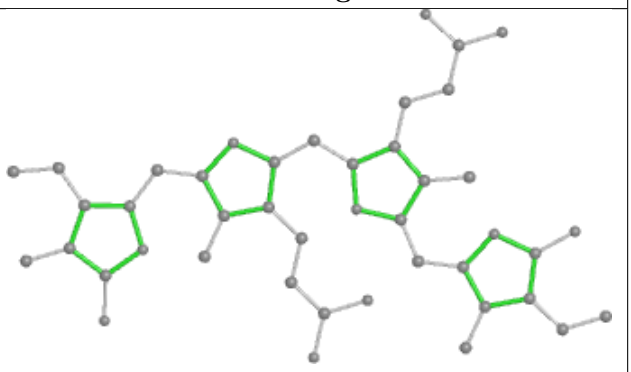
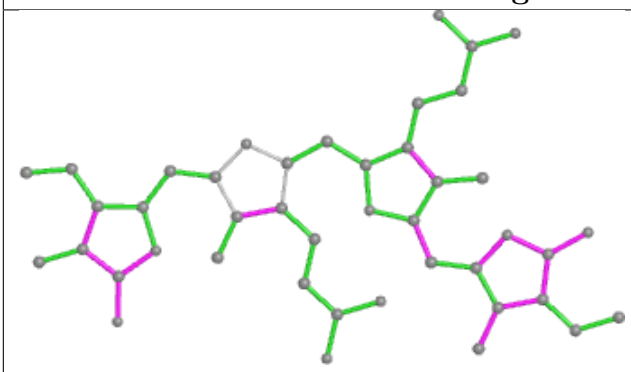


Rings

Ligand CYC bX 201



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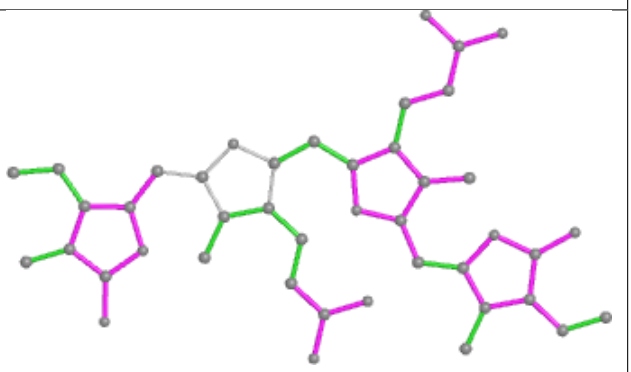

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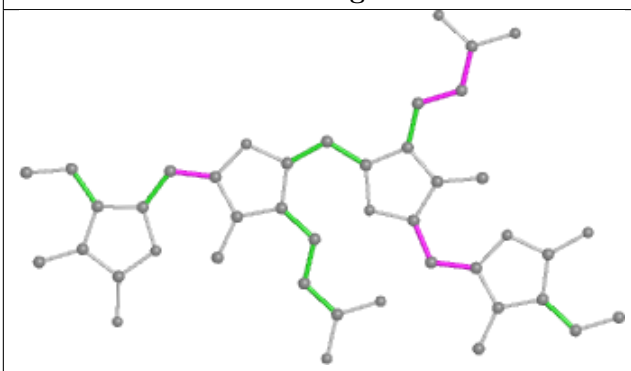
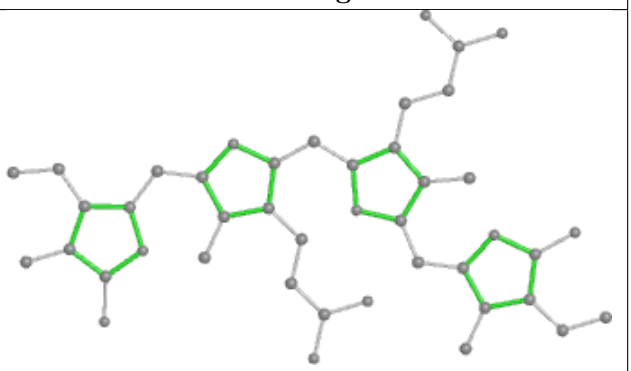
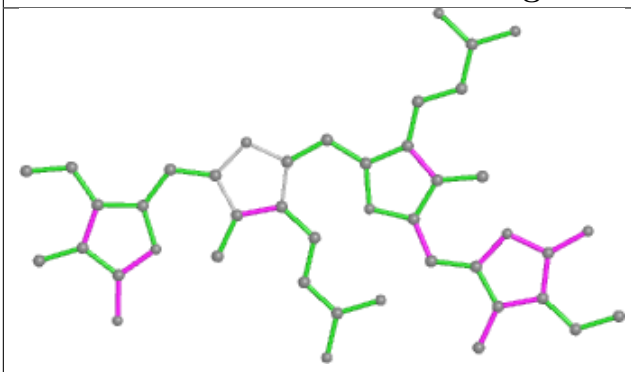


Torsions



Rings

Ligand CYC fI 201



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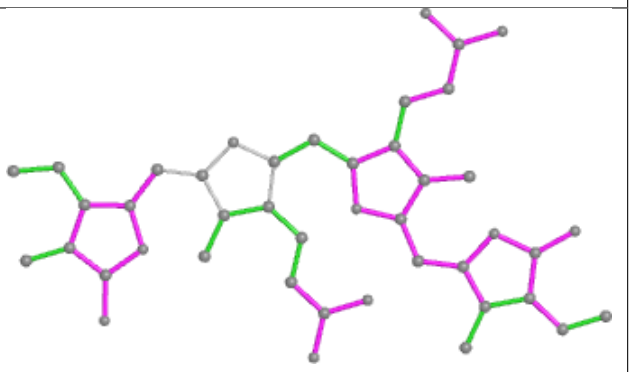
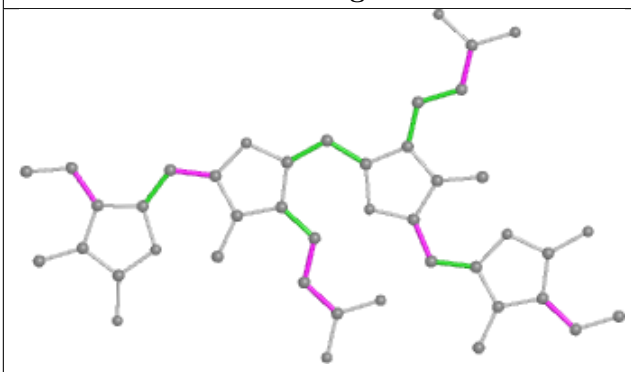


Bond angles



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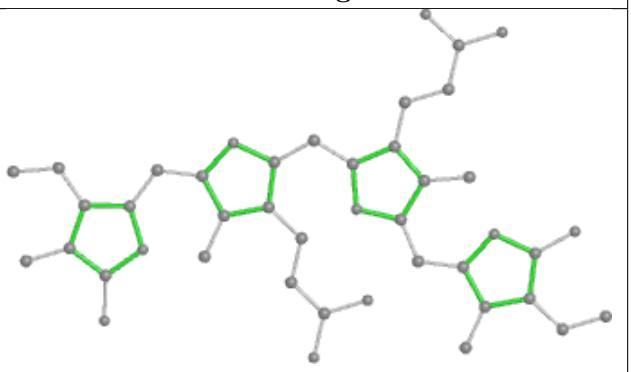
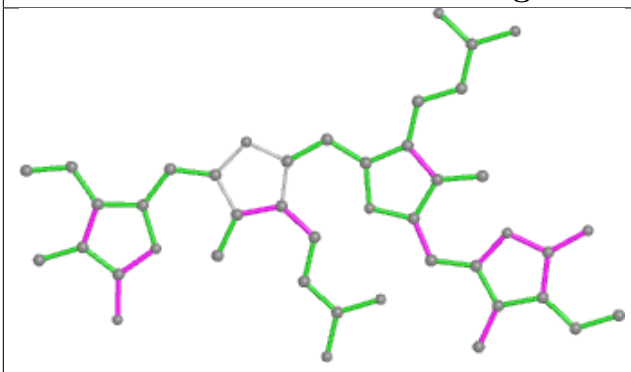


Rings

Ligand CYC aQ 201



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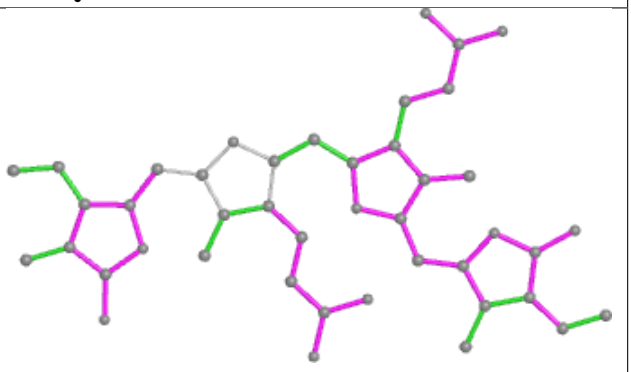
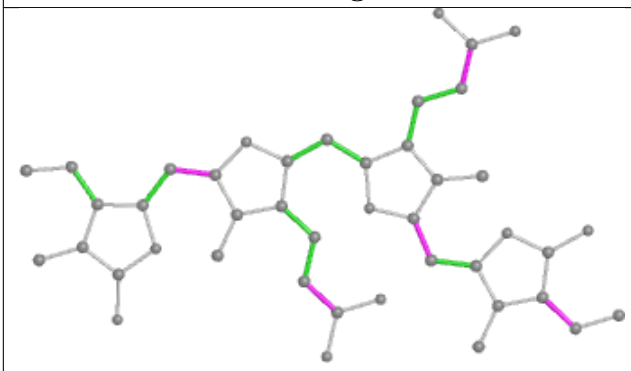


Bond angles



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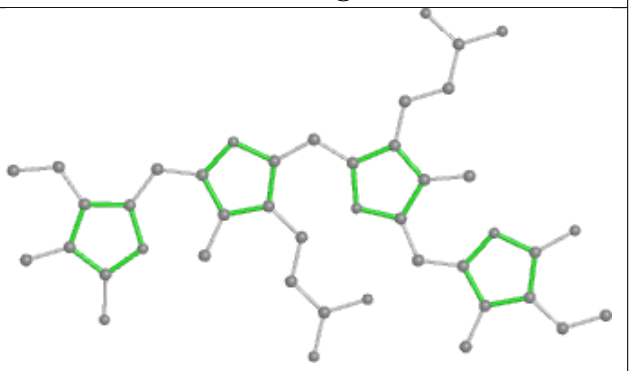
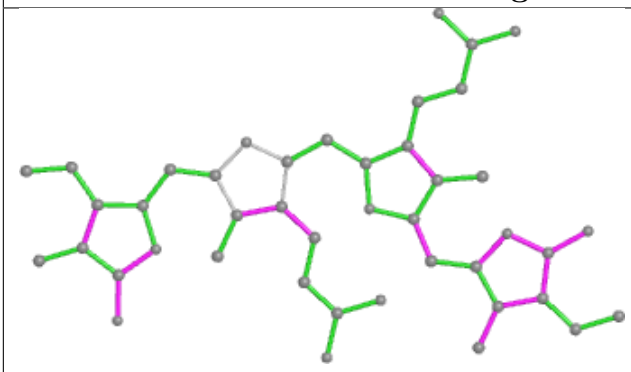


Rings

Ligand CYC dH 201



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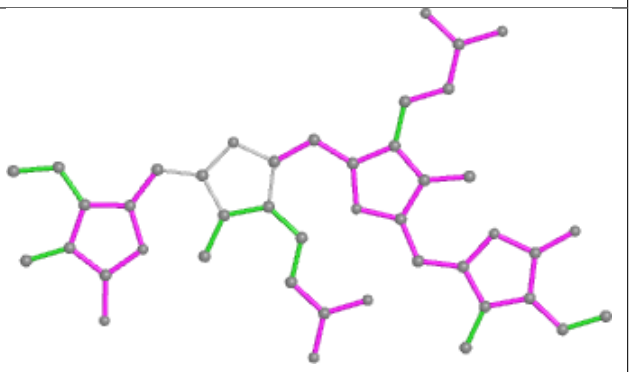

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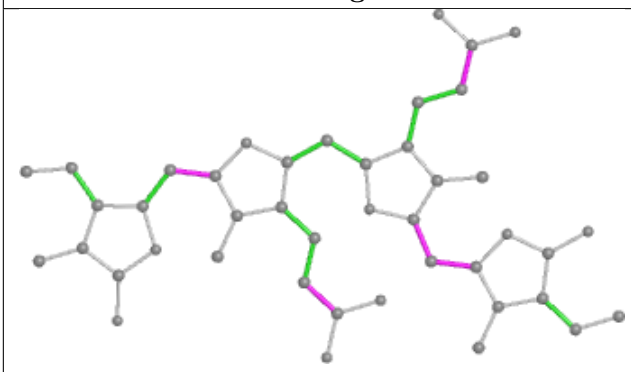

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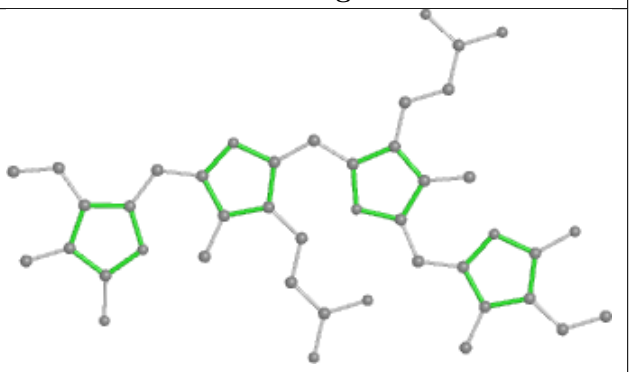
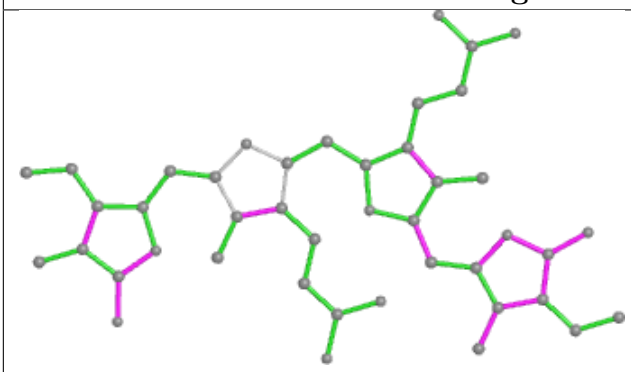


Rings

Ligand CYC bN 201



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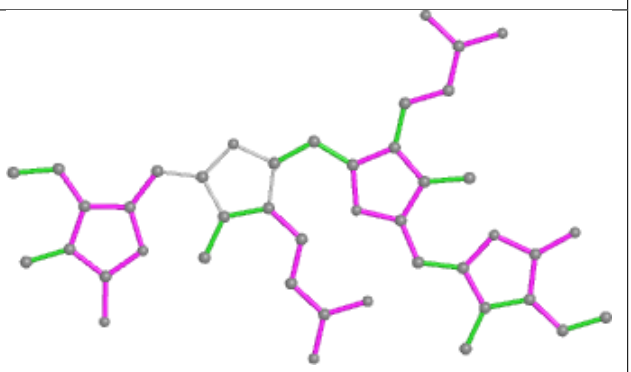
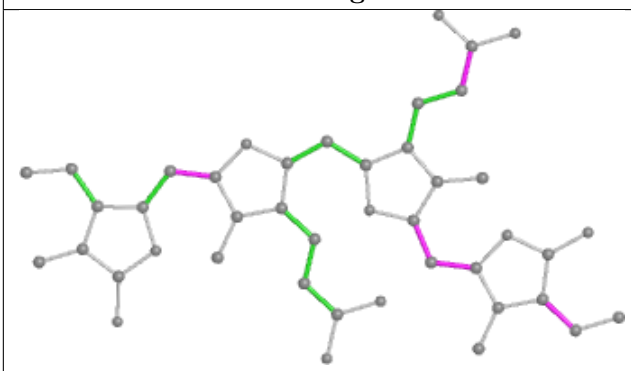
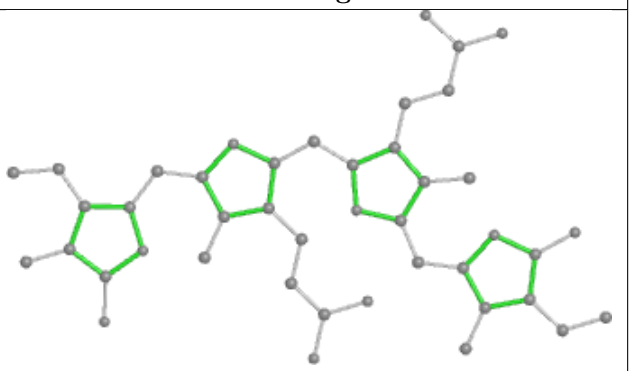


Bond angles

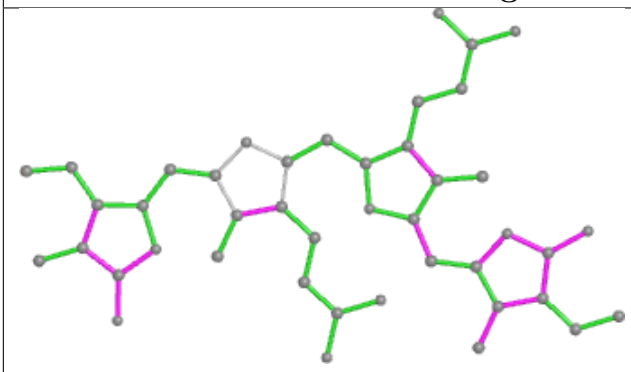


Torsions

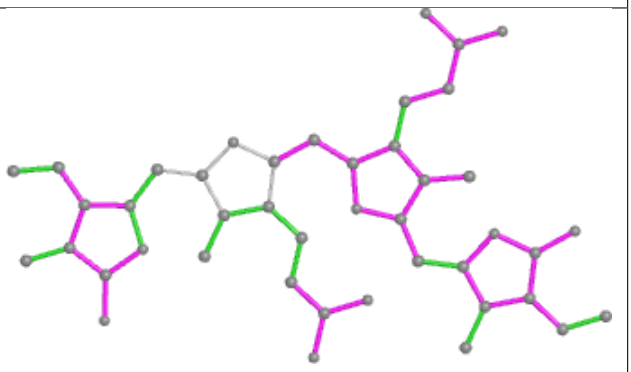


Rings

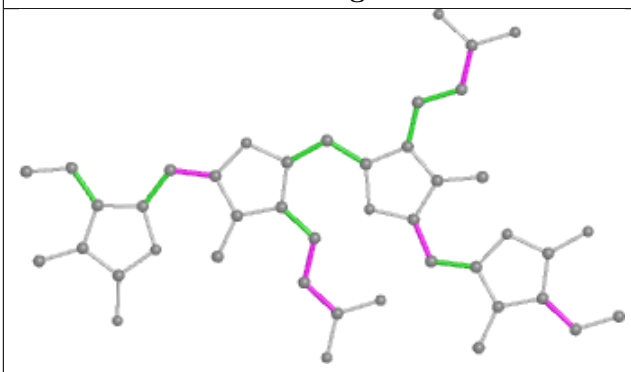
Ligand CYC aM 1202



Bond lengths



Bond angles



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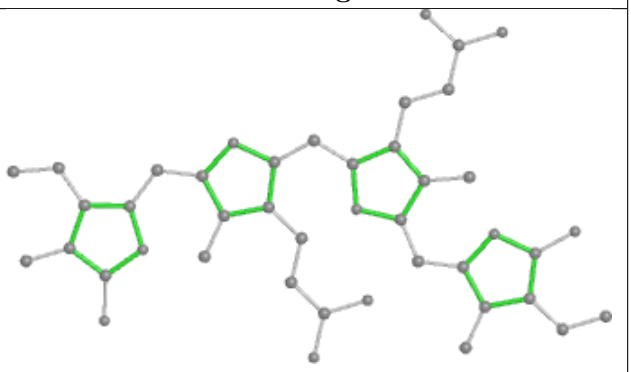
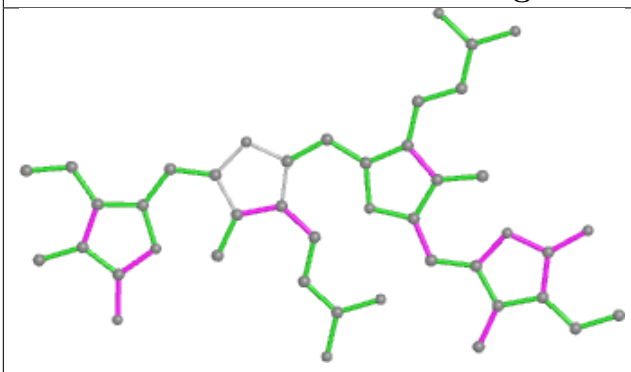


Rings

Ligand CYC eO 201



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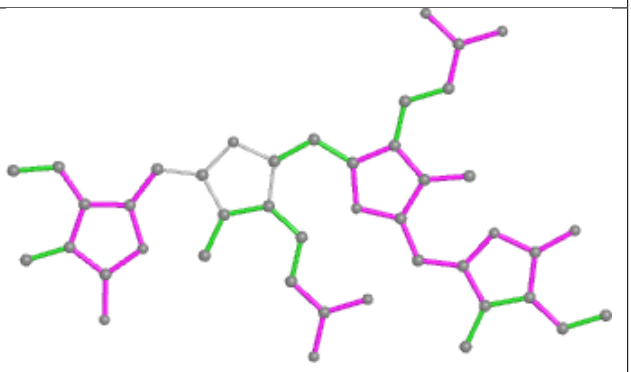
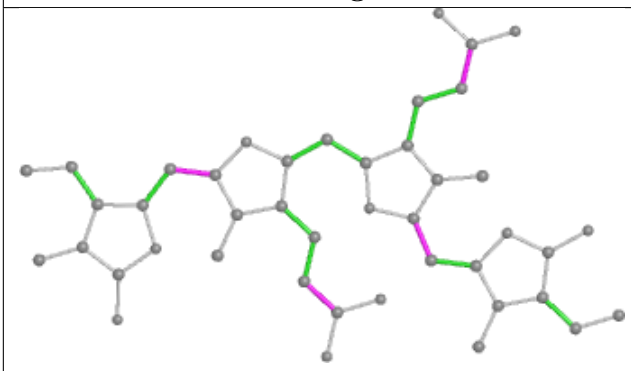
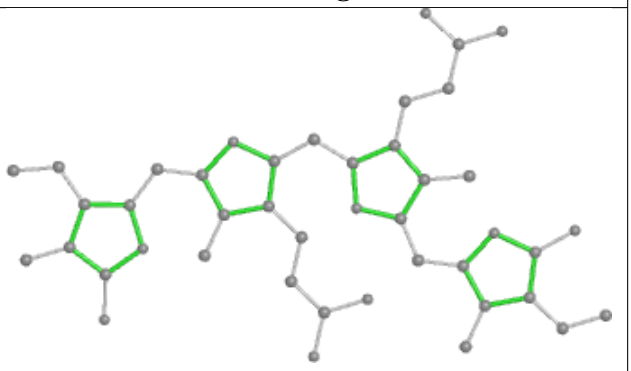


Bond angles

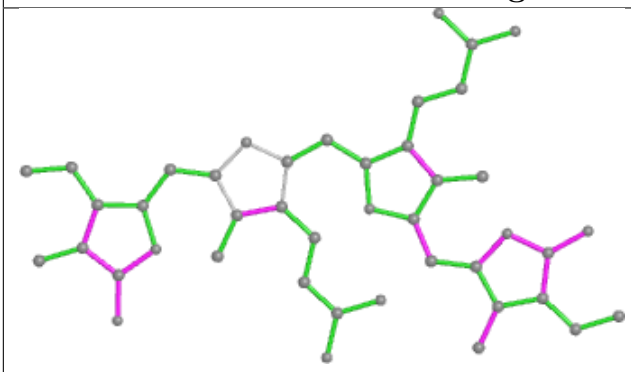


Torsions



Rings

Ligand CYC bM 201



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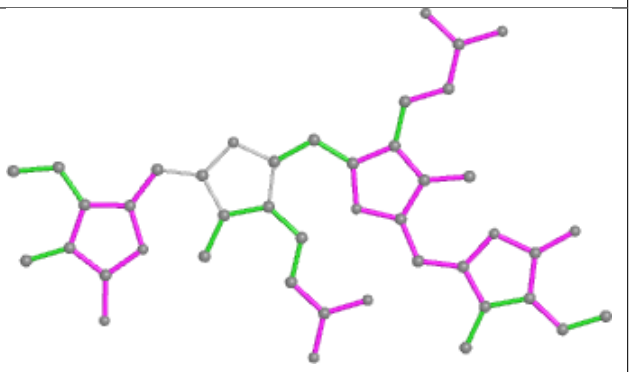
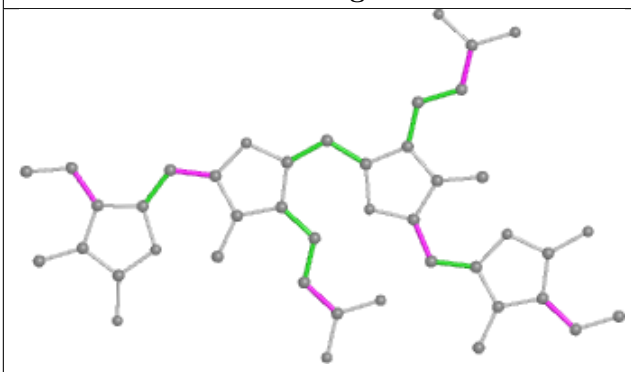
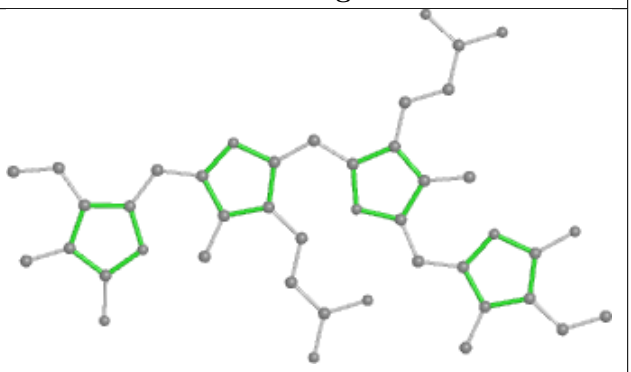


Bond angles

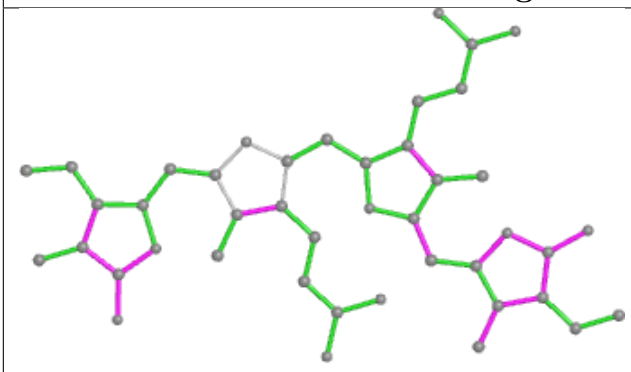


Torsions

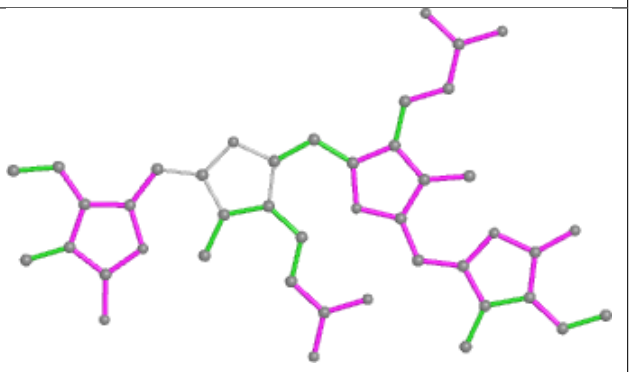


Rings

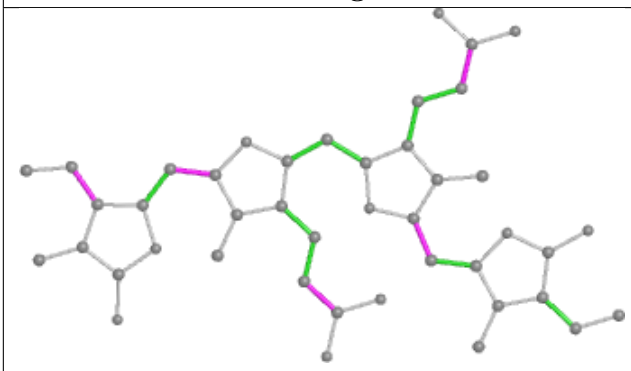
Ligand CYC fG 201



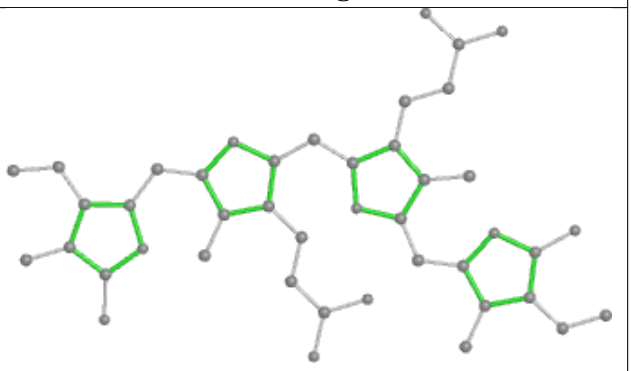
Bond lengths



Bond angles

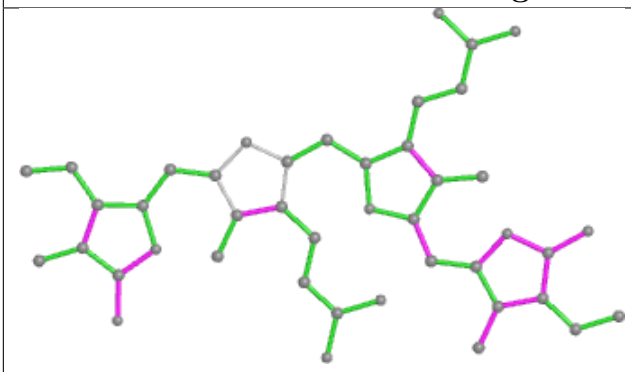


Torsions

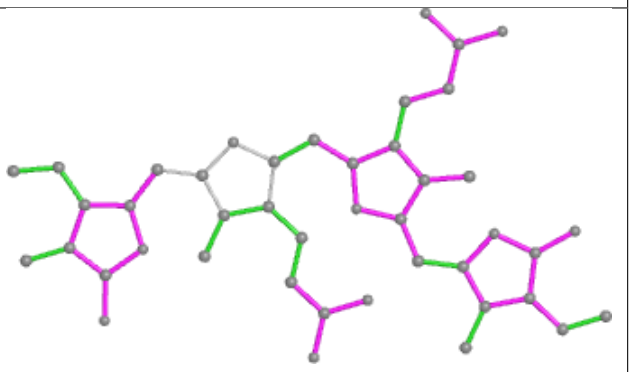


Rings

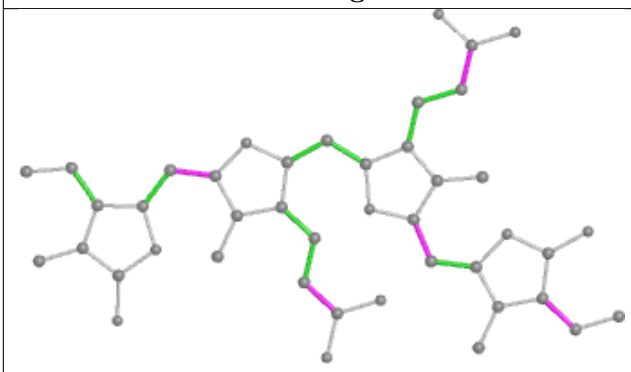
Ligand CYC bR 201



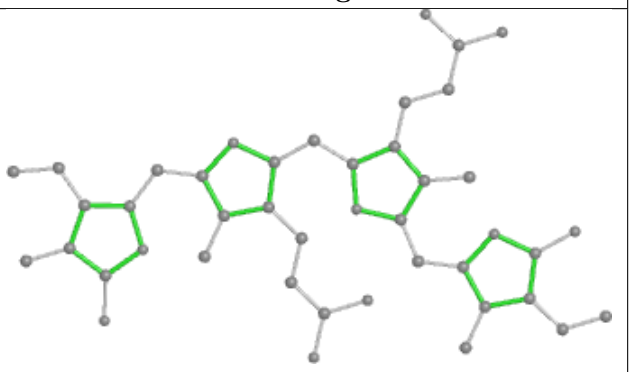
Bond lengths



Bond angles

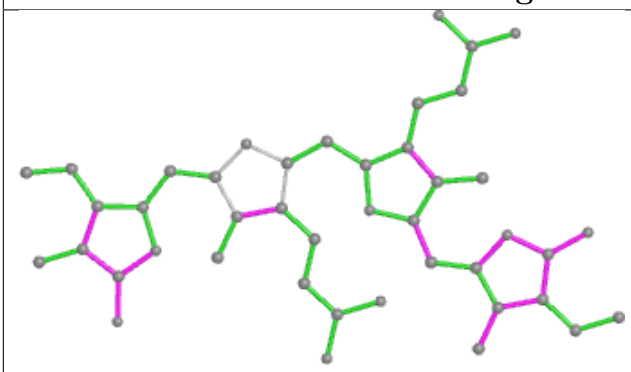


Torsions



Rings

Ligand CYC cF 202



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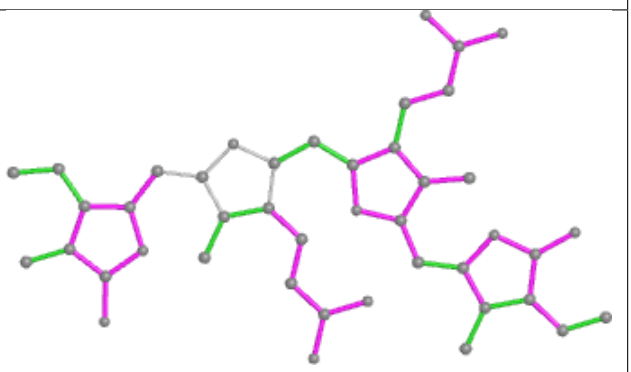
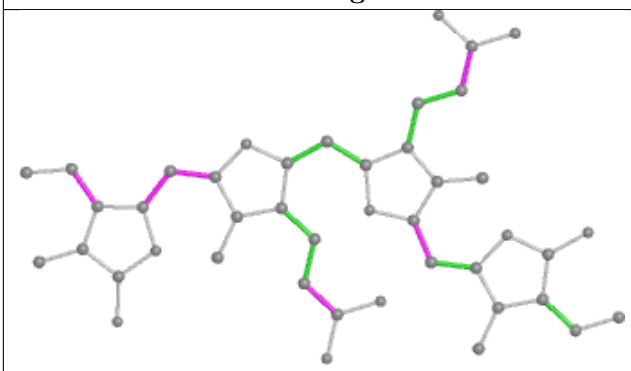
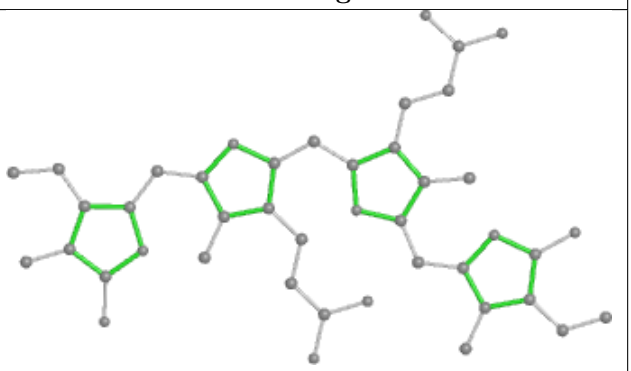


Bond angles

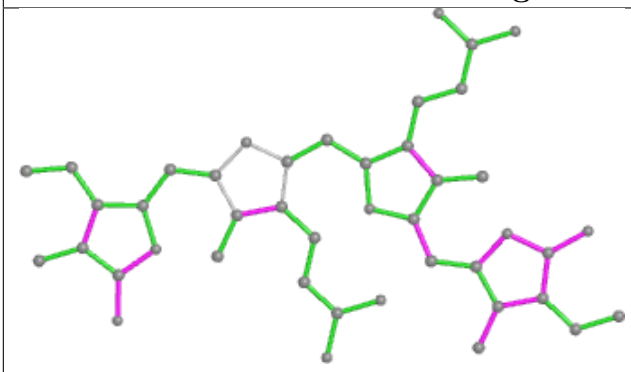


Torsions



Rings

Ligand CYC aD 201



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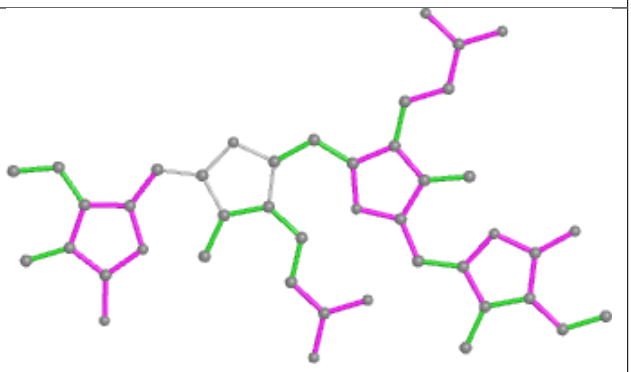
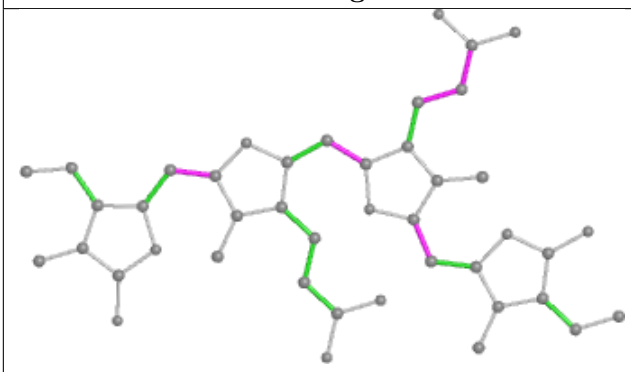


Bond angles



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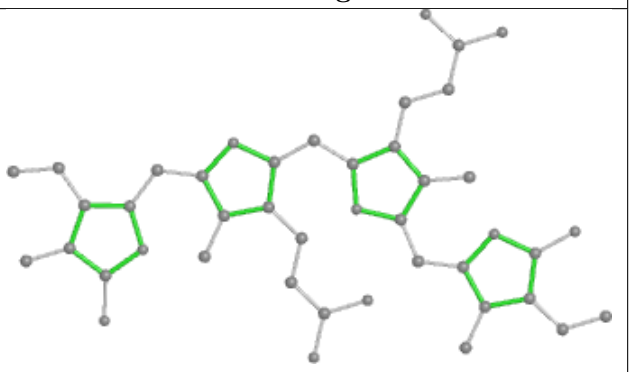
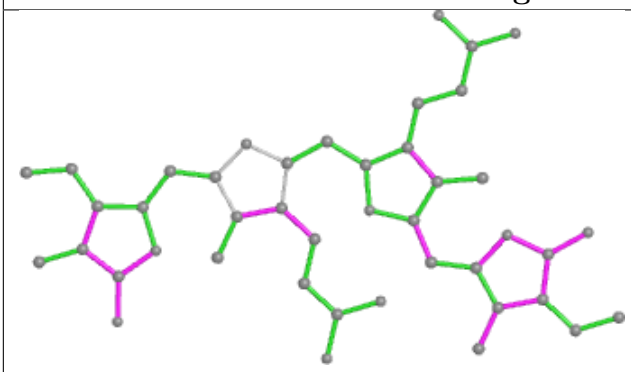


Rings

Ligand CYC aO 201



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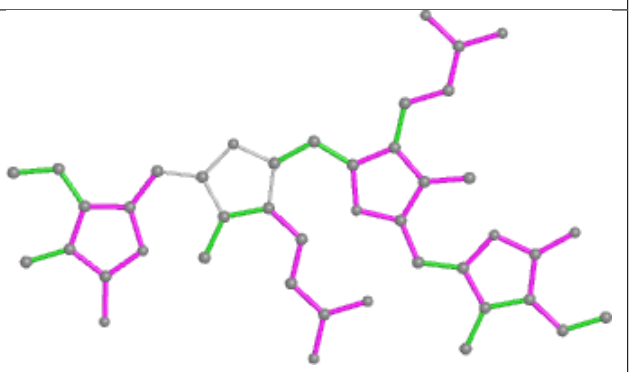

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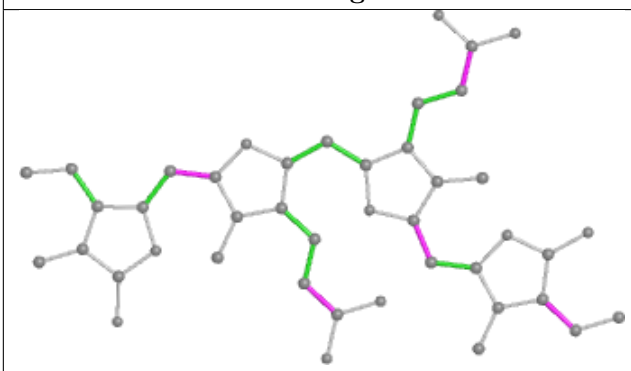

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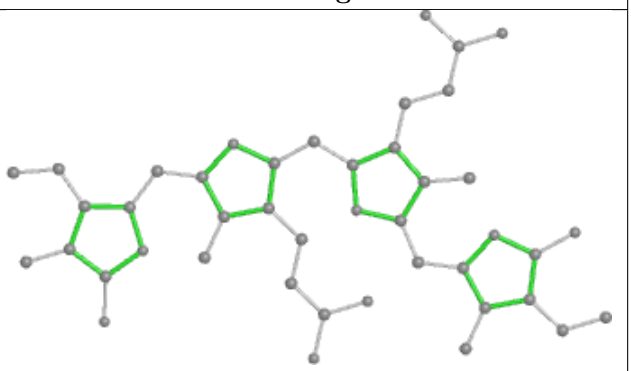
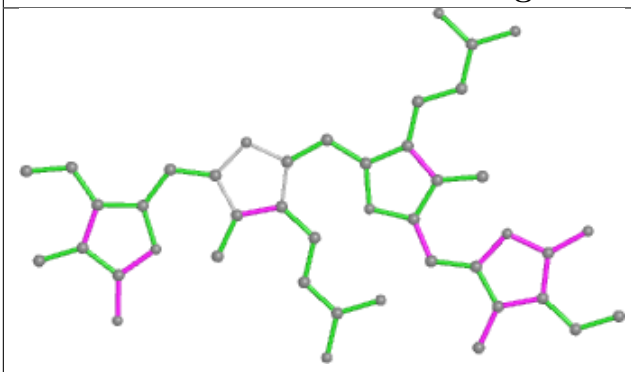


Rings

Ligand CYC eV 201



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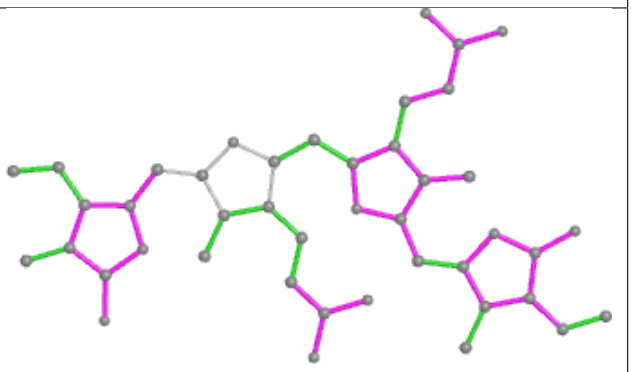

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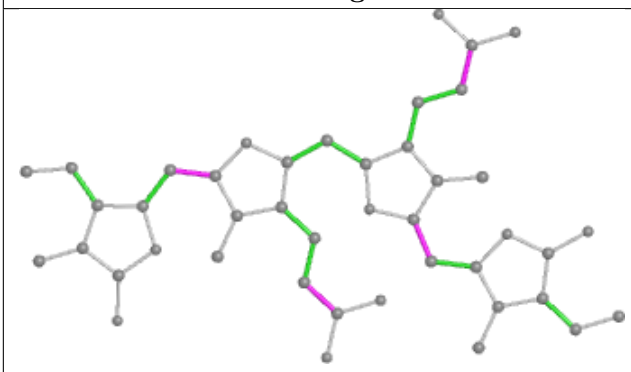

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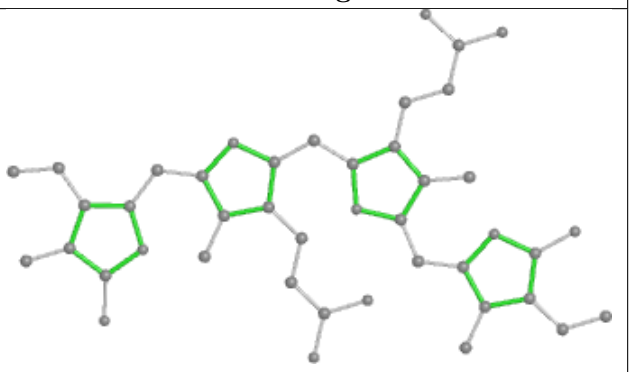
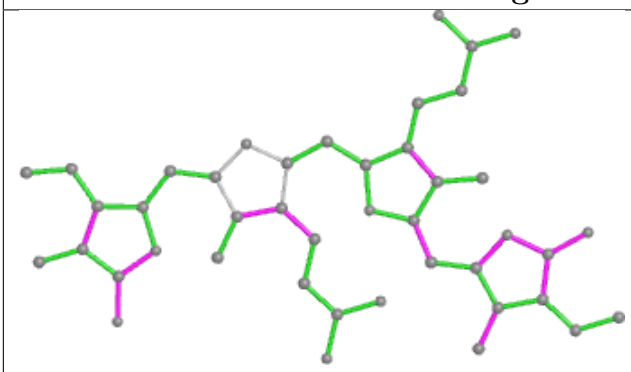


Rings

Ligand CYC dQ 201



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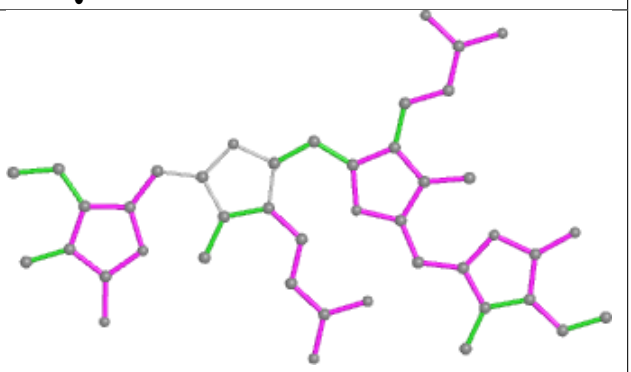
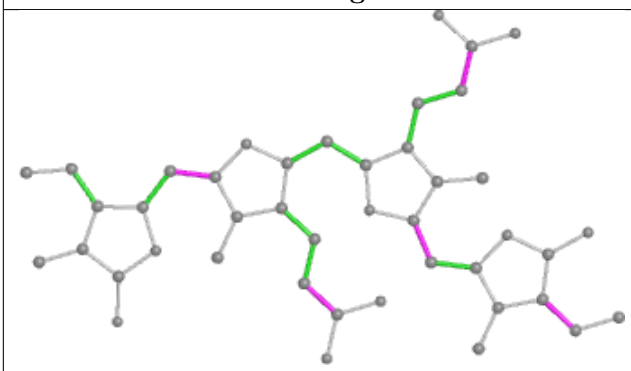


Bond angles



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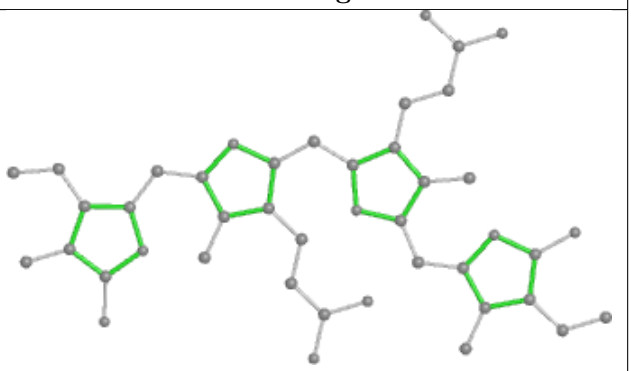
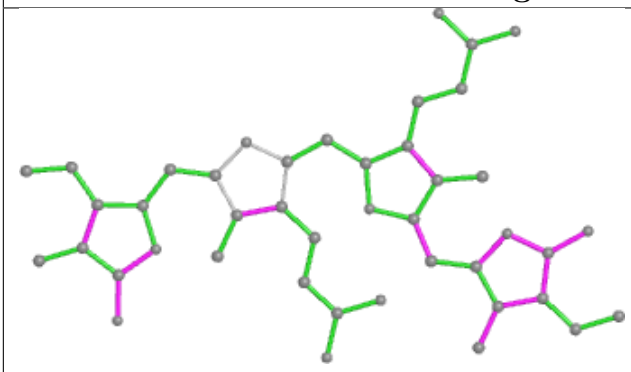


Rings

Ligand CYC cD 202



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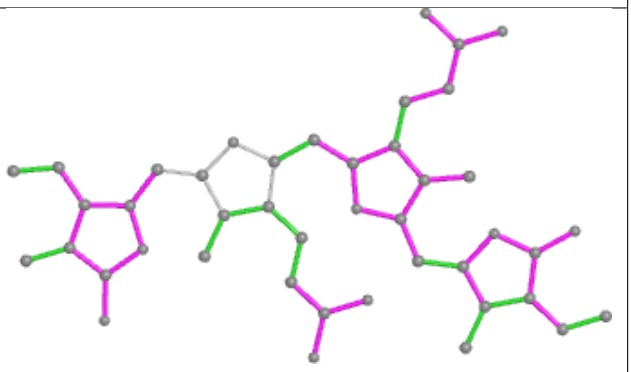
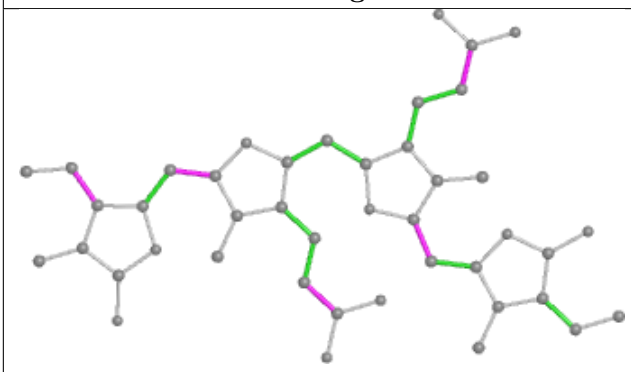


Bond angles



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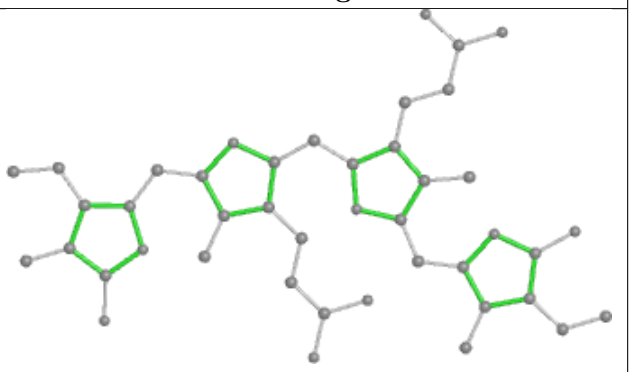
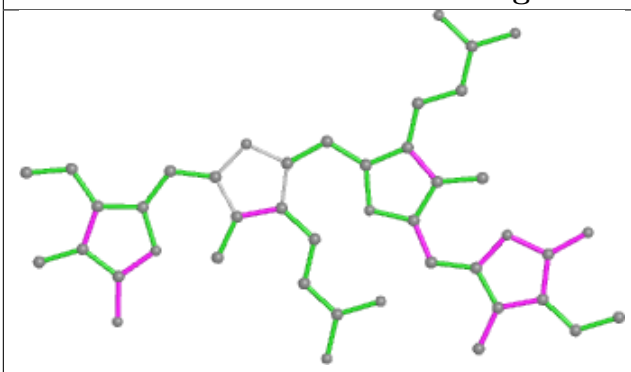


Rings

Ligand CYC aA 201



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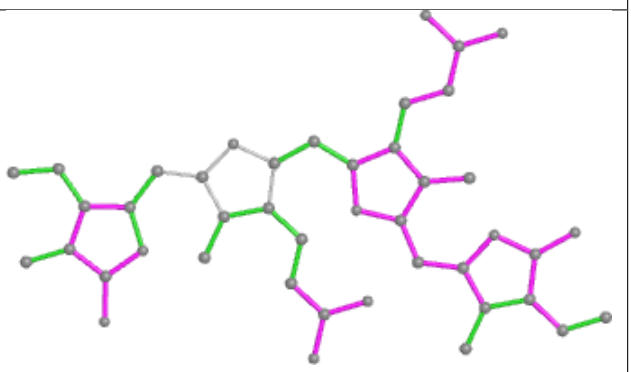

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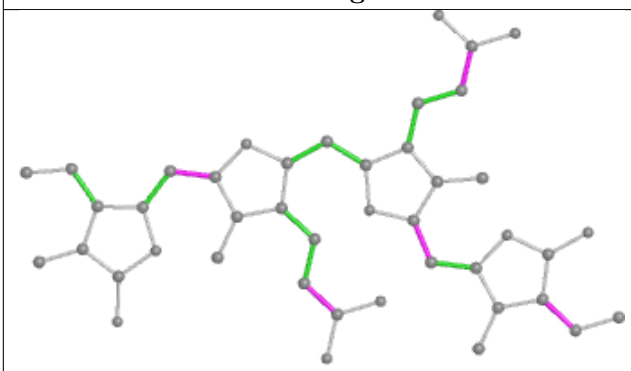

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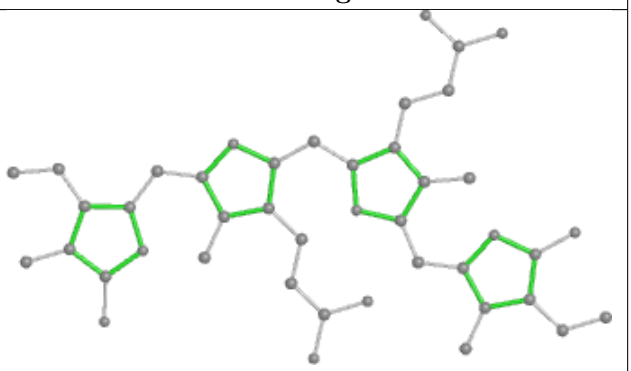
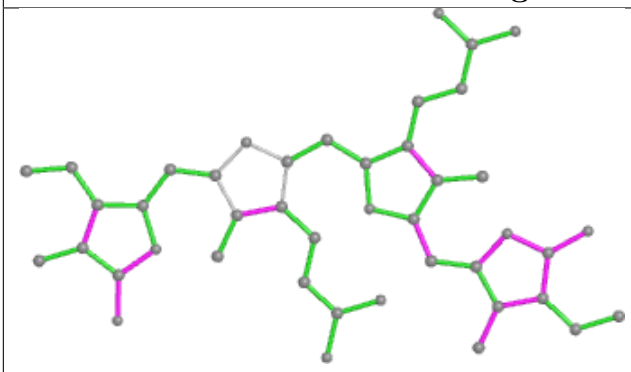
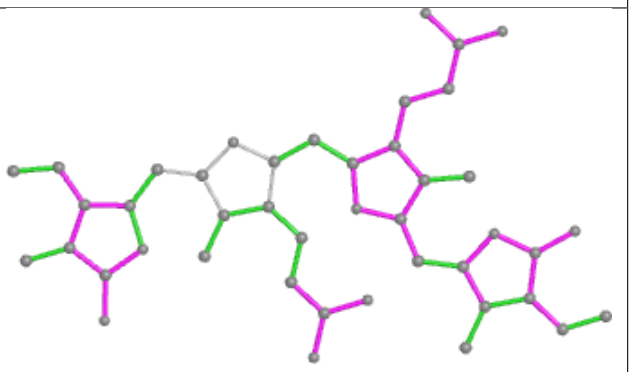


Rings

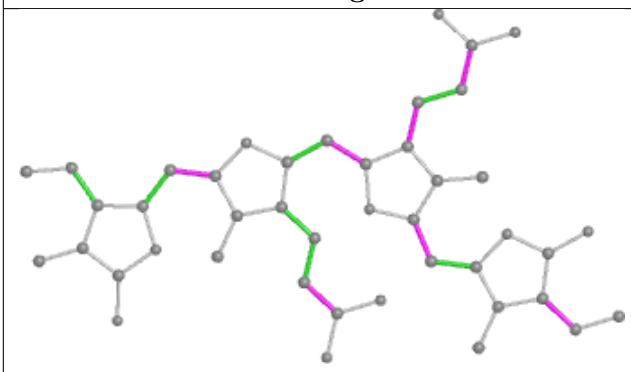
Ligand CYC dG 201



Bond lengths



Bond angles



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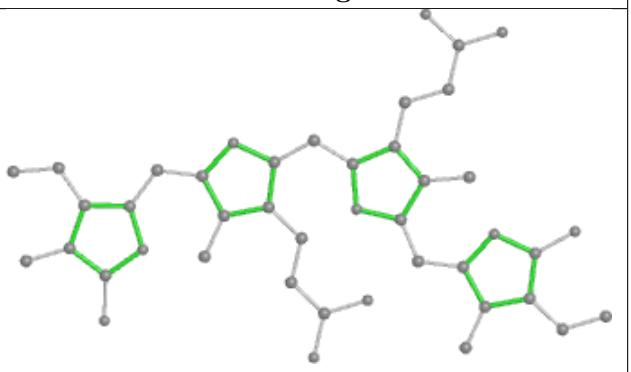
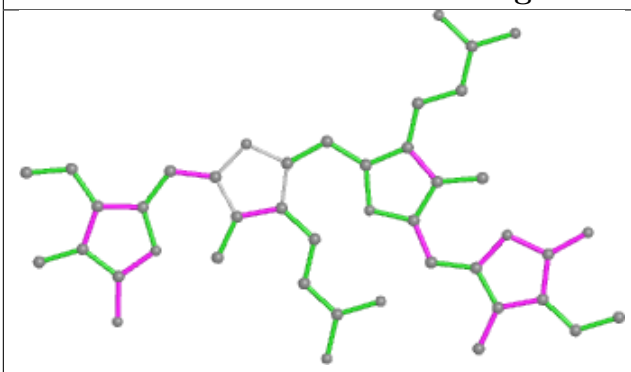


Rings

Ligand CYC eT 201



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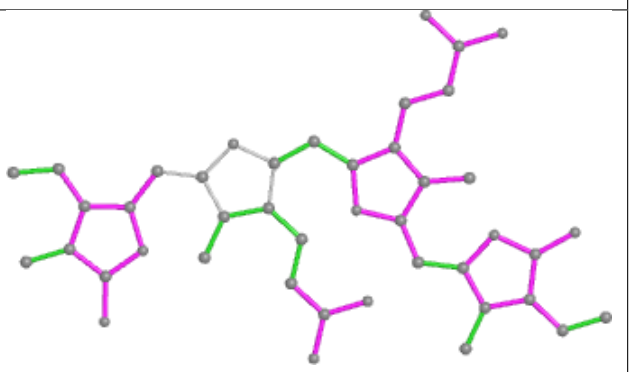
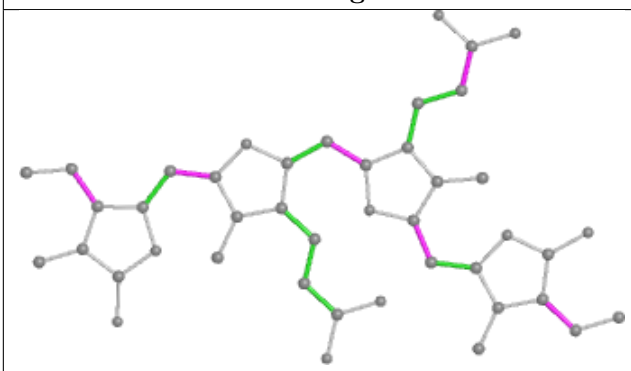
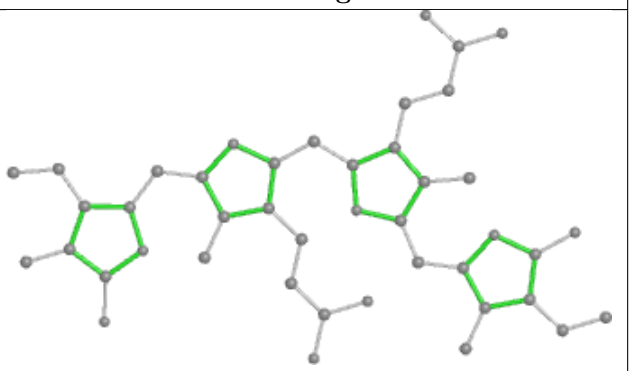


Bond angles

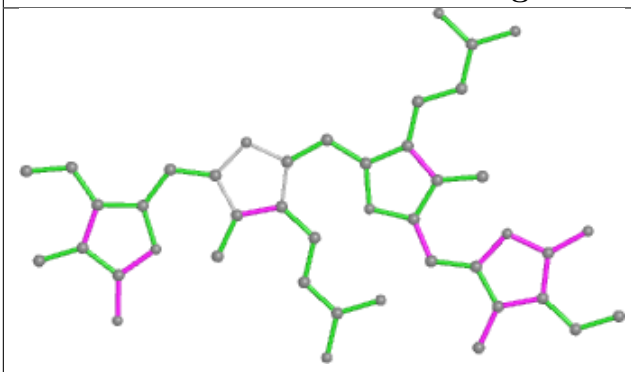


Torsions



Rings

Ligand CYC dD 201



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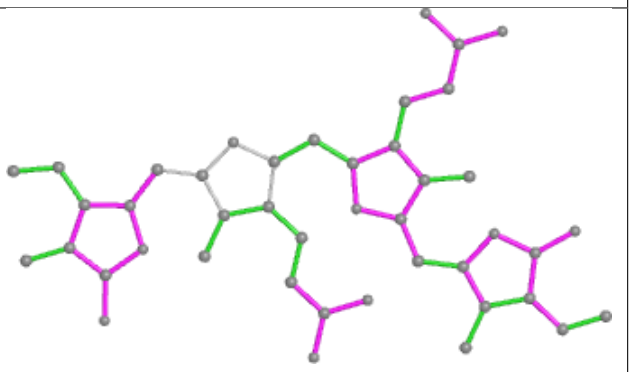
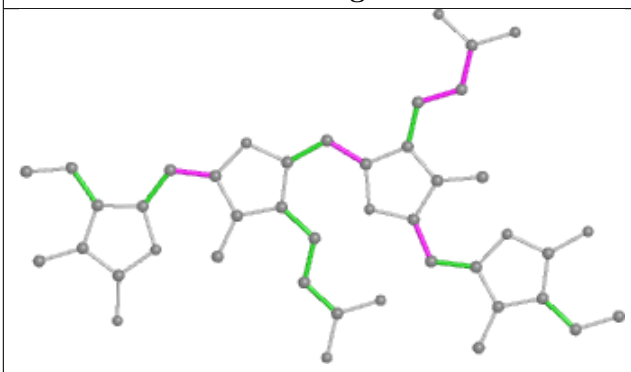
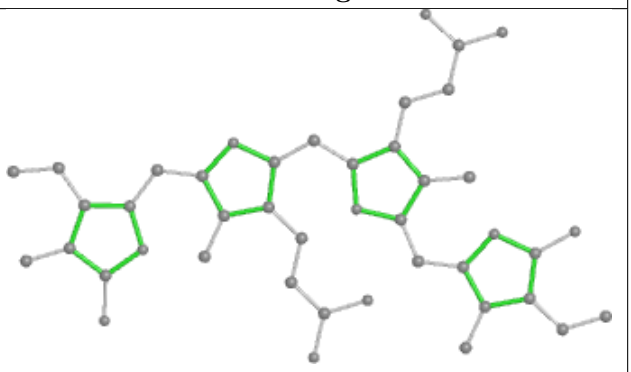


Bond angles

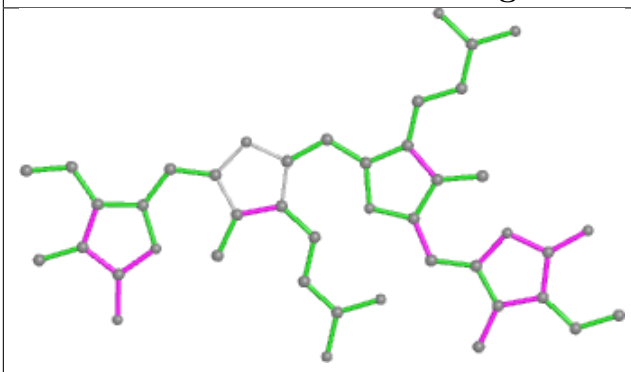


Torsions



Rings

Ligand CYC dM 1203



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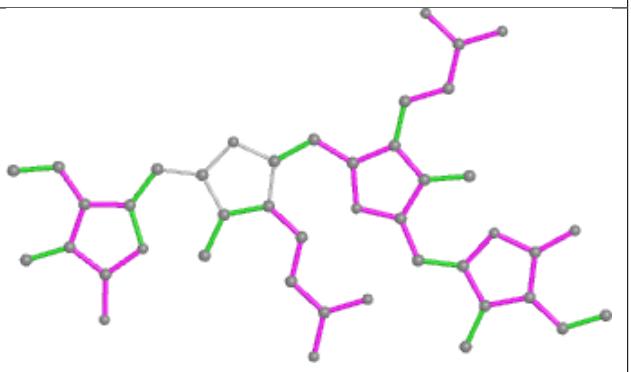
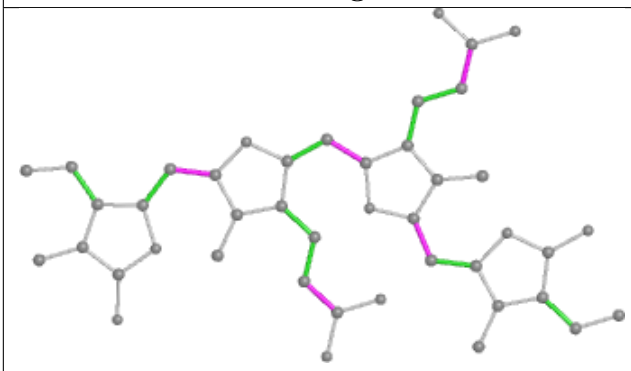


Bond angles



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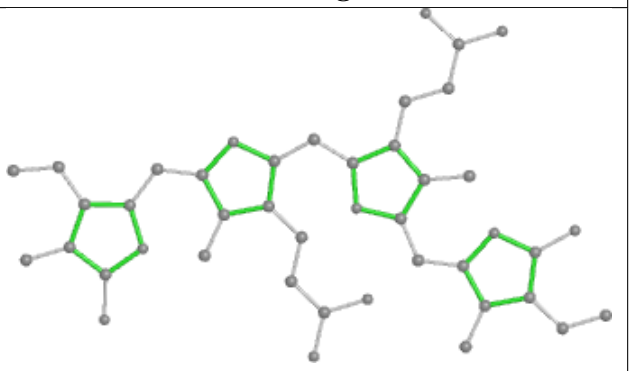
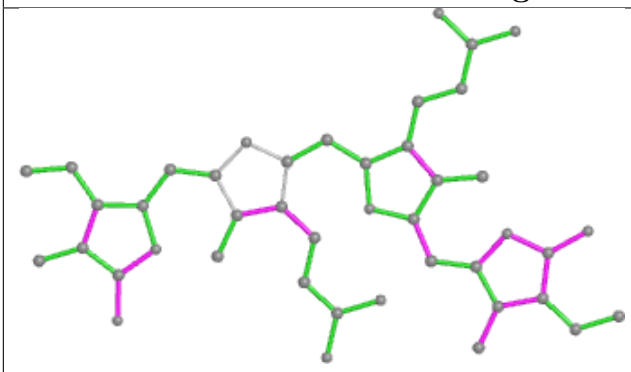


Rings

Ligand CYC aK 201



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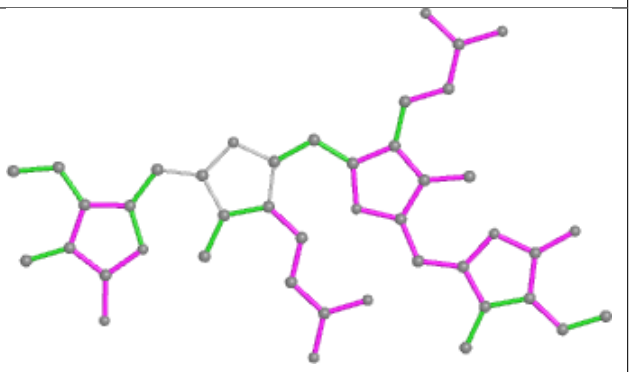
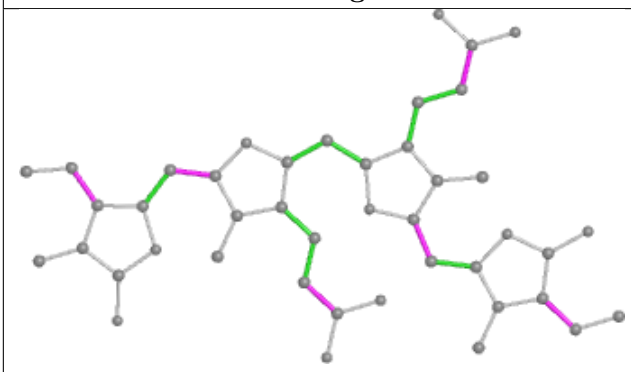
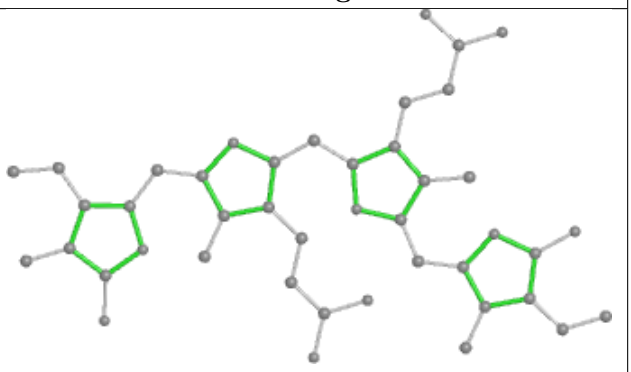


Bond angles

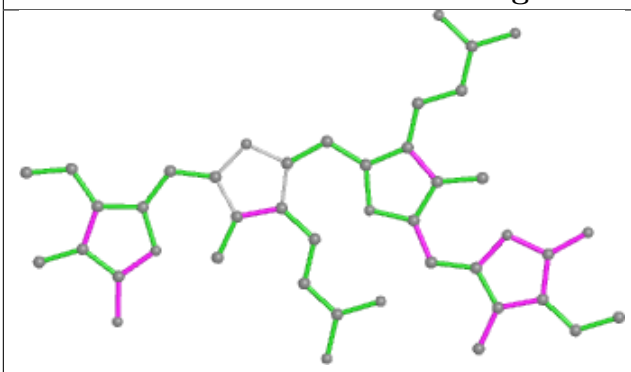


Torsions



Rings

Ligand CYC bV 201



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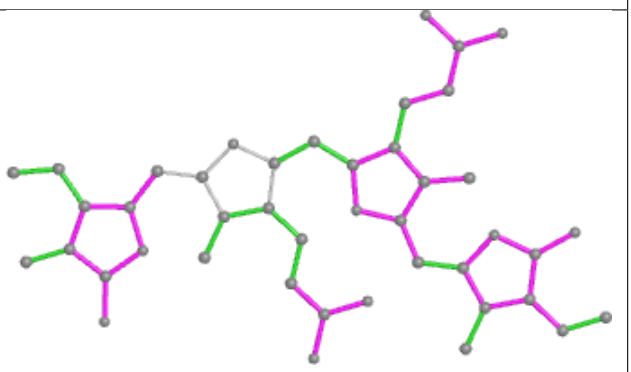
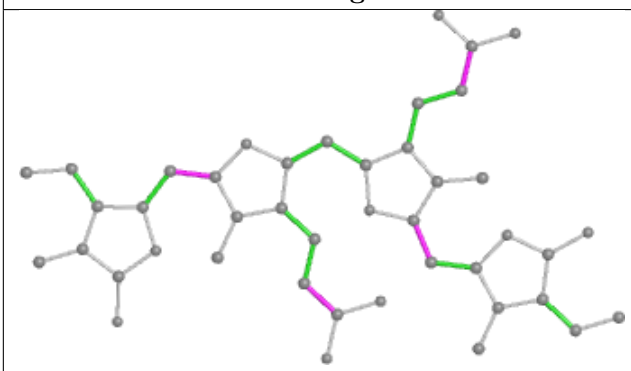


Bond angles



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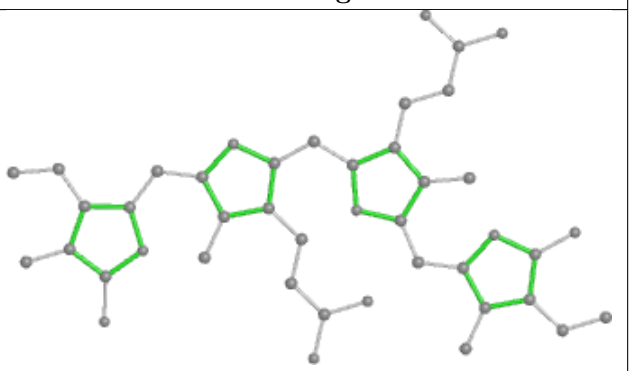
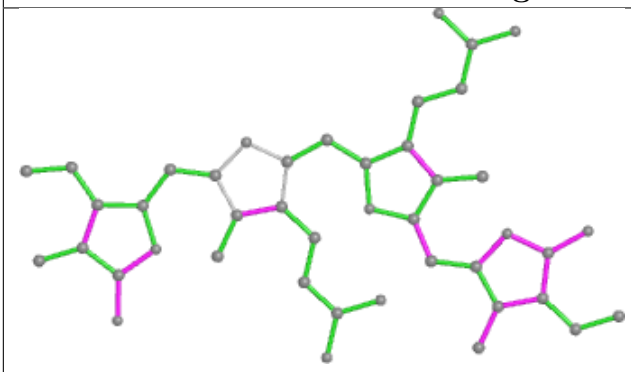
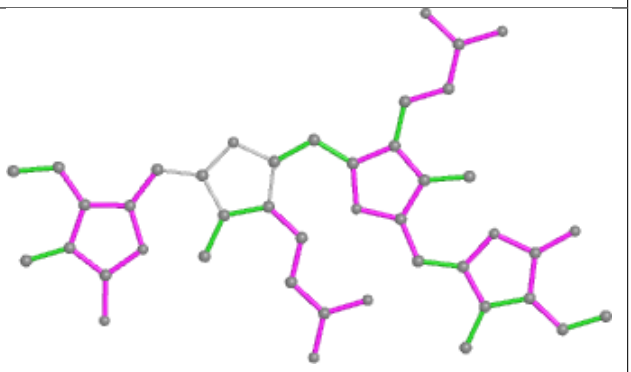


Rings

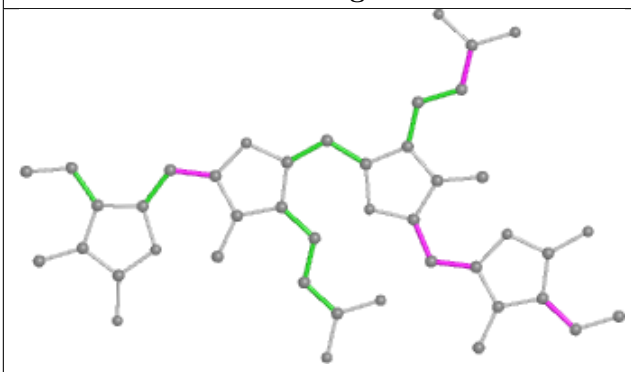
Ligand CYC eN 201



Bond lengths



Bond angles



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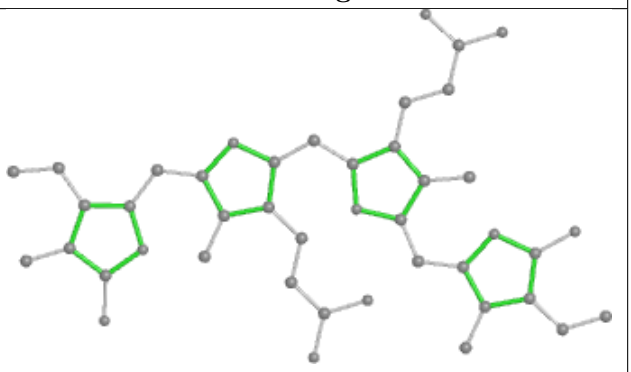
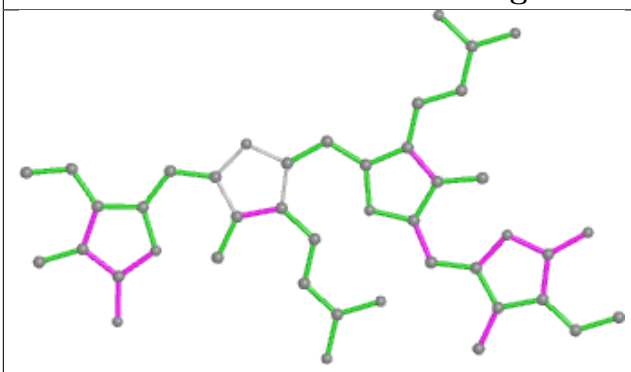
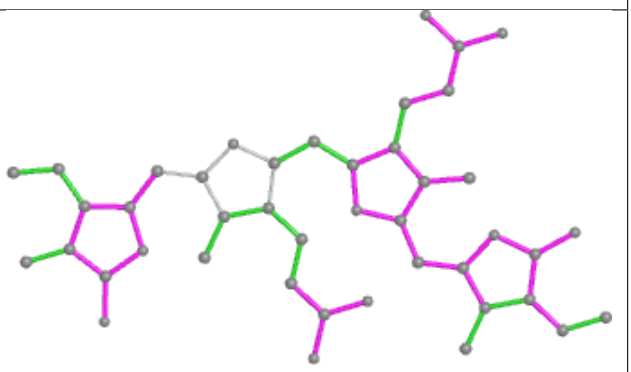


Rings

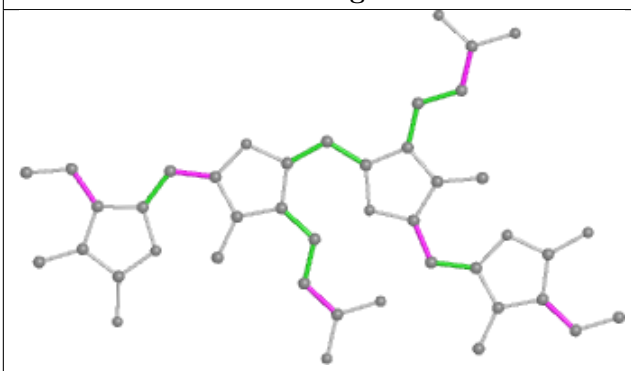
Ligand CYC eM 201



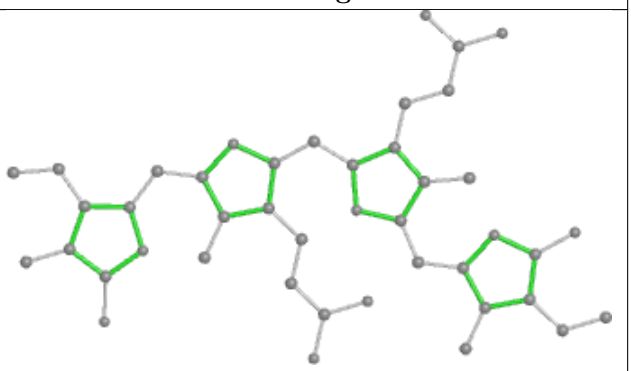
Bond lengths



Bond angles

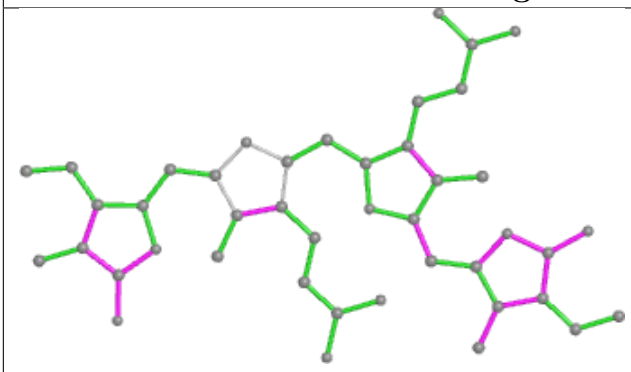


Torsions

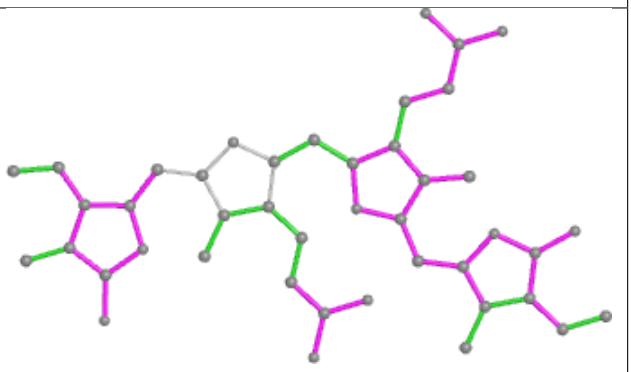


Rings

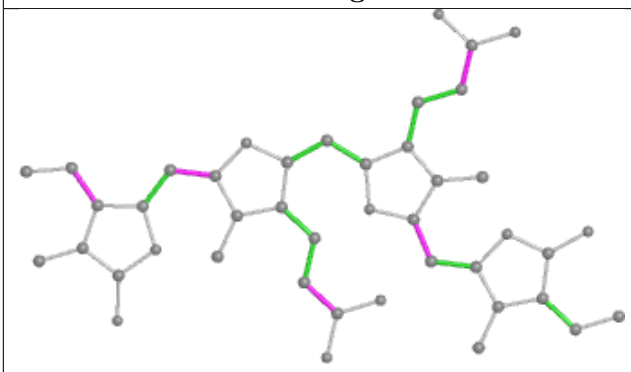
Ligand CYC cG 201



Bond lengths



Bond angles



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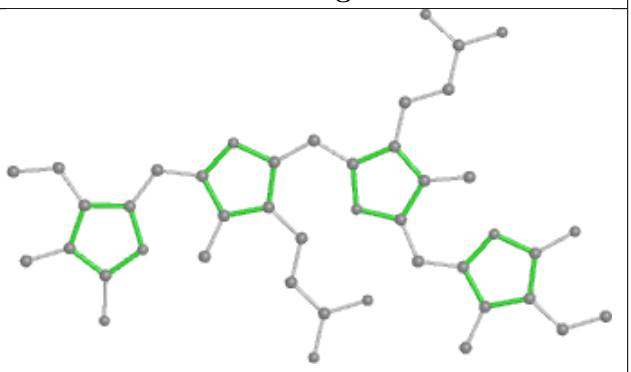
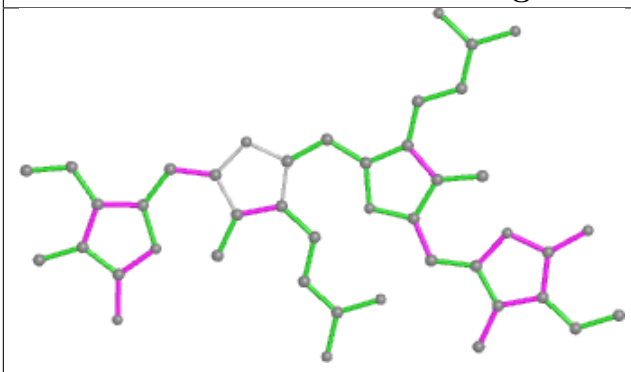


Rings

Ligand CYC bT 201



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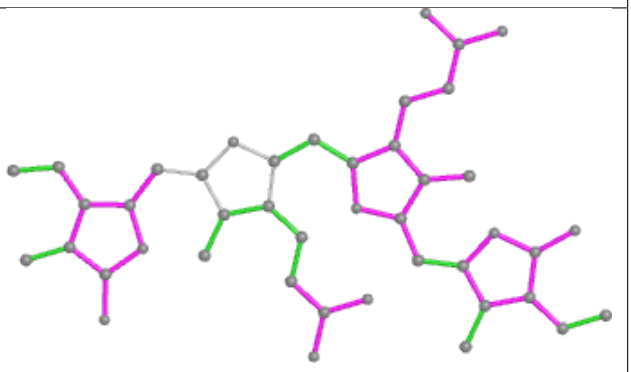

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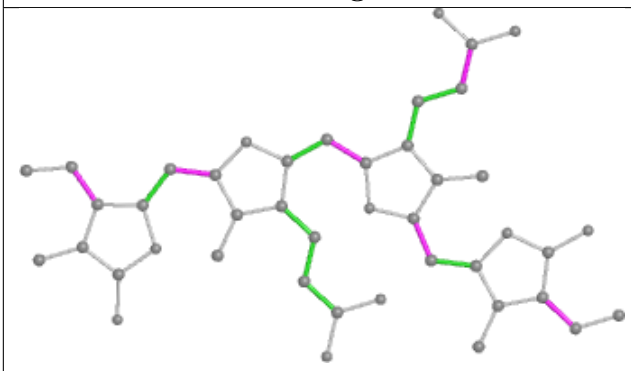
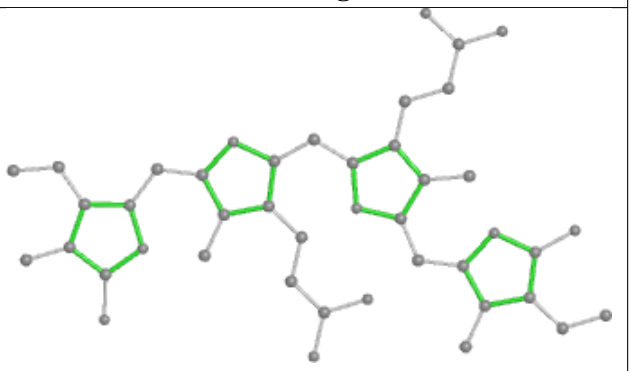
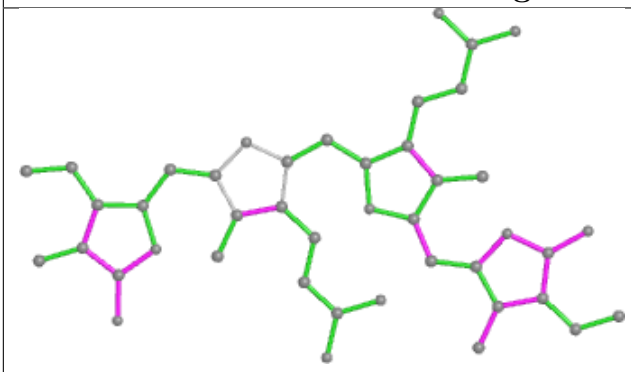


Torsions



Rings

Ligand CYC eX 201



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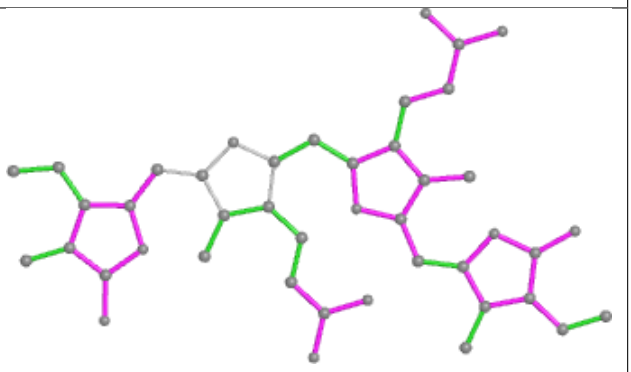
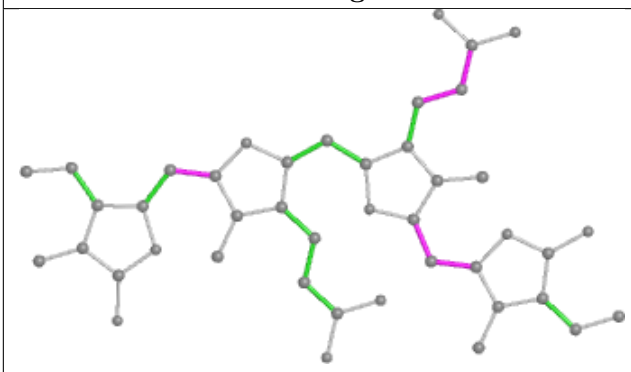
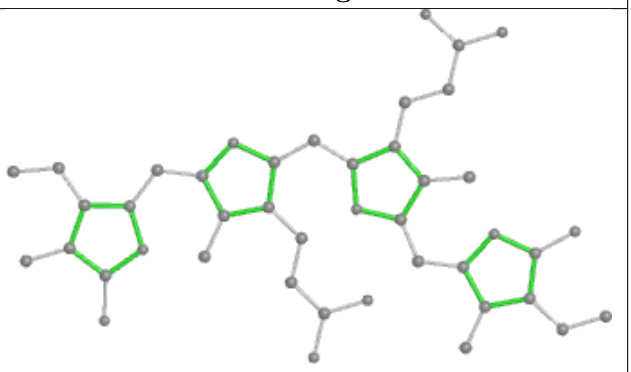


Bond angles

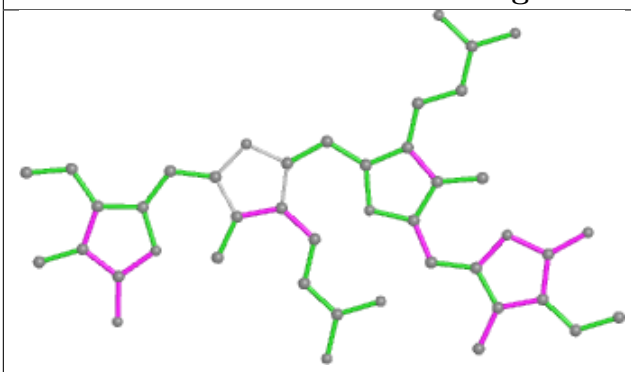


Torsions



Rings

Ligand CYC dO 201



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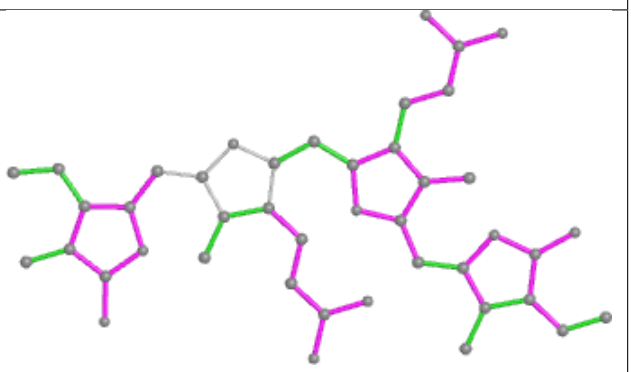
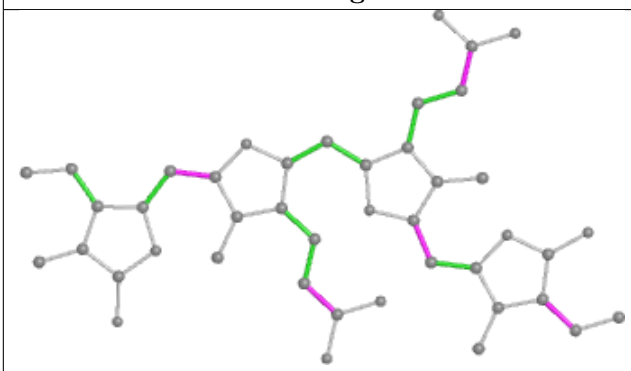


Bond angles



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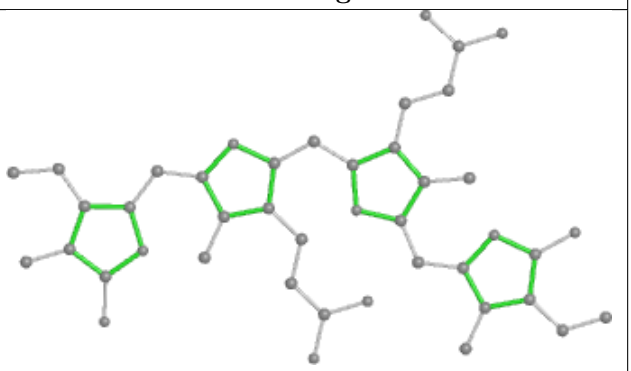
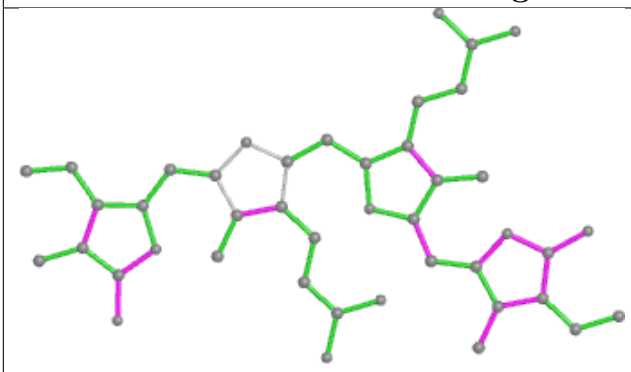


Rings

Ligand CYC dA 201



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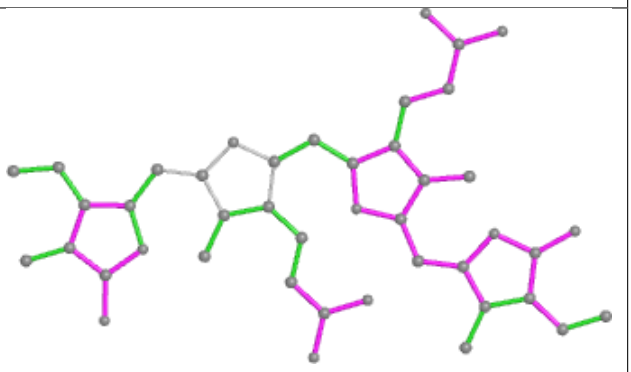
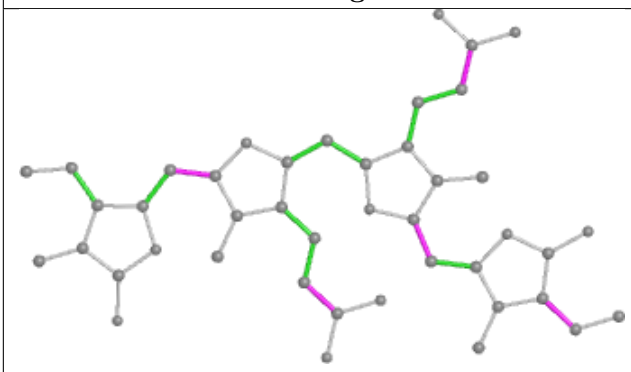


Bond angles



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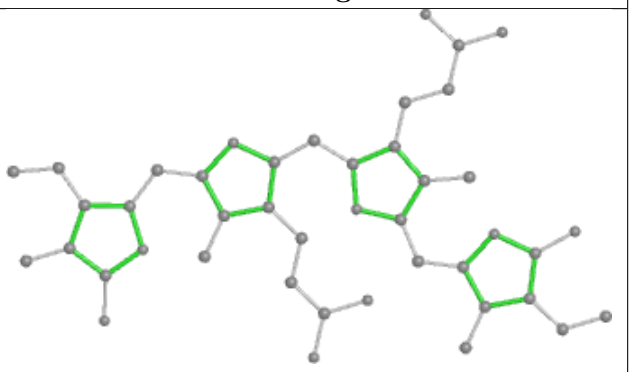
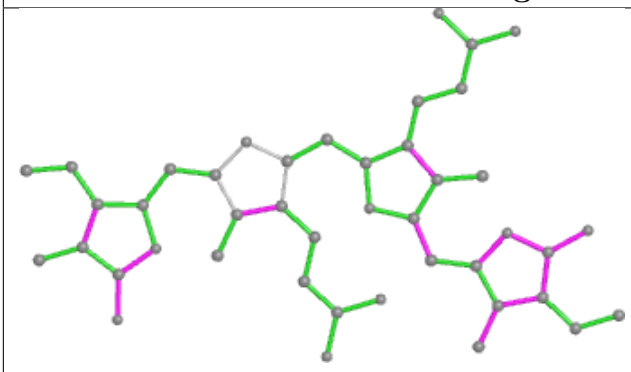


Rings

Ligand CYC dE 201



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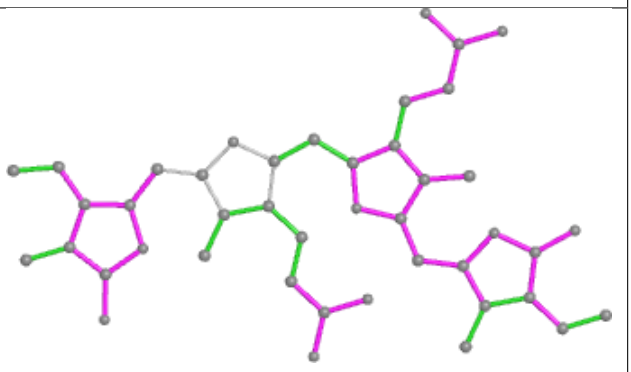
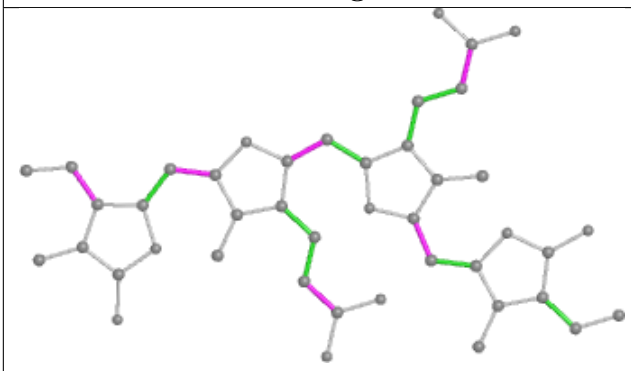


Bond angles



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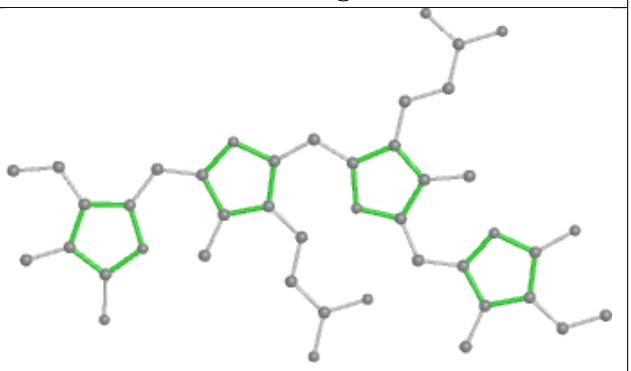
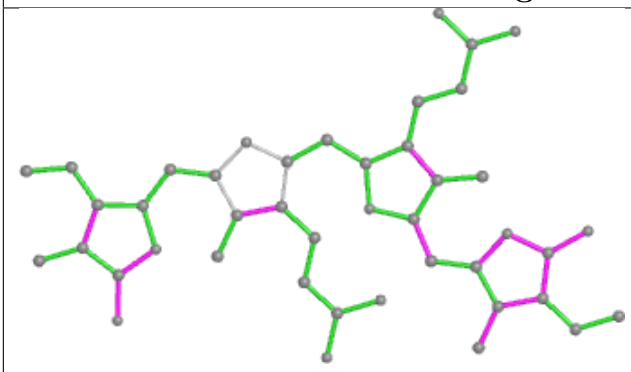


Rings

Ligand CYC aL 201



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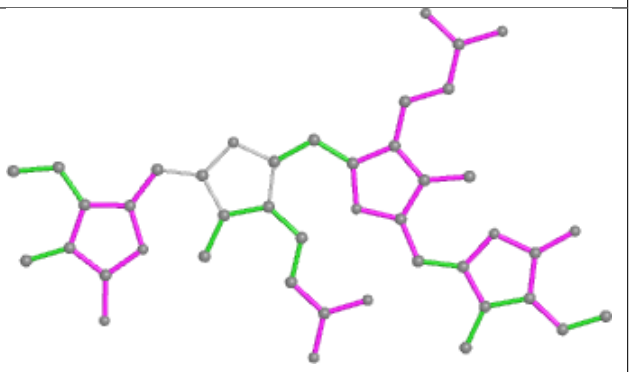

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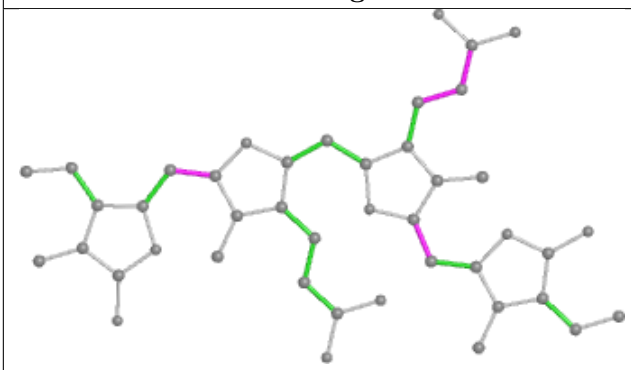
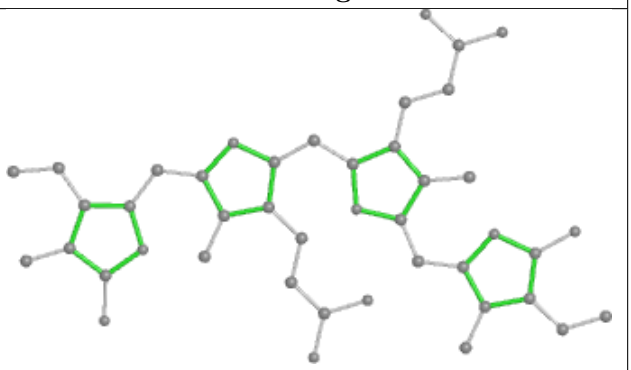
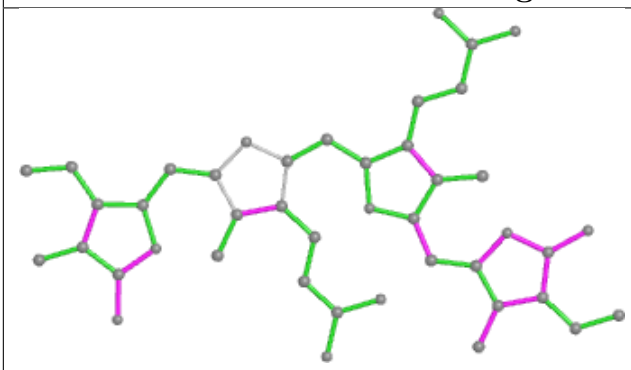


Torsions



Rings

Ligand CYC fD 202



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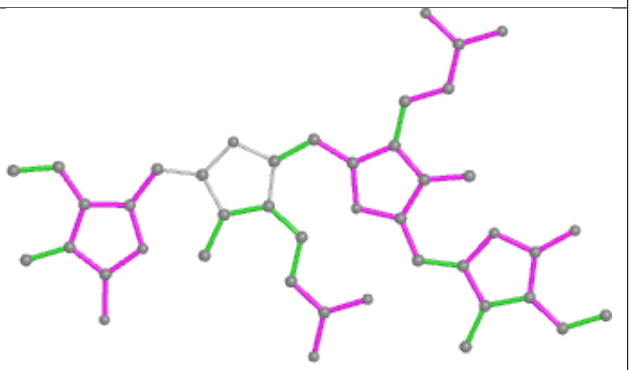
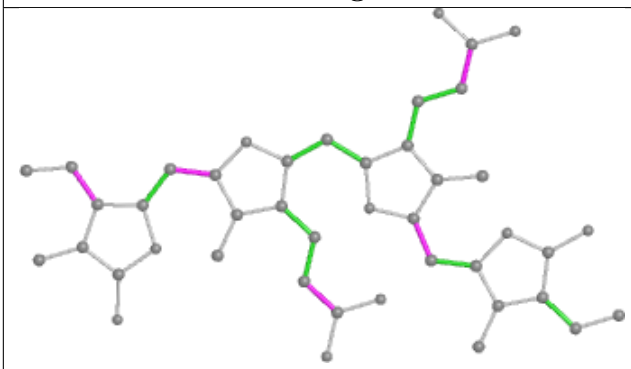
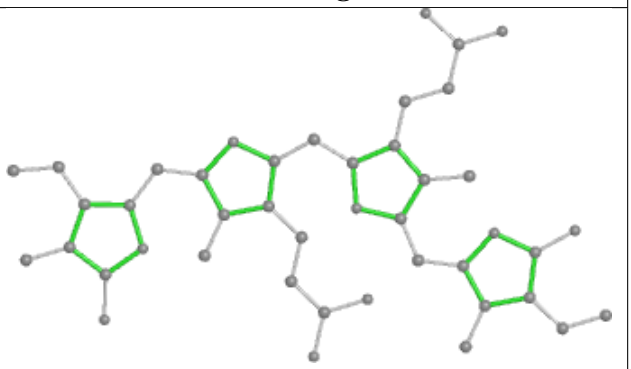


Bond angles

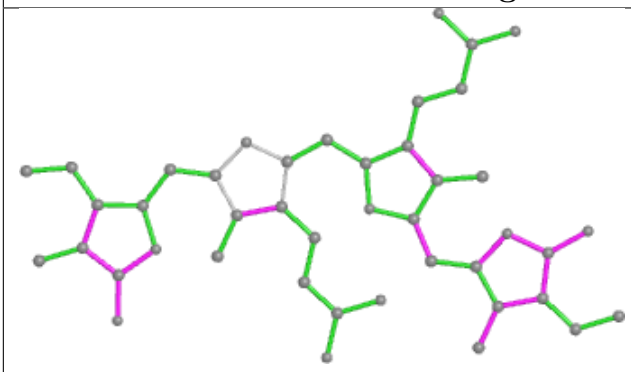


Torsions

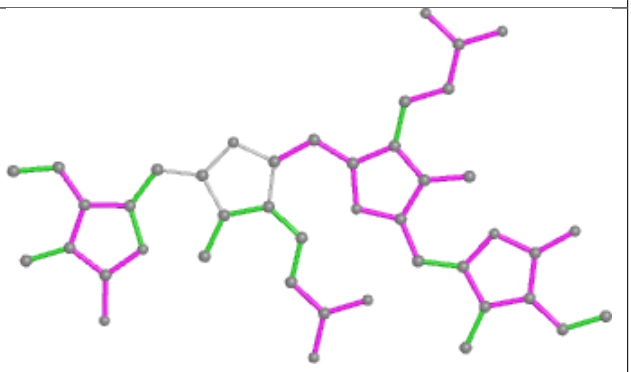


Rings

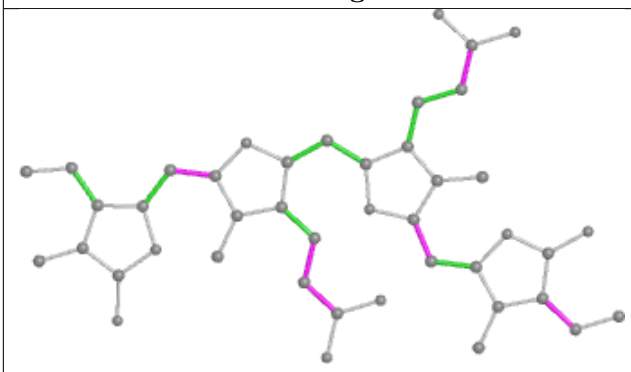
Ligand CYC dM 1202



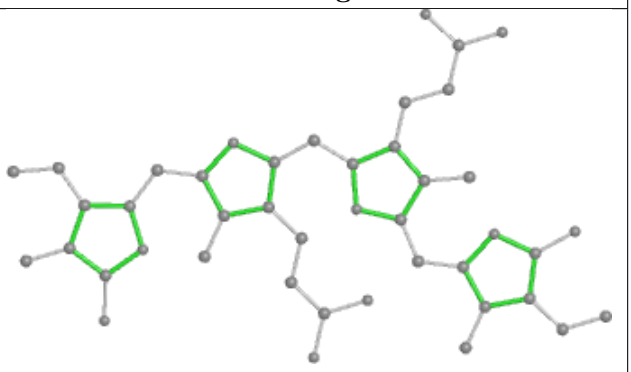
Bond lengths



Bond angles

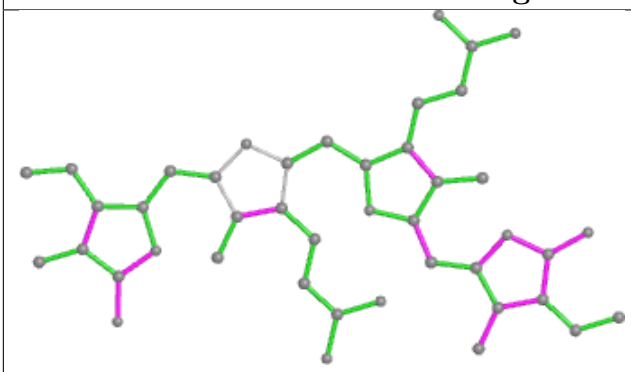


Torsions

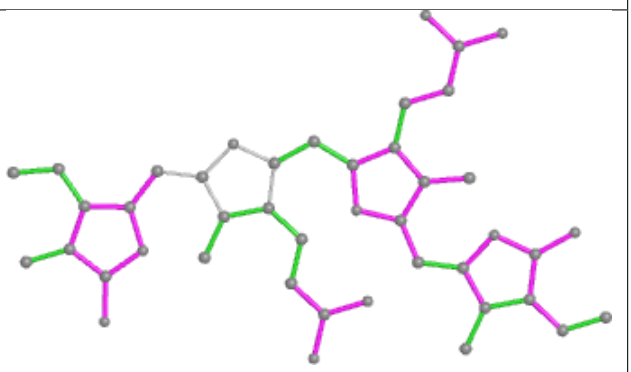


Rings

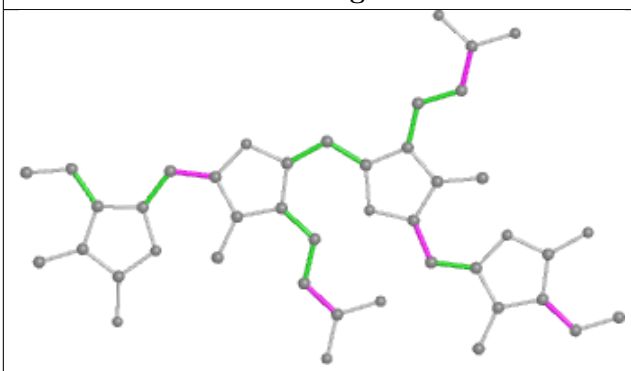
Ligand CYC bP 201



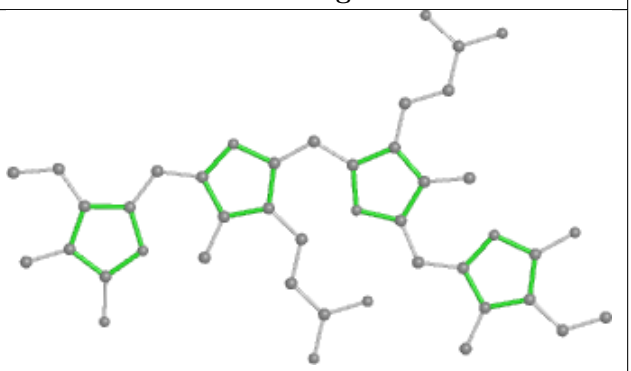
Bond lengths



Bond angles

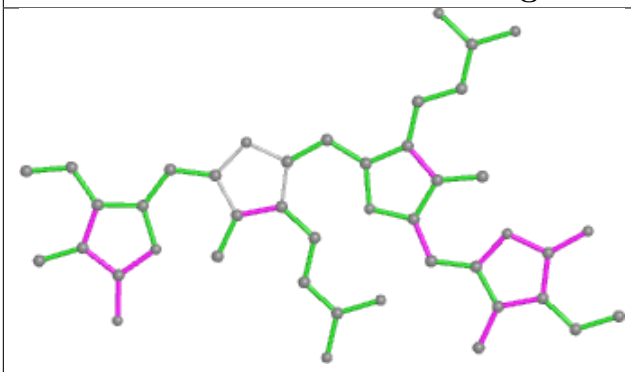


Torsions



Rings

Ligand CYC fJ 201



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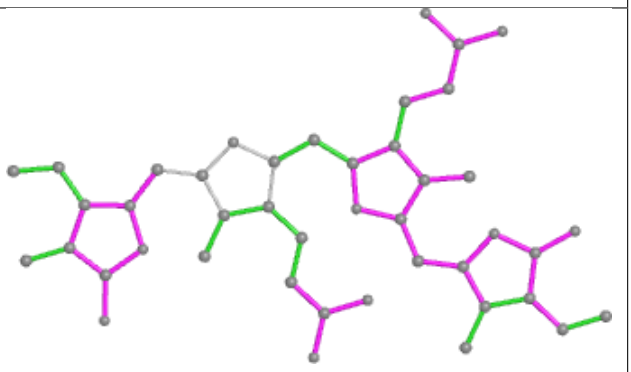
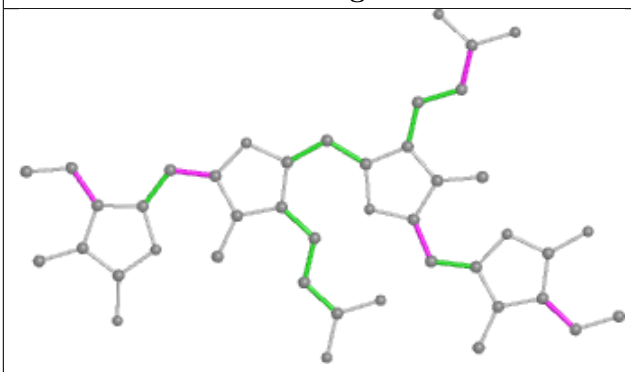


Bond angles



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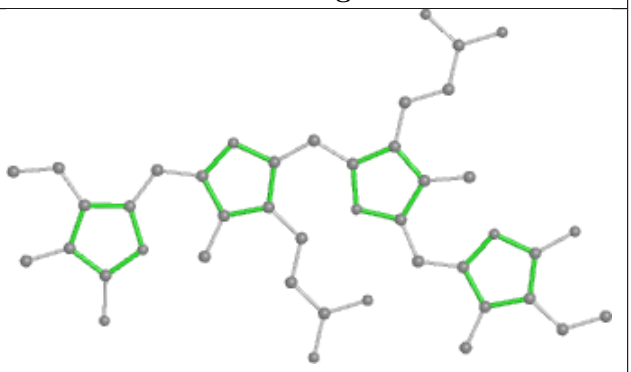
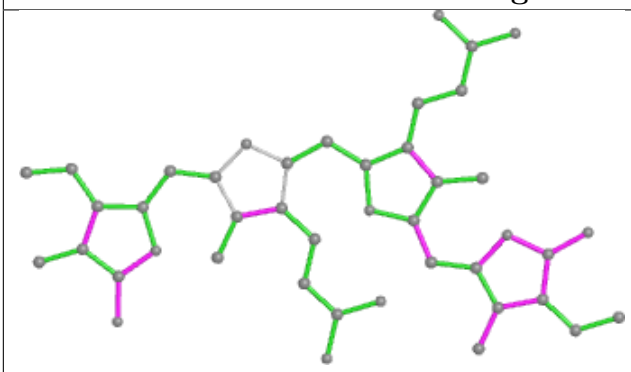


Rings

Ligand CYC dN 201



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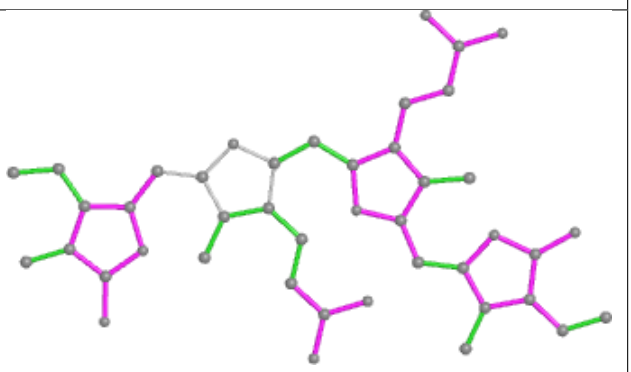
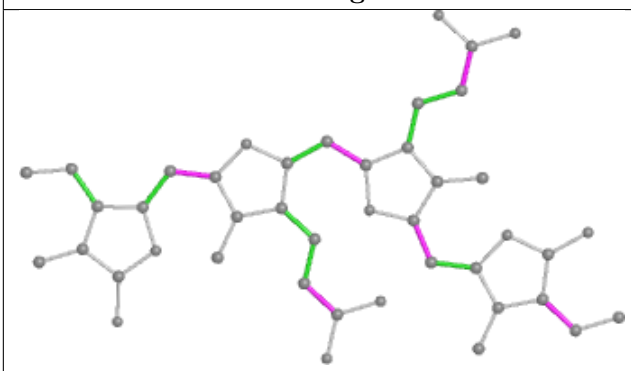
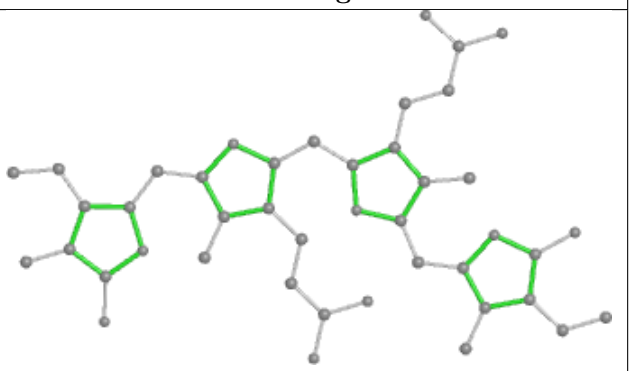


Bond angles

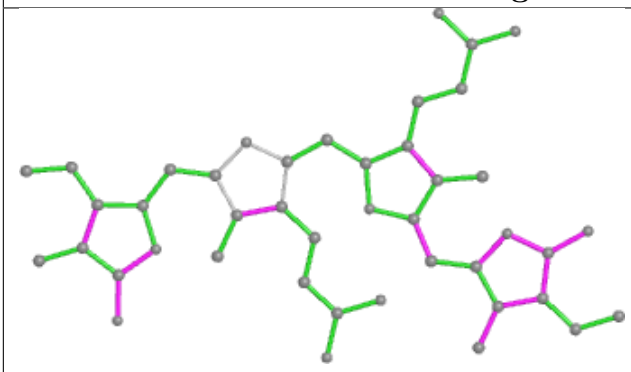


Torsions

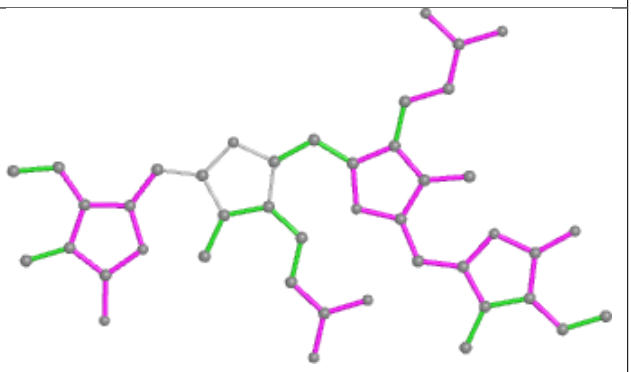


Rings

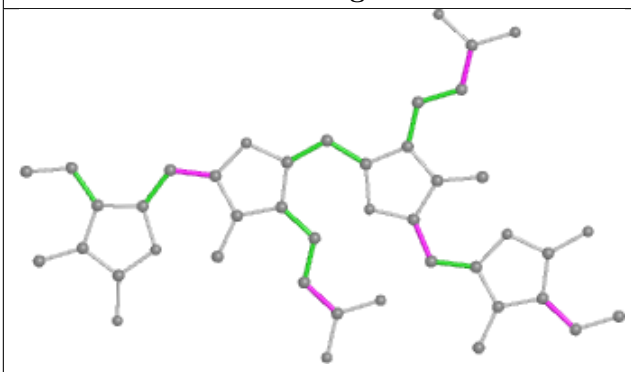
Ligand CYC bU 201



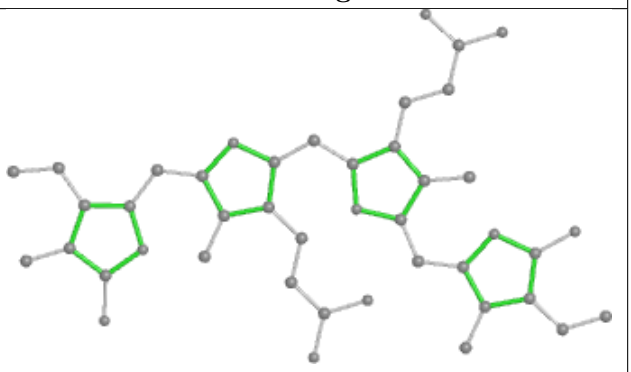
Bond lengths



Bond angles

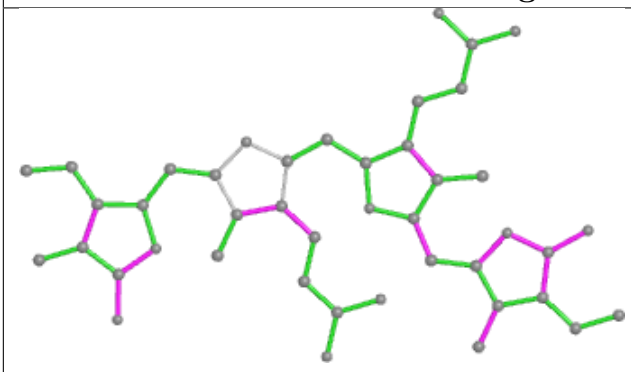


Torsions

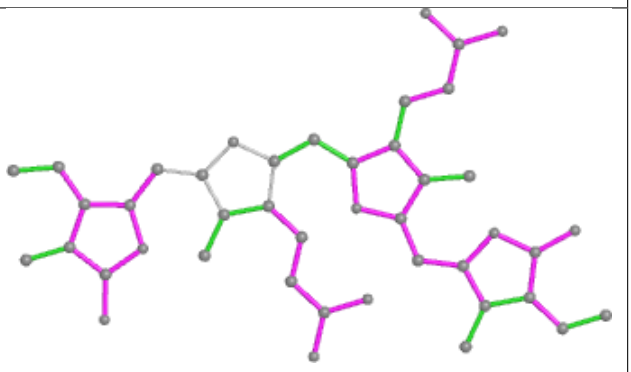


Rings

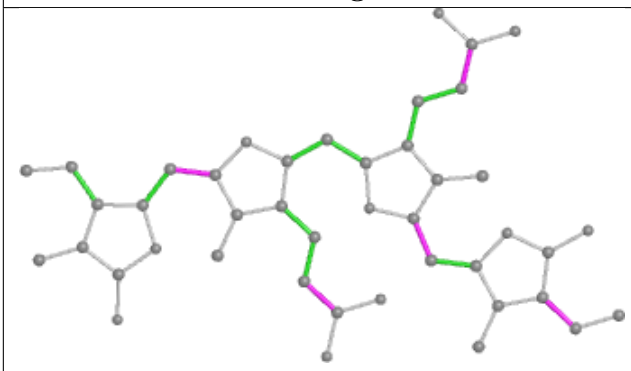
Ligand CYC dI 201



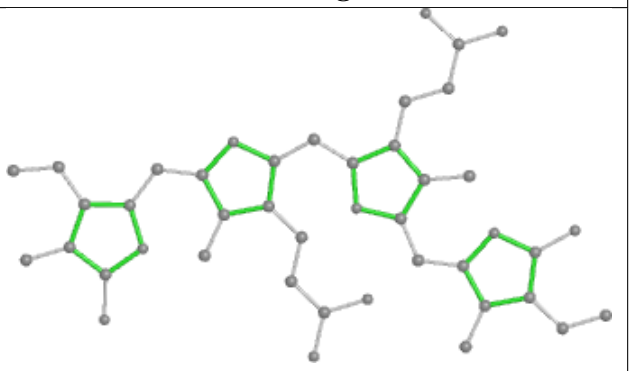
Bond lengths



Bond angles

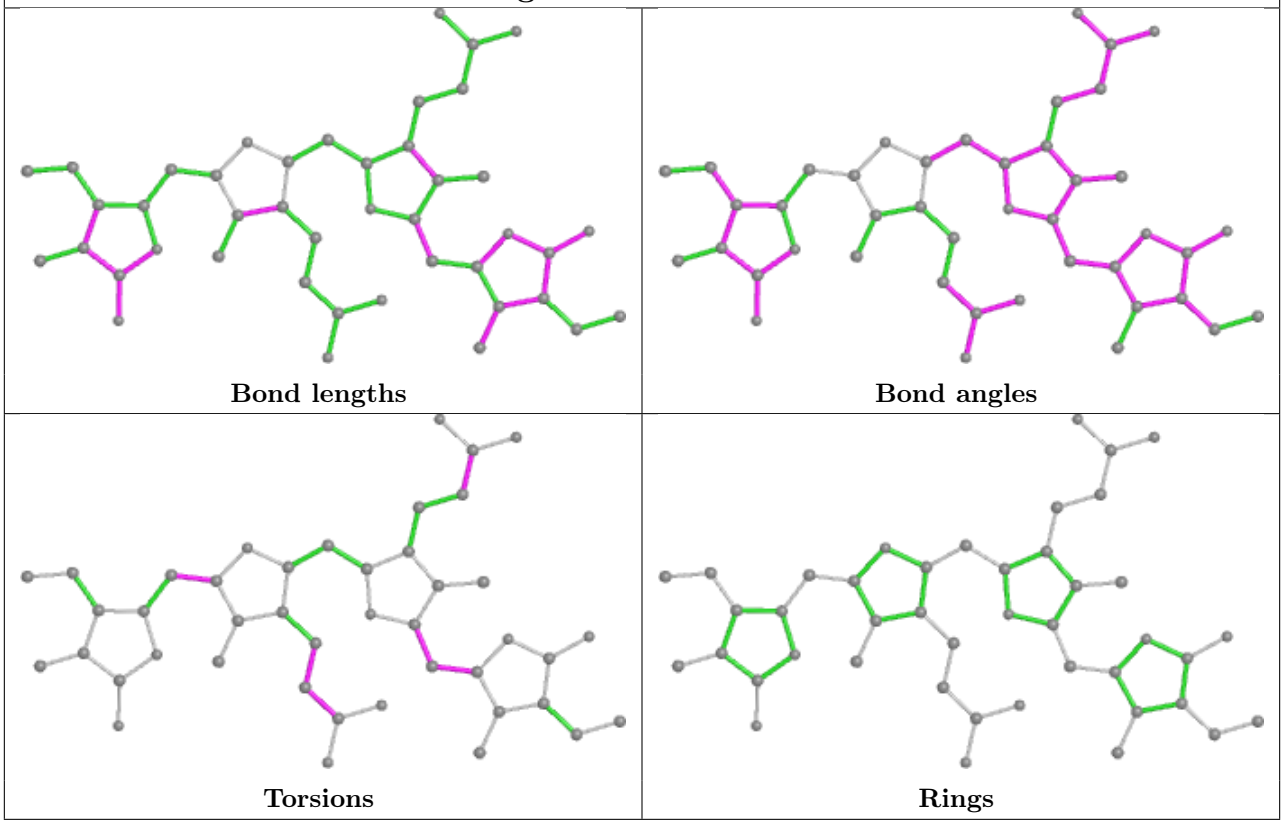


Torsions

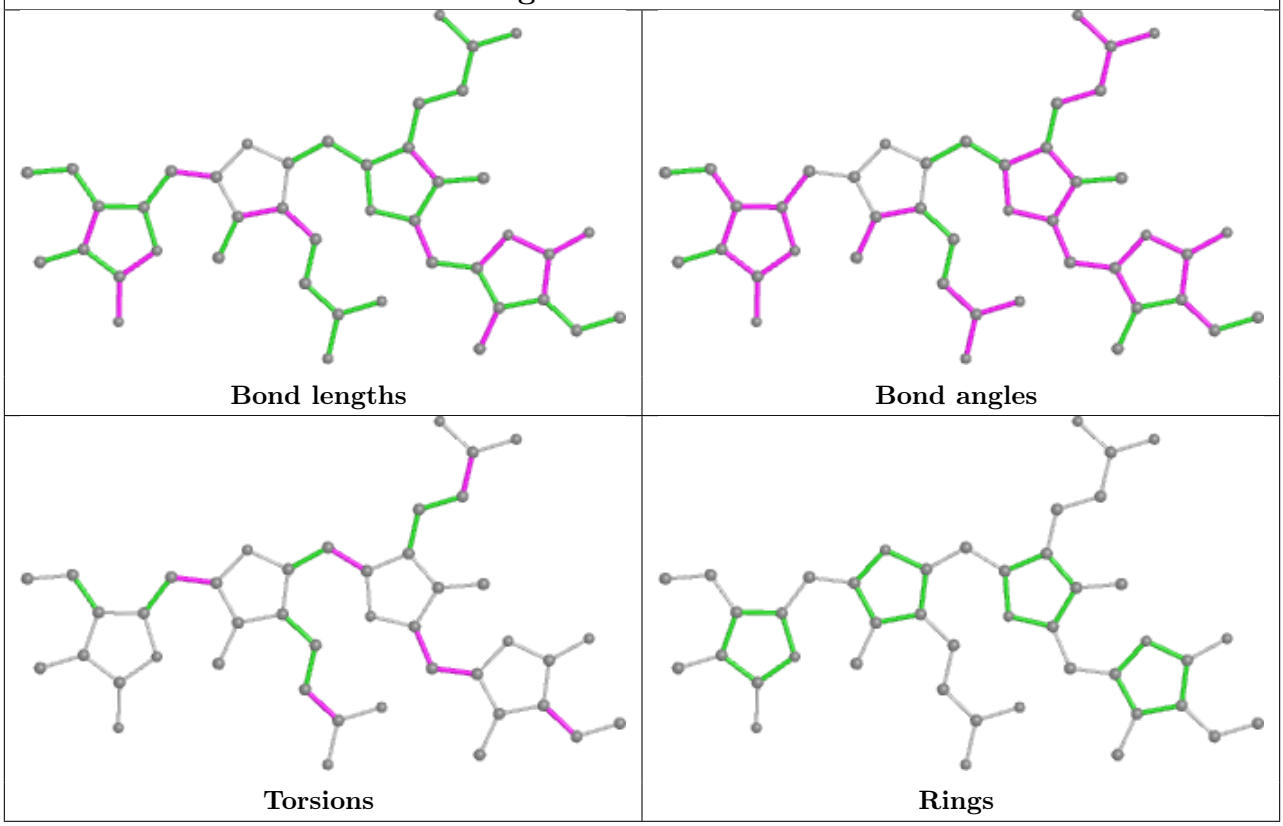


Rings

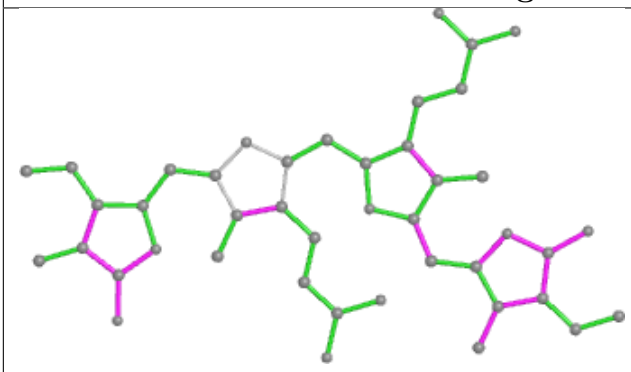
Ligand CYC cL 201



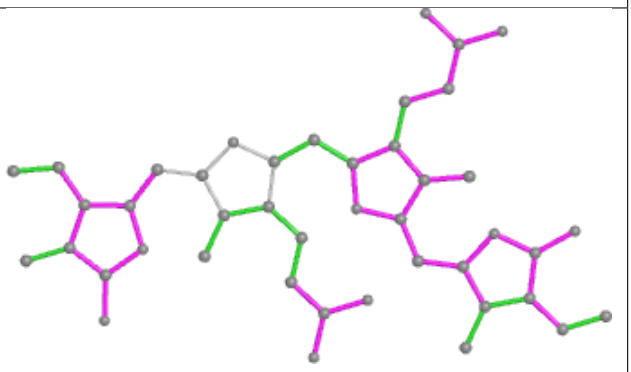
Ligand CYC aJ 201



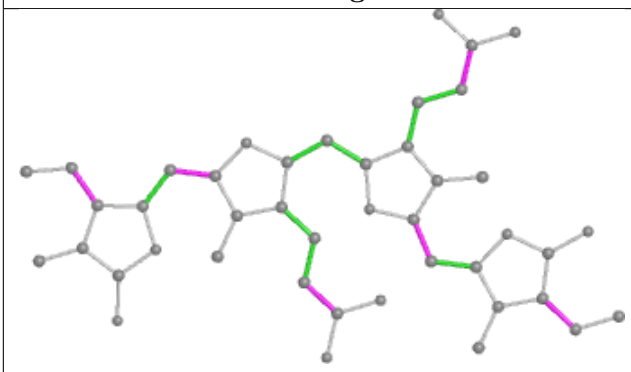
Ligand CYC fB 201



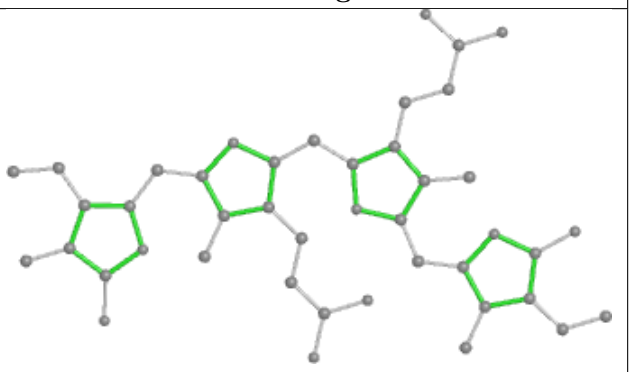
Bond lengths



Bond angles

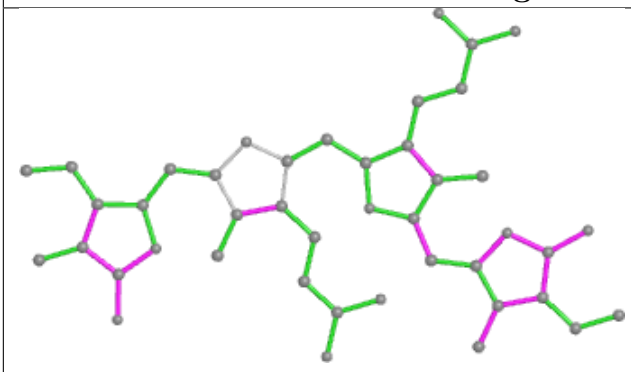


Torsions

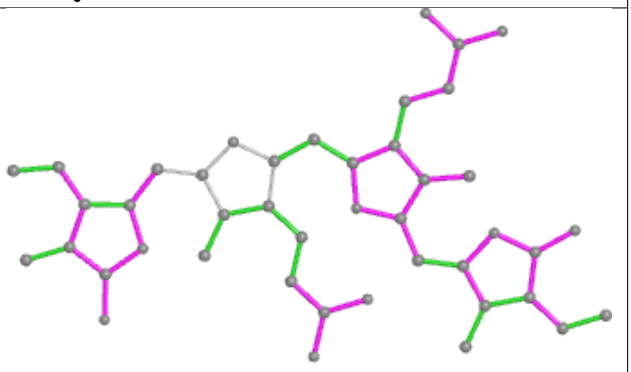


Rings

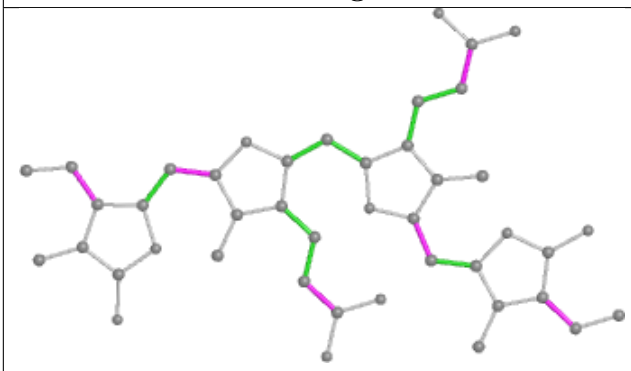
Ligand CYC eQ 201



Bond lengths



Bond angles



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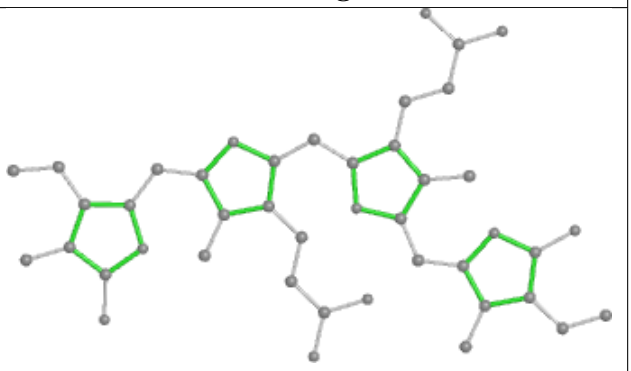
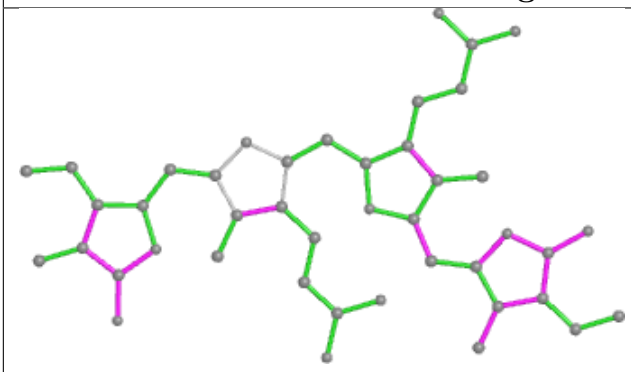


Rings

Ligand CYC cJ 201



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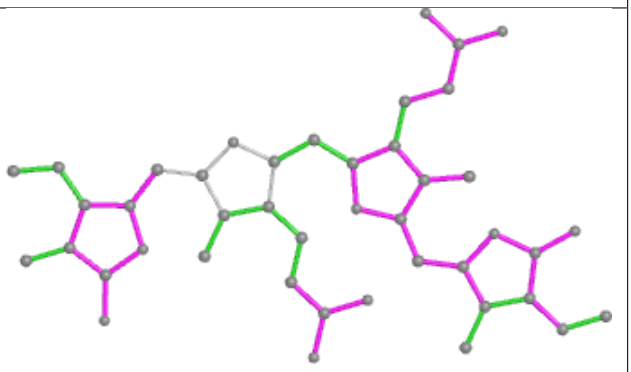
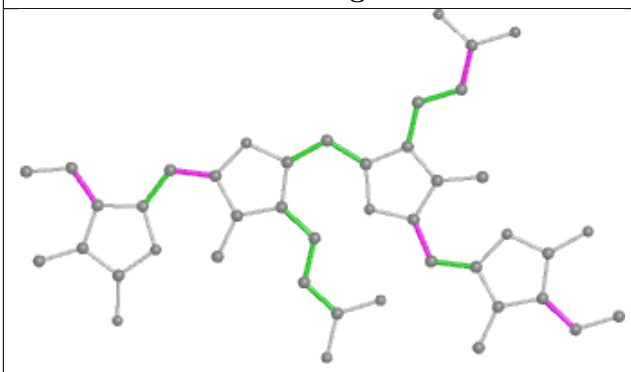
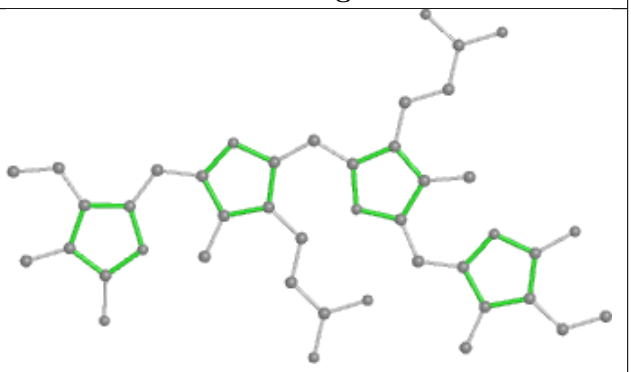


Bond angles

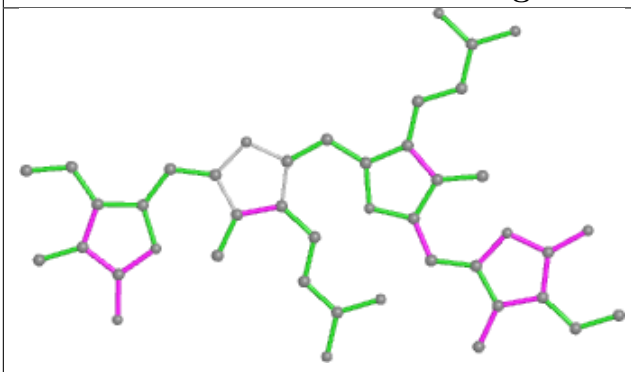


Torsions



Rings

Ligand CYC fM 101



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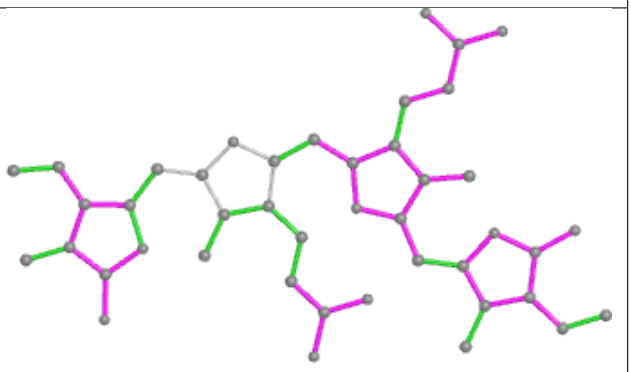
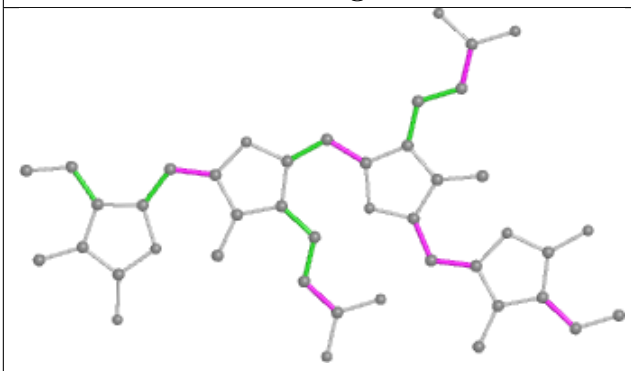


Bond angles



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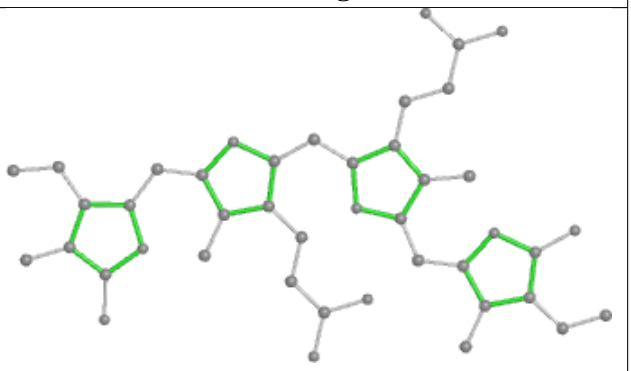
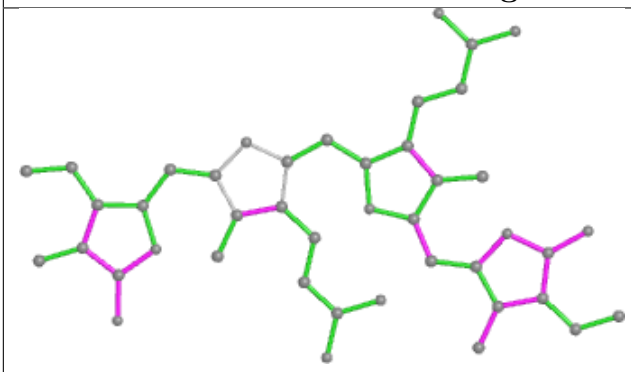
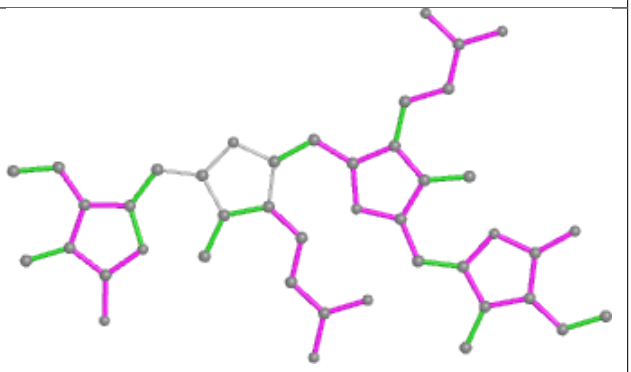


Rings

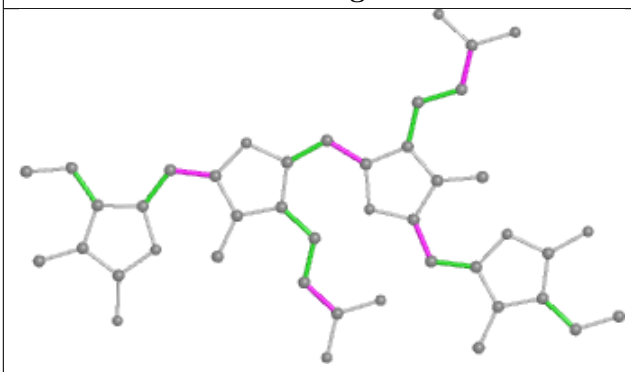
Ligand CYC aM 1203



Bond lengths



Bond angles



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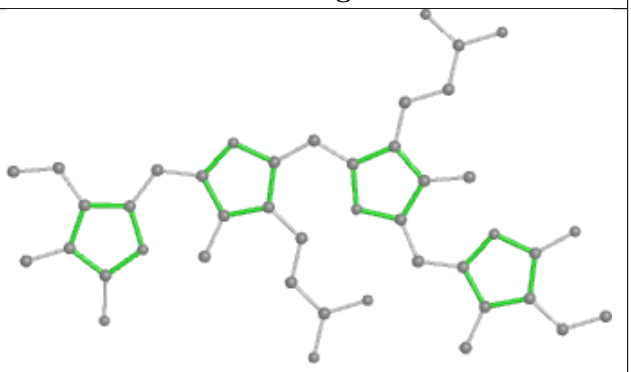
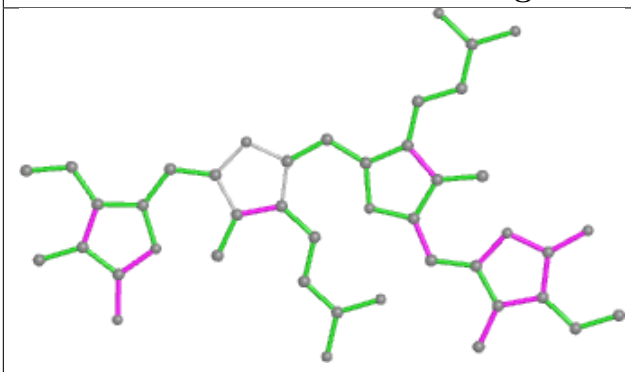


Rings

Ligand CYC dL 201



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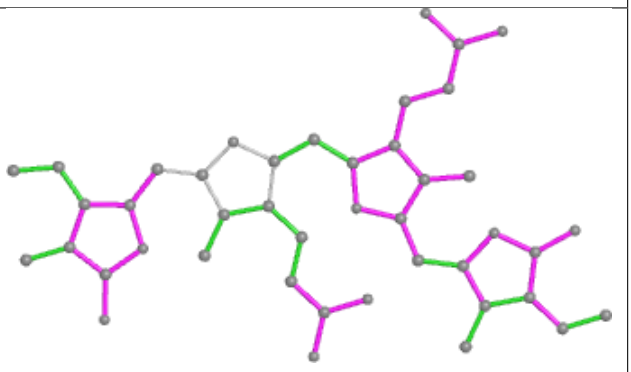
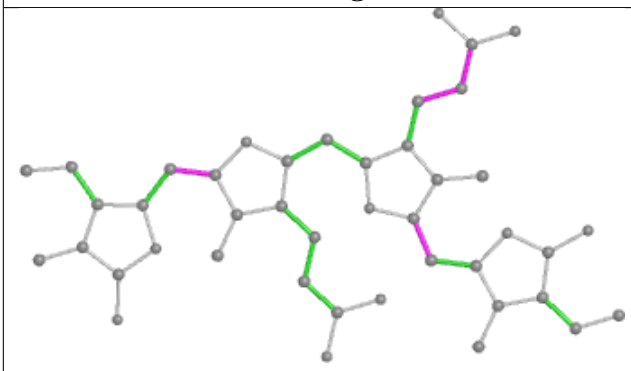


Bond angles



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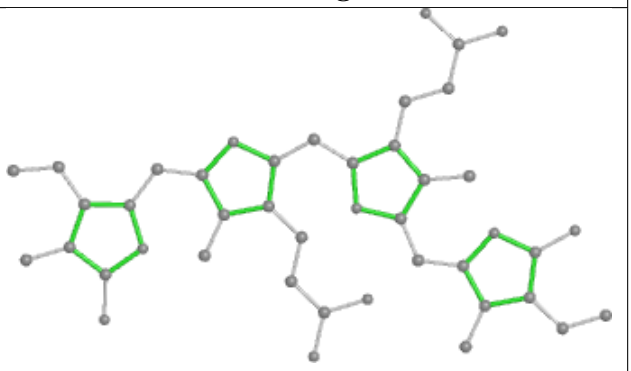
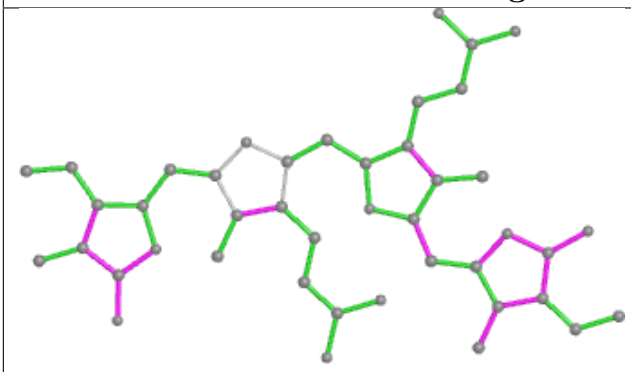


Rings

Ligand CYC eW 201



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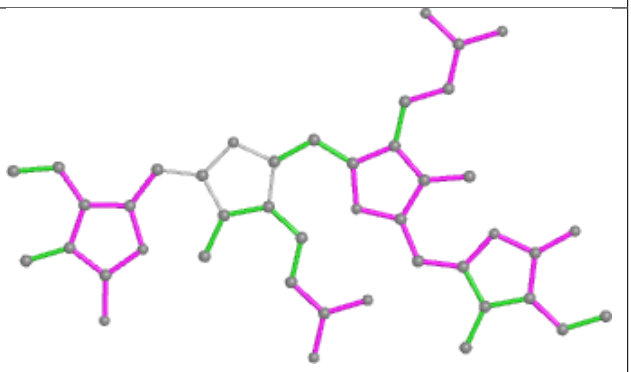
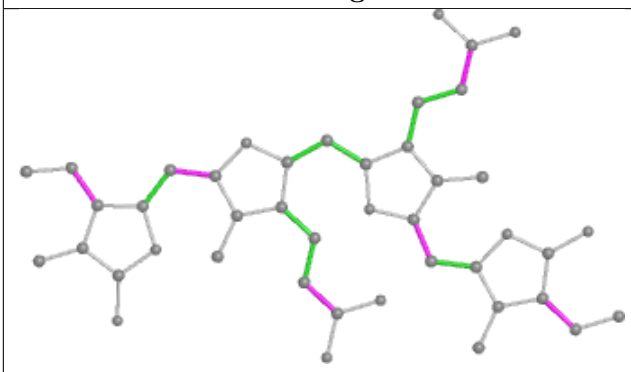


Bond angles



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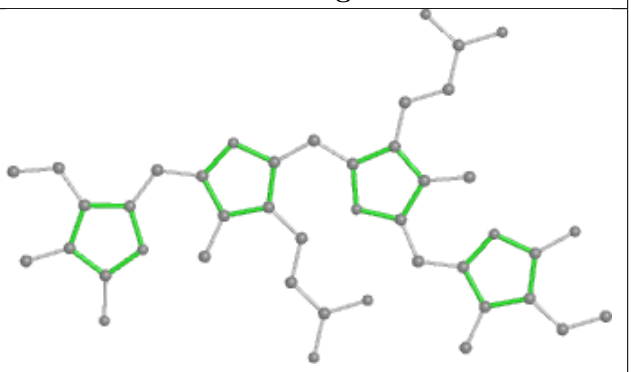
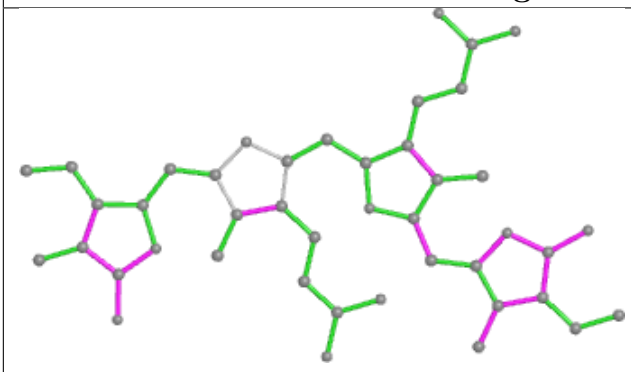


Rings

Ligand CYC cD 201



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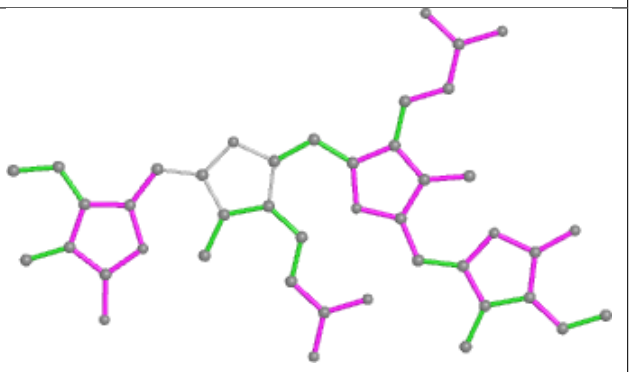
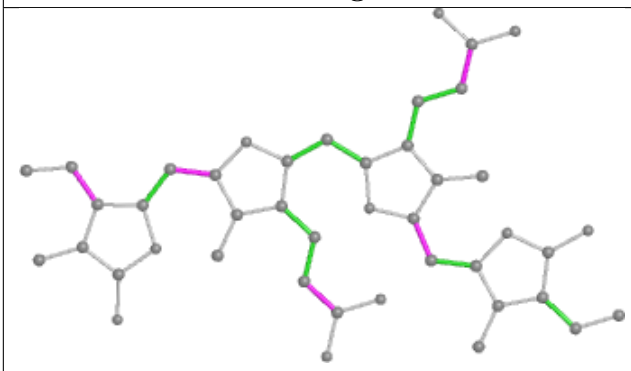
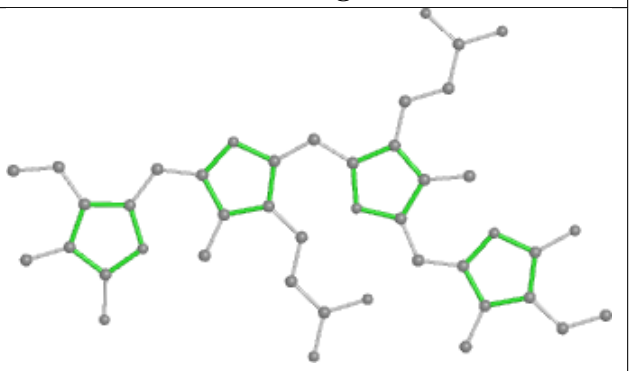


Bond angles

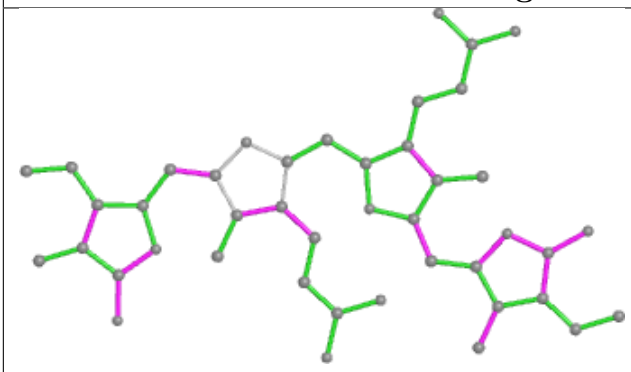


Torsions



Rings

Ligand CYC dJ 201



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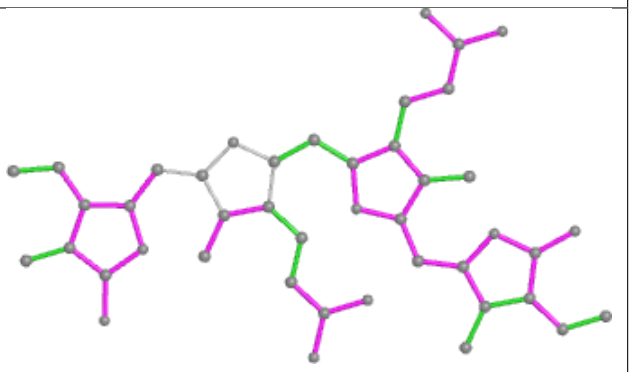
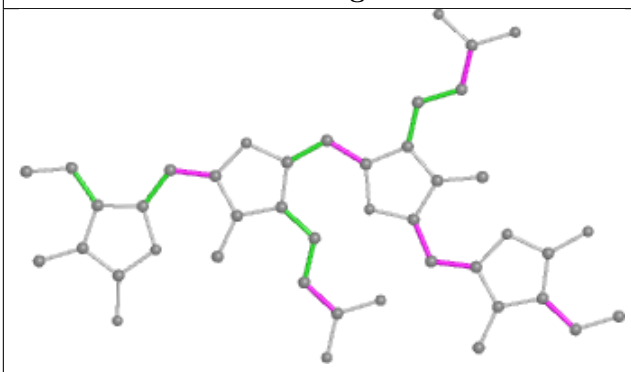
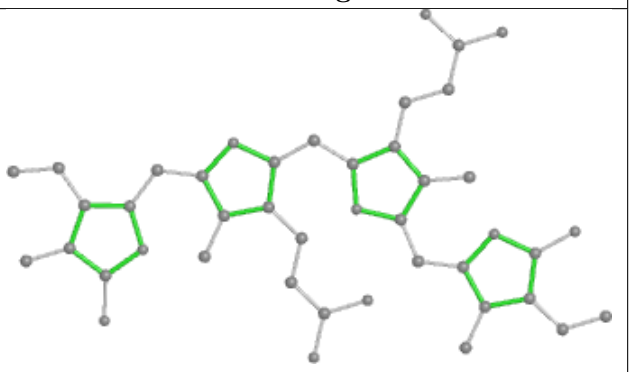


Bond angles

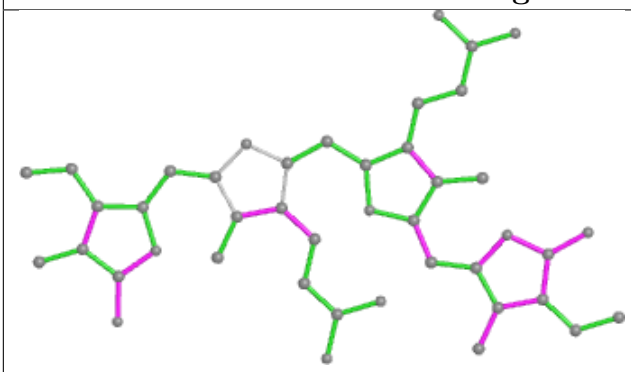


Torsions

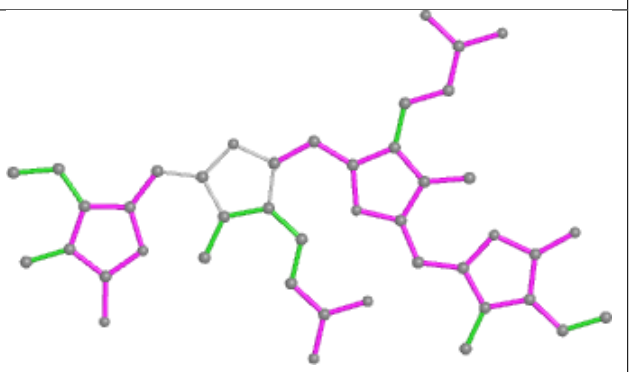


Rings

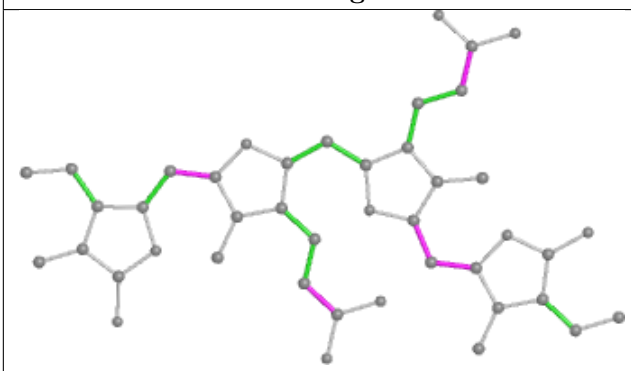
Ligand CYC aH 201



Bond lengths



Bond angles



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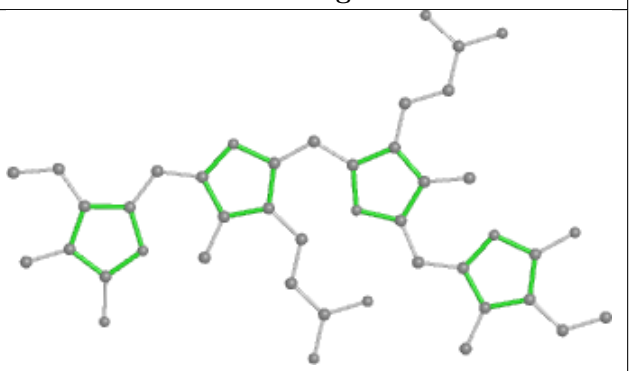
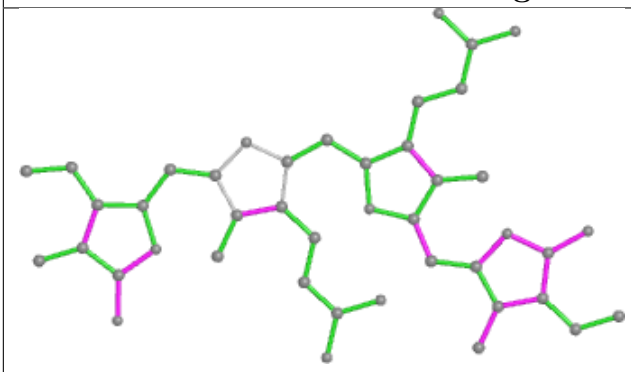


Rings

Ligand CYC eR 201



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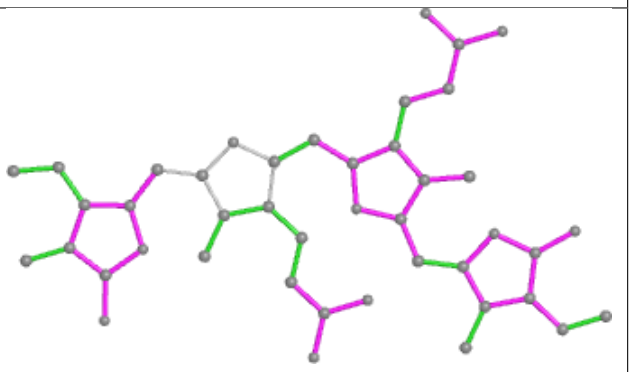
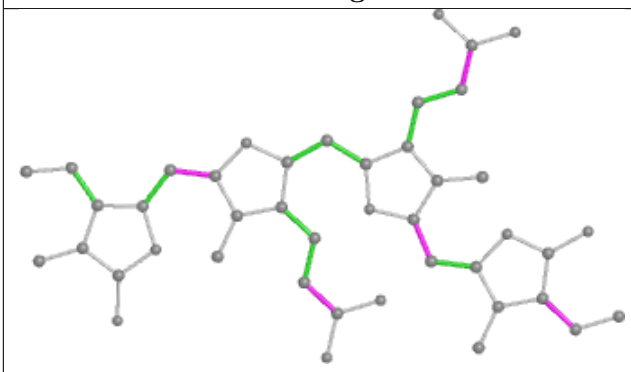
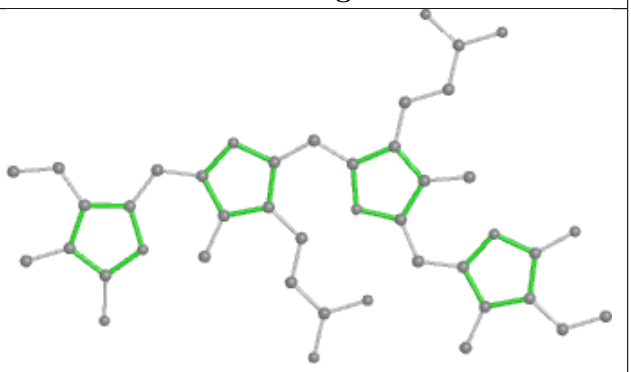


Bond angles

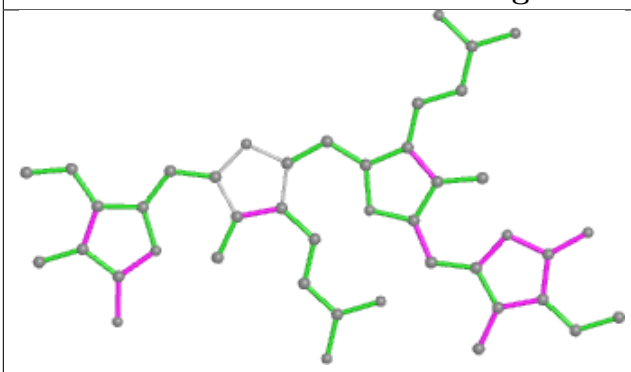


Torsions

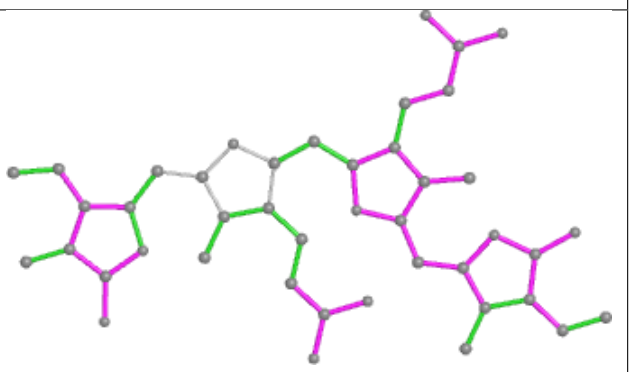


Rings

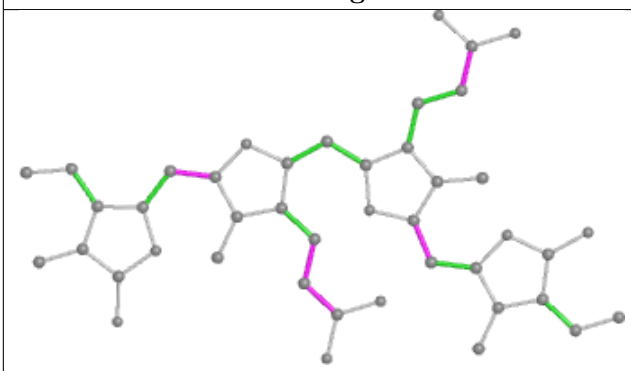
Ligand CYC dC 201



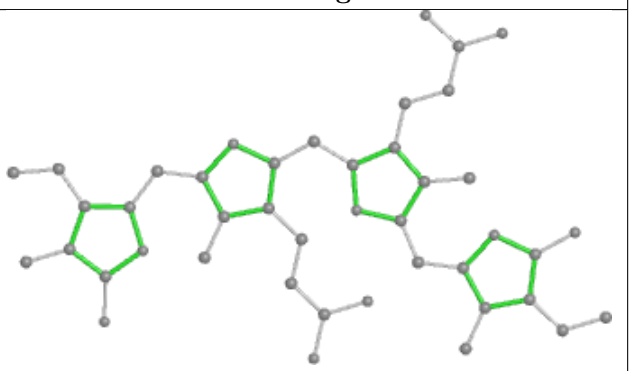
Bond lengths



Bond angles

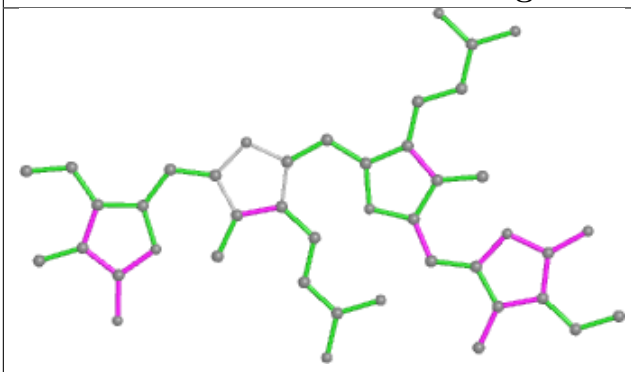


Torsions

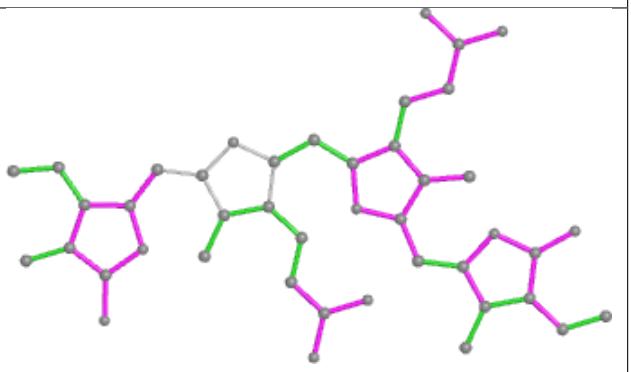


Rings

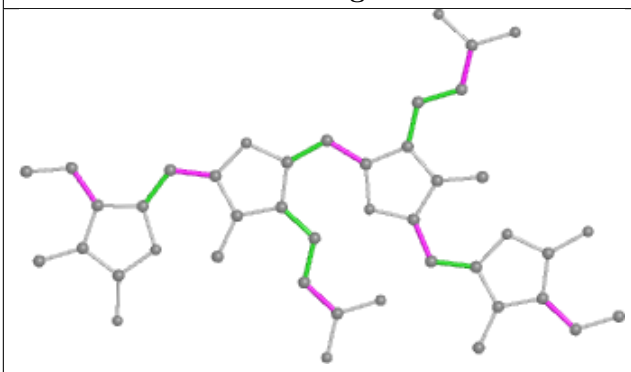
Ligand CYC cF 201



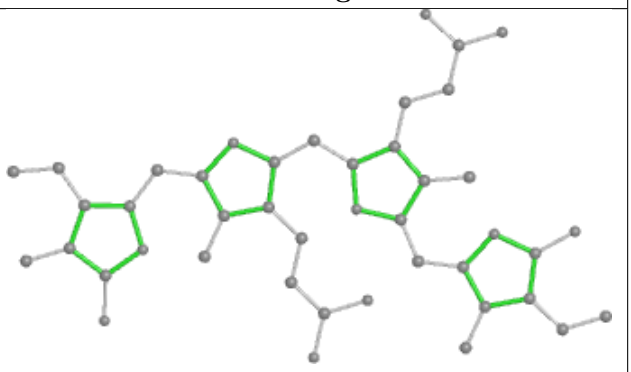
Bond lengths



Bond angles

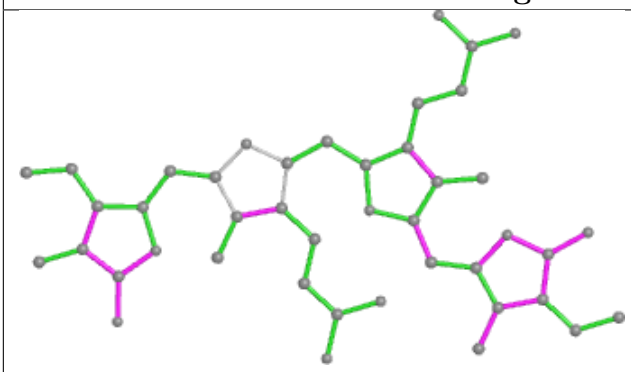


Torsions



Rings

Ligand CYC aB 201



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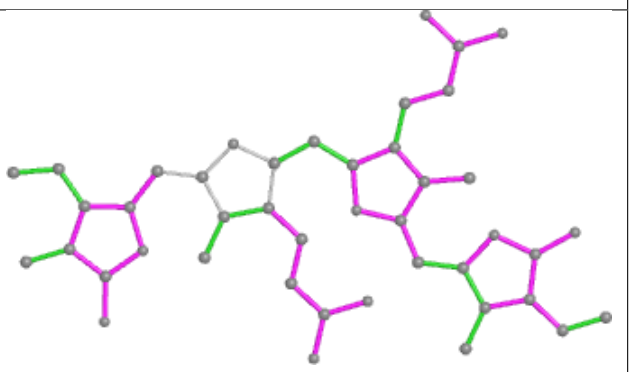
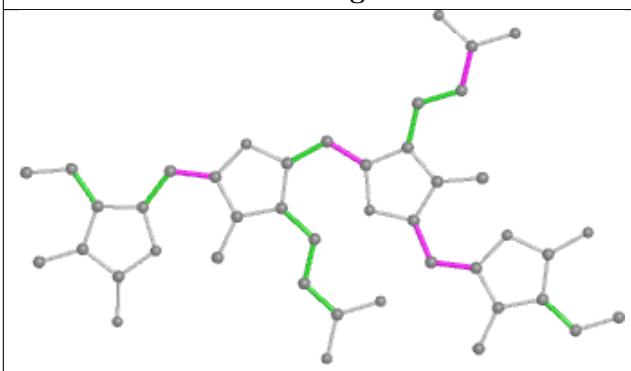
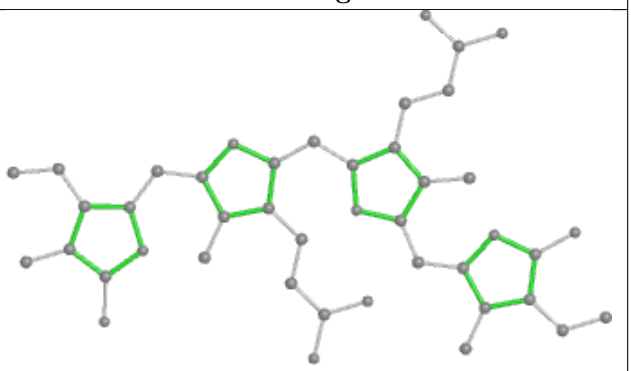


Bond angles

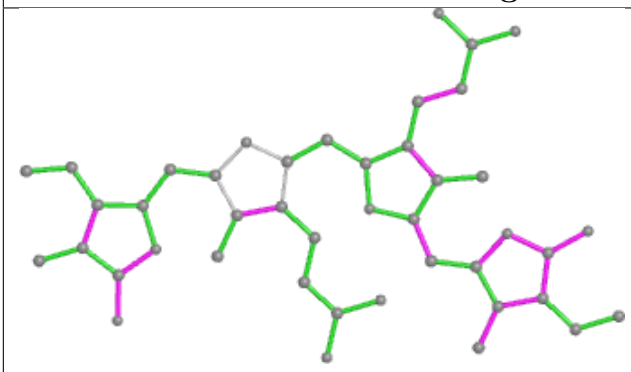


Torsions



Rings

Ligand CYC aM 1201



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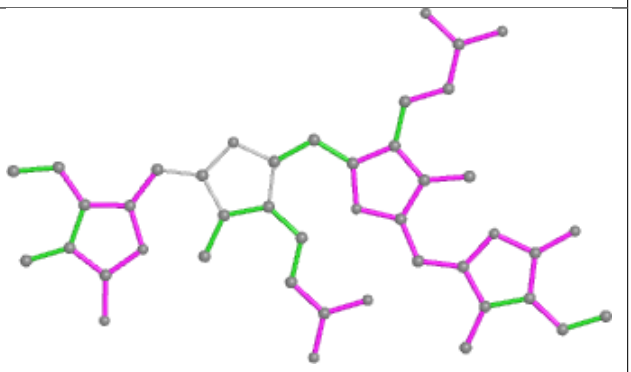
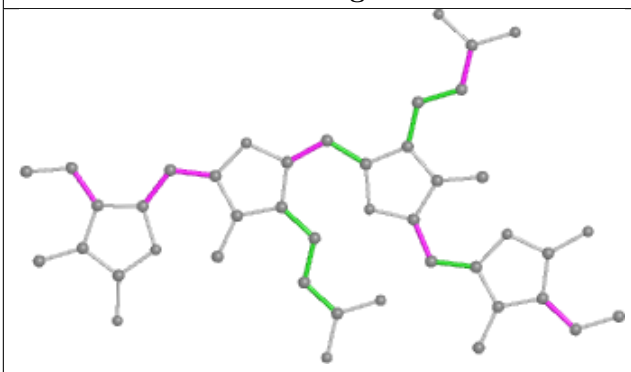


Bond angles



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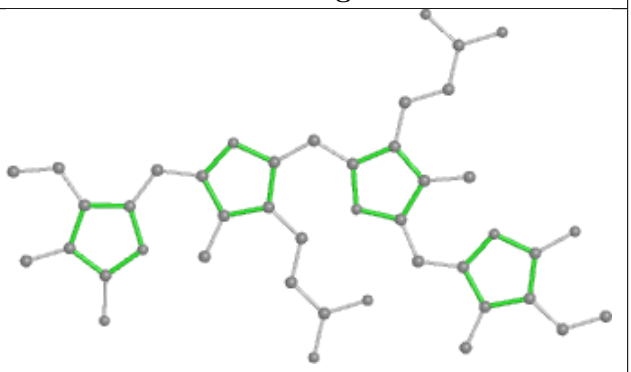
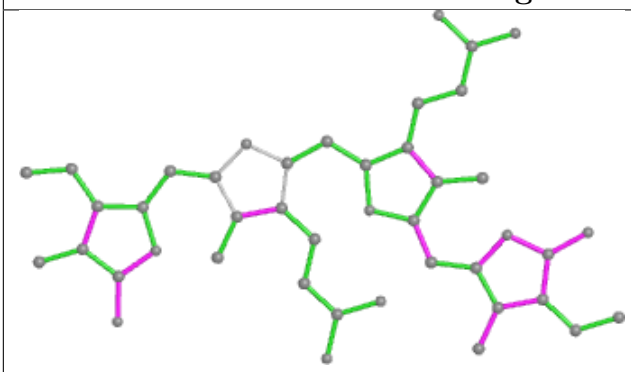


Rings

Ligand CYC bS 201



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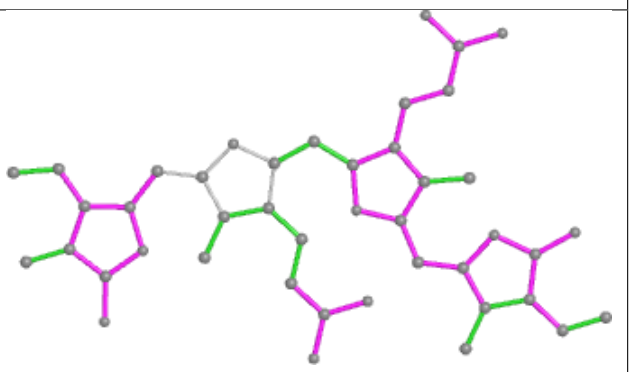

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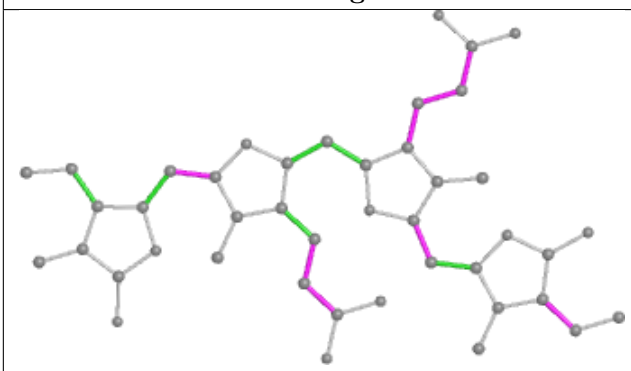

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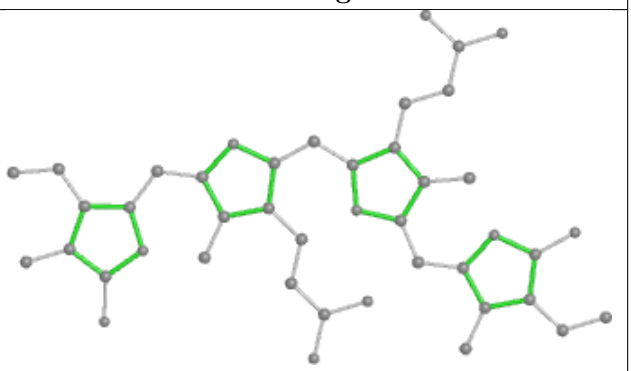
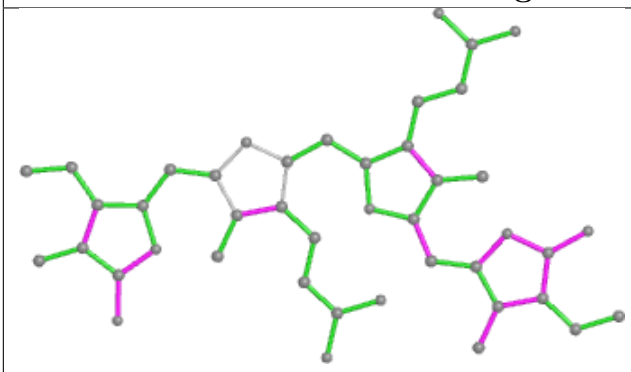


Rings

Ligand CYC eP 201



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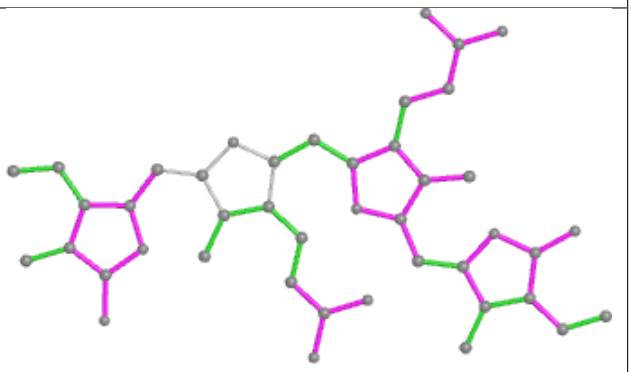

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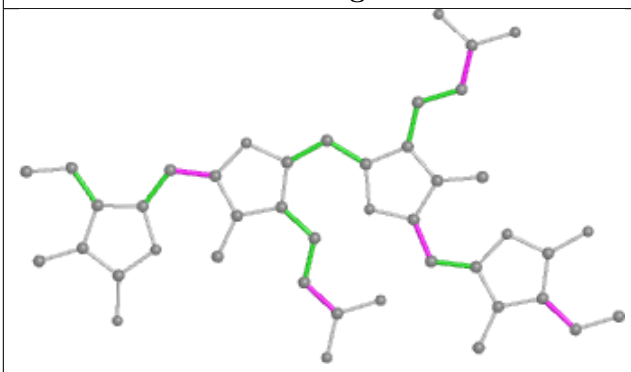

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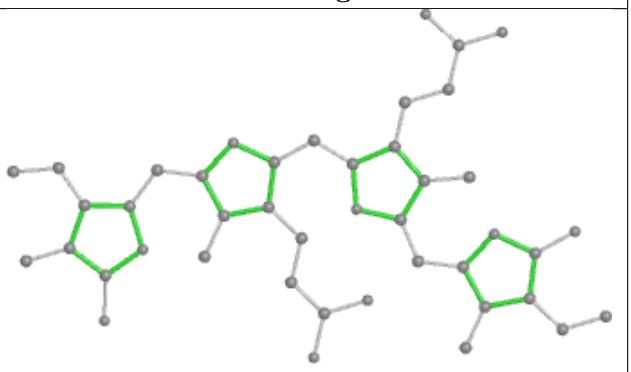
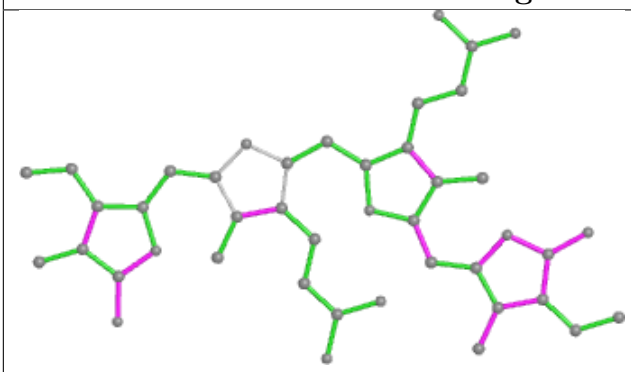
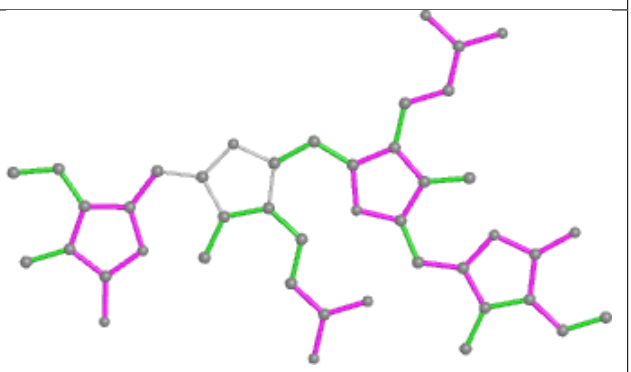


Rings

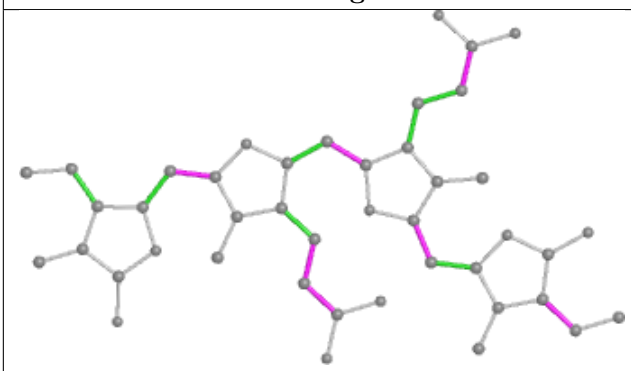
Ligand CYC aF 201



Bond lengths



Bond angles



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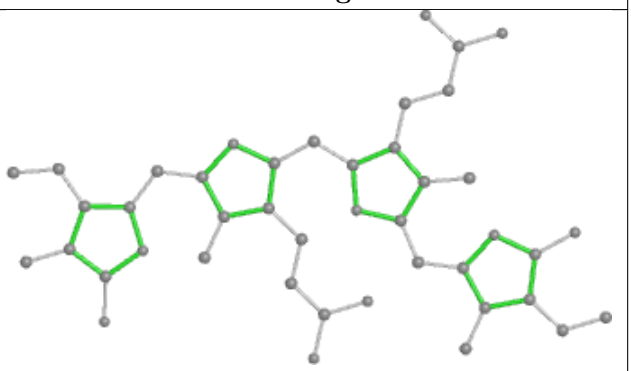
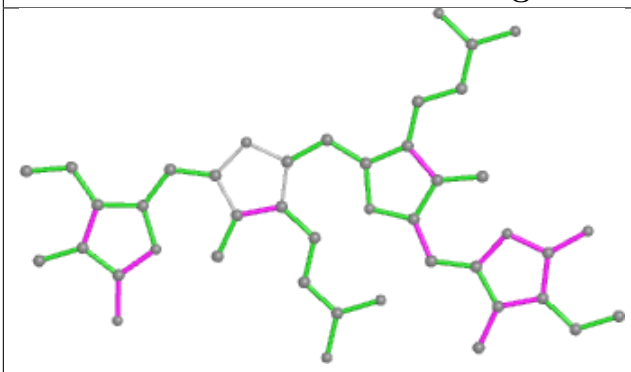


Rings

Ligand CYC aG 201



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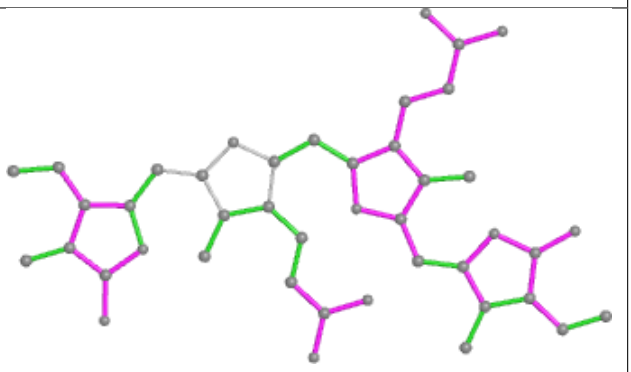
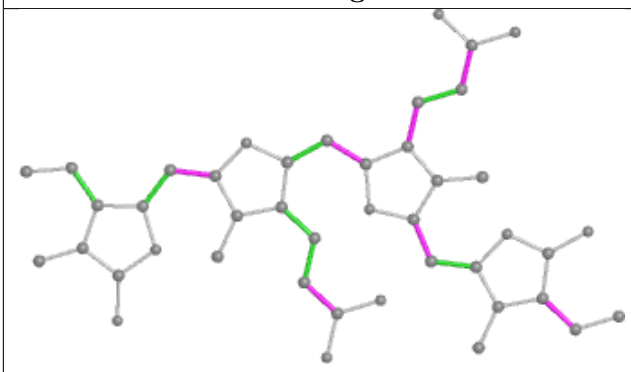


Bond angles



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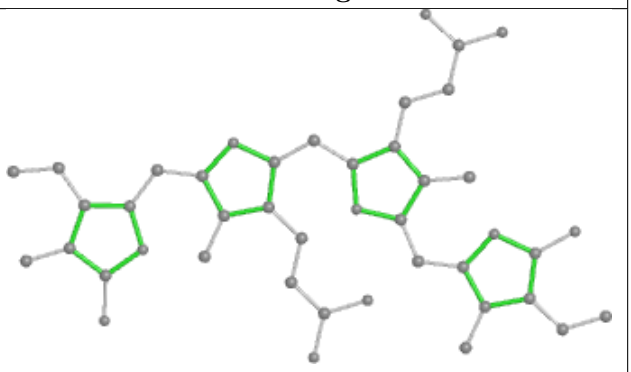
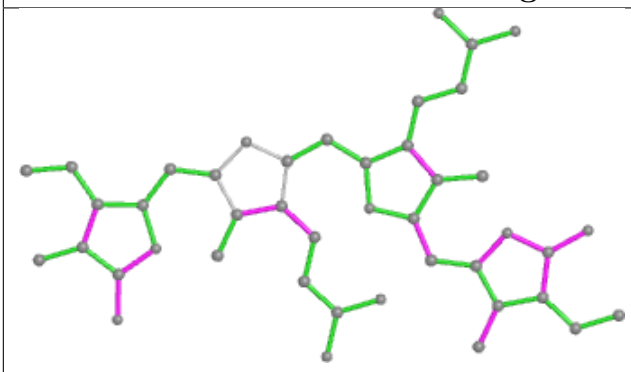


Rings

Ligand CYC aI 201



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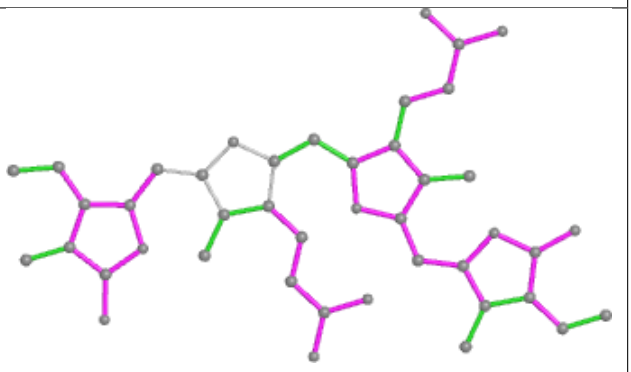
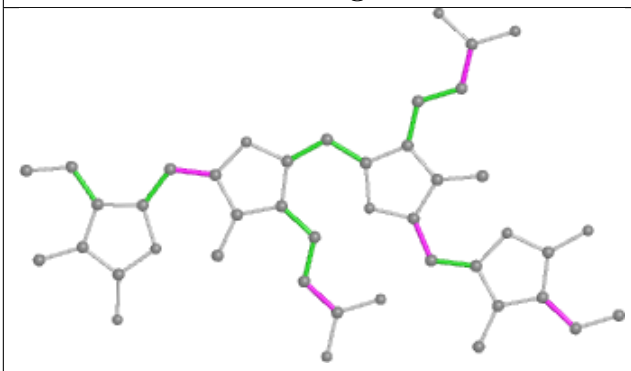


Bond angles



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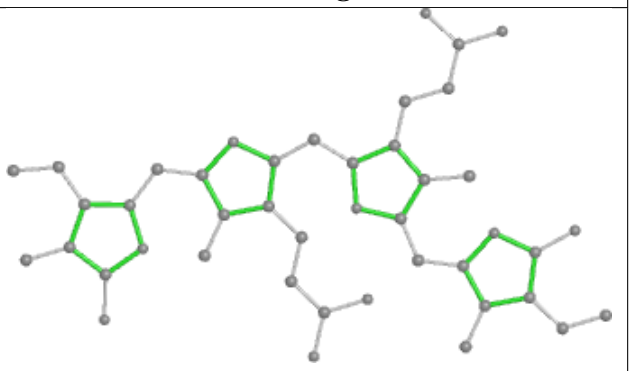
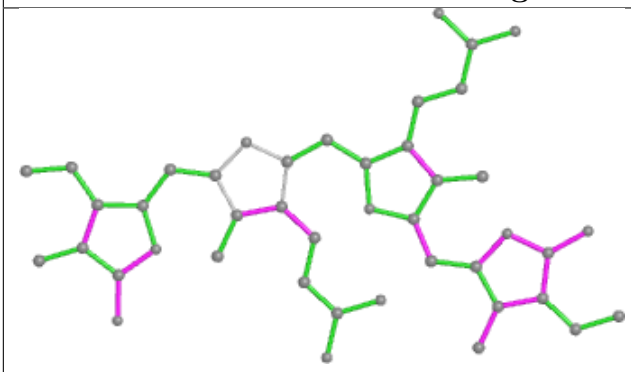


Rings

Ligand CYC dK 201



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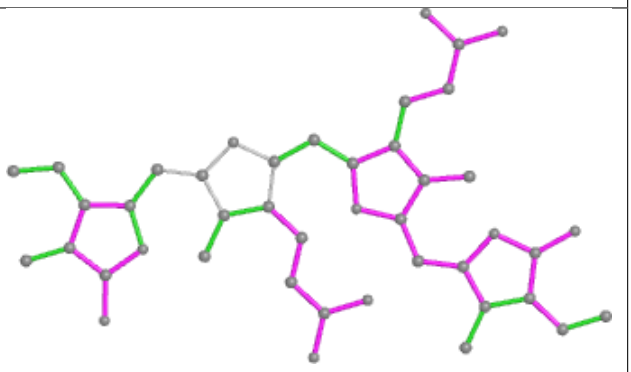
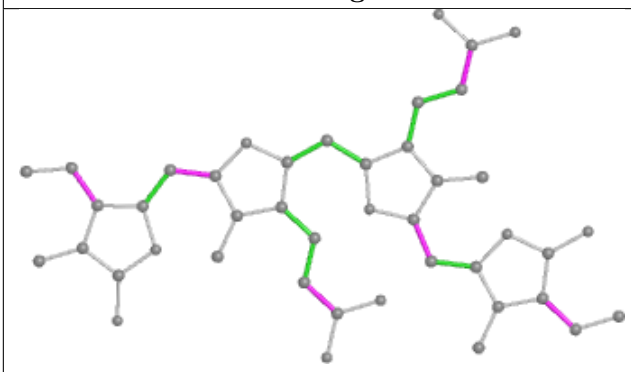


Bond angles



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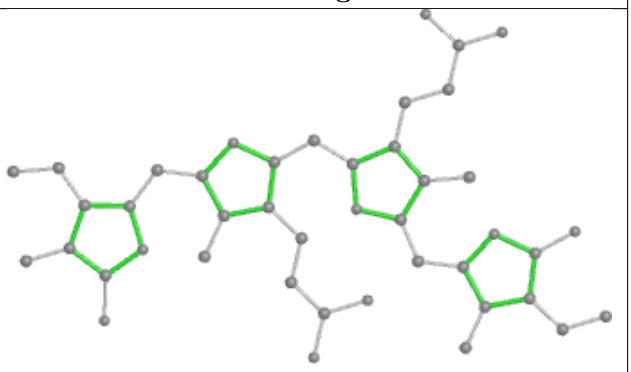
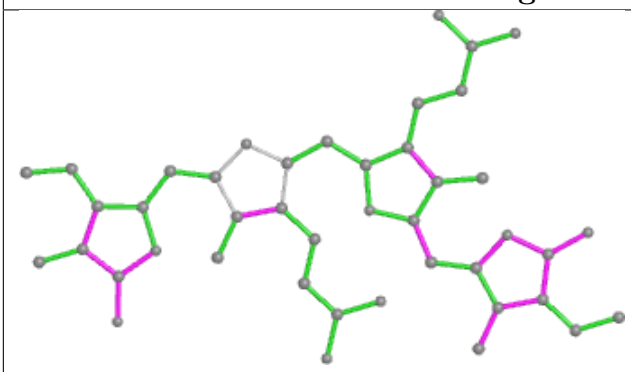


Rings

Ligand CYC fF 201



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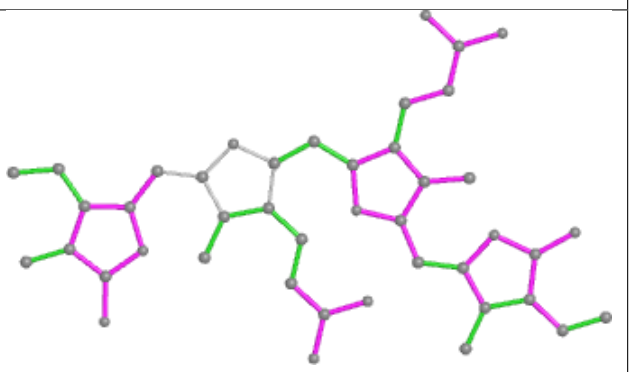
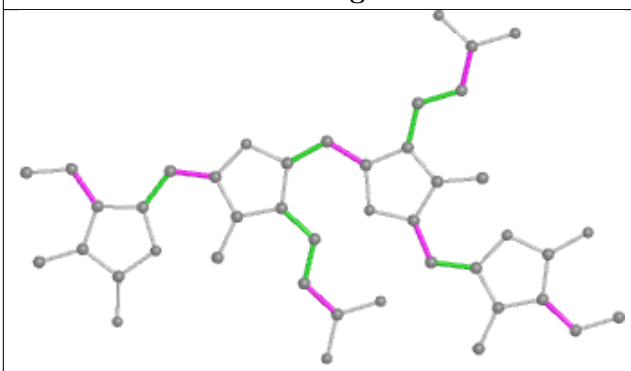


Bond angles



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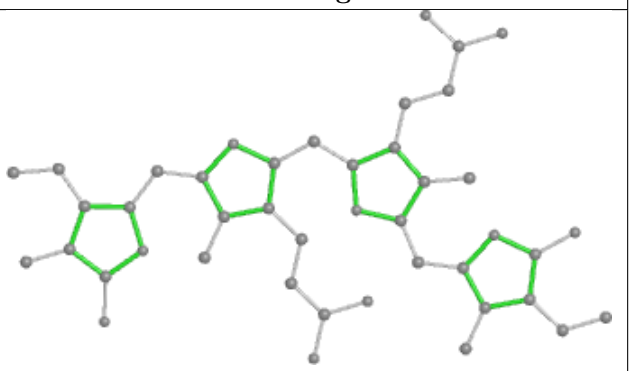
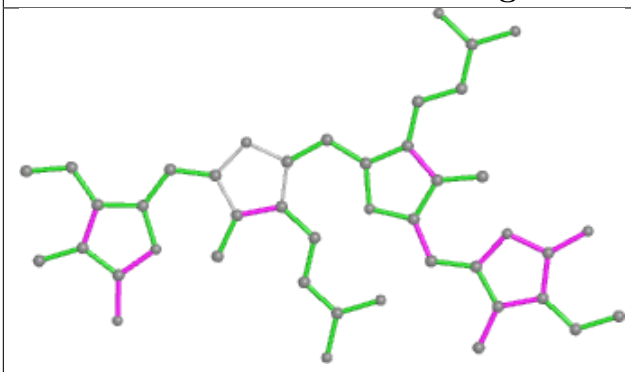


Rings

Ligand CYC dM 1201



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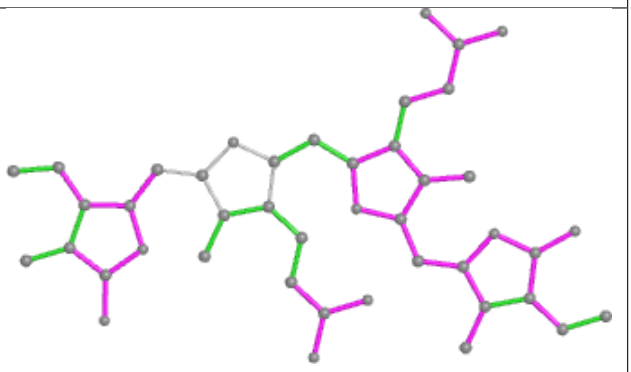
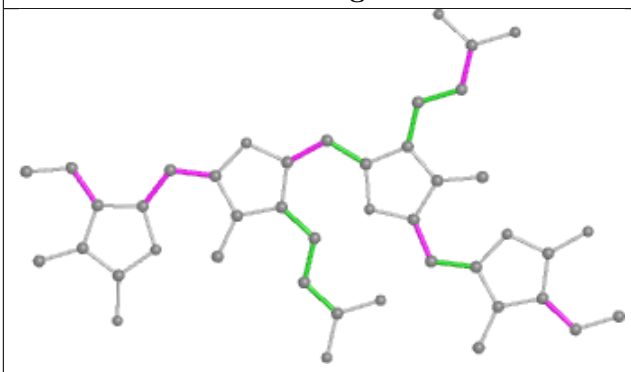
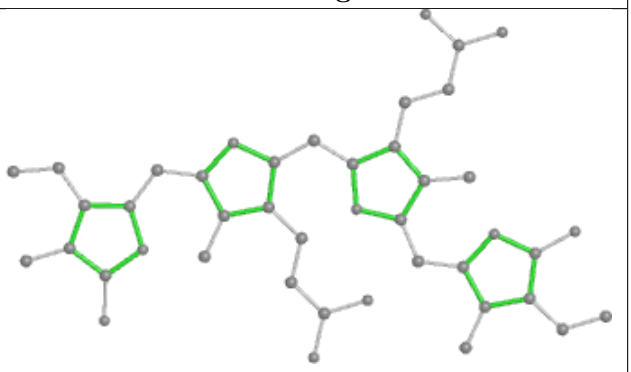


Bond angles

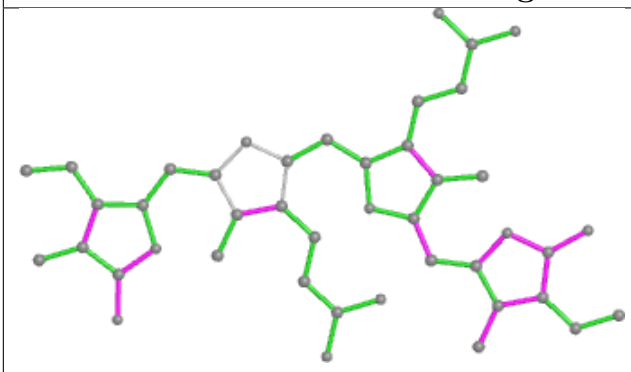


Torsions



Rings

Ligand CYC eS 201



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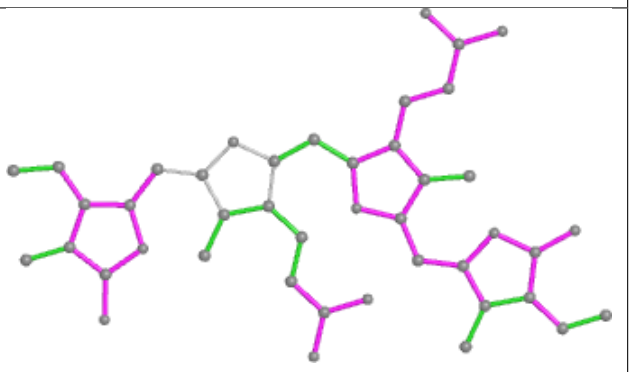
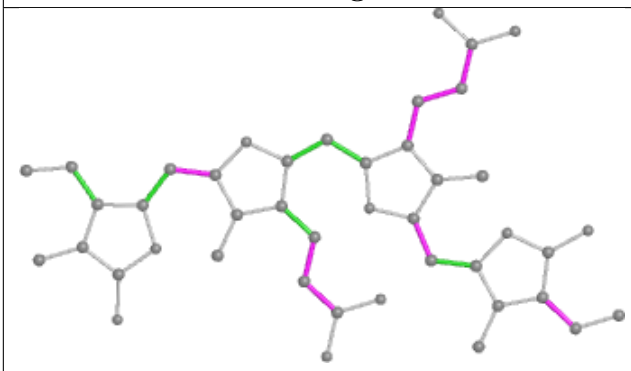
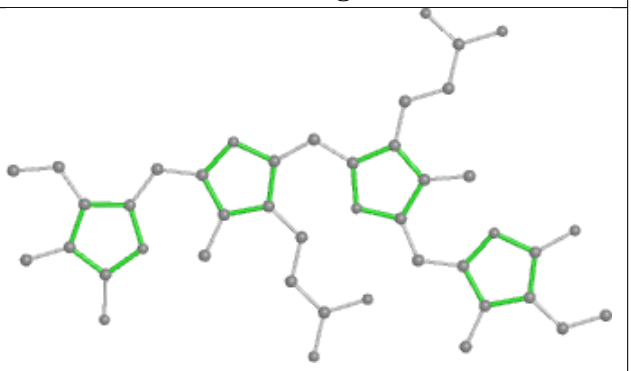


Bond angles

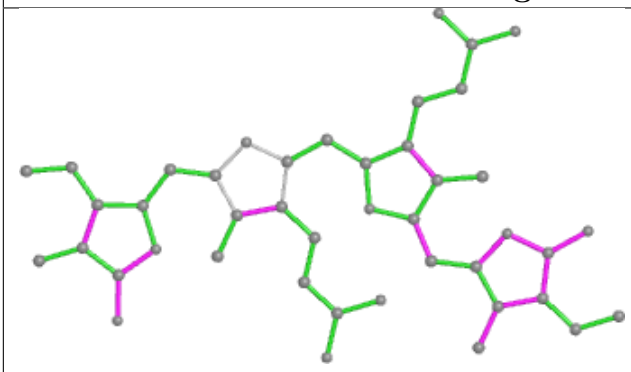


Torsions



Rings

Ligand CYC dF 201



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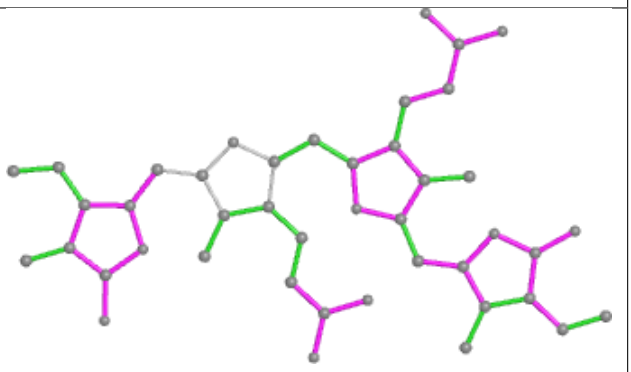
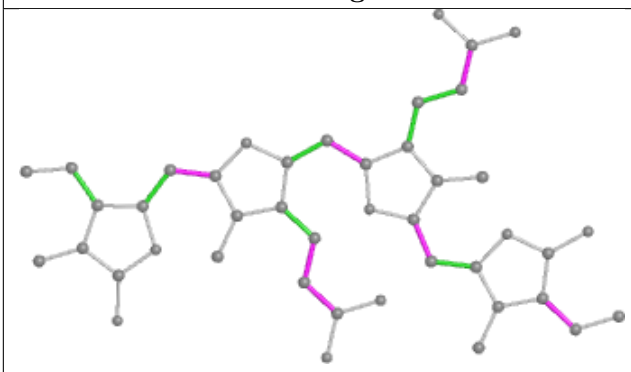


Bond angles



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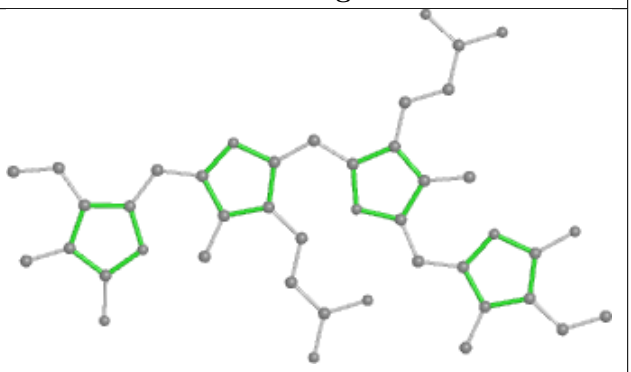
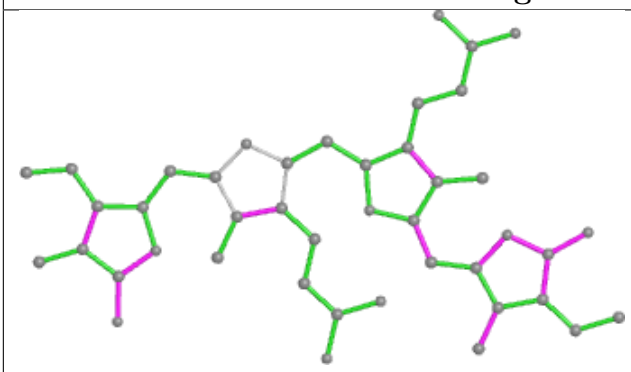


Rings

Ligand CYC aP 201



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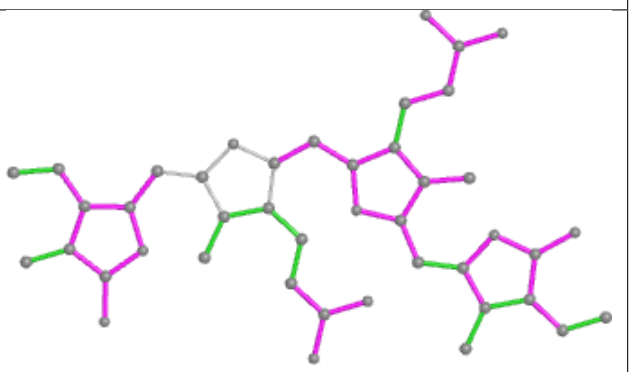
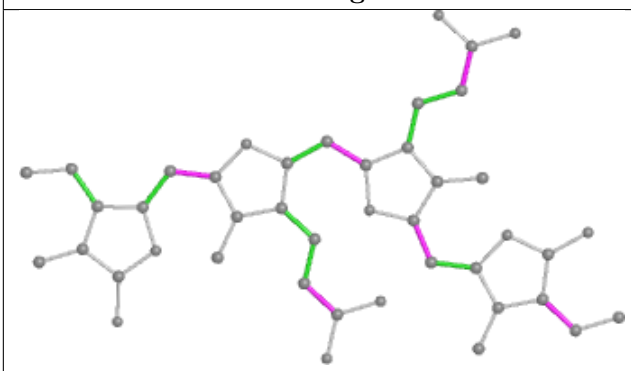
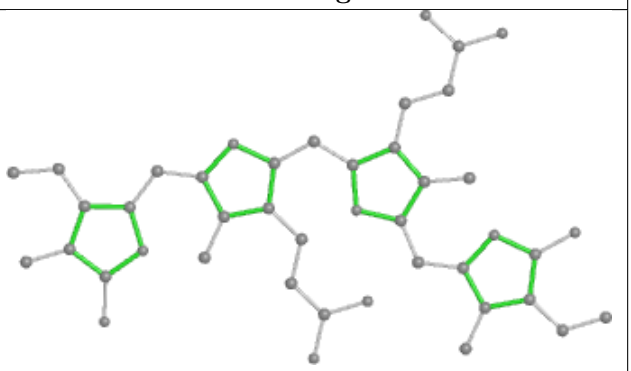


Bond angles

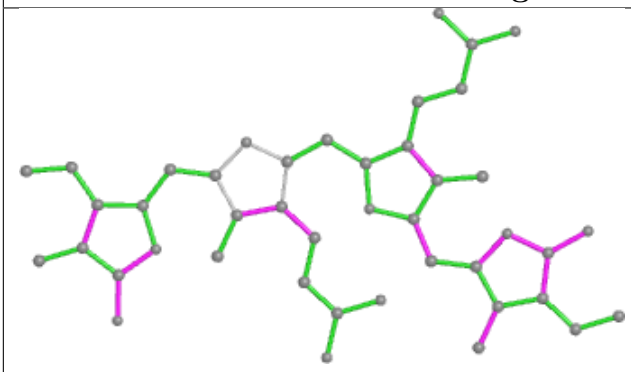


Torsions

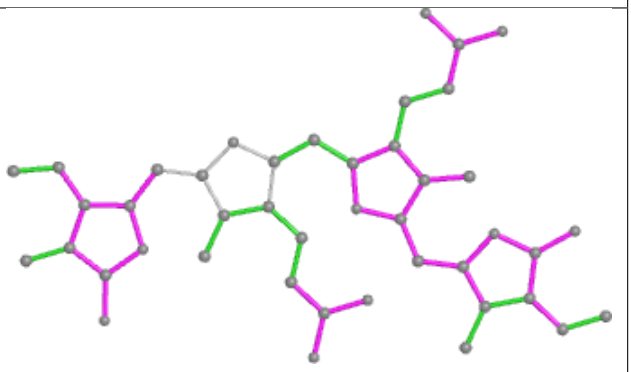


Rings

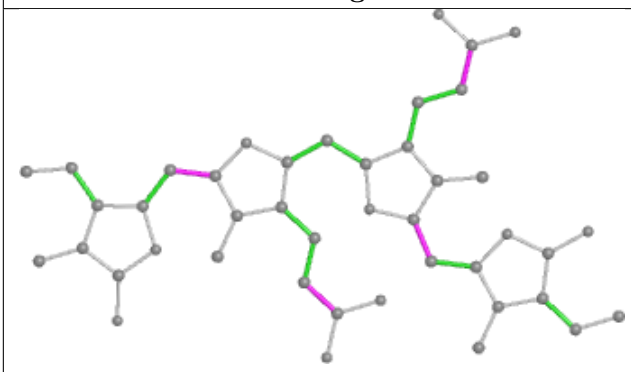
Ligand CYC bO 201



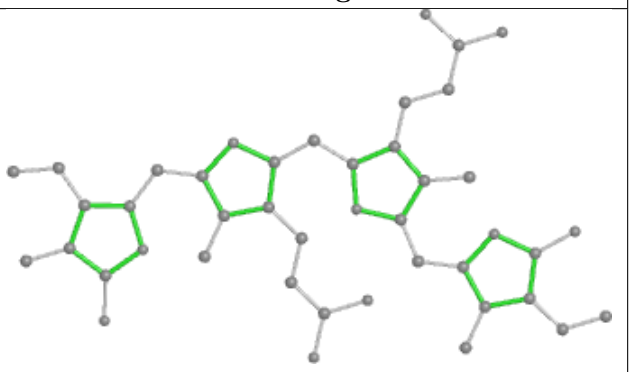
Bond lengths



Bond angles

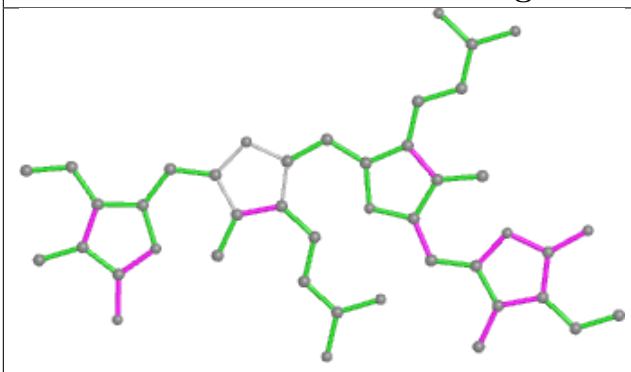


Torsions

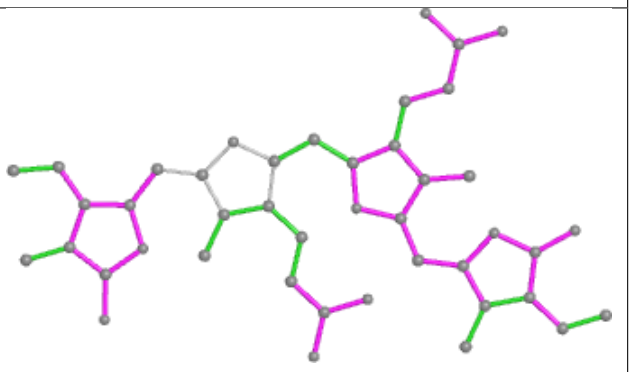


Rings

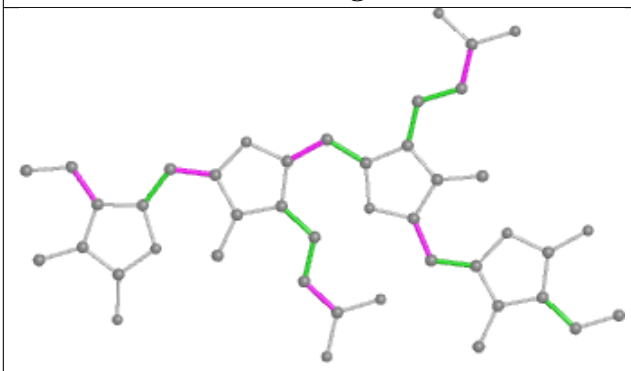
Ligand CYC aE 201



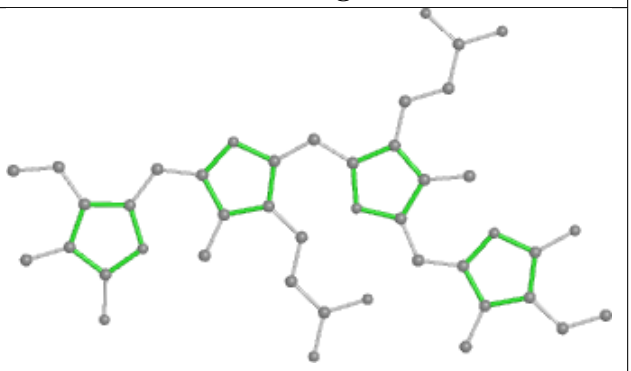
Bond lengths



Bond angles

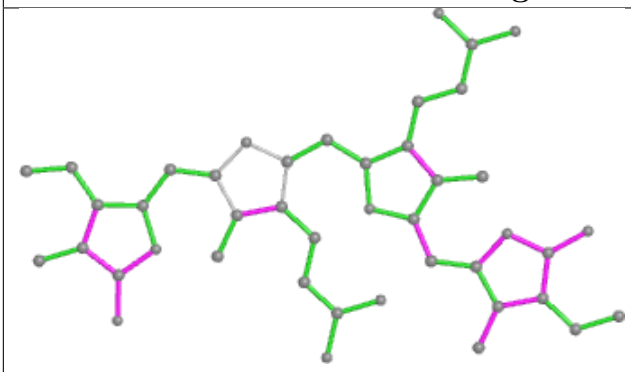


Torsions

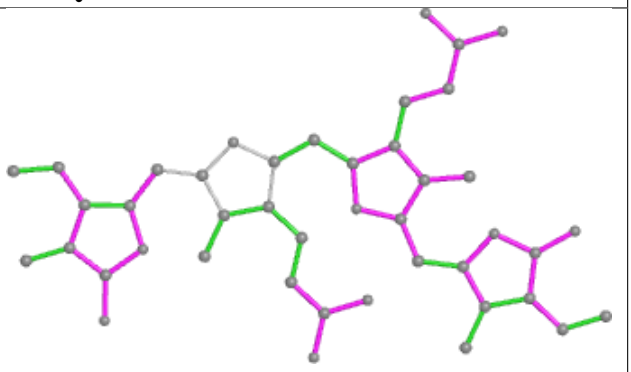


Rings

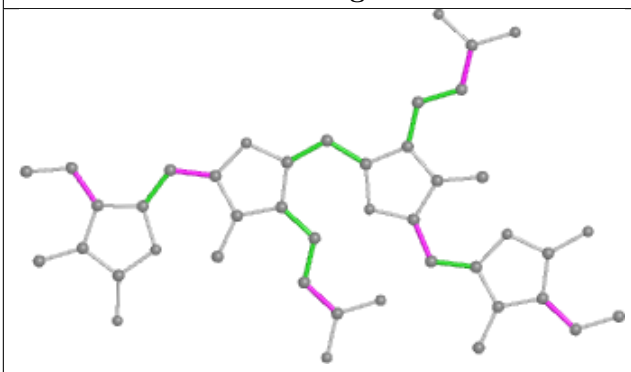
Ligand CYC bQ 201



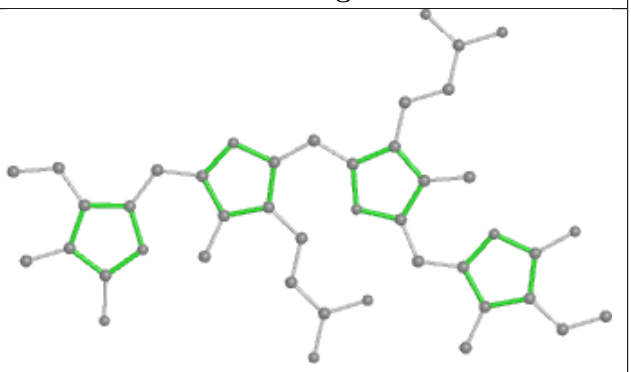
Bond lengths



Bond angles

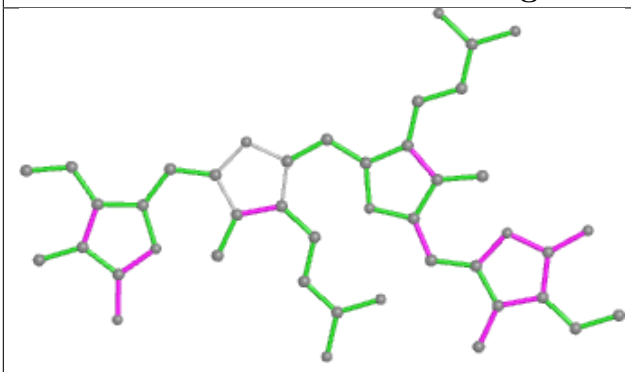


Torsions

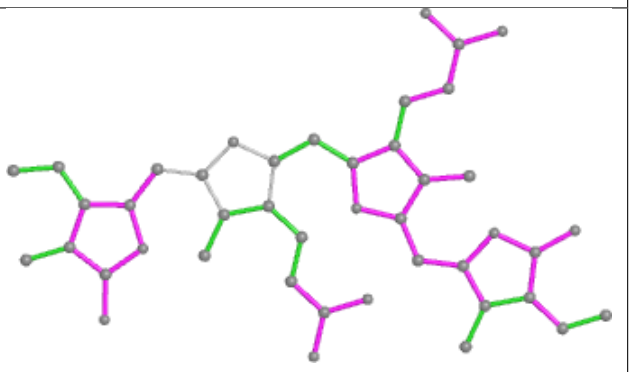


Rings

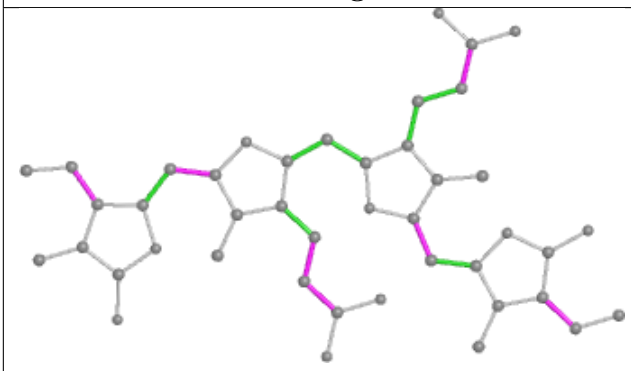
Ligand CYC cI 201



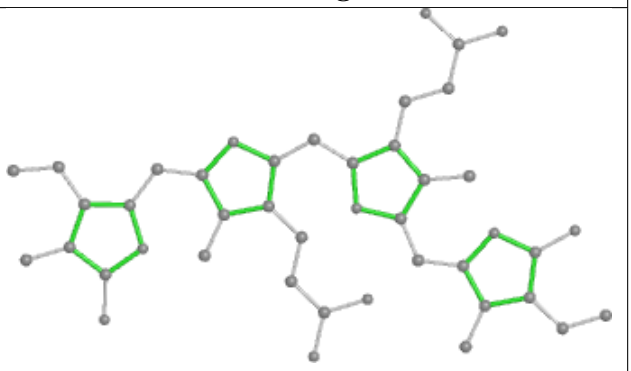
Bond lengths



Bond angles

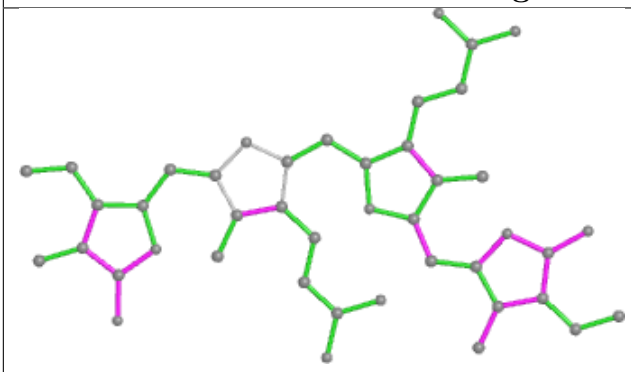


Torsions

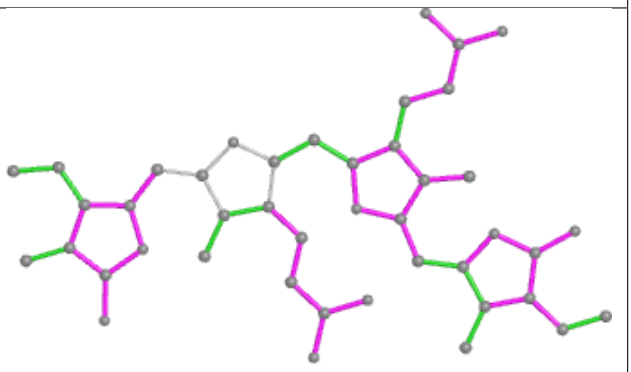


Rings

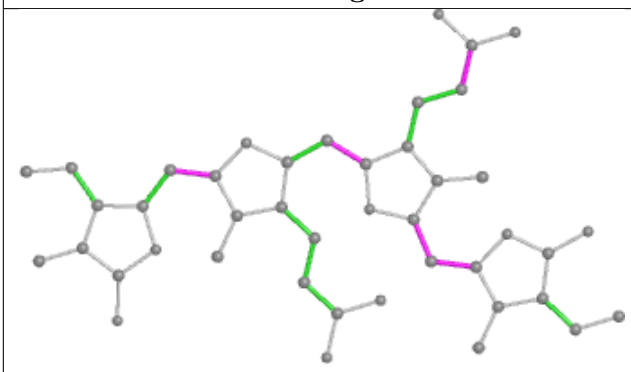
Ligand CYC dB 201



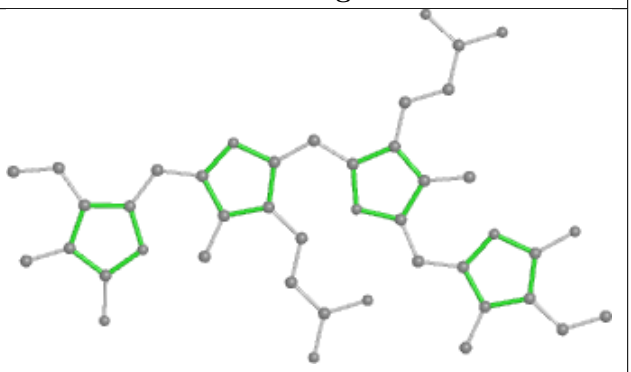
Bond lengths



Bond angles

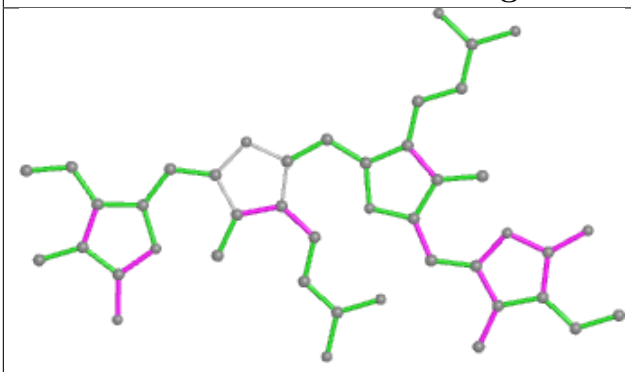


Torsions

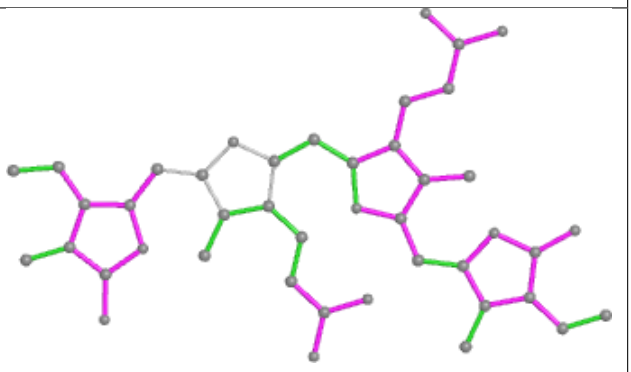


Rings

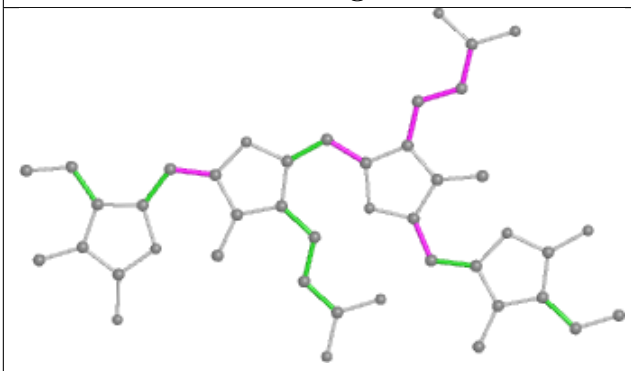
Ligand CYC aM 1204



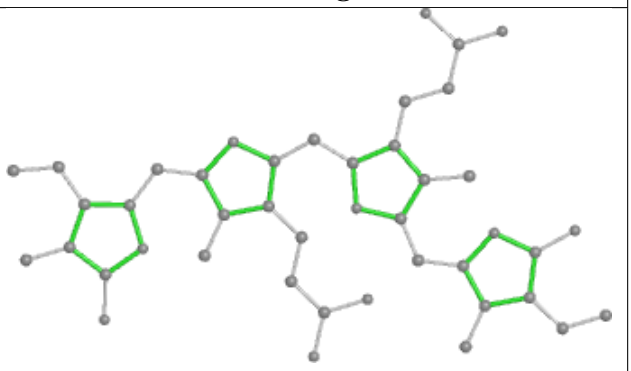
Bond lengths



Bond angles

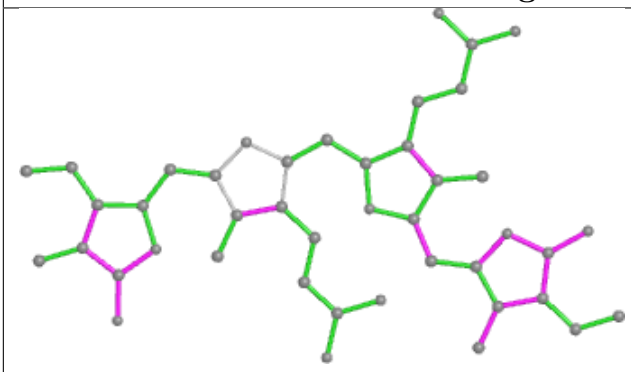


Torsions

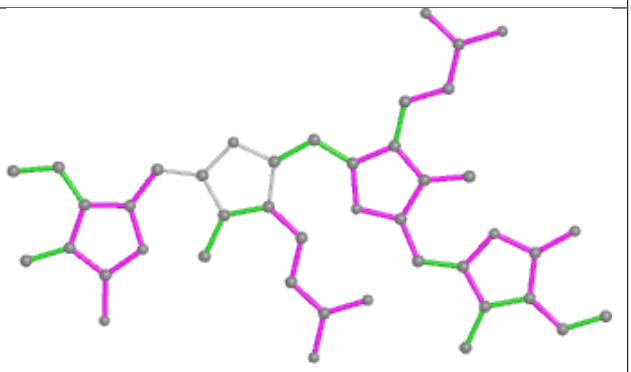


Rings

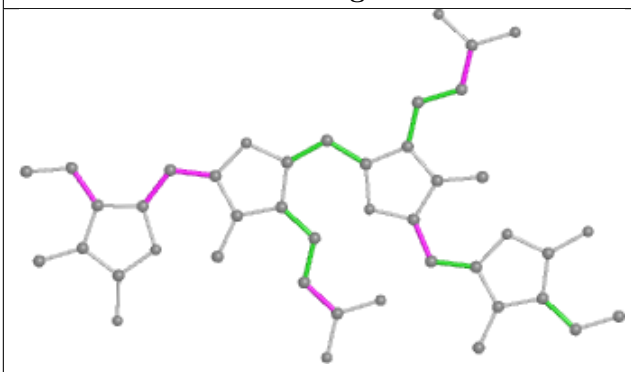
Ligand CYC fF 202



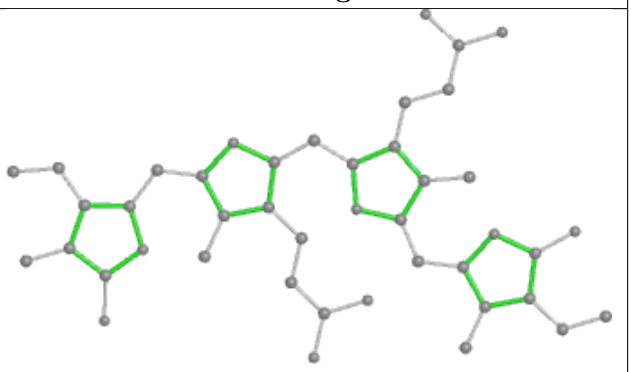
Bond lengths



Bond angles

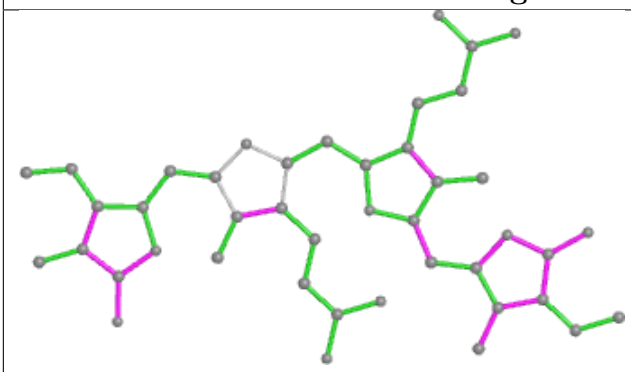


Torsions

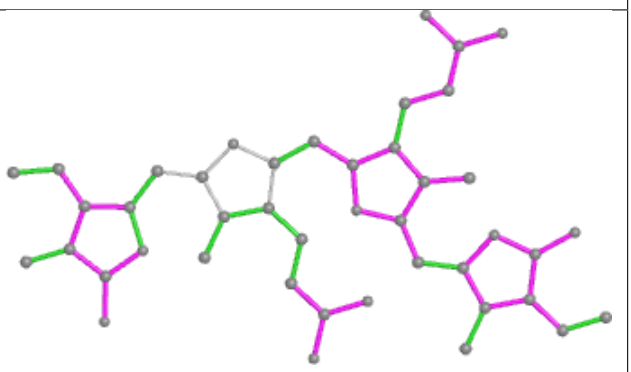


Rings

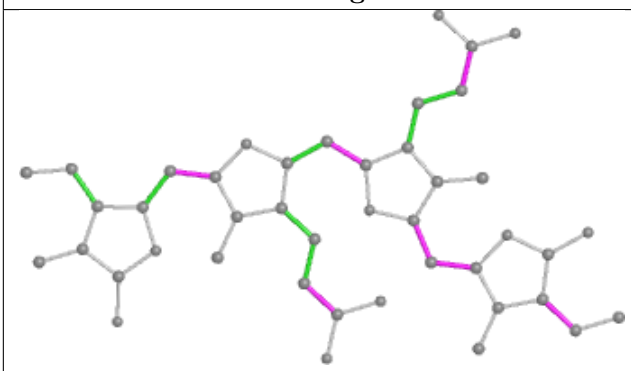
Ligand CYC cM 101



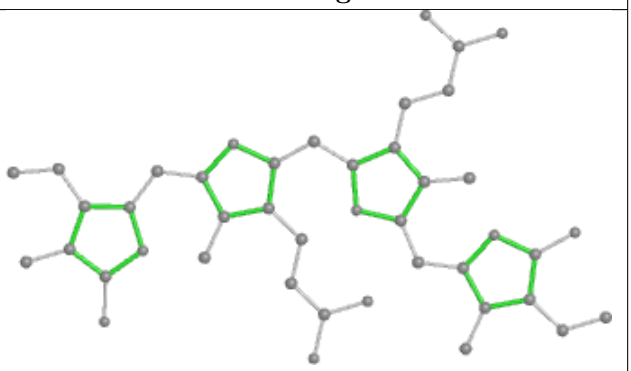
Bond lengths



Bond angles

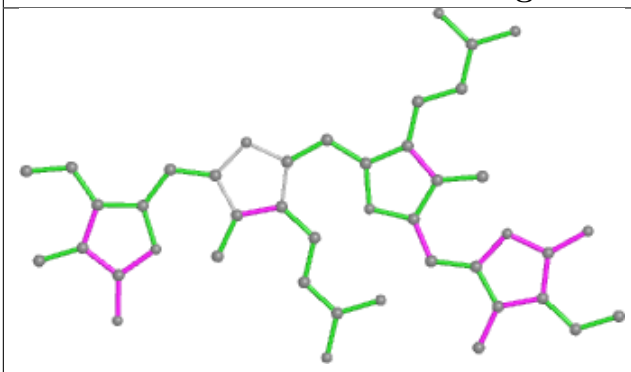


Torsions

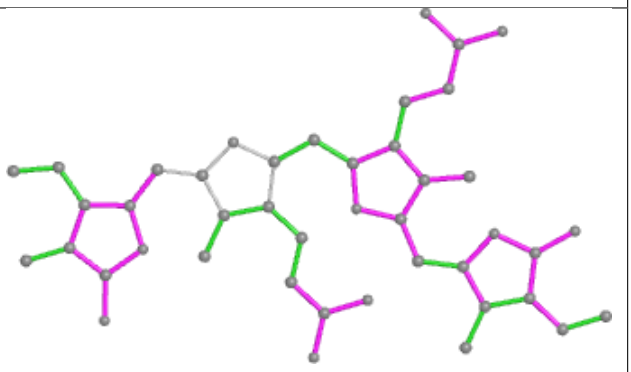


Rings

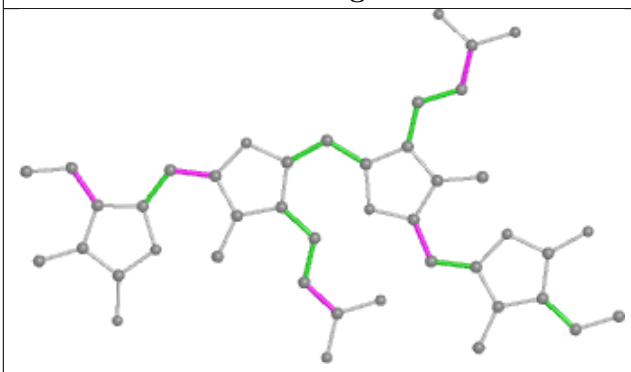
Ligand CYC fD 201



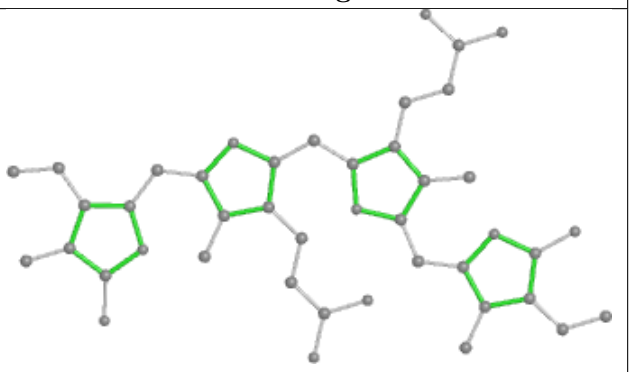
Bond lengths



Bond angles

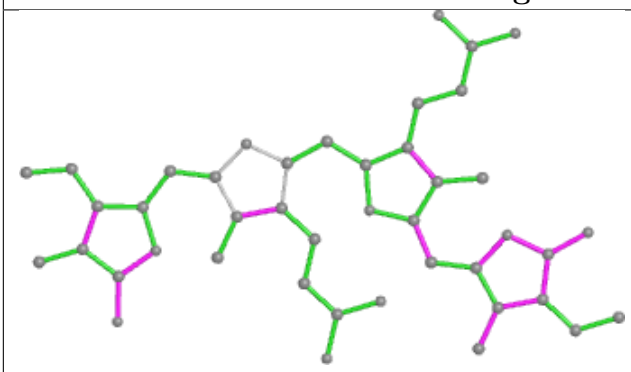


Torsions

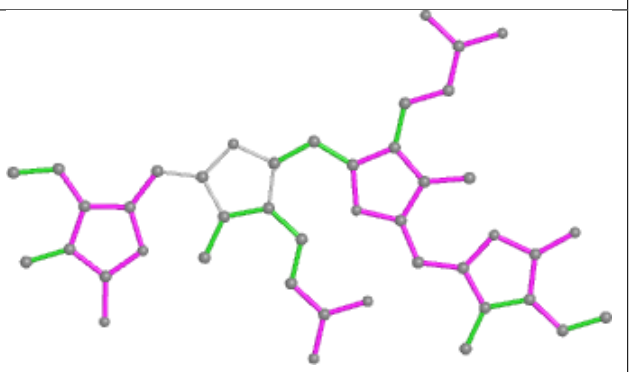


Rings

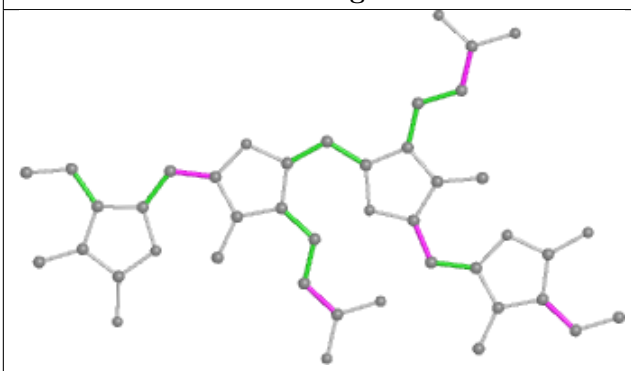
Ligand CYC eU 201



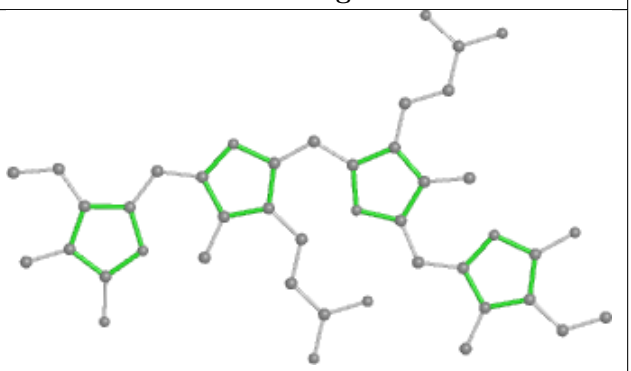
Bond lengths



Bond angles

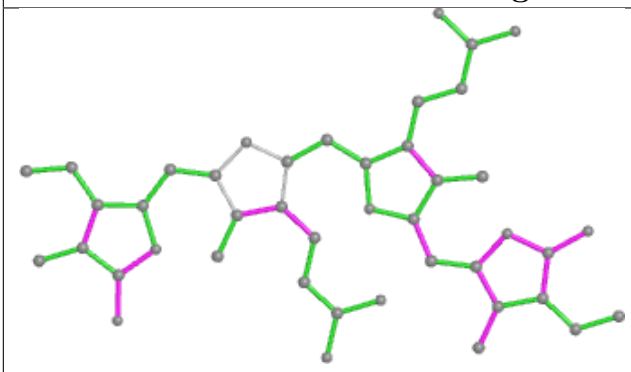


Torsions

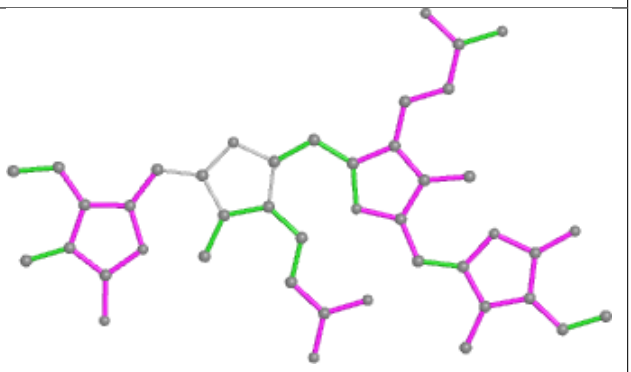


Rings

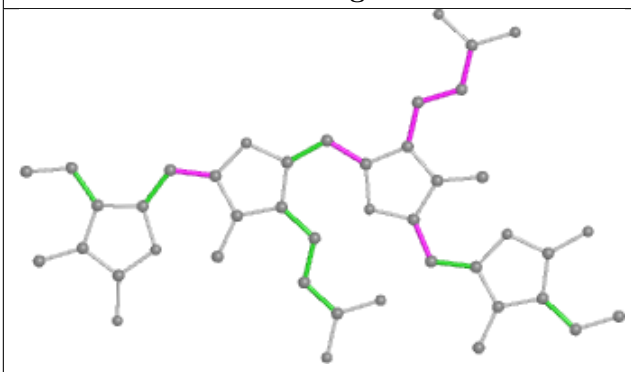
Ligand CYC dR 201



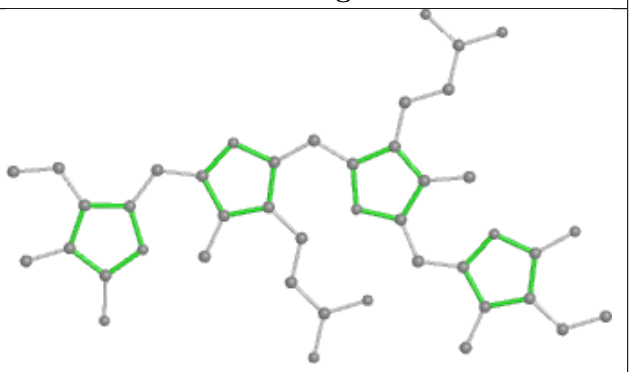
Bond lengths



Bond angles

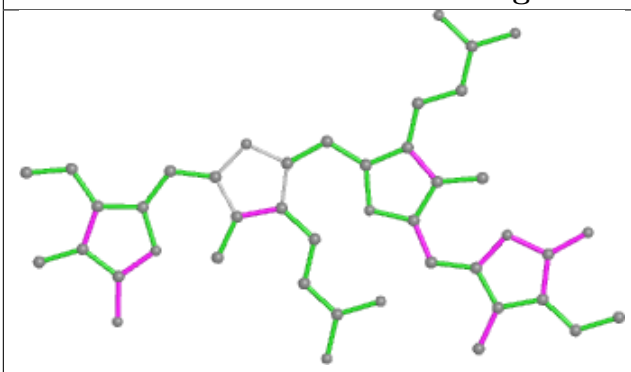


Torsions

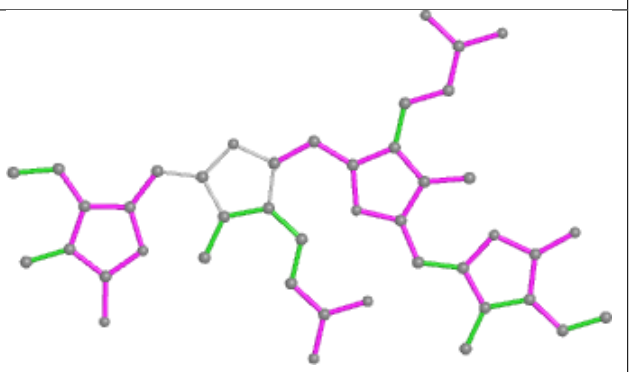


Rings

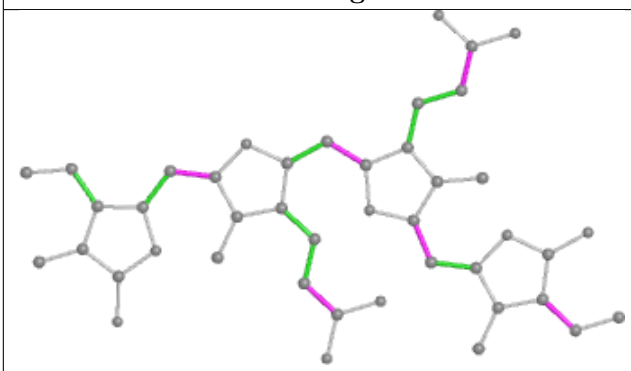
Ligand CYC dP 201



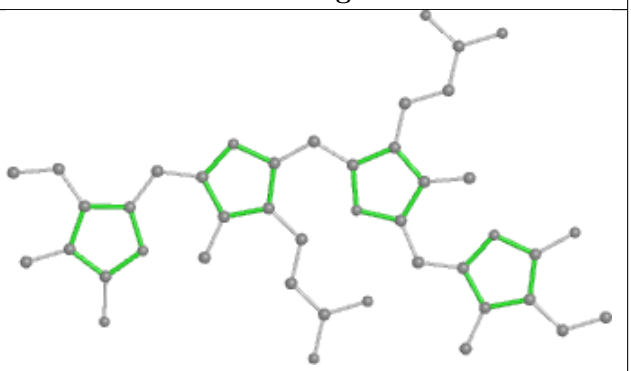
Bond lengths



Bond angles

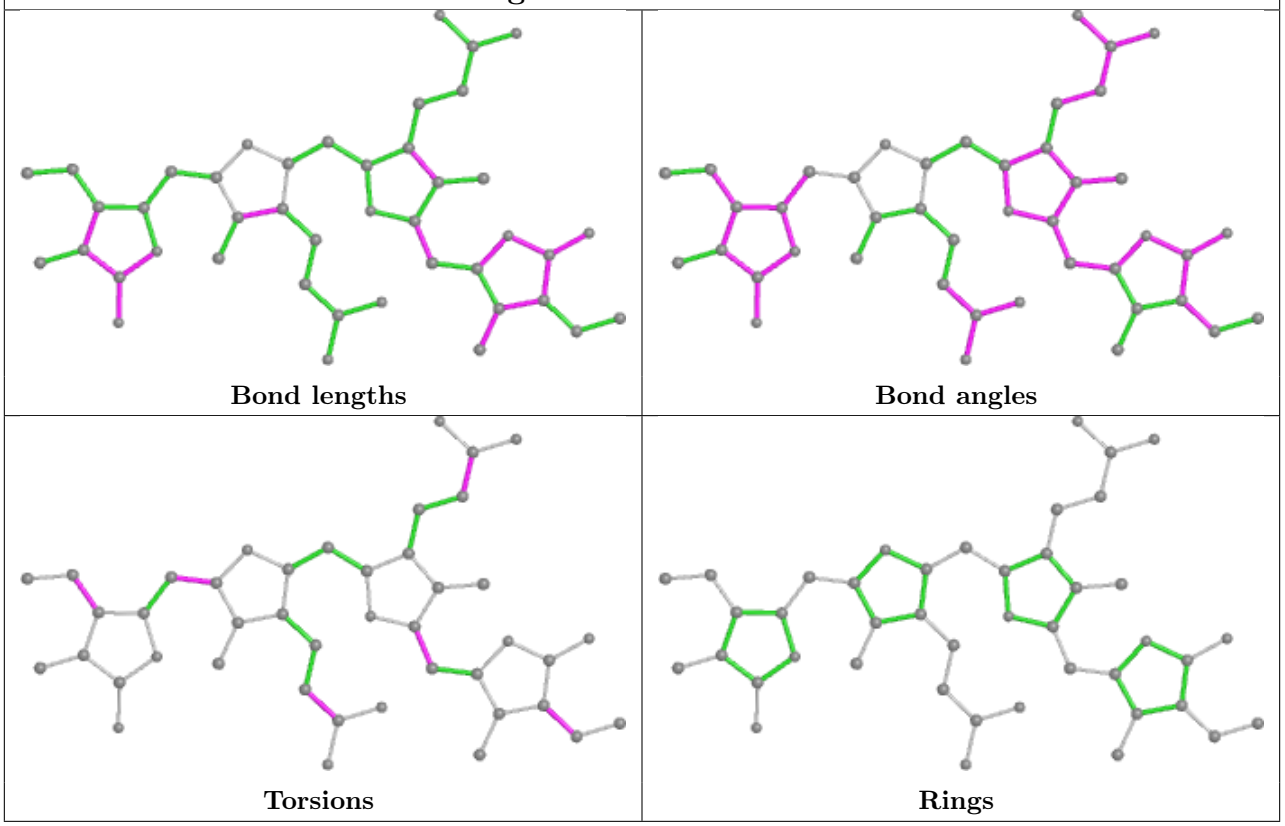


Torsions



Rings

Ligand CYC bW 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

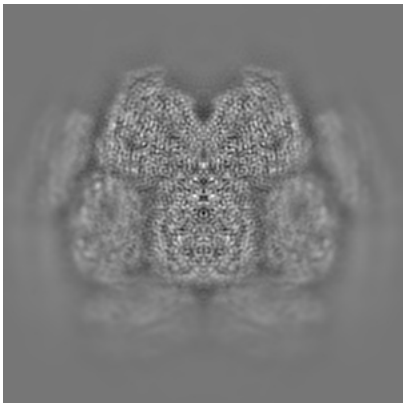
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31944. These allow visual inspection of the internal detail of the map and identification of artifacts.

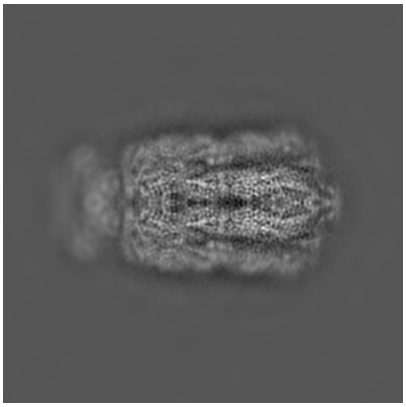
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

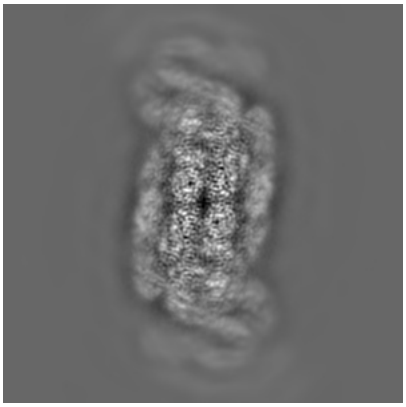
6.1.1 Primary map



X



Y

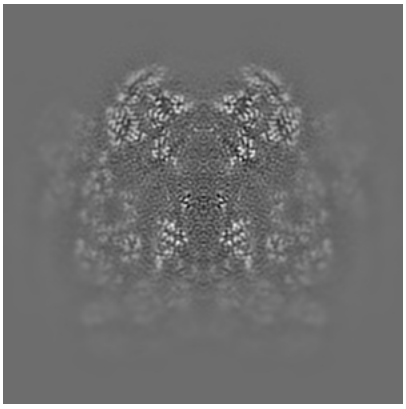


Z

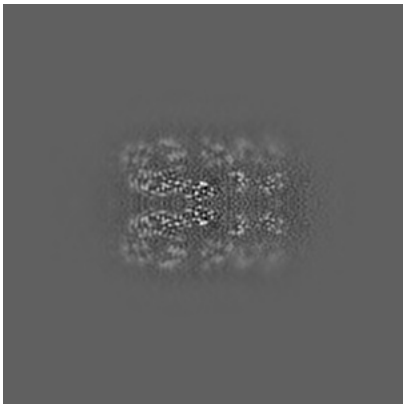
The images above show the map projected in three orthogonal directions.

6.2 Central slices

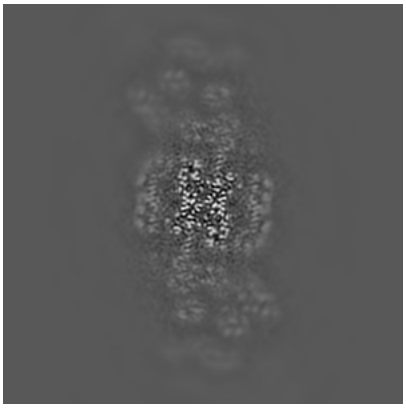
6.2.1 Primary map



X Index: 150



Y Index: 150

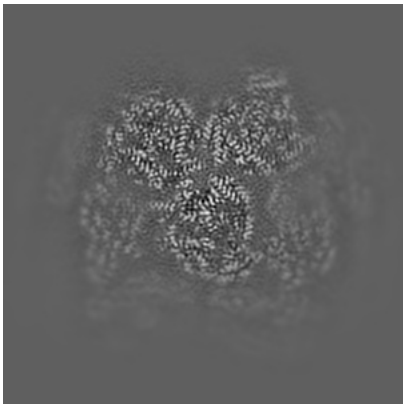


Z Index: 150

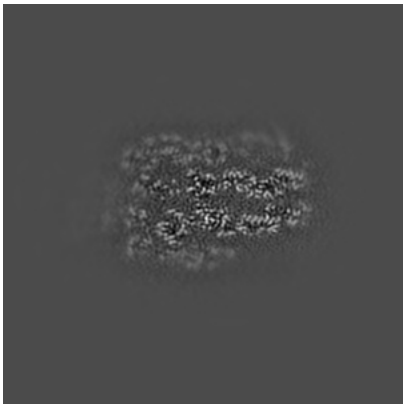
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

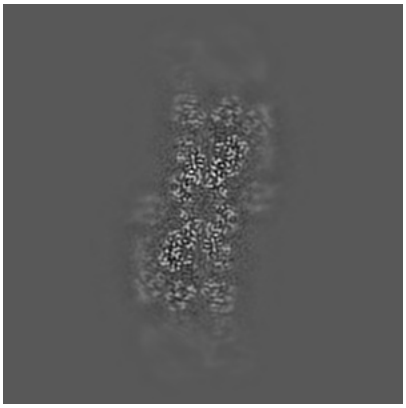
6.3.1 Primary map



X Index: 138



Y Index: 160



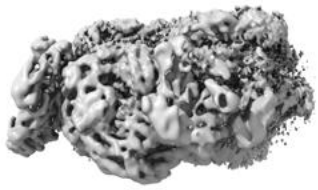
Z Index: 194

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.00612. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

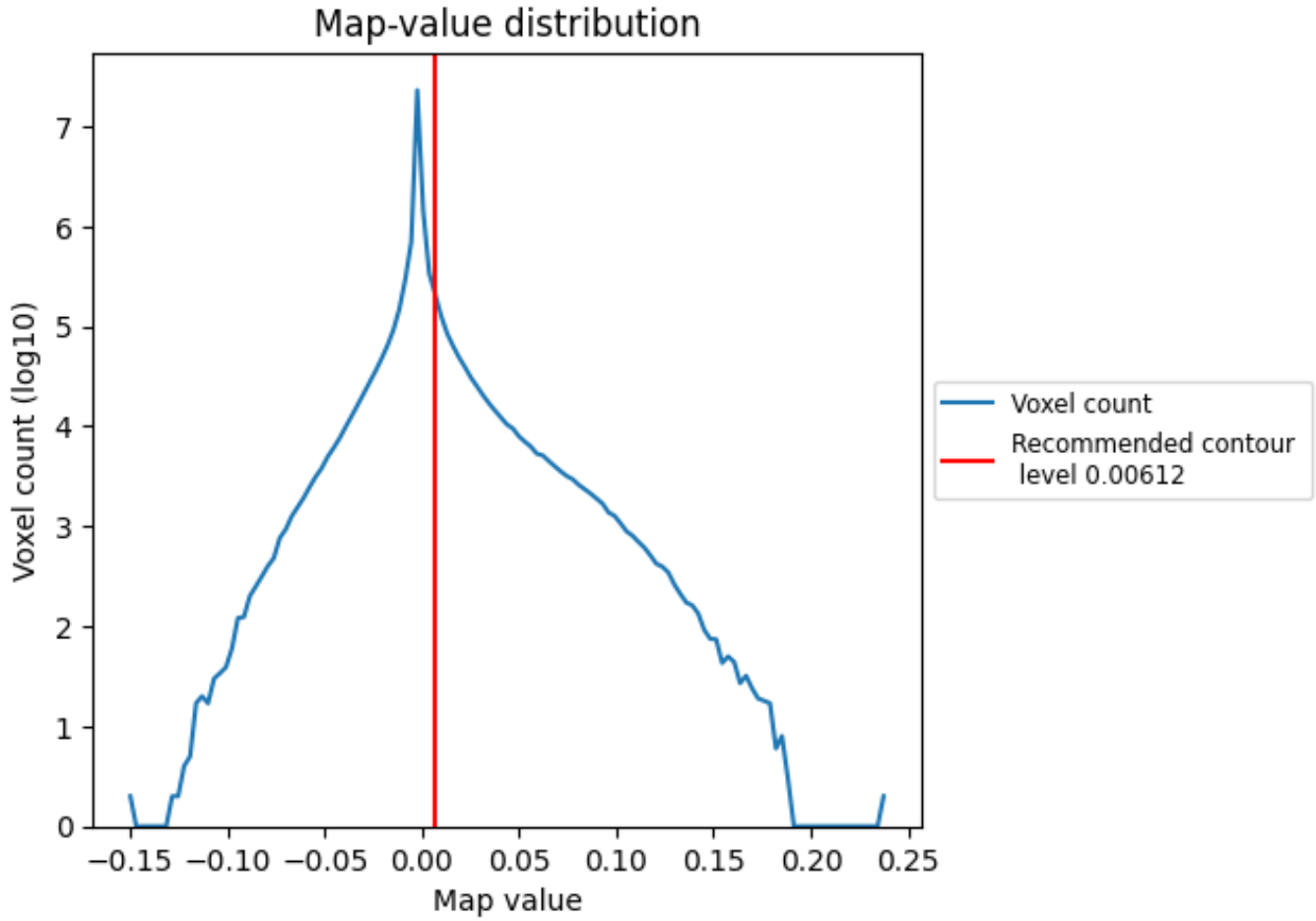
6.5 Mask visualisation (i)

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

7 Map analysis

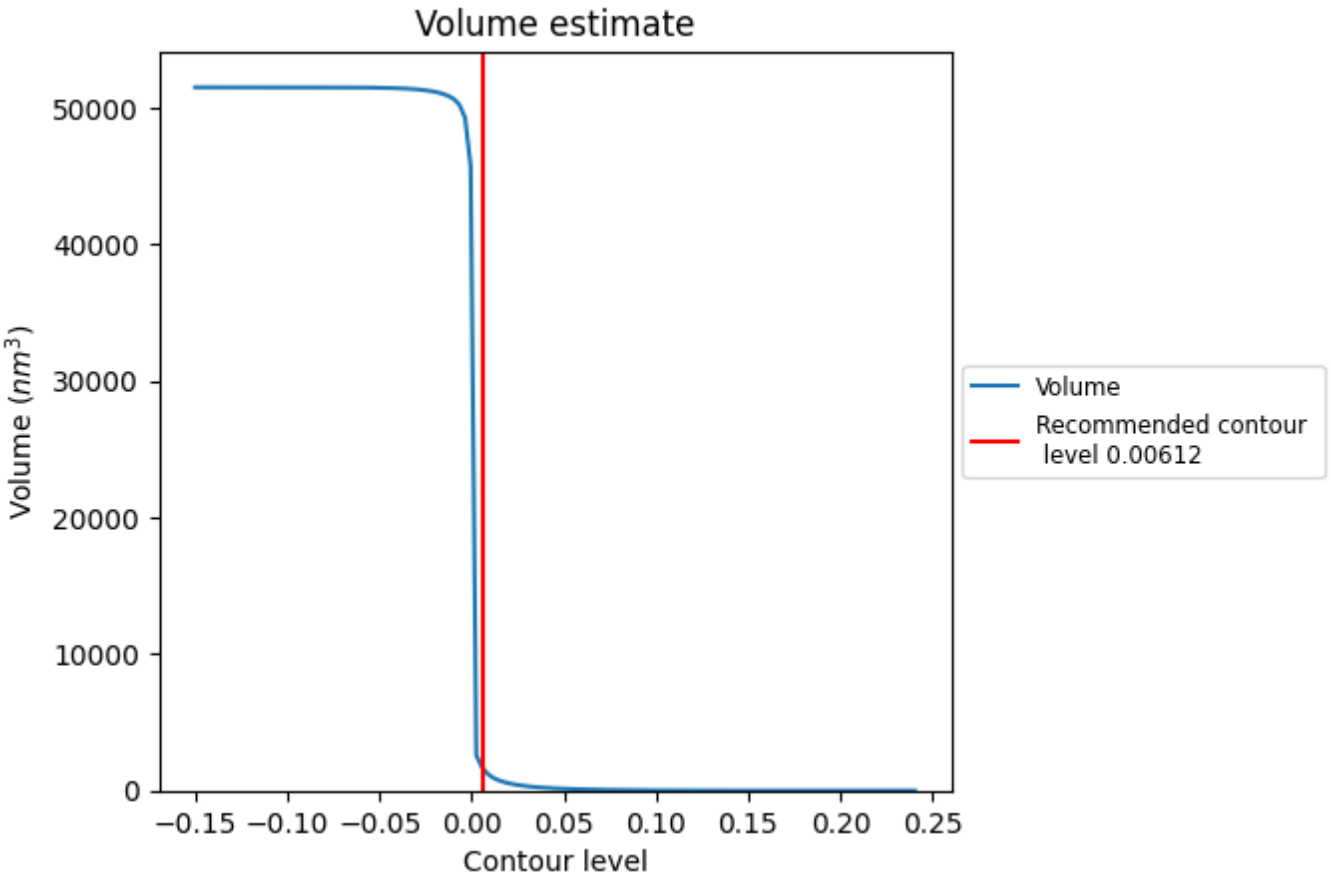
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

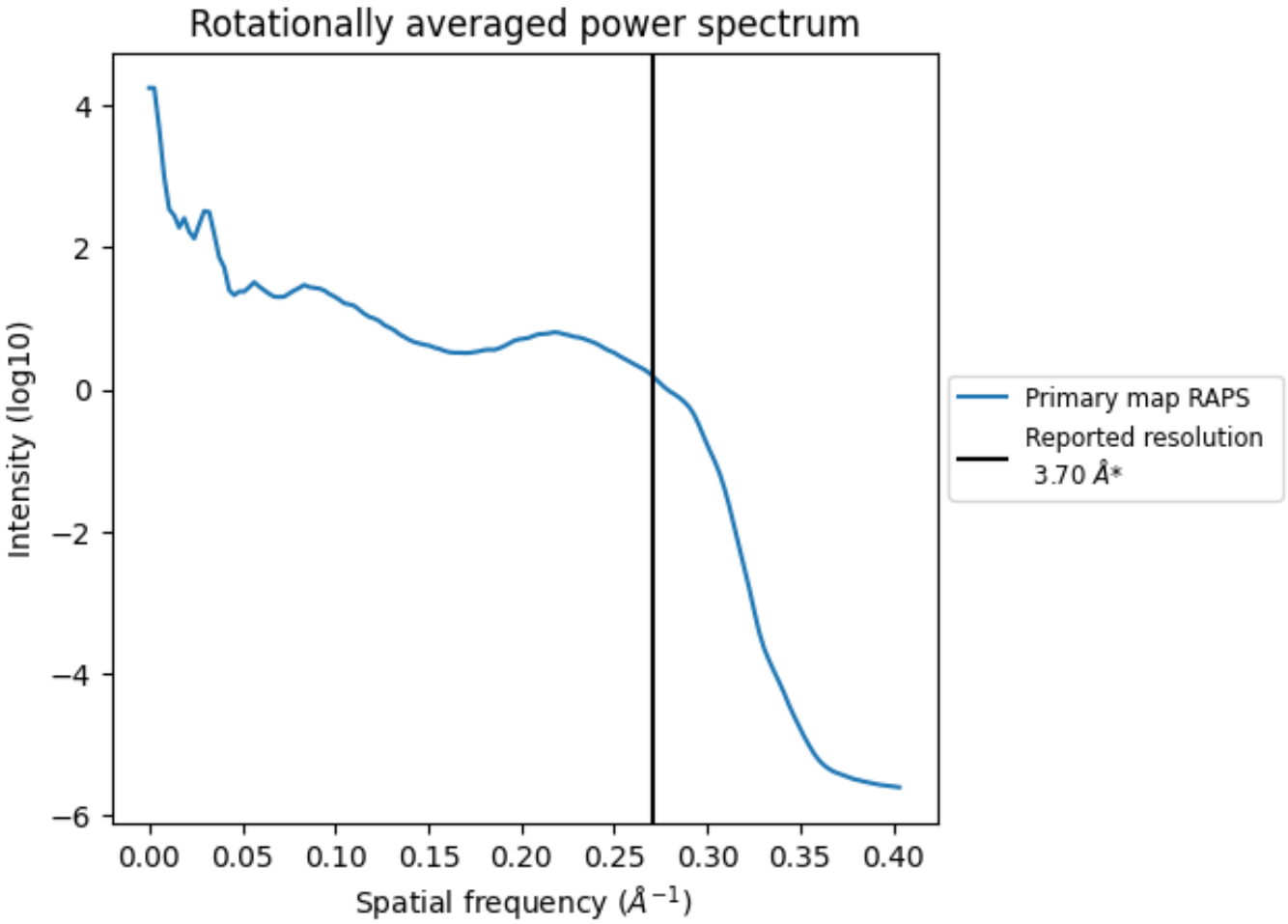
7.2 Volume estimate



The volume at the recommended contour level is 1627 nm^3; this corresponds to an approximate mass of 1470 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)

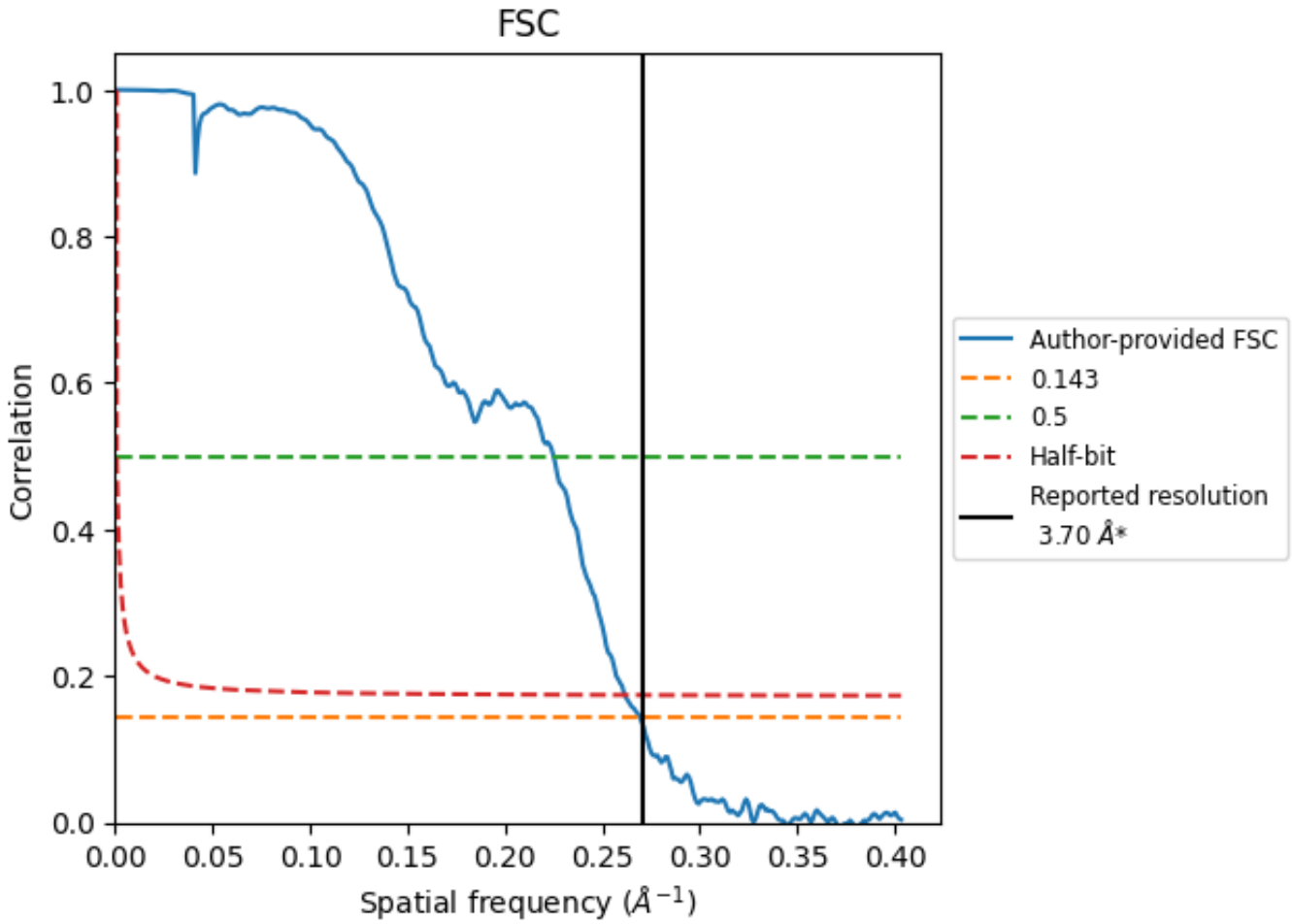


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

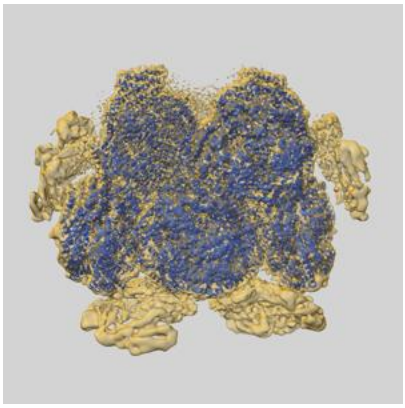
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.45	3.82
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

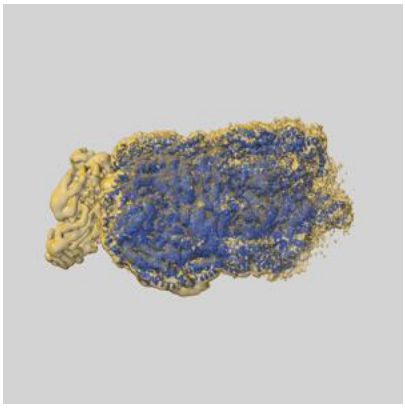
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31944 and PDB model 7VEA. Per-residue inclusion information can be found in section 3 on page 17.

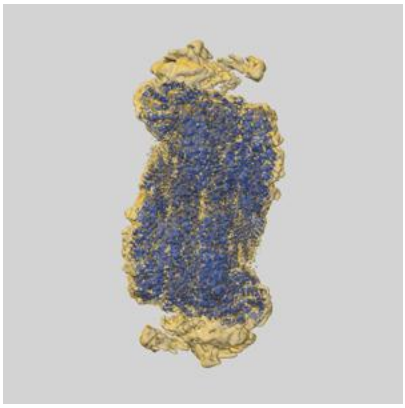
9.1 Map-model overlay



X



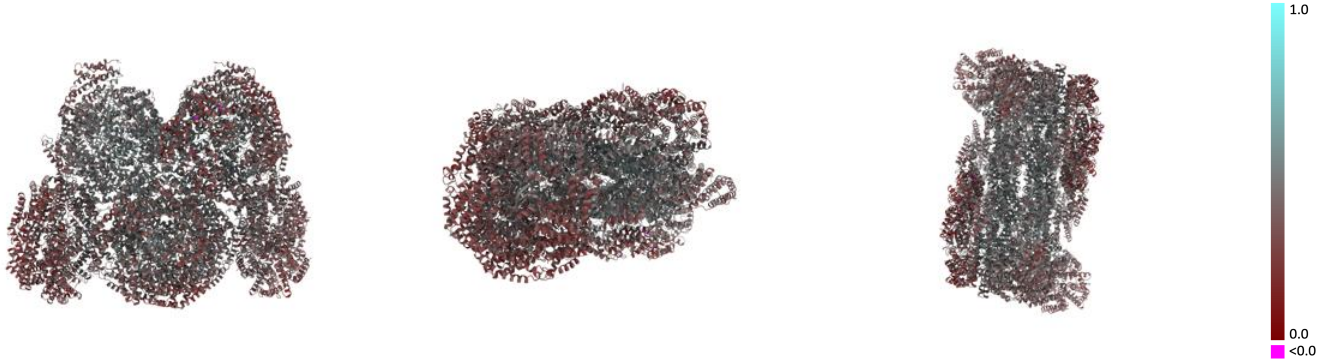
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00612 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.

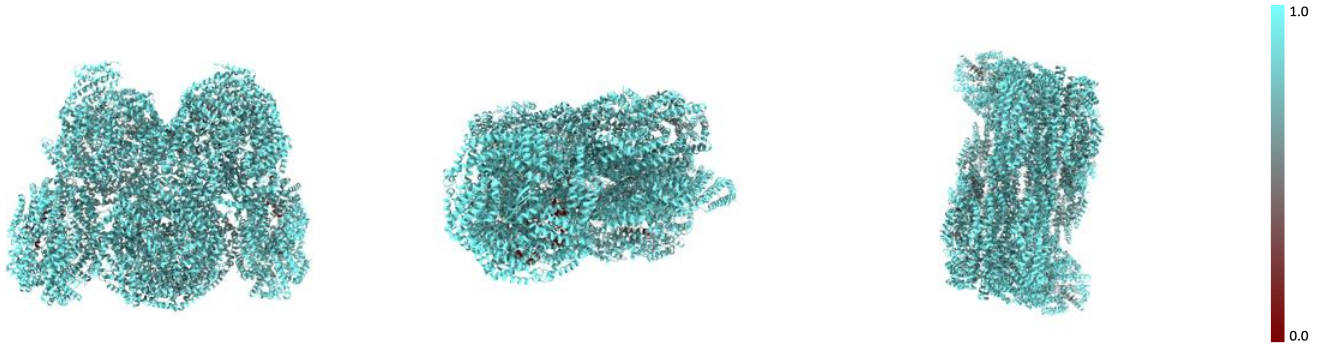
9.2 Q-score mapped to coordinate model



X Y Z

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

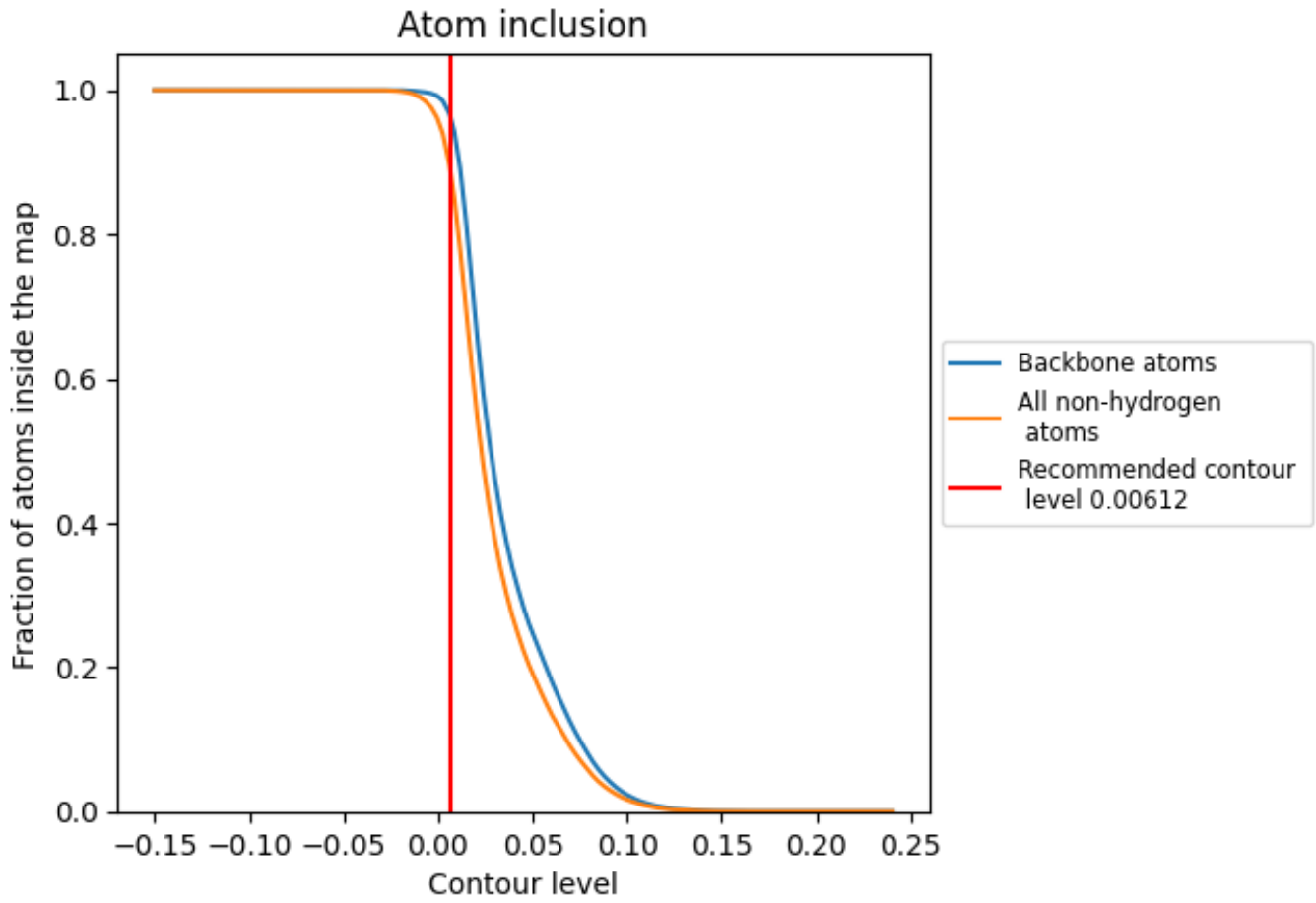
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00612).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00612) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8956	0.4150
aA	0.8292	0.4300
aB	0.8807	0.3300
aC	0.8107	0.3300
aD	0.8491	0.3070
aE	0.7974	0.3490
aF	0.8961	0.3490
aG	0.9249	0.4410
aH	0.9186	0.5100
aI	0.9339	0.5070
aJ	0.9098	0.4930
aK	0.8972	0.4460
aL	0.8941	0.4680
aM	0.9049	0.4640
aN	0.9016	0.4320
aO	0.9042	0.4190
aP	0.9072	0.4950
aQ	0.9412	0.4940
aR	0.9126	0.4670
aS	0.8615	0.3530
bM	0.8991	0.4330
bN	0.9186	0.4960
bO	0.9341	0.4880
bP	0.9023	0.4690
bQ	0.8531	0.3970
bR	0.8885	0.4370
bS	0.8162	0.3310
bT	0.8893	0.3810
bU	0.8231	0.4050
bV	0.8850	0.3580
bW	0.8693	0.3790
bX	0.8902	0.3660
bY	0.8695	0.4530
cA	0.9430	0.3300
cB	0.9539	0.3280

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Chain	Atom inclusion	Q-score
cC	0.9038	0.3350
cD	0.9408	0.4200
cE	0.9374	0.4090
cF	0.9338	0.4040
cG	0.8523	0.2840
cH	0.9584	0.2960
cI	0.9189	0.3210
cJ	0.9704	0.3600
cK	0.9110	0.3890
cL	0.9475	0.3180
cM	0.8855	0.4150
dA	0.8358	0.4320
dB	0.8882	0.3320
dC	0.8176	0.3270
dD	0.8558	0.3110
dE	0.8246	0.3470
dF	0.8927	0.3530
dG	0.9265	0.4430
dH	0.9161	0.5110
dI	0.9364	0.5110
dJ	0.9131	0.4970
dK	0.8939	0.4460
dL	0.8966	0.4670
dM	0.9049	0.4660
dN	0.9057	0.4330
dO	0.9092	0.4210
dP	0.9112	0.4990
dQ	0.9404	0.4940
dR	0.9115	0.4700
dS	0.8862	0.3480
eM	0.8999	0.4320
eN	0.9178	0.4960
eO	0.9317	0.4870
eP	0.9055	0.4750
eQ	0.8506	0.3970
eR	0.8869	0.4350
eS	0.8153	0.3260
eT	0.8868	0.3780
eU	0.8313	0.4070
eV	0.8792	0.3530
eW	0.8693	0.3790
eX	0.8885	0.3620

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Chain	Atom inclusion	Q-score
eY	0.8735	0.4520
fA	0.9442	0.3300
fB	0.9681	0.3290
fC	0.8005	0.3180
fD	0.9398	0.4170
fE	0.9190	0.4070
fF	0.9338	0.4030
fG	0.8269	0.2770
fH	0.9597	0.2970
fI	0.9153	0.3140
fJ	0.9787	0.3500
fK	0.7841	0.3830
fL	0.9105	0.2950
fM	0.8825	0.4070